THE CRYSTAL CHEMISTRY OF KORNERUPINE

by

MARK ALAN COOPER

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in

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THE CRYSTAL CHEMISTRY OF KORNERUPINE

BY

MARK ALAN COOPER

A Thesis/Practicum submitted to the Faculty of Graduate Studies of The University of Manitoba in partial fulfillment of the requirements of the degree

MASTER of SCIENCE

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ABSTRACT

Kornerupine is an accessory sorosilicate mineral found in high-grade metamorphic rocks. It has the general formula (□, Mg, Fe) (Al, Mg, Fe)$_9$ (Si, Al, B)$_5$ O$_{21}$ (OH,F). Previous studies have been unable to arrive at accurate structural formulae and corresponding detailed crystal-chemical relations. Forty seven ferrous-iron kornerupines ($Fe^{3+}/Fe^{2+} \leq 0.5$) from ~35 localities were examined using SREF, EMPA, SIMS and H-extraction line techniques to acquire complete crystallographic and chemical data. EMP data was processed using an anion-normalization scheme whereby cations are scaled to O$_{21}$ (OH + F)$_1$ *pfu*, which is supported by bond-valence arguements and H values from H-extraction line analysis. B and Fe^{3+} quantities were developed *via* site-occupancy refinement at the T(3) and M(4) sites, respectively. Excellent agreement was attained between B values arrived at by SIMS and SREF methods. Site populations for the three tetrahedra, five octahedra and single eight-coordinate site were developed using standard crystal-chemical criteria.

B is fully ordered at the T(3) site [0.0 → 0.9 B *pfu*]. A coupled substitution $^{T(3)}B \rightarrow {}^{T(3)}(Si,Al)$ and $^{T(2)}Si \rightarrow {}^{T(2)}Al$ results in a dramatic reduction in size of the T(3) tetrahedron with a concomitant rotation of the T(2) tetrahedra. Coincident with these geometric changes of the T(2)—T(3)—T(2) tetrahedral trimer is greater chemical variation at all crystallographic sites. A substitutional limit of ~0.9 B and ~1.6 (Fe^{2+}, Mn^{2+}) is proposed for the kornerupine structure. Complete solid-solution for all compositions is indicated, whereby variation in □, 2^+, 3^+ and 4^+ cations can be expressed in terms of Tschermak-type and □-type substitutions, and cation sums are observed from 14.18 to 14.40 *pfu*. The M(4) site is an active participant in most substitutions, where Mg ⇔ (Al, Fe^{3+}) exchange provides important charge-compensation for other substitutions occurring elsewhere in the structure.

Dimensional information provided by cell refinement of powder XRD data in combination with chemical information from EMPA can be incorporated into simple empirical relations that provide accurate values for B, Fe^{2+}, Fe^{3+}, F and H.

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Kornerupine, a high grade metamorphic mineral of upper amphibolite and granulite facies rocks (Grew *et al.*, 1996), has been identified from every continental land mass (App. A and references within). It is a Mg-Al-silicate that contains variable amounts of iron [up to 15 wt.% FeO] (Grew *et al.*, 1995) and boron [up to 4 wt.% B_2O_3] (Grew *et al.*, 1990a; Hawthorne *et al.*, 1995). A metasedimentary origin has been inferred whereby boron likely originated from an influx of marine (Grew *et al.*, 1987b) or evaporitic (Grew, 1988) sediments. The ability of kornerupine to incorporate variable amounts of the light elements H,Li,Be,B and F,Fe[2+/3+] (Grew *et al.*, 1990a) enables it to serve as a valuable indicator of protolith and metamorphic-fluid compositions. Often inconspicuous in hand samples, kornerupine ranges in color from colorless to black. As the color increases in intensity, it is typically comprised of pleochroic olive-green and khaki-brown hues that generally become more saturated with increasing iron content.

The crystal structure of kornerupine was solved by Moore & Bennet (1968). Subsequent structure refinements (see section on previous work) have yielded semi-quantitative structural formulae and have tentatively identified mechanisms of chemical substitution. Details regarding the overall anion chemistry [O,OH,F,(H_2O?)], ferrous/ferric iron distribution, light-element chemistry [esp. B], and absolute ordering of major elements have been lacking. It is evident from the most recent structural study (Klaska & Grew, 1991) that quantitative relationships of various crystal-chemical details between different samples requires a larger and more systematic study. The structural formula resulting from previous structural studies (Moore & Araki, 1979; Moore *et al.*, 1989; Klaska & Grew, 1991) is :

$$^{X}(\square,Fe^{2+},Mg)\ ^{M1,2}(Mg,Fe^{2+})_3\ ^{M3,5}(Al)_4\ ^{M4}(Al,Mg,Fe^{3+})_2\ ^{T1}(Si)_2\ ^{T2}(Si,Al)_2\ ^{T3}(Si,B,Al)\ (O,OH,F)_{22}$$

1.2 Kornerupine nomenclature

Kornerupine was first described from the Fiskenæsset region of Greenland by Lorenzen (1884). Sauer (1886) proposed the name prismatine for a mineral from Waldheim Germany. The two species were compared by Ussing (1889) who concluded that they were the same mineral. Nevertheless, the name prismatine has appeared in the literature for nearly a century. More recently, Grew *et al.* (1996) have shown that kornerupine and prismatine are distinct isostructural minerals distinguished by their B content. The name kornerupine denotes compositions with B < 0.5 atoms per formula unit (*apfu*) and prismatine denotes compositions with B > 0.5 *apfu* based on 22(O,OH,F). When the B-content is unknown, the name kornerupine should be used. The modifiers 'boron-free' and 'boron-poor' can only apply to kornerupine *sensu stricto*, and should be used when B=0 and B < 0.2 *apfu*, respectively (Grew *et al.*, 1996; Friend, 1995). Throughout this work, all samples will be referred to as kornerupine *sensu lato*, unless reference is made specifically to boron-rich samples, in which case the name prismatine will be used.

1.3 Objectives

- Investigate a large sample population of kornerupine specimens using several analytical techniques to acquire precise, accurate, and complete chemical and crystallographic data over the range of compostions known to date.
- Develop a self-consistent understanding of the crystal-chemistry such that complete structural formulae can be written and important substitution mechanisms can be identified.
- Develop simple empirical relations that can be used by other geoscientists to further characterize their kornerupine samples with the aid of widely available equipment.

1.4 Strategic considerations

This section introduces to the reader, within the context of kornerupine crystal-chemistry, several methodological considerations involving large sample populations and the use of multiple analytical techniques.

From a chemical standpoint, kornerupine at first glance appears simple. There are only five major elements (Si,Al,Mg,Fe,B) from which only three (Si,Al,Mg) are essential constituents. Crystallographically, kornerupine is a complex mineral containing three tetrahedral sites, five octahedral sites, and a single eight-coordinate (X) site. There are ten anion sites, of which nine are occupied by O^{2-} and one by $OH^- / F^- / (H_2O?)$. Si and B are tetrahedral occupants, and Mg and Fe occupy the octahedral and X sites. Al is distributed over both tetrahedral and octahedral sites.

With few elements and many sites, there are many possible ordering schemes. One needs to develop a strategy in which each crystallographic site can be sensitized to the quantification of two or more possible elements in order to arrive at a complete structural formula. Further complicating the situation for kornerupine are the following four hurdles:

I. likelihood of encountering iron as both Fe^{2+} and Fe^{3+};

II. one of the sites (X) has a variable vacancy;

III. the possibility of a variable anionic charge, $O(10)=OH^-,F^-,(H_2O?)$;

IV. significant and variable light-element content (up to 1 B *apfu*)

The above hurdles combined with all possible ordering schemes yield an unconstrained problem — there is a variable number of cations that need to be scaled to an anionic charge that itself may also vary. Then for a given anionic charge, all cations can be rescaled for various

Fe^{2+}/Fe^{3+} ratios. The resolution of such a complex system requires that one keep the problem "floating" while sensible constraints are developed, tested for internal consistency with all current data, and then implemented. Results at various intermediate stages should also be compared to, and tested for their viability against, basic crystal-chemical principles from other mineralogical studies. In this manner, a succession of accurate constraints may eventually provide a unique solution and the resultant detailed structural formula. It should be obvious that no single analytical technique is capable of yielding the necessary measurements that are required to complete this task.

When attempting to quantify both major and more subtle crystal-chemical variations, caution must be exercised: (i) in the selection of ancillary analytical techniques; (ii) in combining data from different techniques; (iii) during the sampling and processing of samples. The validity of the constraints, as well as the outcome that evolves from them, is dependant on both the understanding and minimization of error throughout. One must proceed cautiously in that the crystal-chemical hurdles mentioned earlier offer potential degrees of freedom that are inherently capable of incorrectly absorbing analytical errors. Individual measurements need to be assessed for their accuracy (difficult) , and multiple measurements over many similiar samples should retain a high degree of relative precision.

In order to minimize error and maximize internal precision, the following procedures were used in this study :

1) Examine samples using different analytical techniques

This allows one to incorporate information that may only be attainable by specific techniques. The same quantity measured by more than one technique allows assessment of accuracy and fine tuning of the technique itself, which is particularily important for techniques that are in their early developmental stages. In addition, quantities in close agreement when

measured by different techniques, serve to establish what can now be referred to as a known and accurate quantity.

2) Carefully observe sample characteristics at various scales

Sample requirements are different for different techniques, and sample preparation should reflect this fact. Small-scale sampling of optically pure single-crystals that can be analyzed sequentially by non-destructive microbeam techniques may be the best approach. Such crystals are free of extraneous phases (mineral/fluid/gas inclusions ; weathered outer margins ; mineral micro-films coating microfractures), and because they are small, sample heterogeneity (zoning) can be minimized. By analyzing the same small volume by a series of non-destructive techniques, measured values from the different techniques can be directly compared. However, it may not be possible to remove aspects of sample variance entirely. This can be illustrated in the following common practice (which was done for this study) — the single crystal used for the structure refinement is subsequently microprobed. By default, the structure analysis provides an average result for the entire sample volume. The electron microprobing of a handful (often 10) of random point analyses through a narrow cross-section of the crystal can only provide an approximate average compostion.

Bulk sampling, necessary for some analytical techniques (*e.g.*, Mössbauer spectroscopy), can give valuable information (*e.g.*, Fe^{2+}/Fe^{3+} ratios), but the results must be carefully scrutinized in regard to sample contamination and heterogeneity issues. Therefore, results attained by different techniques need to be assessed individually and compared carefully in light of (1) sample considerations, (2) the relative sensitivities, (3) standards and corrections used, and (4) internal instrument precision.

3) Examine many samples covering a wide range in composition

With wider chemical variation, one is more likely to encounter a larger extent of chemical substitution on a given site. Larger ranges of site substitution allow one to document that the substitution occurs, and to develop reliable empirical relations. When the sample data-base is also large, the confidence in the above empirical relations increases , and one is also able to detect minor crystal-chemical perturbations that may be associated with solid-solution gaps or limits. The significance of these two points will become apparent in a later section when discussing the quantification of three components at a single site.

4) Examine all samples simultaneously during data aquisition and data processing

Sometimes referred to "parallel processing *via* the recipe", batch processing of samples offers better efficiency and level of internal precision. This approach usually entails producing similiar samples in a similiar manner and then running them with the same set of operating conditions/standards/corrections on the same instrument over a relatively short span of time. This does not mean that one follows a recipe blindly without regard to individual sample attributes. The recipe itself is a carefully designed procedure that must ensure quality control and also offer flexibility to accomodate sample differences.

1.5 The crystal structure of kornerupine

1.5.1 Previous studies

The crystal structure of kornerupine was solved in the space group Cmcm by Moore & Bennet (1968) with material from Mautia Hill, Tanganyika (R=11.3%). Five octahedral and three tetrahedral sites were recognized, giving 14 cations per 22 oxygen atoms. One of the oxygen sites, O(10), is occupied by an OH group. The B content (1.92wt.% B_2O_3 of McKie, 1965) of this sample was not reported at any of the terahedral sites; however, it is apparent from inspection of the isotropic-displacement parameters that the B resides at the tetrahedral site labelled Si(2) [later named the T(3) site by Moore & Araki, 1979]. The magnitude of the displacement parameter for the atoms at the Si(2) position is more than twice that of the other two tetrahedral sites; this is consistent with an unaccounted lighter substituent at the Si(2) site.

Moore & Araki (1979) refined a synthetic (Werding & Schreyer, 1978) kornerupine (R=5.2%) containing 2.73wt.% B_2O_3. This synthetic sample contains no Fe and provided an opportunity to study the structural sites with one less variable. Moore & Araki (1979) concluded (1) all B resides at T(3); (2) a partly occupied eight-coordinated cation-site, X, occurs at the origin and contains $^1/_3$ Mg and $^2/_3$ □; (3) the O(10) site contains an OH group, providing 1(OH) per 22 oxygens. It was postulated from comparison of various kornerupine data that the O(10) position could vary in compostion from $(O^{2-})_1\ (OH^-)_0$ to $(O^{2-})_0\ (OH^-)_1$ and that this variation couples to an X occupancy from 1 to $^1/_3$, respectively.

Finger & Hazen (1981) clearly demonstrated the ordering of Fe at two of the octahedral sites [M(1),M(2)] by refinement of an Fe-rich kornerupine (12.2 wt.% FeO ; 3.09 wt.% B_2O_3) from the Grenville Province, Ontario (R=4.7%). They suggested that there were no obvious structural limitations on the degree of Fe⇔Mg substitution.

Moore *et al.* (1989) refined another Mautia Hill kornerupine (R=2.7%) and gave further evidence for Fe^{3+} at the M(4) site. They revised their thoughts of the O(10) site to include compositions from $(O^{2-})_1\ (OH^-)_0$ to $(O^{2-})_{1/3}\ (OH^-)_{2/3}$ with a coupled X occupancy from 1 to $^1/_3$, respectively.

Klaska & Grew (1991) refined a B-free kornerupine from the Limpopo belt, South Africa (R=3.4%). They concluded that the T(3) position contains Al in addition to Si, and that all low-B kornerupines likely contain Al in addition to Si and B at T(3). A disordered H-position was located, and an interpretation for both OH and H_2O was given. The O(10) site contains both OH and F, and a discussion involving further substitution by H_2O indicated the possibility of more than 1 H *apfu*. Comparison of the earlier structural studies [Finger & Hazen (1981) **B=0.69** ; Moore & Araki (1979) **B=0.58** ; Moore *et al.* (1989) **B=0.41**] with their study (**B=0** *apfu*), indicates a coupled substitution of B for Si and Al at T(3) and Si for Al at T(2) , and complex substitutions amongst the octahedral sites.

Table 1 summarizes the individual results, as well as inferred ordering for other kornerupine data presented in those studies.

TABLE 1: KORNERUPINE ORDERING SCHEMES FROM PREVIOUS STUDIES

SITE	Moore & Araki (1979) B=0.58	Finger & Hazen (1981) B=0.69	Moore *et al.* (1989) B=0.41	Klaska & Grew (1991) B=0
X	□,Mg,Fe,(Na,Ca)	□,Mg,Fe	□,Mg	□,Mg,Fe
M(1)	Mg,Fe	Mg,Fe	Mg	Mg,Fe
M(2)	Mg	Mg,Fe	Mg,Al	Mg
M(3)	Al	Al	Al,Mg	Al
M(4)	Al,Mg,Fe^{3+},(Ti,Cr^{3+})	Al,Fe^{3+},Mg	Al,Mg,Fe^{3+}	Al,Mg
M(5)	Al	Al	Al	Al
T(1)	Si	Si	Si	Si
T(2)	Si,Al	Si,Al	Si,Al	Al,Si
T(3)	B,Si	B,Si	Si,B	Si,Al
O(10)	O^{2-} / OH^-	OH^-	O^{2-} / OH^-	OH^- / F^- / (H_2O?)

1.5.2 Structure description

Moore & Araki, (1979) described the kornerupine structure as a complex densely organized structure comprised of two kinds of layers oriented parallel to (010). Layer **A** (Fig. 1) is based on walls of edge-sharing and corner-sharing octahedra. These walls are four octahedra wide along [100], run parallel to [001], and link together along [100] *via* edge-sharing distorted cubes which contain the X cation. All of the central cation sites within layer **A** [X, M(3), M(5)] have fractional coordinates $y = z = 0$ and are symmetrically constrained to lie on the c-glide plane ($y = 0$). The octahedral wall comprised of M(3) and M(5) octahedra is corrugated along [001], in that rows [100] of corner sharing oxygens undulate above and below the *c*-glide plane.

Above and below ($y \approx \pm 0.15$) is layer **B** (Fig. 2), consisting of the M(1), M(2), M(4) octahedral sites and the T(1), T(2), T(3) tetrahedral sites. The octahedra link to form chains along [100] by edge-sharing in the sequence —M(1)—M(4)—M(2)—M(4)—M(1)—, and also by corner-sharing between M(1) octahedra. The octahedral chains are linked in the [001] direction through corner-sharing with T_2O_7 [T(1)-T(1)] and T_3O_{10} [T(2)-T(3)-T(2)] tetrahedral units that alternate along [100].

The linkage between layers **A** and **B** is shown in Figure 3. The octahedra of both layers nestle neatly together to form a compact edge-sharing cluster. The *n*-glide parallel to (010) at $y = {}^1/_4, {}^3/_4$ relates two **B** layers (**B**,**B′**) that link by edge-sharing between M(1) octahedra of layer **B** and T(2) tetrahedra of layer **B′**, and by corner-sharing between M(4) octahedra of layer **B** and T(1) tetrahedra of layer **B′**. The structure repeats along *b* in the fashion ...**ABBABBA**...

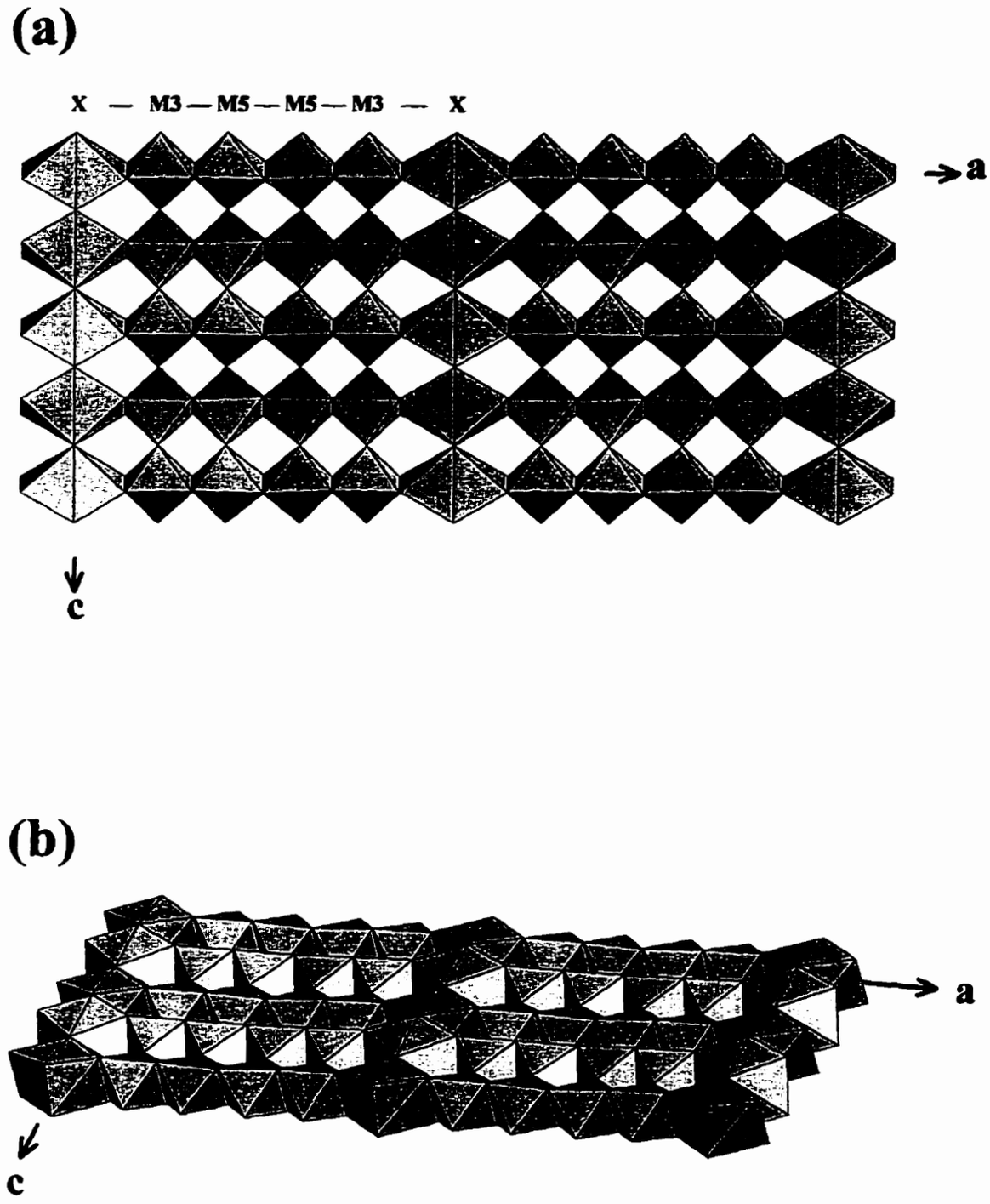


Figure 1: The structure of kornerupine (a) The A layer projected down [010]. (b) Perspective view of A layer.

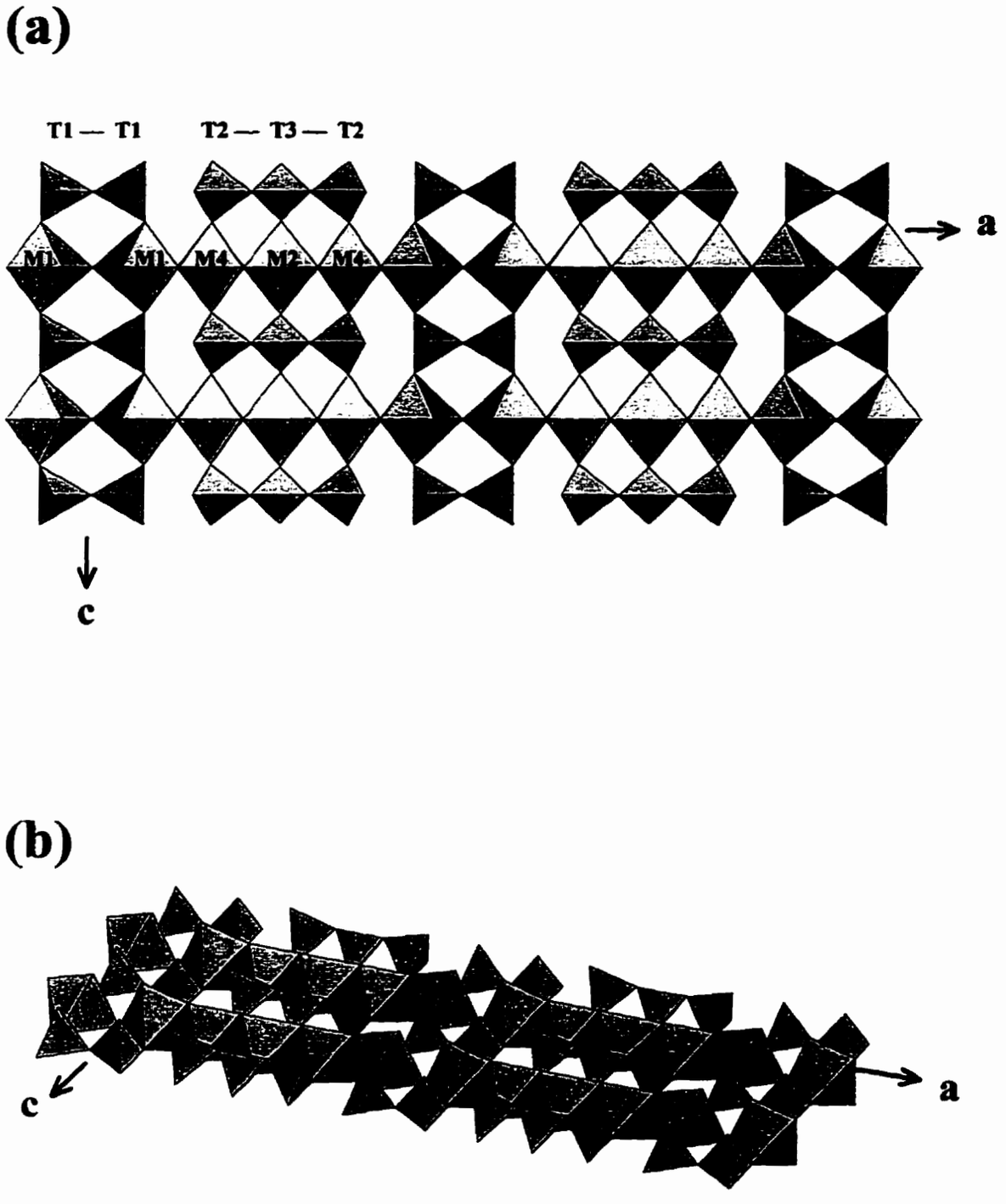


Figure 2: The crystal structure of kornerupine (a) The **B** layer projected down [010]. (b) Perspective view of **B** layer.

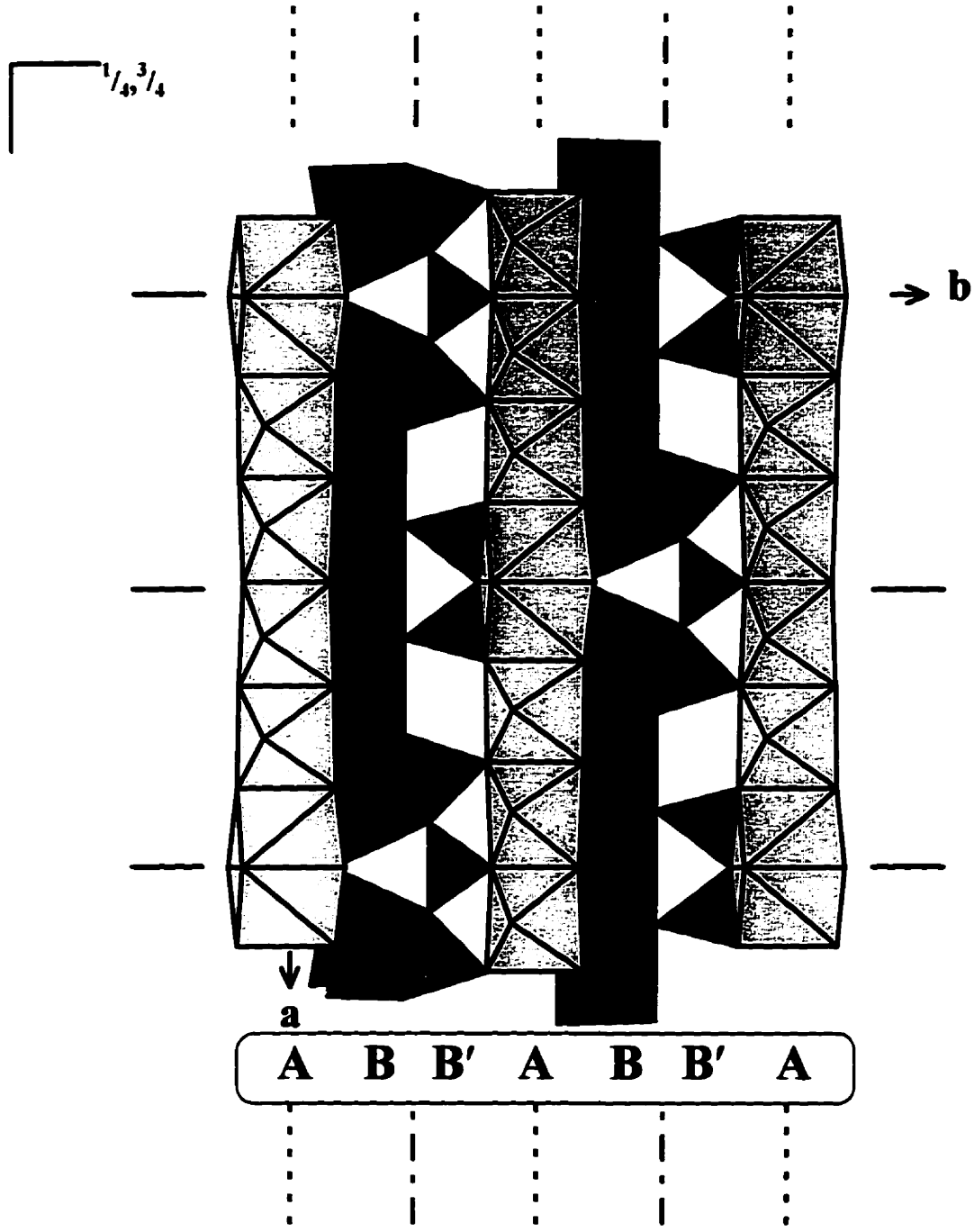


Figure 3: The kornerupine structure projected down [001]. **A**-layer components are light grey and reside on the *c*-glide plane (010) at $y = 0,{}^{1}/_{2}$. **B**-layer components are dark grey and relate to each other across the *n*-glide plane (010) at $y = {}^{1}/_{4},{}^{3}/_{4}$. Along the *c*-axis (perpendicular to the page), **A**-layer components are at $z = 0,{}^{1}/_{2}$; **B**-layer components are on the mirrors (001) at $z = {}^{1}/_{4},{}^{3}/_{4}$. The *C*-centered cell is marked by the X sites.

CHAPTER 2

EXPERIMENTAL METHODS

2.1 Analytical techniques

2.1.1 General information

The particulars involving the analytical techniques used for this study , including the specific information gained *via* the technique, are listed below in Table 2.

TABLE 2: TECHNIQUES USED IN THIS STUDY

TECHNIQUE	LOCATION	ANALYST	INFORMATION
(1) Electron microprobe analysis (EMPA)	University of Manitoba	Cooper, M.A. Chapman, R.	relative weight fractions of major (Si,Al,Mg,Fe) and minor (Cr,V,Ti, Mn,F) elements
(2) Structure refinement (SREF)	University of Manitoba	Cooper, M.A.	electron totals at crystallographic sites. Interatomic distances and angles
(3) Secondary-ion mass spectrometry (SIMS)	CNR-CSCC, Pavia, Italy	Bottazzi, P., Ottolini, L.	weight fraction of the element B
(4) H-extraction line	University of Saskatchewan	Kyser, K.	weight fraction of the element H

2.1.2 Sample preparation

The microbeam techniques listed in Table 2 [(1),(2),(3)] , were used for the same single-crystal for each kornerupine in the sequence (2)→(1)→(3). A prudent crystal-selection process was used because kornerupine typically contains microfractures, altered growth margins and a wide variety of inclusions. Under a binocular microscope, an equidimensional crystal fragment, typically 0.2-0.3mm in size, free of cracks, with uniform color and high optical clarity, was chosen. The fragment was always extracted a suitable distance from any growth margin in order

to avoid softer low-temperature alteration products. A pre-screening with the optical microscope eliminated unsuitable crystals displaying anomalous extinction or containing inclusions. Crystals that passed the selection process were then transferred to a Nonius air grider and subsequently abraded to produce spherical shapes in order to minimize X-ray absorption anisotropy. Each rounded crystal was glued to the end of a glass fiber fitted within a split brass pin. This brass-pin assembly is then easily mounted onto the goniometer head of the four-circle X-ray diffractometer. After completion of the intensity-data collection, the crystals were detached from the glass fibers and fixed to one-inch plexiglass disks with a thermal setting epoxy (PETROPOXY™). The surface was polished and carbon-coated in preparation for EMPA. The same sample disks, containing samples K1→K32, were later sent to Pavia, Italy for SIMS analysis.

For the seven samples (K2,K5,K6,K22,K23,K25,K32) used in the determination of H, the same screening procedure was used to accumulate 30-50mg of pure material. These grain separates were ground to fine powder using a clean (ultrasonically washed) mortar and pestle, and then sent to the University of Saskatchewan for analysis by H-extraction line. It should be noted that only seven of the then 32 available (K1→K32) samples were used for this technique for one simple reason : sample quality control. The majority of kornerupine specimens tend to be less than ideal candidates for the selection of bulk pure (>99.9%) material.

2.2 Electron–microprobe analysis (EMPA)

Electron-microprobe analysis was done on a CAMECA SX-50 instrument using back-scattered electron (BSE) imaging and energy-dispersive spectrometry (EDS) for qualitative assessment, and wavelength-dispersive spectrometry (WDS) for aquiring quantitative chemistry. All crystals were initially prescreened using BSE imaging to check for element zonation ; none was detected for any crystal. Next, an ED spectrum was collected for each crystal in order to identify all sample X-ray emission lines and thereby ensure complete element coverage during subsequent WDS analysis.

Standards were selected such that they (i) provide suitable calibration ranges ; (ii) minimize matrix corrections ; and (iii) have proven precision based on successful cross analysis with other standards and overall long-term lab use. The following standards and spectrometer crystals were used for Kα spectral lines: Si, diopside, PET; Al, kyanite, TAP; Mg, olivine, TAP; Fe, fayalite, LiF; Na, albite, TAP; Mn, spessartine, LiF; V, VP_2O_7, LiF; Ti, titanite, LiF; Ca, diopside, PET; K, orthoclase, PET; Cr, chromite, PET; F, fluor-riebeckite, TAP. WDS was done with the following operating conditions: 15 kV excitation voltage; 20 nA sample current; 20 s peak count time; 10 s background count time. Ten random points were analyzed per crystal using a beam diameter of 2 microns. Data reduction was done with the ϕ (ρZ) method (Pouchou & Pichoir, 1984, 1985).

2.3 Crystal structure analysis

2.3.1 Structure refinement (SREF)

Intensity data were collected on a Siemens P3 single-crystal diffractometer using graphite-monochromated Mo *Kα* X-radiation. The crystals were optically aligned within the X-ray beam, and 25 reflections from a rotation photo were centered. The cell parameters and orientation matrix were derived by least squares-refinement of the setting angles of the centered reflections. Crystal quality was assessed at this stage *via* the profiles of Bragg diffraction peaks and cell-parameter standard deviations, with rejection of unsuitable candidates. A single asymmetric unit of intensity-data was collected (4→60° 2θ; θ-2θ scan mode; 96 steps; 2.2° 2θ scan range; 4→30° 2θ/min. variable scan rate). Two standard reflections were collected every 50 measurements to monitor instrument stability. After the intensity-data set was collected, a second data set was collected in order to aquire information regarding the absorption behavior so that an empirical absorption correction could be applied. It consisted of eleven strong reflections uniformly distributed with regard to 2θ and measured over 10° intervals of ψ (the azimuthal angle corresponding to rotation of the crystal about its diffraction vector) from 0→360°ψ.

The Siemens SHELXTL (PC version) system of programs was used throughout this study. Data reduction included scaling on the standard reflections and applying standard drift, Lorentz, polarization, and background corrections. These data were then corrected for absorption using the the ψ-scan data with the crystal modelled as an ellipsoid. The resulting data were reduced to structure factors and used for full-matrix least-squares structure refinement. The structure was refined on F^2 using neutral scattering factors, absorption coefficients, and anomalous dispersion corrections from the *International Tables for Crystallography* (1992) for all cations. Ionized scattering factors were used for oxygen [O^{2-}] (Azavant & Lichanot, 1993) and fluorine [F^-] (*International Tables for Crystallography*, 1992).

2.3.2 Rationale for refining on F^2

Refinements based on F_o^2 are less common than those using $|F_o|$ [usually with $|F_o| > 4\sigma(|F_o|)$] , and therefore some comments are warranted regarding the decision to use F_o^2.

Because all data are used during refinement on F_o^2 , there is a greater data-to-parameter ratio as compared to that using $|F_o|$ with $|F_o| > 4\sigma(|F_o|)$. This results in lower esd's for refined parameters as well as reducing systematic error (which originates from ignoring weak data) that introduces bias which mainly affects the atomic-displacement parameters (Hirshfeld & Rabinovich, 1973; Arnberg *et al.*, 1979). This point is relevant to kornerupine in that ~150 of 1200 unique reflections collected fall into this weak data [$|F_o| < 4\sigma(|F_o|)$] category (App. B).

The effects of a variable extinction parameter are often significant for the refining of atom parameters of "gemmy" minerals with low mosaic spread. The extinction phenomenon usually expresses itself as unpredictable and unreasonable behavior in the refining atom displacement parameters. Experienced crystallographers can usually detect this behavior in the latter stages of isotropic refinement, and then insert a refining extinction parameter to correct for it. Left untreated, severe extinction will result in non-positive-definite anisotropic-displacement parameters and a biased refinement result. The F_o^2-refinement software (SHELXL-93; G.M. Sheldrick, unpubl. data) uses an improved expression for modelling extinction as compared to that of the older $|F_o|$-refinement software (Larson, 1970; section 2.3.3). This is applicable to kornerupine in that the magnitude of the refined extinction parameter ranges from insignicant to moderately large values (App. B).

Another fundamental difference between the refinement packages is contained in the weighting expression. Weighting in the F_o^2 refinement is handled in a more sophisticated expression that reduces statistical bias (Wilson,1976; section 2.3.3). The software refines weight parameters that give a flat analysis of variance, and then outputs these coefficients so that the

user can incorporate them into the weight command for the next phase of refinement. Refining weights in the older F_o software often leads to convergence difficulties as well as statistical bias from the weighting expression itself.

The comments in favor of refinement using F_o^2 have so far been based solely on statistical correctness; an important cosmetic advantage also favors the F_o^2 refinement, in the way the instruction file is constructed. During the later stages of kornerupine refinement, most of the cation sites are assigned multiple scattering-factors. Each of these sites must have the atom positional and displacement parameters constrained to be equal. The $|F_o|$-refinement software requires that each of these refining parameters be constrained through assignment of a common free-variable — a very clumsy and laborious task considering the number of free variables required. The F_o^2-refinement software uses a much simplier strategy to accomplish this task — all positional and displacement parameters are constrained using short site-label equivalence commands. This last point may be difficult to appreciate until the need arises to edit 50 refinement instruction files several times during the process of incorporating multiple site-occupants into the refinement. With recent advances in computing power, the actual run-time of the least-squares (once the rate determining step) is now a trivial procedure [50 kornerupines involving 120 parameters/1200 data and 6 cycles of least-squares refinement each, can be refined in a sequential batch job on a modest Pentium-PC in 20 minutes]. Such improvements help to make (SREF) a simple and efficient process that can be easily applied to large scale structure studies.

2.3.3 Refinement expressions

The form of the equations for the residual indices, extinction correction, and anisotropic displacement parameters are as follows:

$$R_1 = \Sigma(|F_o|-|F_c|) / \Sigma|F_o|$$

$$wR_2 = [\Sigma w(F_o^2-F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$$

$$w = 1/ [\sigma^2(F_o^2) + (a\times P)^2 + (b\times P)] \quad \text{,where a \& b are refineable parameters}$$

$$P = [\{\max(0,F_o^2)\} + 2F_c^2] / 3$$

An extinction parameter **X** is refined, where

$$F_c^* = kF_c[1+0.001\times \mathbf{X}\times F_c^2\times\lambda^3 / \sin(2\theta)]^{-1/4}$$

(k is the overall scale-factor)

Atom displacement parameter forms:

for isotropic U:

$$\exp(-8\pi^2 U[\sin(\theta) / \lambda]^2$$

for anisotropic U_{ij}:

$$\exp[-2\pi^2(h^2a^2U_{11}+k^2b^2U_{22}+l^2c^2U_{33}+2hkabU_{12}+2hlacU_{13}+2klbcU_{23})]$$

where U_{eq} is one-third of the trace of the orthogonalized U_{ij} tensor.

2.4 Secondary-ion mass spectrometry (SIMS)

Kornerupine samples [K1→K32] were analyzed on a CAMECA IMS-4F ion-microprobe at CNR-CSCC, Pavia for B using Conventional Energy-Filtering (CEF). The experimental details are given in Hawthorne *et al.* (1995) and Ottolini *et al.* (1993).

2.5 H-extraction line

Kornerupine samples [K2, K5, K6, K22, K23, K25, K32] were analyzed at the University of Saskatchewan according to the procedure of Kyser and O'Neil (1984).

CHAPTER 3

SREF / EMPA SYNERGY

3.1 Introductory comments

This chapter describes the iterative process by which results from SREF and EMPA can be combined in order to develop needed constraints. As mentioned in an earlier section (1.4), these constraints are required to reduce the number of unknowns during the allocation of specific elements to specific sites in the structure. It should be emphasized that this process involves the simultaneous processing of data from all kornerupine samples. The following sections address the following topics:

(1) how to best process the raw EMPA data;

(2) indirectly deducing B and Fe^{3+} contents;

(3) assigning the tetrahedral occupants;

(4) assigning octahedral occupants

The last section contains: (i) a flow chart illustrating the sequence of steps used; (ii) an accompanying chart giving the details of the scattering-factor assignments for each refinement stage.

3.2 Formula calculation

In order to cast the chemical information from EMPA into useable form, a normalization scheme must be applied to the relative weight-fractions of the oxides. In addition to choosing either a cation or anion normalization scheme, there is also the issue of partitioning Fe among its two valence states, as well as contending with the "missing" B_2O_3 (and often H_2O) value.

The main problem with developing a cation-normalization scheme stems from the fact that the X site is populated by appreciable vacancy in the presence of cations that are difficult to assess. This point can be explained by comparing the nine-coordinate X site in tourmaline to the eight-coordinate X site in kornerupine. The standard practice used to assign occupants to the X site in tourmaline is to probe (EMPA) for the alkalis [Ca,Na,K] and then assign them all to the X site, the remainder being filled by vacancy. It is simple to verify the correctness of this procedure for tourmaline by comparing the observed scattering at the X site to the alkali content from EMPA; so far, various investigators have reported reasonably good agreement (Burns *et al.*, 1994; Foit, 1989; Grice *et al.*, 1993; MacDonald *et al.*, 1995a, 1995b, 1993; Taylor *et al.*, 1995), thereby ruling out the possibility of other cation substituents at X. For kornerupine, the alkali contents reported (Grew *et al.*, 1990a) have always been extremely minor, and total Na+Ca can account only for a marginal proportion of the total scattering observed at X. It has therefore been deduced that the observed electron-density at X is primarily the result of occupation by various mid-sized divalent cations [Fe^{2+}(Mn^{2+}),Mg] (section 1.5.1). It is also known that Fe and Mg disorder over several of the octahedral sites [M(1),M(2),M(4), Finger & Hazen, 1981; Moore *et al.*, 1989]. In the presence of variable vacancy, the Fe and Mg contents cannot be directly assessed at the X site by occupancy refinement. Therefore, the correct assignment of Fe^{2+} and Mg to X is dependant on the accuracy in assigning these elements to several other sites first. The

four structural studies done prior to this work (section 1.5.1) collectively show a variable number of X cations ranging from 0.20 to 0.37 atoms. Although the error in assessing the exact number of X atoms remains significant, it is likely that the cation occupancy is indeed variable. Hence this rules out the possibility of using a simple cation-normalization scheme to process the EMP data.

Although the decision was made to use an anion-normalization scheme, some discussion involving its merit is also required. All investigators agree that 21 of the 22 O sites *pfu.* in kornerupine are occupied solely by O^{2-}. Complexity arises in assessing the occupancy of the O(10) position, in which the following occupants have been proposed: O^{2-}, OH^-, F^-, (H_2O?). The presence of F and a disordered H belonging to an OH group has been established (Grew *et al.*, 1990a; Moore & Araki, 1979; Klaska & Grew, 1991) by chemical / spectroscopic / structural studies. The quantification of an OH content has been a much more difficult task; results to date, indicate that it is a variable quantity, differing between various kornerupines. The recent study by Klaska & Grew (1991) suggested the possibility of H_2O at the O(10) site. Taken in their entirety, all previous studies would extend the H content from $0 \rightarrow 1^+$ *apfu.* , corresponding to an anionic charge from 44^- to $\leq 43^-$ *pfu* (section 1.5.1). The O(10) site lies on a mirror plane ($x = 0$) and is symmetrically bonded to two M(1) sites (related by the mirror) on one side, and by two X sites on the opposite side that lie on the mirror (Figs.1,3). A local arrangement with both M(1) and both X sites occupied, would contribute approximately $^1/_3$ valence units (*vu*) from each of the bonds to the O at O(10). Receiving a total of $^4/_3$ *vu* would leave the O at the O(10) site significantly underbonded, and therefore O^{2-} is unlikely to occur at the O(10) site. The H position (Klaska & Grew, 1991) lies very close to the X site (X—H , 1.17Å). With both X sites occupied, it is not possible for a H to also bond to the O at O(10). If one of the X sites were vacant, then there is room for a single H atom [*i.e.*, O(10) = OH] and the O at the O(10) site would receive $^1/_3$

(×3) + 1 = 2 *vu*, and its bond-valence requirements would be satisfied. If both of the X sites were locally vacant, then there is room for two H atoms to bond to the O at the O(10) site. Geometrically, this configuration of the H's about the O(10) position is consistent with the geometry of an H_2O group (Klaska & Grew, 1991). The O is receiving from the two M(1) sites $^1/_3$ (×2) = $^2/_3$ *vu* — could two H's also bond to the same O ? Yes; the mineral kieserite, $Mg(SO_4)(H_2O)$, contains corner-sharing chains of Mg octahedra that have bridging H_2O groups (Hawthorne *et al.*, 1987). However, although the possibility of H_2O may exist, it has not yet been conclusively identified in kornerupine (Klaska & Grew, 1991). It therefore seems reasonable to *tentatively* process the EMP data using an anion-normalization scheme based on O_{21} $(OH+F)_1$. Considering the refractory nature of kornerupine, the small quantity of H in question, and the sample-quality problems often encountered, it is quite probable that reported H quantities are based on some of the most erroneous measurements associated with kornerupine chemical investigation. The apparently variable H-content reported by others is therefore considered by this author to be based, at least in part, upon unreliable data. A later section (5.3) discussing results from this study will re-address the local-ordering possibilties in the vicinity of O(10) in more detail.

With the anion normalization scheme in place [O_{21} $(OH+F)_1$], there remain two quantities that must be determined before the chemical data can be processed correctly into cations *pfu*, namely B and Fe^{3+}. Because the total number of cations remains unconstrained, values for both B and Fe^{3+} are required.

3.3 B and Fe^{3+} *via* SREF

3.3.1 A first approximation

B is fully ordered at the T(3) site (1.5.1). Also located at the T(3) site are Si and Al (Klaska & Grew, 1991). In order to extract an accurate B value from the structure refinement, the T(3) site needs to be quantitatively characterized in terms of its three constituents. This cannot be done directly within the refinement, as only two dependant occupancy factors can be coupled to a single crystallographic site. The previous structural studies (1.5.1) suggest that Al is a minor component at T(3) (except when B approaches zero). The electron signatures for the three species are Si=14e; Al=13e; B=5e. Therefore, the best way to set up the initial site-refinement for T(3) is to couple the Si occupation factor to the B occupation factor so as to maintain a high contrast between the two prominent refining scattering species (*i.e.*, 14e *vs.* 5e), and exclude the Al scattering factor which is very similiar to that of Si (*i.e.*, 13e *vs.* 14e). This style of refinement will give a first approximation of the B content.

Fe^{3+} is fully ordered at the M(4) site (1.5.1). Also located at M(4) are Al and Mg. Al is dominant over Mg, and both are similiar in scattering power (Al = 13e; Mg = 12e) as compared to Fe (26e). Therefore, the best way to set up the initial site-refinement for the M(4) site is to couple the Fe occupancy factor to the Al occupancy factor, and exclude the Mg scattering-factor contribution [analogous to the strategy at T(3)].

After running the above "primary refinement" step (Fig.4, Table 3), it will then be possible to process the EMP data (using the B and Fe^{3+} from SREF) into an initial working set of cations *pfu*.

3.3.2 Fine-tuning the tetrahedral B, Si and Al

In order to improve the B value that evolves from the structure refinement, the Al content at T(3) needs to be assessed and then modelled in the refinement by incorporating the Al scattering factor at T(3). The other tetrahedral sites also need to be properly modelled in terms of Si/Al distribution so that the overall refinement is better scaled. The Al content at T(3) can be arrived at in the following manner:

(1) from the results of the initial refinement, approximate B and Fe^{3+} values are used to process the EMP data and provide the number of Si cations *pfu*;

(2) All Si resides at the three tetrahedral sites. Because the total Si and B *pfu* values are known, the Al content *pfu* for the tetrahedra can be arrived at by difference: 5 - Si - B = $^{[4]}$Al;

(3) the three occupants in question (B, Si, Al) have mutually distinctive radii (0.11; 0.26; 0.39Å), respectively (Shannon, 1976). Isomorphous substitution by these elements is then recorded in the bond-length information. From the quantities ($^{[4]}$Si, $^{[4]}$Al, $^{T(3)}$B) and the bond-length details, the Si/Al partitioning for all tetrahedra can be calculated.

Subtle bond-length variations are often overlooked or dismissed in their importance in studies that involve only a handful of refinements. In larger studies, these subtle variations can take on new meaning when all data is processed simultaneously. The importance of simultaneous processing cannot be overstated in properly identifying and characterizing systematic variations in observed bond-lengths. Further details involving the Si/Al partitioning over the three tetrahedral sites are now given. Klaska & Grew, (1991) have clearly documented the presence of Al at T(2) and T(3). Their Figure 5 shows a minor ⟨T(1)–O⟩ variation for the four kornerupines

presented, and this author attributes this bond-length variation to the presence of minor Al at T(1) (especially at low B values). Therefore, the Si/Al partitioning was applied to all three tetrahedral sites in this study. Next, some assumptions concerning the T(1) site were used. The shortest ⟨T(1)–O⟩ observed for all kornerupines in this study (1.618 Å) (App. G.2) corresponds to 100% Si at T(1). The bond-length variation at T(1) conforms to isomorphous substitution by minor Al that emulates a *hard-sphere packing* model. Therefore the intercept (y = 1.618 at Al = 0) and slope (= 1) have been fixed for the ⟨T(1)–O⟩ *vs.* constituent radii (r), and Si and Al coefficients can now be calculated for all observed ⟨T(1)–O⟩ distances. With the Si/Al partitioning complete for T(1) , the T(2) and T(3) sites can now be processed. The ⟨T(2)–O⟩ distances observed in this study range from 1.646 to 1.698 Å (App. G.2). Application of the strategy used for T(1) is inappropriate for T(2) because: (1) it is clear from the ⟨T(2)–O⟩ variation that significant Al substitution occurs, and (2) it is unlikely that 1.646 Å corresponds to complete Si occupancy of the T(2) site. The complicated situation at T(3) also excludes any assumptions of total occupancy by one of B, Si, Al for a given ⟨T(3)–O⟩. Without the possibility of further constraint, the partitioning of Si and Al to T(2) and T(3) will have to be done in a mutually dependant fashion. Various combinations of intercept and slope (near 1) were imposed on the T(2) site. For each selection of intercept/slope combination, all $^{T(2)}$Si and $^{T(2)}$Al values are recorded. The amount of Si to assign to T(3) is calculated from $^{T(3)}Si = {}^{EMP}Si - {}^{T(1)}Si - {}^{T(2)}Si$; because there is a tentative B value from the initial refinement, the Al to assign to T(3) can be arrived at by difference. For each T(2) intercept/slope selection, resulting ⟨T(3)–O⟩ *vs.* r relations were assessed using least-squares techniques (*i.e.*, monitoring correlation coefficients of the linear regressions). Graphical comparisons of T(3) results were also used to track outlier points on ⟨T(3)–O⟩ *vs.* r plots. In this manner, the T(2) intercept/slope combination that gave the best fit for T(3) was determined.

From the ⟨T–O⟩ *vs.* *r* relations at [T(1),T(2),T(3)] , all of the following quantities were output: $^{T(1)}Si$, $^{T(1)}Al$, $^{T(2)}Si$, $^{T(2)}Al$, $^{T(3)}Al$. These quantities were then entered into the next series of refinements as fixed occupancy factors. At T(3), the coupling of variable Si and B occupancy factors was maintained so that the Si and B could now readjust in the presence of Al. The subsequent change in the refined B occupancy is most significant for kornerupines with greater Al at T(3). After completing this series of refinements ("secondary refinement"; Fig.4, Table 3), the new B values [and possibly newly adjusted Fe^{3+} values at M(4)] were used to recalculate new Si *pfu* values from the EMP data. Then the steps above used to calculate the Si/Al distribution for each tetrahedron were repeated. These Si and Al quantities were then updated in the refinements, and another stage of least-squares refinement was done. The entire sequence ("TETRAHEDRAL CYCLE"; Fig.4) was then iterated to self-consistency.

This rather-involved process of iteratively adjusting tetrahedral occupants by using SREF electron and bond-length criteria tied to EMP results, has three important outcomes :

- the tetrahedra are well characterized;
- B has changed in status from unknown variable to tentative constraint;
- the octahedral Al contents are tentatively constrained *via* $^{[6]}Al = {}^{EMP}Al - {}^{[4]}Al$

Also, the site refinement at M(4) involving Fe and Al coupled-occupancy factors, has provided an approximate Fe^{3+} that has improved the Si *pfu* quantity by better scaling cations during the processing of EMP data.

3.3.3 Fine-tuning Fe^{3+} at M(4)

In order to improve the Fe^{3+} value that evolves from the structure refinement, the Mg content at M(4) needs to be assessed and then modelled in the refinement through inclusion of the Mg scattering factor. In addition to Al at the M(4) site, previous investigators report that the M(3) and M(5) sites are entirely populated by Al (1.5.1). The M(3) and M(5) sites would then contribute 4 Al *pfu*. No significant Al has ever been proposed for the M(1), M(2), or X sites. At the completion of fine-tuning the tetrahedra (3.3.2), the quantity $^{[6]}Al$ was determined. The Al to be assigned to M(4) can be arrived at by difference: $^{M(4)}Al = {}^{[6]}Al - 4$. At this stage, the complete Al distribution has been determined. In the refinements, the Al contents of T(1), T(2), T(3), M(3) and M(5) are all tentatively constrained with fixed occupancy factors. It then seems reasonable to fix the Al occupancy factor at M(4), because the M(4) site is merely accepting the remainder of the Al from the EMP data not accounted for by the other sites. In addition to the Al, fixed occupancy-factors corresponding to the Ti, V and Cr contents from EMP data are also inserted at the M(4) site. The remaining M(4) electron density is then able to partition itself between refining Mg and Fe. The reason for not fixing the Mg, and then refining Al against the Fe is simple — there is no way to accurately determine what fixed Mg value should be used. This stems from the fact that both Mg and Fe can mutually occupy the X site in addition to a variable amount of vacancy. Therefore, the Mg content at X cannot be directly determined from the refinement, and a Mg population for M(4) cannot be estimated.

The results of the above series of refinements ("tertiary refinement"; Fig.4, Table 3) provide newly modified Fe^{3+} values [and possibly changed B values]. When these new Fe^{3+} ($\pm$B) values are used to re-process the EMP data, the cations *pfu* are rescaled and the Si value is subject to change. Therefore, the TETRAHEDRAL CYCLE is repeated to make appropriate reajustments to the tetrahedral occupants. "Tertiary refinement" is then repeated with updated

fixed-occupancy factors for $^{M(4)}$Al. Another pass through the TETRAHEDRAL CYCLE followed by "tertiary refinement" gave no further change in Fe^{3+} or B values, so the process was stopped. All tetrahedral and octahedral sites are now in chemical synchronization with the EMP data. The last remaining task is to assign the residual Fe^{2+} and Mg (from the EMP data) to the X site.

During the presentation of the individual kornerupine sites in the next chapter, it will become apparent that some sites will require additional readjustment of occupants. Further modifications to the strategy presented here will then be discussed.

TABLE 3: SITE-SCATTERING SPECIES AT VARIOUS REFINEMENT STAGES

SITE	Primary Refinement	Secondary Refinement	Tertiary Refinement
X	Mg	[Na Ca] Mg	[Na Ca] Mg
M(1)	Mg Fe	Mg Fe	Mg Fe
M(2)	Mg Fe	Mg Fe	Mg Fe
M(3)	[Al]	[Al]	[Al]
M(4)	Al Fe	Al Fe	[Ti V Cr] [Al] Mg Fe
M(5)	[Al]	[Al]	[Al]
T(1)	[Si]	[Si] [Al]	[Si] [Al]
T(2)	Si	[Si] [Al]	[Si] [Al]
T(3)	Si B	[Al] Si B	[Al] Si B
O(10)	O^{2-} F^-	O^{2-} F^-	O^{2-} F^-

square brackets designate fixed occupancy factors

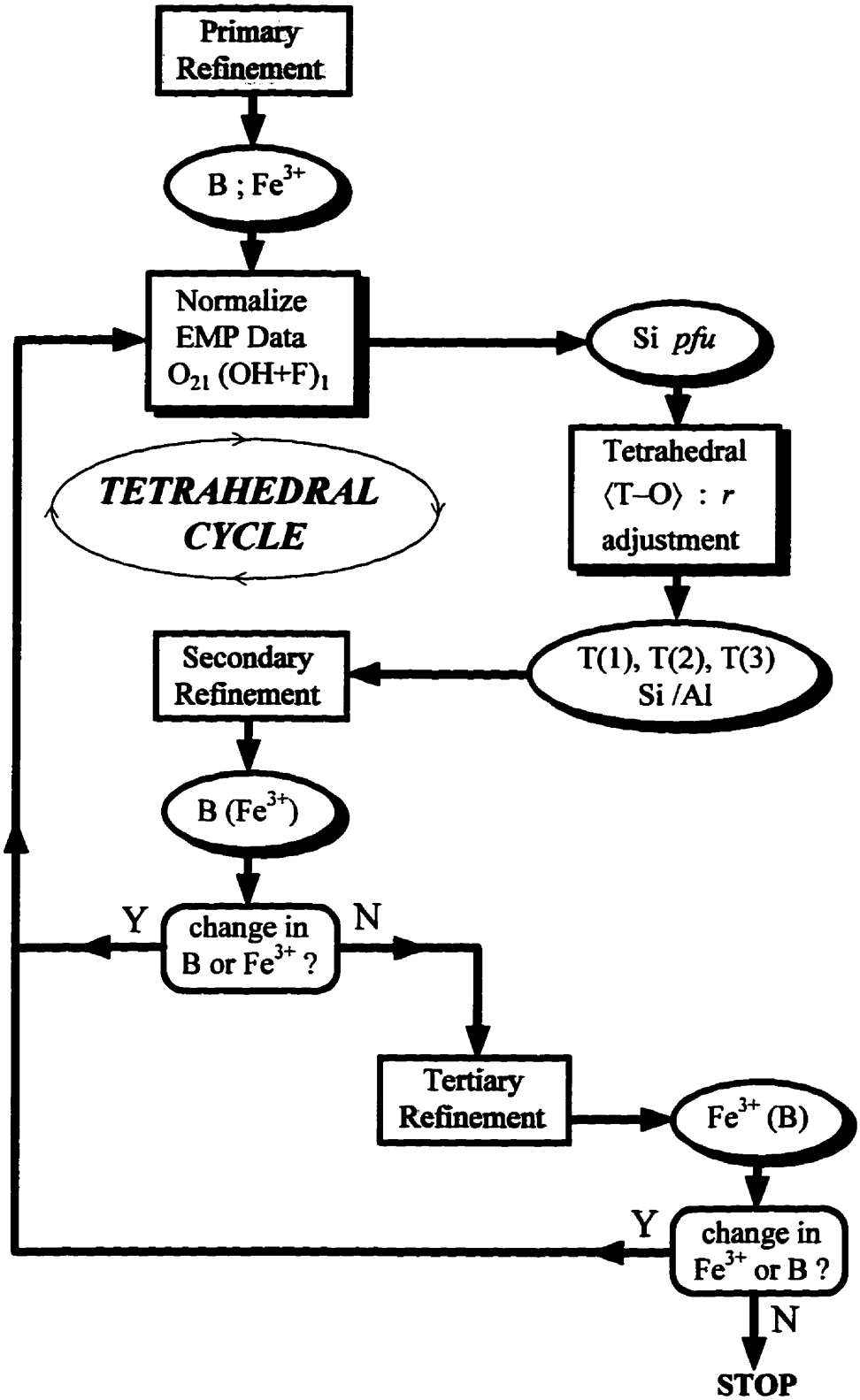


Figure 4: Flow chart illustrating the EMP—SREF synergy.

CHAPTER 4

ASSIGNMENT OF SITE POPULATIONS

4.1 Tetrahedral sites

The final assignments of Si, Al, and B to the three tetrahedral sites T(1), T(2), and T(3) are presented in Figures 5, 6, and 7 (App. F). Observed ⟨T(1)–O⟩ distances vary from 1.618 to 1.632 Å and correspond to site populations ranging from $Si_{1.000}Al_{0.000}$ to $Si_{0.900}Al_{0.100}$, respectively (Fig.5). Observed ⟨T(2)–O⟩ distances vary from 1.646 to 1.698 Å and correspond to site populations ranging from $Si_{0.899}Al_{0.101}$ to $Si_{0.508}Al_{0.492}$, respectively (Fig.6). Observed ⟨T(3)–O⟩ distances vary from 1.505 Å to 1.665 Å, and reflect the following maximum ranges in site occupants : $B_{(0.016\rightarrow0.880)}$, $Si_{(0.057\rightarrow0.727)}$, $Al_{(0.053\rightarrow0.299)}$ (Fig.7).

During the fine-tuning of tetrahedral occupancies (3.2.2), the T(1) and T(2) site-occupancies were constrained, such that there was absolute adherence to intercept/slope values associated with ⟨T–O⟩ : *r* relations. In doing this, all relative error was associated with the ⟨T–O⟩ : *r* relation at the T(3) site. Because this error distribution is inappropriate, all relative error was subsequently reapportioned among the tetrahedral sites in accordance with the respective site-multiplicities. Linear-regression analysis was then used to derive the ⟨T–O⟩ : *r* relation. For each tetrahedral site, a slope, *y*-intercept and correlation coefficient were computed (Figs.5,6,7). The *y*-intercepts (1.36-1.37) and slopes (1.00-1.02) are in excellent agreement ($r^2 = 0.927$-0.998) with usual O^{2-} radii (Shannon, 1976) and a *hard-sphere packing* model. The esd's for individual T–O bond distances are all ≤ 0.002 Å, and the resulting standard deviations on ⟨T–O⟩ distances are ≤ 0.001 Å. Error bars dipicting two standard deviations ($2\sigma \approx 0.002$ Å) are placed in the upper left corners of Figures 5-7. Error associated with ⟨M–O⟩ and ⟨X–O⟩ distances is represented in identical fashion.

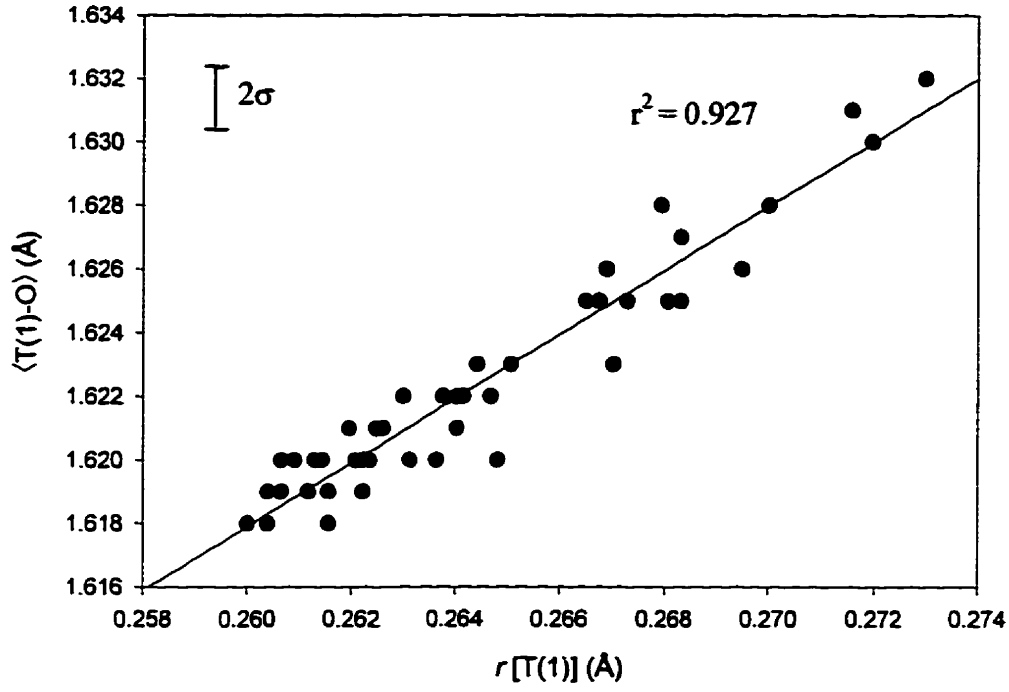


Figure 5: Relationship between ⟨T(1)-O⟩ and constituent T(1) cation radius. The regression line has the form: ⟨T(1)-O⟩ = 1.0074(*r*) + 1.3560.

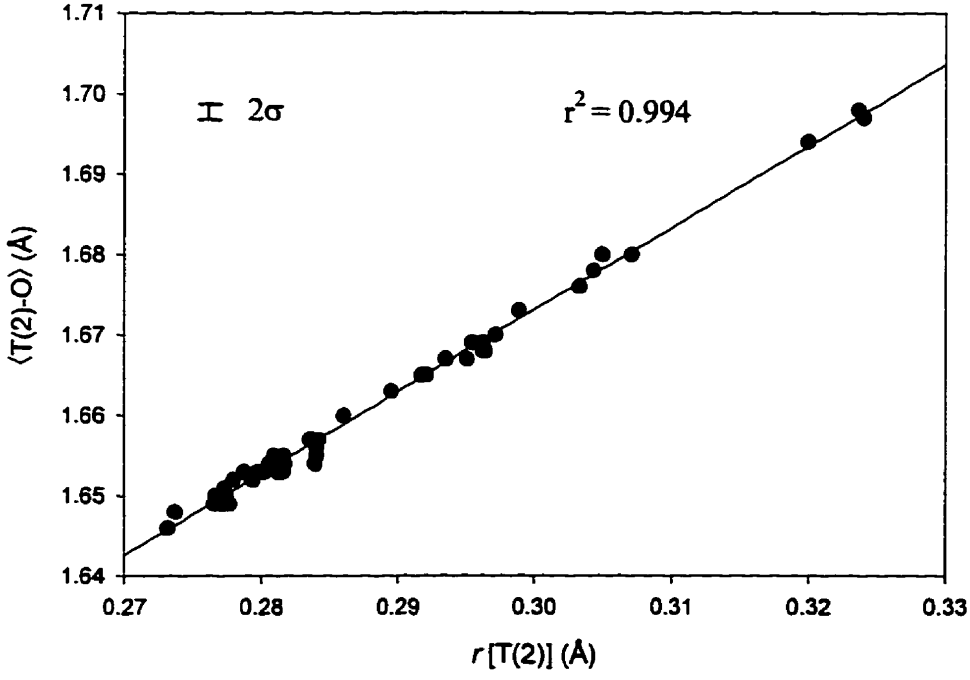


Figure 6: Relationship between ⟨T(2)-O⟩ and constituent T(2) cation radius. The regression line has the form: ⟨T(2)-O⟩ = 1.0176(*r*) + 1.3679.

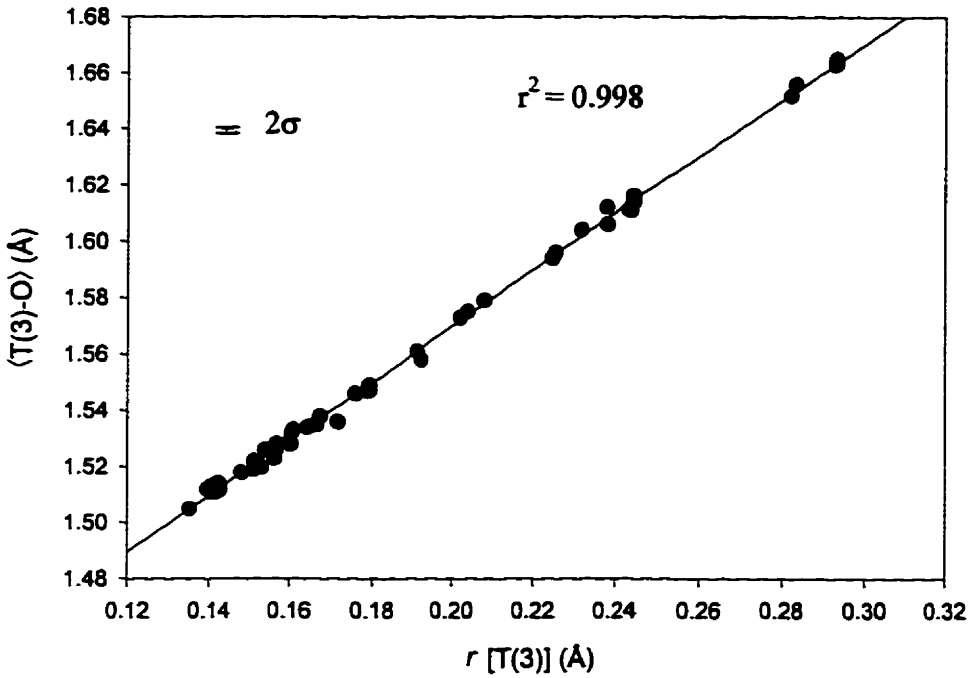


Figure 7: Relationship between ⟨T(3)-O⟩ and constituent T(3) cation radius. The regression line has the form: ⟨T(3)-O⟩ = 1.0039(*r*) + 1.3692.

4.2 Octahedral sites

4.2.1 Preliminary M(2)-site assignment

In accordance with the site scattering species given in Table 3, all refinement stages used an M(2) site modelled by coupled occupancy of Mg and Fe scattering factors. The constituent radii, *r*[M(2)], calculated from these site occupancies are plotted against the observed ⟨M(2)-O⟩ distances (Fig.8). The data define a field that can be outlined by an acute scalene triangle (dashed ; *A,B,C*). With decreasing Fe, the triangular field opens, and near a constituent radius of 0.72 Å ('Mg end-member'), there are positions plotting over a continuous range in ⟨M(2)-O⟩ from ~2.095 to ~2.075 Å (along $\overline{AC}$). The cation at M(2) bonds to O^{2-} at the O(2), O(3), and O(8) positions (App. G.1). The O(3) position is coordinated by 3 cations, and O(2) and O(8) are coordinated by 4 cations each, giving an average empirical O^{2-} radius of 1.373 Å (Shannon, 1976). Adding this O^{2-} radius to the empirical Mg radius of 0.72 Å gives a sum of 2.093 Å. This is close to observed ⟨M(2)-O⟩ values in the vicinity of the triangle vertex *A*. Data that follow the $\overline{AB}$ side of the triangle approximate a slope of 1. Therefore, predicted isomorphous substitution of Fe^{2+}(0.78 Å) for Mg(0.72 Å) at the M(2) site is conformable with data lying along $\overline{AB}$, with positions near *A* representative of the Mg end-member. How does one account for positions lying appreciably below $\overline{AB}$, especially near vertex *C* ? Positions plotting below $\overline{AB}$ have ⟨M(2)-O⟩ distances that are shorter than those predicted by a simple binary Fe^{2+}⇔Mg substitution. This can be explained in terms of a third occupant at M(2) having a shorter empirical radii than Mg(0.72 Å). The two most plausible candidates are Fe^{3+}(0.645 Å) and Al(0.535 Å). By examining data near vertex *C*, we can rule out Fe^{3+} because results of the occupancy refinement at M(2) showed no appreciable Fe for *these* samples. Furthermore, it is assumed that Fe^{3+} is absent at M(2) for all samples. It is therefore concluded that the variation in observed ⟨M(2)-O⟩

distances can be best represented by M(2) site occupants Mg, Fe^{2+} and Al. Adding Al into the aggregate-radius calculation will result in smaller constituent radii (r) that will cause affected positions to plot to the left of current positions on Figure 8. Adjusted in this manner, positions currently below $\overline{AB}$ will then conform to the linearity of $\overline{AB}$.

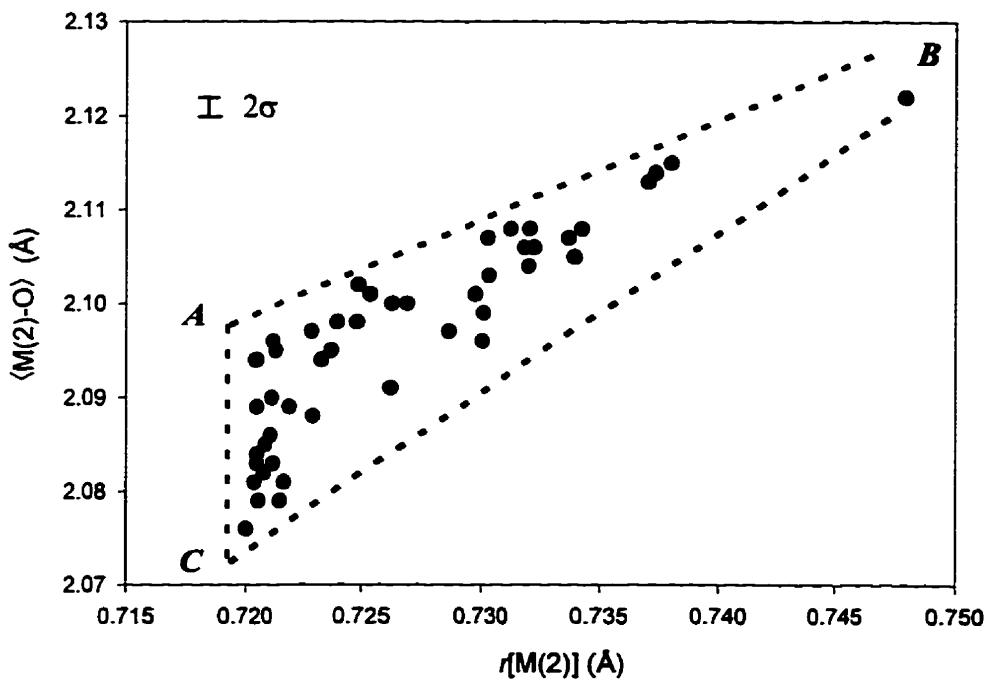


Figure 8: Relationship between ⟨M(2)-O⟩ and constituent M(2) cation radius. The constituent radii, r[M(2)], are calculated using Mg and Fe^{2+} radii and refined Mg and Fe occupancies.

4.2.2 Preliminary M(3) and M(5) site assignments

In accordance with the site-scattering species given in Table 3, all refinement stages have the M(3) and M(5) sites modelled with fixed Al-occupancy factors. At the completion of the secondary-refinement stage, three independent refinement procedures were conducted to test M(3) and M(5) site electron totals. During these tests, the following styles of occupancy refinement were tried: (1) M(3) occupancy fixed , M(5) refining; (2) M(3) occupancy refining , M(5) fixed; (3) both M(3) and M(5) occupancies refining. At the completion of each test, the refined occupancy factors were examined. In all cases, the refined occupancy factors for M(3) and M(5) showed no appreciable deviation from 13 electrons. From this point onward, the M(3) and M(5) sites were therefore modelled with the Al scattering factor and fixed ideal occupancies. Previous investigators have also reported Al as the only significant occupant of the M(3) and M(5) sites (1.5.1). If M(3) and M(5) contain only Al, ⟨M(3)-O⟩ and ⟨M(5)-O⟩ distances should reflect this. Figure 9 shows the variation in ⟨M(3)-O⟩ and ⟨M(5)-O⟩ distances for all kornerupines in this study. The plotted positions are paired vertically, in that a pair of ⟨M(3)-O⟩ and ⟨M(5)-O⟩ values originate from the same sample. All pairs were then sorted according to ⟨M(3)-O⟩ values, such that observed ⟨M(3)-O⟩ distances increase progressively from left to right across the diagram. ⟨M(3)-O⟩ distances range from 1.921 to 1.931 Å (App. G.2). A very weak correlation between increasing ⟨M(3)-O⟩ and ⟨M(5)-O⟩ distances may exist. If the variation in ⟨M(3)-O⟩ distances (Δ=0.01 Å) proved to be significant, is there a simple explanation to account for it ? Arguements could be put forth that would attribute the ⟨M(3)-O⟩ variation to minor steric adjustments in response to neighboring bond-configurations. On the other hand, if the variation were in response to a second occupant, there is only one reasonable choice for that substituent, namely Mg. This last point is explained in the following manner. If ⟨M(3)-O⟩ distances near 1.93 Å were coupled to 100% Al occupancy, then a substituent smaller than Al(0.535 Å) would be

required to give ⟨M(3)-O⟩ distances near 1.92 Å. However, this is impractical, because Al is the smallest octahedral cation recorded from chemical analysis (App. H). ⟨M(3)-O⟩ distances near 1.92 Å could correspond to 100% Al occupancy, the 0.01 Å increase in bond length resulting from a substituent of larger radius than Al. Small amounts of Mg (0.72 Å ; 12 electrons) substituting for Al (0.535 Å ; 13 electrons) would increase M(3)'s average aggregate radius without significantly perturbing the site's electron total. Supporting evidence for minor Mg substitution at the M(3) and M(5) sites is presented in the next section.

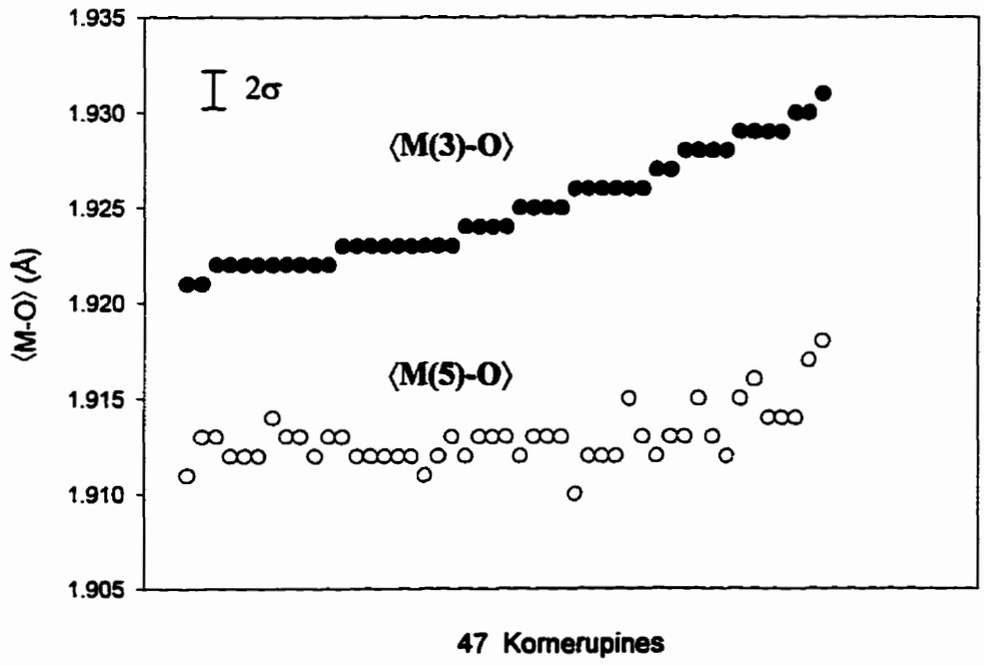


Figure 9: ⟨M(3)-O⟩ (filled circles) and ⟨M(5)-O⟩ (open circles) sample pairs for all 47 kornerupine samples, sorted according to increasing ⟨M(3)-O⟩ values.

4.2.3 Adjusting the M(2), M(3) and M(5) site populations: rationale

When a comparison is made between the M(2) and M(3,5) sites, there is good correlation between the proposed Al content of M(2) and the proposed Mg content of M(3,5). Figure 10 shows an approximate 1 : 1 relation between the proposed $^{M(2)}$Al (*pfu*) and $^{M(3)+M(5)}$Mg (*pfu*). The Al proposed for M(2) is that which will bring about linearity to the ⟨M(2)-O⟩ *vs* *r*[M(2)] plot, and the Mg proposed for M(3) and M(5) will do the same for the corresponding plots for M(3) and M(5).

Of particular interest with regard to kornerupine is the highly variable B content, and the influence that this may have for other crystal chemical parameters. When the proposed Al content of M(2) is plotted against B content (Fig.11), there is a strong inverse correlation. Admittedly, the small range in ⟨M(3)-O⟩ and ⟨M(5)-O⟩ distances in Figure 9, and the narrow spread of ⟨M(2)-O⟩ distances in Figure 8, may seem negligible at first glance. However, the prominent correlations displayed on Figures 10 and 11 clearly indicate that these minor variations in ⟨M-O⟩ distances contain quantitative site-occupancy information. Proving with absolute certainty that minor amounts of a given element actually occur at a specific site is often a very difficult task in complex structures. A strong arguement in support of the substitution comes from improved mutual agreement between other sites that are affected. For this reason, final site populations for M(2) are calculated using Mg, Fe^{2+} and Al.

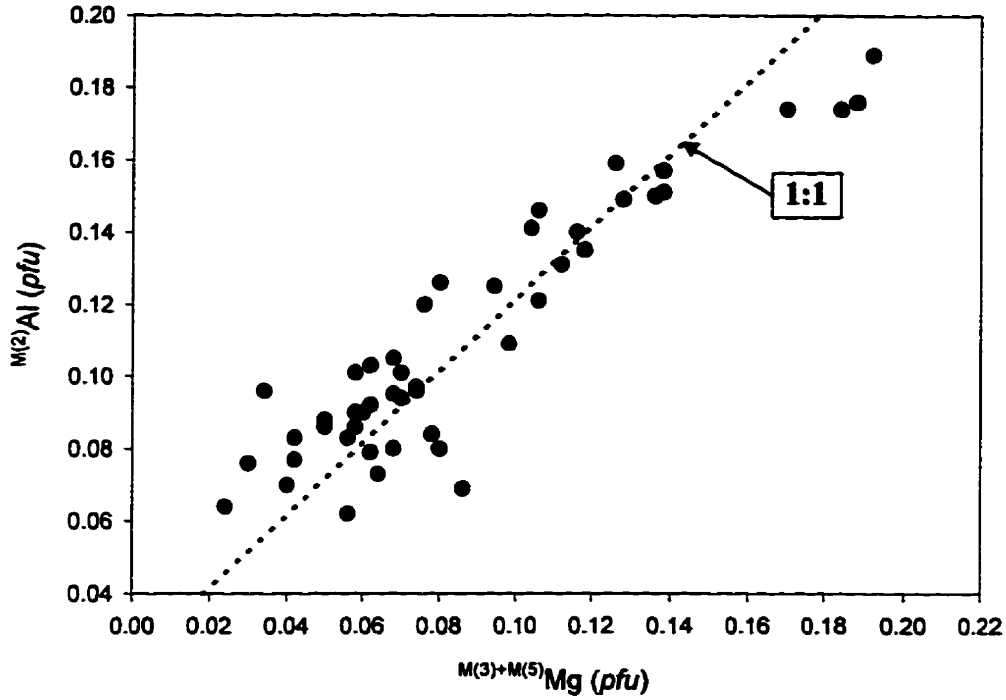


Figure 10: Proposed Al contents of the M(2) site (*pfu*) plotted against the proposed Mg contents of both the M(3) and M(5) sites (*pfu*).

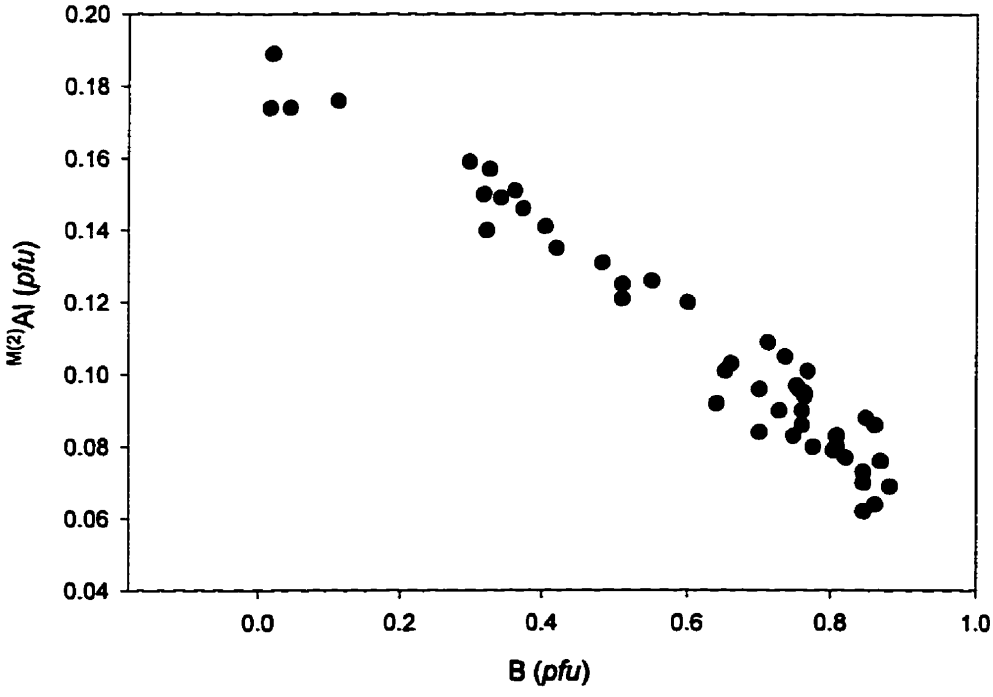


Figure 11: Proposed Al contents of the M(2) site (*pfu*) plotted against the B contents of the T(3) site (*pfu*).

4.2.4 Final M(2), M(3), M(4) and M(5) site assignments

During the tertiary-refinement stage (Table 3), the M(2) site-occupancy is refined in terms of Mg and Fe, the M(4) site in terms of Mg and Fe (in the presence of fixed Al, Cr, Ti and V), and the M(3) and M(5) sites are constrained with fixed Al-occupancies. The tertiary-refinement procedure was not further modified to reflect changes to M(2), M(3) and M(5) (4.2.3) for the following reasons: (1) incorporating very minor amounts of Al at a Mg-dominated site [M(2)], or minor Mg at an Al-dominated site M(3,5), will have a negligible effect on the refinement because of the similiarity in Al and Mg scattering factors; (2) because the relation between the proposed $^{M(2)}Al$ and $^{M(3)+M(5)}Mg$ is near 1:1 (Fig.10), there is little need to change the fixed-Al occupancy factor currently assigned to the M(4) site [$^{[6]}Al = {}^{M(3)}Al + {}^{M(5)}Al + {}^{M(2)}Al + {}^{M(4)}Al$]. Modifying the current tertiary-refinement strategy further is therefore unlikely to produce any significant change. The final M-site-assignment procedure that now follows, however, does not assume a 1:1 relation between $^{M(2)}Al$ and $^{M(3)+M(5)}Mg$, or that the currently fixed Al-occupation factor at M(4) is invariant. The assumptions that were used are : $^{M(4)}[Fe^{3+},Cr,V,Ti]$, $^{M(2)}Fe^{2+}$ and $^{[6]}Al$ are all known at this stage. Therefore, only the Mg/Al ratio needs to be optimized over M(2), M(3), M(4) and M(5) such that all ⟨M–O⟩ *vs* constituent-radii plots approximate linearity. This Mg/Al optimization over the four sites was done as follows :

(1) Start with the M(3) and M(5) sites. Assume a slope of 1 for the relation between ⟨M-O⟩ and constituent radii. Select various appropriate intercept values and record the calculated $^{M(3)}Al$, $^{M(3)}Mg$, $^{M(5)}Al$, and $^{M(5)}Mg$ populations.

(2) Move to the M(4) site. Test a range of slope/intercept combinations corresponding to various Mg/Al distributions. For each slope/intercept combination selected, the

resulting Mg/Al for the M(2) site will be determined, in that all $^{[6]}$Al not yet assigned to M(3), M(5) or M(4), goes to M(2).

(3) The newly generated ⟨M(2)-O⟩ *vs* *r*[M(2)] plot is then compared to the preliminary plot (Fig.8) for relative improvement or deterioration.

This entire cycle (1→3) was repeated several tens of times for various starting intercepts at M(3) and M(5). Many scenarios were tested involving: (i) Mg at M(3) ±Mg at M(5); (ii) no Mg at either M(3) or M(5); (iii) Mg at both M(3) and M(5). For each of these conditions, several choices in M(3) and M(5) intercept allowed testing over quite varied $^{M(3)+M(5)}$Al. When the Al/Mg site distributions are assessed in this sequence (1→3), there are two important factors that work together to help the results :

- the data near $\overline{AB}$ on the original ⟨M(2)-O⟩ *vs.* *r*[M(2)] diagram (Fig. 8) cannot move much. It was already determined (4.2.1) that these positions were in relatively good agreement with empirical (cation + anion) radii. The main objective was to shift positions lying below $\overline{AB}$ sufficiently to the left (Al replacing Mg) so as to conform to the linearity of $\overline{AB}$.
- because the Al/Mg adjustments were handled in the sequence M(3),M(5)→M(4)→ M(2), there is an enhanced relative sensitivity attached to the process. This results from the relative multiplicities of the crystallographic sites involved, namely 2:2:2:1 for M(3) : M(5) : M(4) : M(2) respectively — small changes to M(3), M(5) and M(4) result in large changes to M(2).

The subsequent adjustments at M(3), M(5) and M(4) that gave the most appropriately adjusted M(2) result, represents the best Al/Mg M-site distribution. Slight changes to the fixed

quantity $^{M(4)}$Al were updated in the last stage of tertiary-refinement. This was done as a precautionary measure, because there existed a potential for the $^{M(4)}$Fe occupancy value to marginally change as a result of a changed $^{M(4)}$Al occupation factor. Because the Fe at M(4) is present as Fe^{3+}, a change in refined Fe occupancy would necessitate recalculation of the EMP data. However, no further change in Fe occupancy occurred at the M(4) site for any of the kornerupine refinements.

Now that Al/Mg values have been optimized for the M(3), M(5), M(4) and M(2) sites, the last remaining task is to properly distribute the relative error associated with the above partioning process among the four sites (*i.e.*, based on relative site-multiplicities). After error adjustments, the assigned site populations for M(2), M(3), M(4), and M(5) were complete (Figs. 12-15) (App. F). Observed ⟨M(3)–O⟩ distances vary from 1.921 to 1.931 Å and correspond to site populations ranging from $Al_{0.995}Mg_{0.005}$ to $Al_{0.942}Mg_{0.058}$, respectively (Fig.12). Observed ⟨M(5)–O⟩ distances vary from 1.910 to 1.918 Å and correspond to site populations ranging from $Al_{0.994}Mg_{0.006}$ to $Al_{0.960}Mg_{0.040}$, respectively (Fig.13). Observed ⟨M(2)–O⟩ distances vary from 2.076 to 2.122 Å , and reflect the following maximum ranges in site occupants : $Mg_{(0.448\rightarrow0.909)}$, $Fe^{2+}_{(0.000\rightarrow0.466)}$, $Al_{(0.062\rightarrow0.189)}$ (Fig.14). Observed ⟨M(4)–O⟩ distances vary from 1.943 to 1.979 Å , and reflect the following maximum ranges in site occupants : $Al_{(0.571\rightarrow0.890)}$, $Mg_{(0.096\rightarrow0.315)}$, $Fe^{3+}_{(0.000\rightarrow0.174)}$, $Ti_{(0.000\rightarrow0.014)}$, $Cr^{3+}_{(0.000\rightarrow0.014)}$, $V^{3+}_{(0.000\rightarrow0.010)}$ (Fig.15). Linear regression analysis for the M(2), M(3) and M(4) sites gave reasonable intercept values for all sites ; however, slope values of 0.98 and 0.93 for M(2) and M(3) respectively, are quite different than the 0.78 slope of M(4). An analogous situation occurs at the M(2) site in amphiboles where the slope of the ⟨M(2)–O⟩ *vs.* constituent radii plot has a similiarly shallow slope (Hawthorne, 1983).

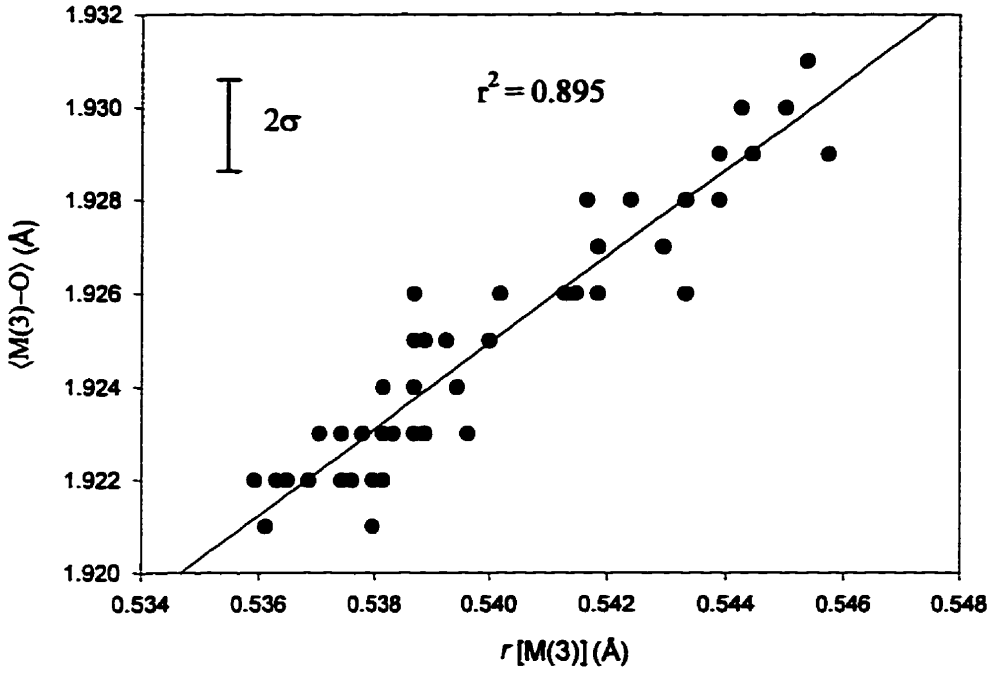


Figure 12: Relationship between ⟨M(3)-O⟩ and constituent M(3)-cation radius. The regression line has the form ⟨M(3)-O⟩ = 0.9276 + 1.4241.

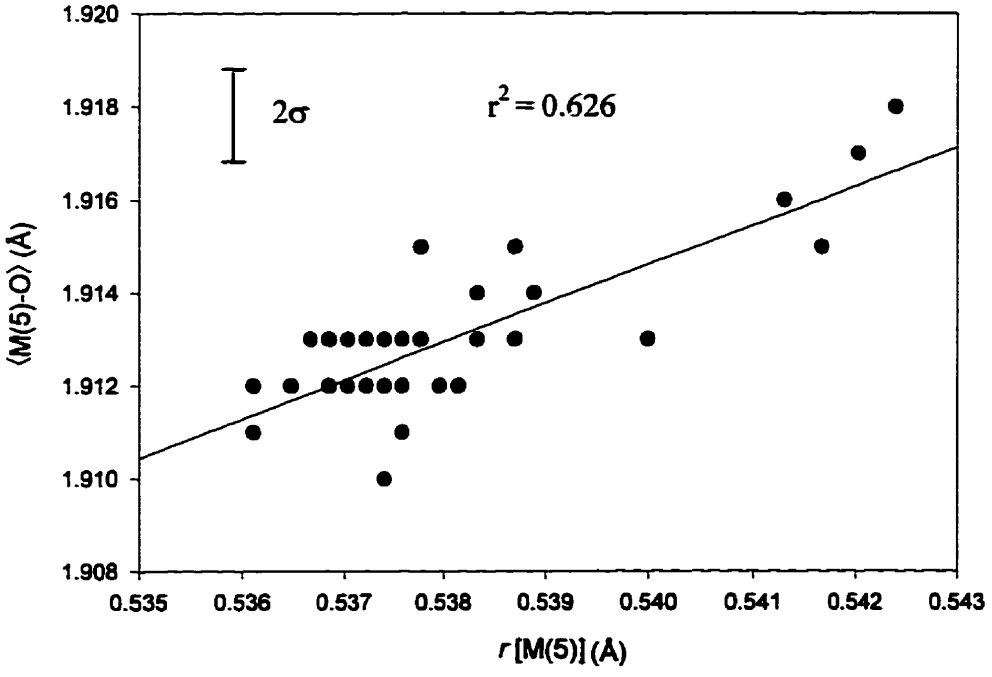


Figure 13: Relationship between ⟨M(5)-O⟩ and constituent M(5)-cation radius. The regression line has the form ⟨M(5)-O⟩ = 0.8363 + 1.4631.

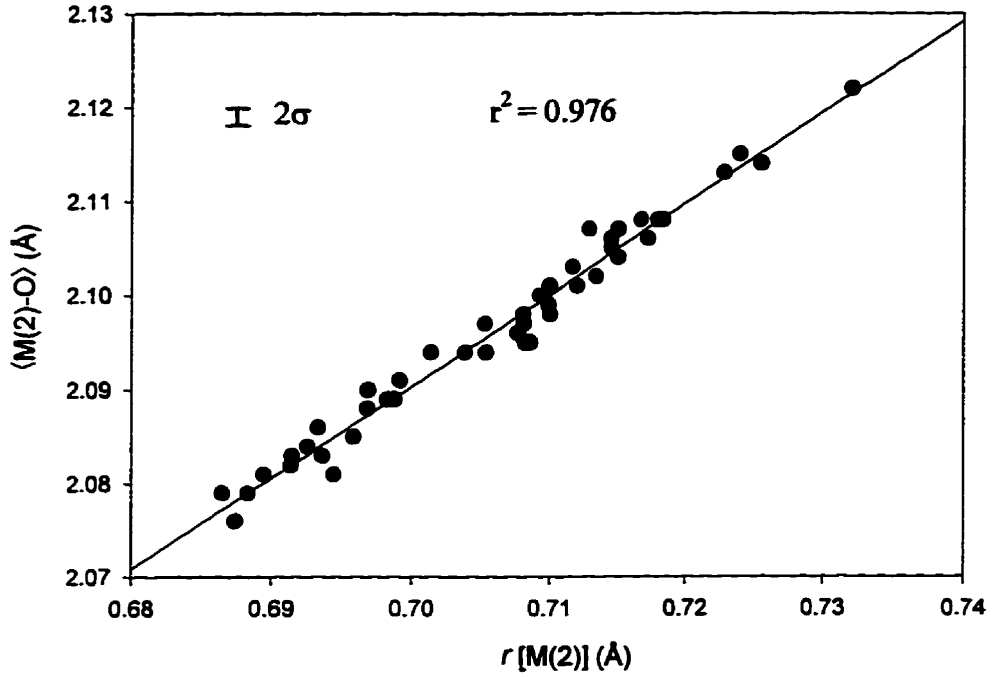


Figure 14: Relationship between ⟨M(2)-O⟩ and constituent M(2)-cation radius. The regression line has the form ⟨M(2)-O⟩ = 0.9722 + 1.4098.

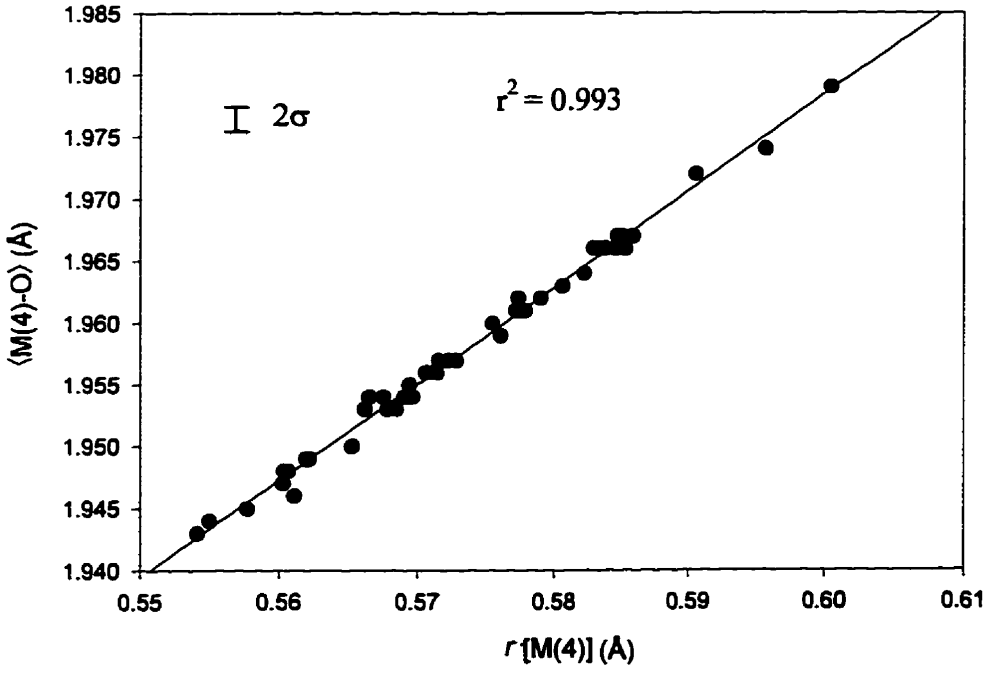


Figure 15: Relationship between ⟨M(4)-O⟩ and constituent M(4)-cation radius. The regression line has the form ⟨M(4)-O⟩ = 0.7802 + 1.5103.

4.2.5 The M(1) site

In accordance with the site-scattering species given in Table 3, all refinement stages have the M(1) site modelled with Mg and Fe scattering factors. The ⟨M(1)–O⟩ *vs.* constituent-radius plot (Fig. 16) is constructed using the refined Mg and Fe occupancies and standard empirical radii for Mg(0.72 Å) and Fe^{2+}(0.78 Å). Plotted positions are corrected for anion size-differences resulting from F⇔OH substitution at the O(10) site. The variation in ⟨M(1)–O⟩ distance spans 0.014 Å (2.111 to 2.125 Å) and the variation in site occupants ranges from $Mg_{0.994}Fe^{2+}_{0.006}$ to $Mg_{0.646}Fe^{2+}_{0.354}$ (App. F). Taken in their entirety, all data conform rather poorly ($r^2 = 0.48$) to a linear relation between ⟨M(1)–O⟩ and *r*[M(1)]. The samples represented in Figure 16 have been subdivided into 3 groups based on their B contents (*pfu*) : open circle = $0 \rightarrow {}^1/_3$ B; circle with cross = ${}^1/_3 \rightarrow {}^2/_3$ B; filled circle = ${}^2/_3 \rightarrow 1$ B. The sample group with the greatest B content (shown by the filled circles) delineates a reasonable correspondence between ⟨M(1)–O⟩ and *r*[M(1)]. The extent of this relation is marked on Figure 16 with a dashed line and the letters *A* and *B* (slope ~0.7). Positions plotting near *A* are characterized by ⟨M(1)–O⟩ distances of ~2.112 Å and constituent radii of ~0.72 Å (*i.e.*, Mg). By comparison, a constituent radii of 0.72 Å at the M(2) site coincides with an observed ⟨M(2)–O⟩ distance of 2.110 Å (Fig. 14). Therefore, good relative agreement exists between observed ⟨M–O⟩ distances and a constituent radius of 0.72 Å for both the M(1) [near *A*] and M(2) sites. The data corresponding to the lowest B content (open circles) deviate significantly from the relation $\overline{AB}$ (Fig. 16) ; a less pronounced deviation is shown by the data corresponding to intermediate B content (circles with crosses). Multiple-regression analysis using the constituent radii *r*[M(1)] and B content (*pfu*) as independent variables gives a much improved overall relation ($r^2 = 0.85$) with the observed ⟨M(1)–O⟩ distances. This is illustrated in Figure 17, where the coefficients derived from multiple

regression are multipled by their respective independent variable quantities, and the result is plotted against the observed ⟨M(1)–O⟩ distances.

The M(1) site links *via* the bridging-oxygen O(10) to another M(1) site (Figs.2,3). The O(5)–O(7) edge of the M(1) octahedron is shared with the T(2) tetrahedron (Fig. 3). The widespread chemical variation associated with the T(2)–T(3)–T(2) tetrahedral trimer (*i.e.*, B, Si, Al) is closely tied to the M(1) site through these shared O(5)–O(7) edges. It is therefore postulated that B–Si–Al variations over the tetrahedral trimer induce a steric response from the M(1) octahedron that, in addition to $Mg \Leftrightarrow Fe^{2+}$ substitution at M(1), accounts for the variation seen in ⟨M(1)–O⟩ distances.

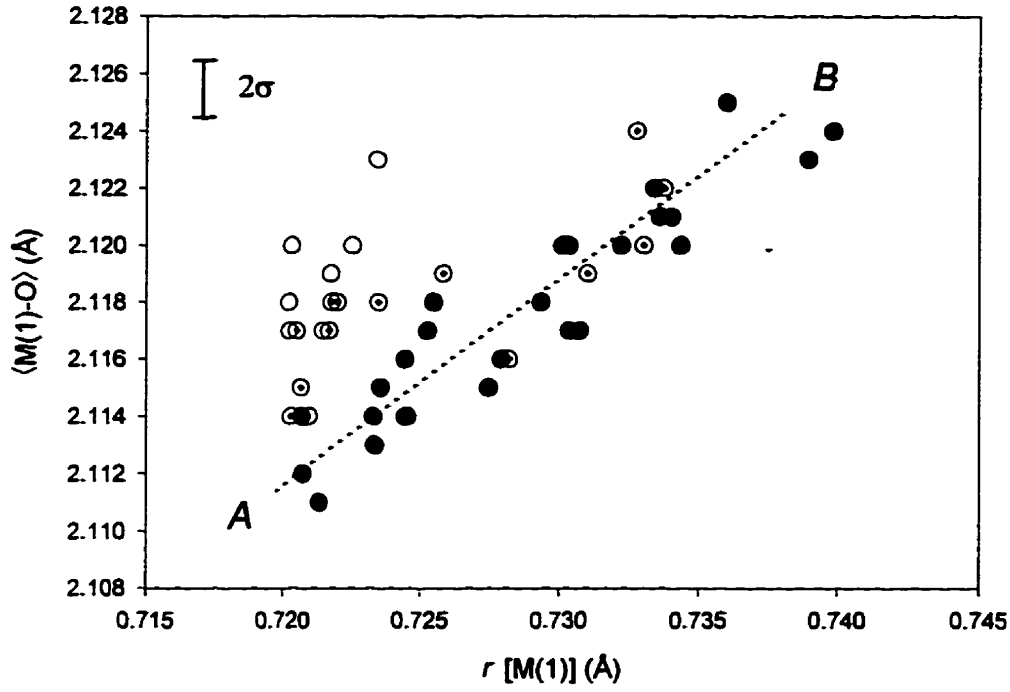


Figure 16: Relationship between ⟨M(1)-O⟩ and constituent M(1)-cation radius. Open circle = 0→$^1/_3$ B ; circle with cross = $^1/_3$→$^2/_3$ B ; filled circle = $^2/_3$→1 B.

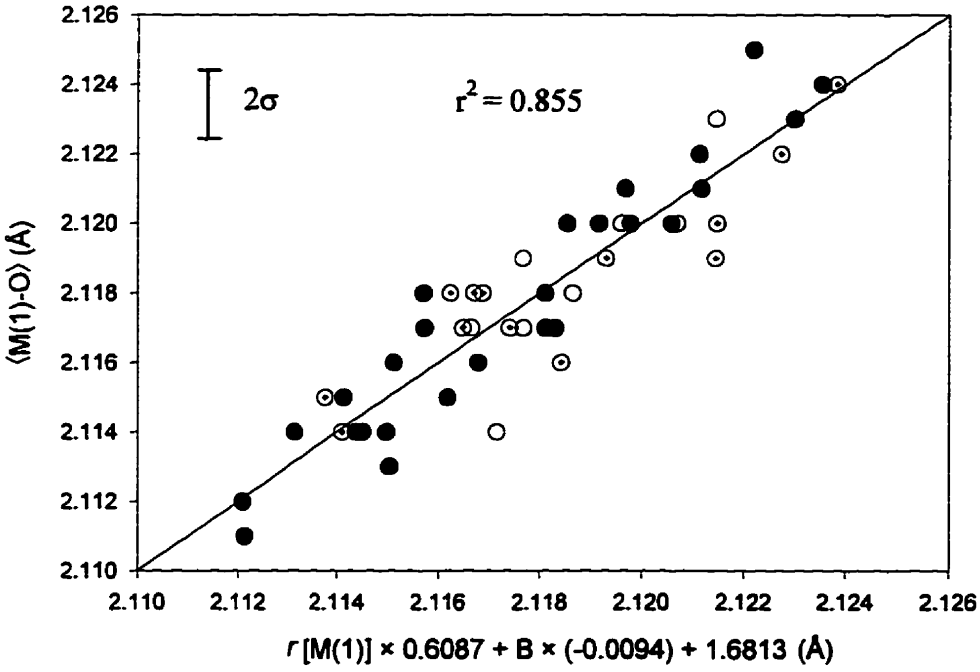


Figure 17: Relationship between ⟨M(1)-O⟩ and the $\langle M(1)\text{-}O\rangle_{predicted}$ from multiple regression using *r*[M(1)] (Å) and B(*pfu*) as independent variables. Symbols as in Fig.16.

4.3 The X site

Of all the crystallographic sites in kornerupine, the eight-coordinate X site represents the most difficult situation in which to quantify the respective occupants. This results mainly from the variable vacancy (□) occurring at X. Interpretation of mean bond-lengths and refined occupancies becomes a much more difficult task when variable □ is involved. The X-site occupants are composed of Na, Ca and Mn (from EMP data) plus the Fe^{2+} and Mg remaining after the octahedral assignments, together with sufficient □ to fill the site. The ⟨X–O⟩ distances are plotted against □ in Figure 18. With increasing □, there is an apparent convergence in the pattern of data points at ⟨X–O⟩ ≈ 2.415 Å and 82% □ (accentuated with dashed lines). It therefore seems reasonable to calculate an approximate radius for □, using the ⟨X–O⟩ distance of 2.415 Å and a typical oxygen radius of 1.37 Å (*i.e.*, 2.415 Å - 1.37 Å = 1.045 Å). The various sizes for the proposed X occupants (C.N. = 8), in ascending order, are: Mg = 0.89 Å; Fe^{2+} = 0.92 Å; Mn^{2+} = 0.96 Å; □ = 1.045 Å; Ca = 1.12 Å; Na = 1.18 Å. All Mn from EMPA was presumed to order at the X site as Mn^{2+}. Also, note that during EMPA, K was analyzed for but not detected. It is quite plausible that K (1.51 Å) is too large to be accomodated at X. The ranges proposed for these various X-occupants are as follows: $□_{0.597\rightarrow0.815}$; $Mg_{0.073\rightarrow0.393}$; $Fe^{2+}_{0.000\rightarrow0.231}$; $Mn^{2+}_{0.000\rightarrow0.038}$; $Na_{0.000\rightarrow0.034}$; $Ca_{0.000\rightarrow0.012}$ (App. F). The ⟨X–O⟩ distances are plotted against the constituent radii in Figure 19 (plotted positions are corrected for anion-size differences resulting from F⇔OH substitution at the O(10) site). Taken in their entirety, all data conform poorly (r^2 = 0.29) to a linear relation between ⟨X–O⟩ and *r*[X]. As was done for the M(1) site, the samples represented in Figure 19 were subdivided into the same three groups based on B content (*pfu*): open circle = $0\rightarrow{}^1/_3$ B; circle with cross = $^1/_3\rightarrow{}^2/_3$ B; filled circle = $^2/_3\rightarrow1$ B. The sample group with the greatest B content (shown by the filled circles) delineates a reasonable correspondence between ⟨X–O⟩ and *r*[X]. The extent of this relation is marked on

Figure 19 with a dashed line and the letters *A* and *B* (slope ~0.75). The data corresponding to lowest B content (open circles) deviate significantly from the relation $\overline{AB}$ (Fig. 19), and a less pronounced deviation is shown by the data corresponding to intermediate B content (circles with crosses). One might expect a possible relation between ⟨X–O⟩ and B, because the large X polyhedron is likely somewhat susceptible to steric influences from neighboring regions of the structure due to the 60-80% vacancy at X. Extreme B–Si–Al substitutional ranges presented in section 4.1 for the T(2)–T(3)–T(2) tetrahedral trimer certainly provide potential for steric influence on neighboring sites. Another factor that likely contributes to variations in interatomic distances in the vicinity of X is the H-bonding that involves the O(10) and O(9) positions [O(10)—H·····O(9) ; Klaska & Grew, 1991]. The relation F + OH = 1 suggests that, because F ranges from 0→0.48 *pfu* (App. H), variable H-bonding would occur. Multiple-regression analysis using the three independent variables *r*[X], B and F gives a much improved correlation ($r^2 = 0.897$) with ⟨X–O⟩ distances. This is illustrated in Figure 20, where the coefficients derived from multiple-regression analysis are multiplied by their respective independent-variable quantities, and the result is plotted against the observed ⟨X–O⟩ distances.

So far, The X-site occupants have been discussed in terms of what cations were available to put at X, following the octahedral assignments. Assessment of ⟨X–O⟩ distances show that these cations are conformable with the variation in ⟨X–O⟩ (Fig. 20). Additional supporting evidence for these cation assignments is contained in the X-ray scattering (electron total) at the X site. If the cations proposed for X are correct, analogous electron-totals should be derived at X from the structure refinements. The X-ray scattering at X was modelled in the following manner:

(1) fix Ca and Na occupancies at X to agree with Ca and Na from EMPA;

(2a) insert the Mg scattering factor at X, refine the occupancy factor. Record results;

(2b) insert the Fe scattering factor at X, refine the occupancy factor. Record results

The proposed X-occupants consist mainly of Mg and Fe^{2+} over a wide range of Mg/Fe ratios (App. F). Due to the large electron difference between Mg(12e) and Fe(26e), the two species have significant differences in X-ray scattering. Thus, refinement results will give different electron totals that evolve from the use of Mg *vs.* Fe scattering factors at the X site. In order to assess the scattering at X in an unbiased manner, two separate refinements were run: (1) with the Mg scattering factor (2a); (2) with the Fe scattering factor (2b). The correct scattering must fall somewhere between these two extremes. The electron totals for all proposed X-cations are plotted against the X-electron totals refined in Figure 21. The lengths of the horizontal bars reflect the difference between electron totals arrived at using the Mg and Fe scattering factors, respectively, in addition to ± 1 sigma for these respective electron totals. The dashed line drawn through the data is a 1:1 reference line. For all data (47 kornerupines) plotted in this manner on Figure 21, the relative agreement between the proposed and observed electrons agrees within half an electron. A factor that contributes to lower precision in observed bond lengths and X-ray scattering is related to the uncertainty at the X site scattering center as reflected in the variation in atomic-displacement parameters of the X cation. The U_{11} displacement parameter is especially prominant in this regard; its value can be up to 10x that associated with the octahedral cations. These 47 kornerupies have a maximum Fe^{3+}/Fe^{2+} ratio of 0.45 (App. F), and are referred to as the 'ferrous-iron kornerupines' in this study. Samples K4, K48 and K51 are all from Bamble, Norway (App. A); they have distinctively higher Fe^{3+}/Fe^{2+} ratios (~2.5) and plot in the vicinity of the ● symbol (Fig.21). Sample K44 (App. A) is from Mautia Hill, Tanganyika (• symbol) and has the greatest Fe^{3+}/Fe^{2+} ratio (~7.7) encountered in this study.

The samples from Bamble, Norway plot significantly off the 1:1 reference line on Figure 21. Their plotted position indicates that there is insufficient X-ray scattering at X to account for the proposed X cations. Assuming that the EMPA is complete and accurate, and that the X-ray

scattering at the cation sites is also accurate, the two most plausible ways to account for this discrepancy are:

(1) the Fe^{3+}/Fe^{2+} ratio is too low; increasing Fe^{3+} will reduce the cations proposed for X;

(2) the H-content is too low; increasing H will reduce the cations proposed for X

Increasing Fe^{3+} would require the incorporation of Fe^{3+} at M(1), M(2) or X, as all Fe at M(4) is designated as Fe^{3+} already. The M(2) site is smaller than M(1) (*cf.* Figs.14&17), it already contains minor Al (4.2.4), and therefore would be the preferred site for Fe^{3+}. However, the X-ray scattering at M(2) suggests a maximum Fe content of 0.03 *apfu* — an insignificant amount. Fe^{3+} is unlikely to order at the larger divalent M(1) site, or at the X site. Therefore, a re-interpretation of octahedral assignments is unlikely to bring about the needed adjustment in Fe^{3+}.

In considering (2) above, the EMP results for the Bamble, Norway, samples show that F is below its detection limit. Therefore, the formula calculation is effectively based on 1 H *pfu* (*i.e.*, F + OH = 1). In order to increase the H above 1 *apfu*, H_2O must be present at O(10) as there are no other possible H-donor sites (1.5.1).

Of the two options available to reduce the cations proposed for X to conform with the X-ray scattering at X, I favor the incorporation of H_2O at O(10) over the assignment of Fe^{3+} to M(1), M(2) or X. Greater oxidizing conditions are favorable for H_2O incorporation, and therefore consistent with this hypothesis (pers. comm., Ed Grew). As H_2O remains a controversial occupant in kornerupine, I was reluctant to include the more oxidized samples from Bamble, Norway (K4, K48, K51) and Mautia Hill, Tanganyika (K44) into the rigorous treatment involving the 47 ferrous-iron kornerupines — self consistency within the mean bond length *vs.* constituent radii relations may have been compromised through inclusion of wrongly interpreted data from the ferric-iron kornerupines.

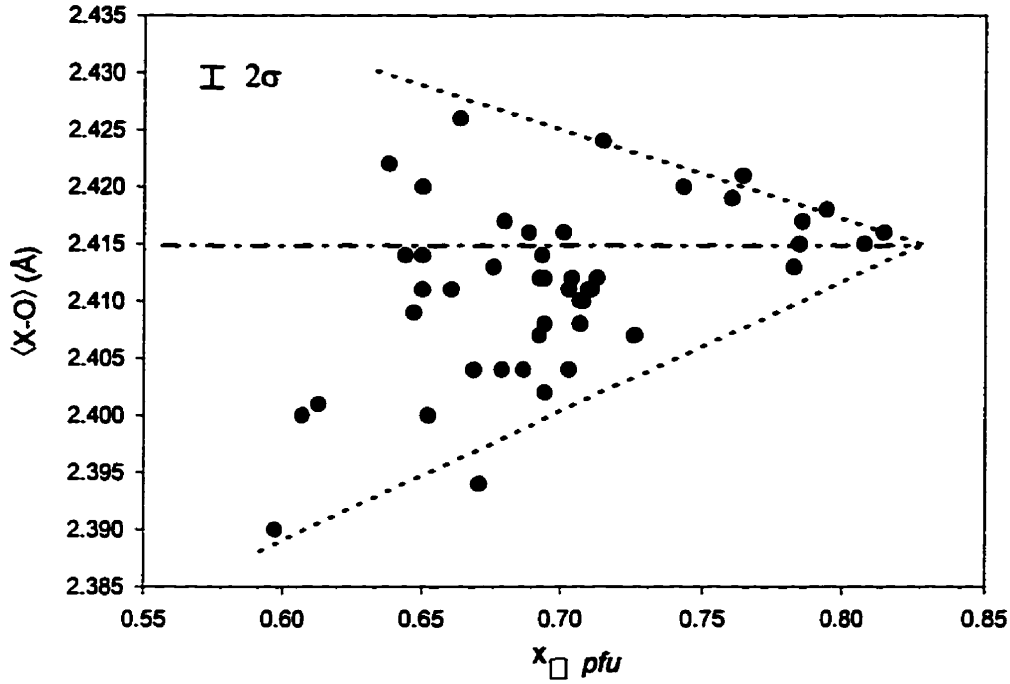


Figure 18: Relationship between ⟨X-O⟩ and vacancy at X ($^{X}\square$). Convergence of data points at ⟨X-O⟩ ≈ 2.415 Å and $^{X}\square \approx 0.82$.

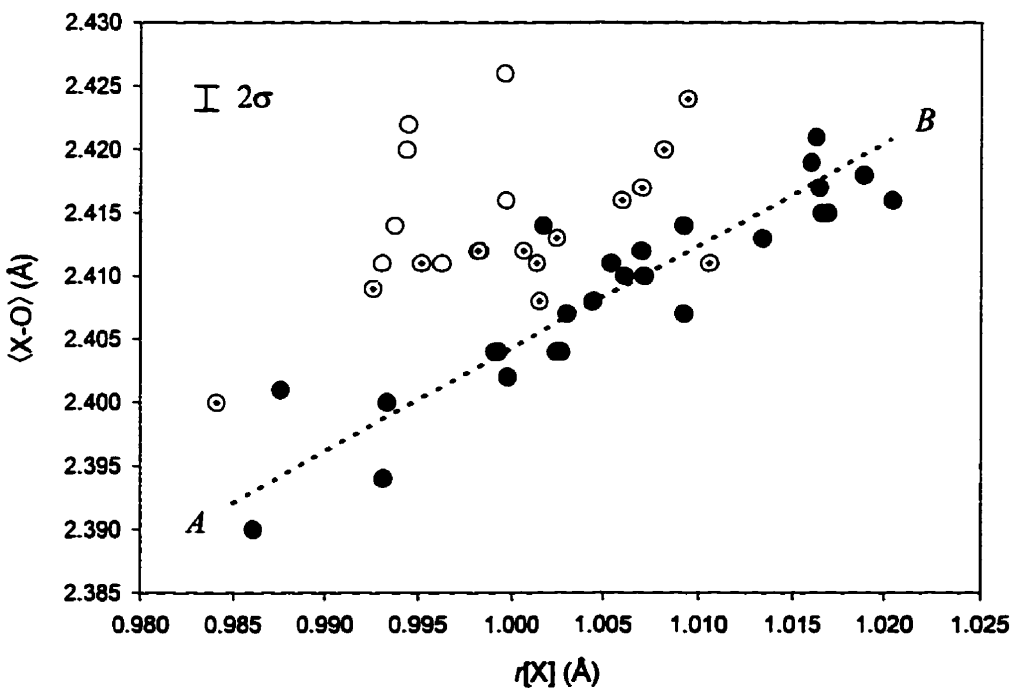


Figure 19: Relationship between ⟨X-O⟩ and constituent X-cation radius.
Open circle = $0 \rightarrow {}^{1}/_{3}$ B ; circle with cross = ${}^{1}/_{3} \rightarrow {}^{2}/_{3}$ B ; filled circle = ${}^{2}/_{3} \rightarrow 1$ B.

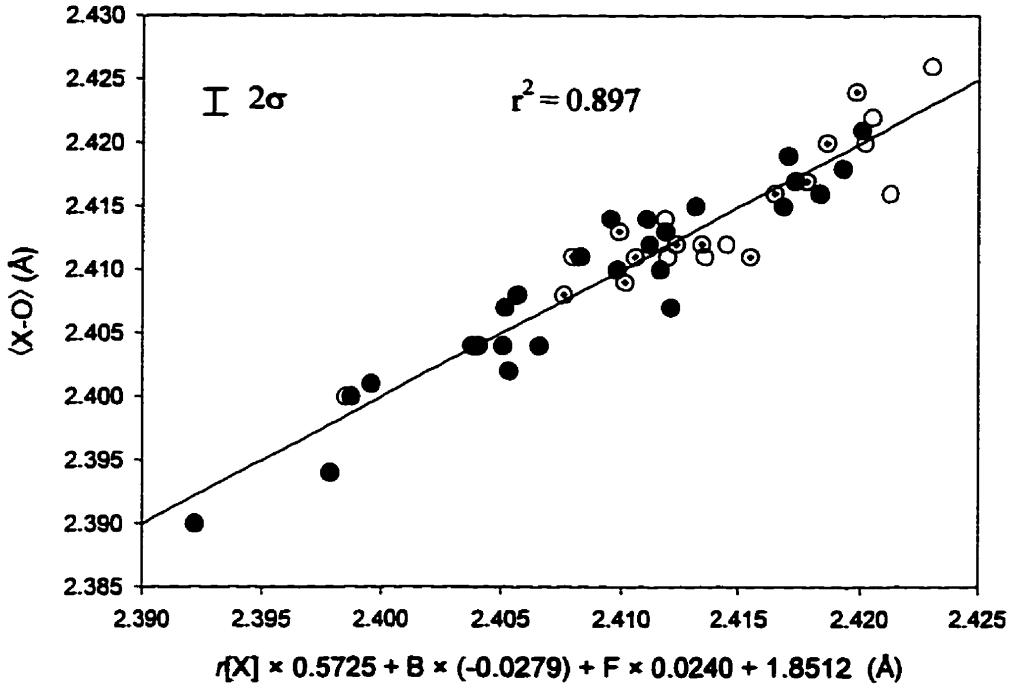


Figure 20: Relationship between ⟨X-O⟩ and the $\langle X\text{-}O\rangle_{predicted}$ from multiple regression using *r*[X] (Å), B(*pfu*) and F(*pfu*) as independent variables. Symbols as in (Fig.19).

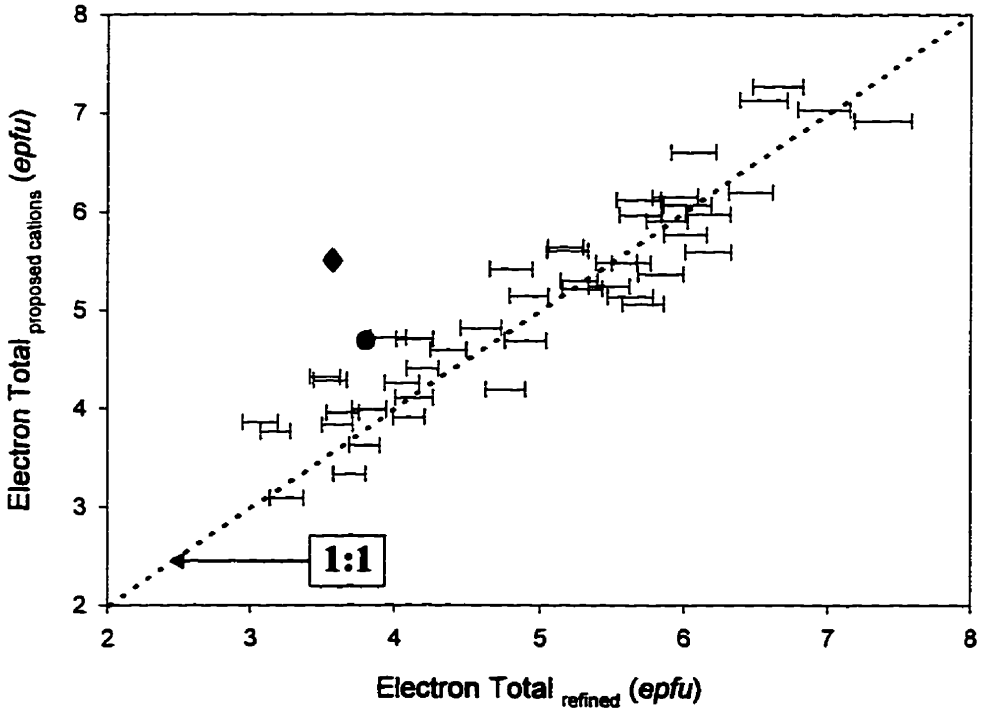


Figure 21: Relationship between X-site electrons from proposed cations and X site electrons refined. ♦ (K4, K48, K51) ; • (K44).

CHAPTER 5

KORNERUPINE CRYSTAL CHEMISTRY

5.1 Kornerupine chemistry

5.1.1 Major variations

The range in oxide (weight percent ; wt.%) and ion (*apfu*) content for the 47 ferrous-iron kornerupines is presented in Table 4 (App. H).

TABLE 4: KORNERUPINE OXIDE (wt.%) AND ION (*apfu*) RANGES

OXIDE	Wt. %	ION	*apfu*
SiO_2	28.53 → 32.38	Si^{4+}	3.55 → 3.88
Al_2O_3	37.75 → 49.57	Al^{3+}	5.60 → 7.16
B_2O_3*	0.08 → 4.21	B^{3+}	0.02 → 0.88
MgO	10.81 → 21.74	Mg^{2+}	2.06 → 3.92
FeO	— → 12.09	Fe^{2+}	— → 1.29
Fe_2O_3**	— → 3.63	Fe^{3+}	— → 0.35
MnO	— → 0.35	Mn^{2+}	— → 0.04
V_2O_3	— → 0.20	V^{3+}	— → 0.02
Cr_2O_3	— → 0.28	Cr^{3+}	— → 0.03
TiO_2	— → 0.30	Ti^{4+}	— → 0.03
Na_2O	— → 0.14	Na^{+}	— → 0.03
CaO	— → 0.09	Ca^{2+}	— → 0.01
F	— → 0.94	F^{-}	— → 0.37
H_2O***	0.75 → 1.23	H^{+}	0.63 → 1.00
		Cation Sum	14.18 → 14.41

* boron *via* SREF at T(3)

** ferric-iron *via* SREF at M(4)

*** anion normalization based on (F + OH = 1) for 22 oxygens

— near detection limits and less than 0.01 *apfu*

The maximum variation for the major elements, expressed as wt.% oxides, as follows is: Al_2O_3 (11.8%); MgO (10.9%); FeO (12.1%); B_2O_3 (4.1%); SiO_2 (3.9%). All minor elements, expressed as wt.% oxides, are below 0.5%. The highest F value measured is 0.94 wt.% F; corresponding calculated wt.% H_2O values (*i.e.*, F + OH = 1) are from 0.75 to 1.23%.

Of the 5 *apfu* available at the three tetrahedral sites, Si occurs over a range of 0.33 *apfu* (*i.e.*, 3.55 to 3.88 *apfu*). In addition to Si, B (0.02 to 0.88 *apfu*) also resides at the tetrahedra [specifically T(3)]. For the octahedral and X sites, the range in Mg spans 1.86 *apfu* and the range for Fe^{2+} is 1.29 *apfu*. Al occurs at both the octahedral and tetrahedral sites over a net range of 1.56 *apfu*. The octahedra contain an additional trivalent species, Fe^{3+}, up to 0.35 *apfu*.

Processing of the oxides from EMPA using the anion normalization scheme [O_{21} (F + $OH)_1$] results in cation totals ranging from 14.18 to 14.40 *apfu*, and a maximum F content of 0.37 *apfu*. The corresponding vacancy calculated for X ranges from 0.60 to 0.82 *pfu*.

The total anion charge is 43^- *pfu* [*i.e.*, $21(O)^{2-}$ + $1(OH,F)^{1-}$] and therefore the cation charge is constrained to be 43^+ *pfu*. The tetrahedral and octahedral sites contain 14 cations *pfu* [$T(1)_2$ + $T(2)_2$ + $T(3)_1$ + $M(1)_2$ + $M(2)_1$ + $M(3)_2$ + $M(4)_2$ + $M(5)_2$], and the X site, primarily occupied by Mg and Fe^{2+}, contains from 0.18 to 0.40 cations *pfu*. As a result, there are a variable number of cations that must sum to 43^+ *pfu*. To maintain this overall charge of 43^+ *pfu*, the variable cation content of X is coupled to changes in the ratio of 2^+ : 3^+ : 4^+ cations in the rest of the structure. This relationship between variable number of cations and maintenance of constant 43^+ charge *pfu* is shown in Figures 22 and 23. In Figure 22, the 2^+ cation total is plotted against the 4^+ cation total. Variation in 4^+ cations corresponds to variation in Si as no other significant tetravalent cations are present. The 2^+ cation total reflects the sum Mg + Fe + Mn (Ca values are insignificant). In a similiar manner, the 3^+ cation total (Al + B + Fe + Cr + V + $[Ti^{4+}]$) is plotted against the 4^+ cation total (Si) in Figure 23. Parallel dashed lines drawn through the plotted

positions are equipotential lines of constant □. Substitutions involving adjustments to $2^+/3^+$ cation ratios with changing Si (4^+) can potentially follow many paths through the data. If the substitution occurs with no change in cation total, then the substitution path must parallel the dashed lines [*i.e.*, a Tschermak-type $2(3^+) \Leftrightarrow (4^+) + (2^+)$ substitution]. All other substitution paths that do not parallel the series of dashed lines involve an additional coupled substitution with □ at the X site. Substitution paths oriented at a high angle to the □-equipotential lines will involve significant coupled substitution with □. A substitution path perpendicular to the dashed lines has a slope of -8 in Figure 22 and a slope of 4 in Figure 23 — its equation $8(2^+) \Leftrightarrow 4(3^+) + (4^+) + 3(□)$ is valid over a maximum of $0.60 \leq □ \leq 0.82$. The distribution of data in Figures 22 and 23 show the lowest and highest Si compositions occurring at $\sim^2/_3$ □. Over the maximum range in Si, the Tschermak-type substitution is able to accomodate changes in 2^+, 3^+ and 4^+ cations without involving a coupled □ substitution. With increasing □ (*i.e.*, 2/3 □ → 0.85 □), possible substitution paths through the data corresponding to the Tschermak-type substitution become progressively shorter in length; at □ ≈ 0.85, the distribution of data may imply that the Tschermak-type substitution is unlikely to occur. In summary, the Tschermak-type substitution is potentially most extensive at relatively low □, and substitutions involving X-site □ are potentially most extensive at intermediate Si compositions.

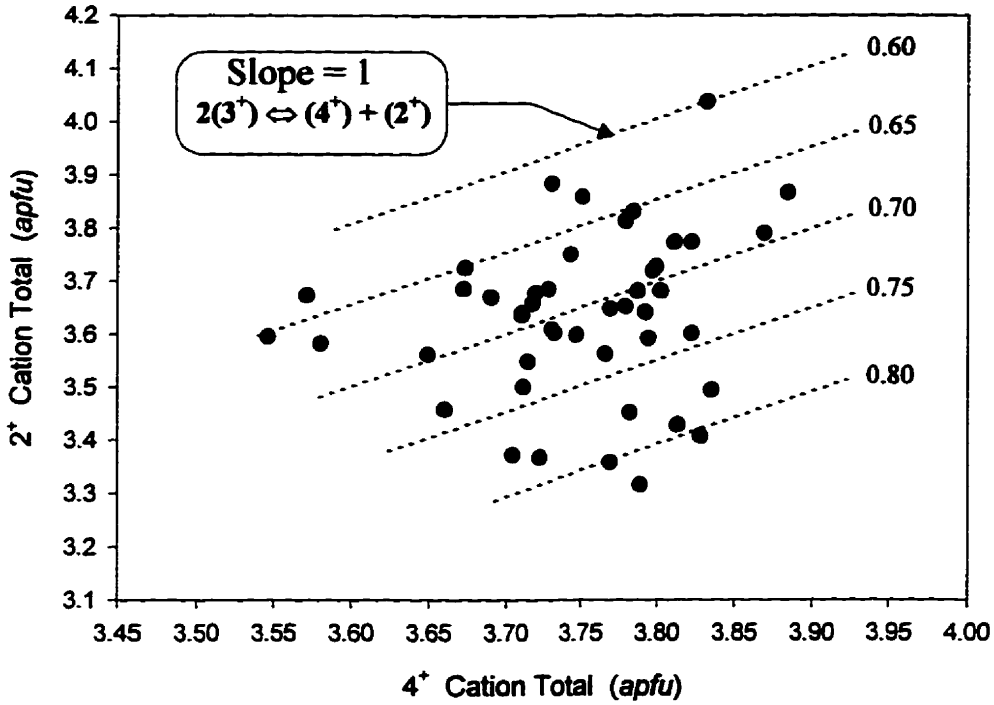


Figure 22: 2^+-cation total (Mg + Fe + Mn) *apfu* plotted against the 4^+-cation total (Si) *apfu*. Dashed lines are equipotential lines representing the □ *pfu*.

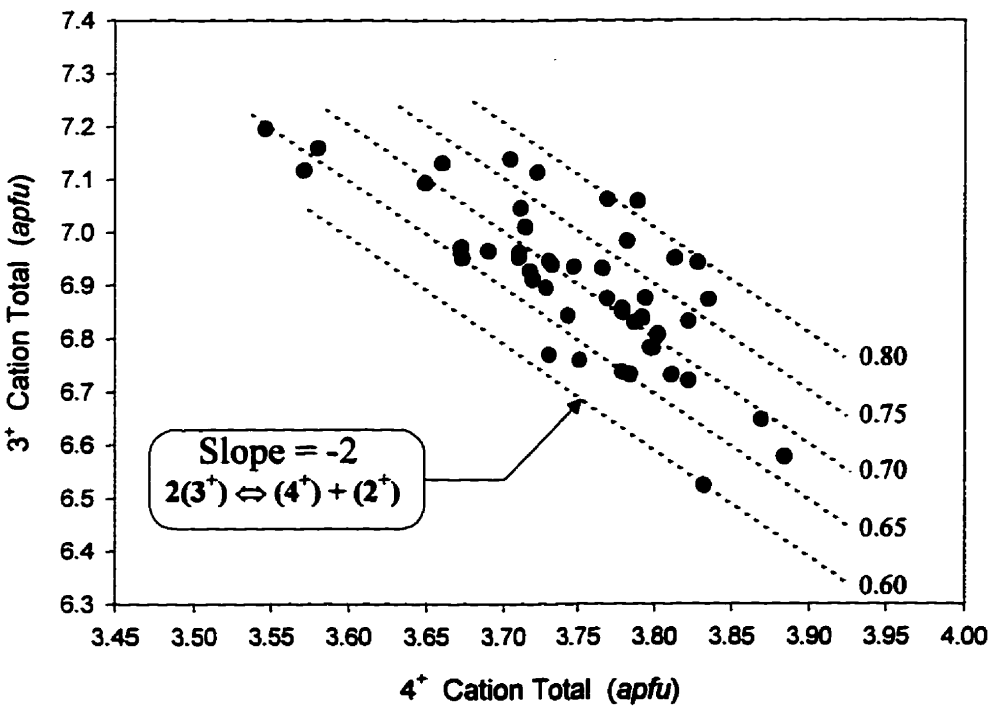


Figure 23: 3^+-cation total (Al + B + Fe + Cr + V + $[Ti^{4+}]$) *apfu* plotted against the 4^+-cation total (Si) *apfu*. Dashed lines are equipotential lines representing the □ *pfu*.

There is a positive correlation between B and Si, and B-rich compositions only occur at moderate-to-high Si content (Fig. 24). Dashed boundary lines enclose the data within a parallelogram (*ABCD*) that outlines the maximum range in Si and B contents for the tetrahedra. For a given B content, Si may vary up to ~0.2 Si *apfu* (*e.g.*, $\overline{AB}$ or $\overline{CD}$). At an Si value of ~3.7 *apfu*, the largest range in observed B occurs (*i.e.*, $\overline{BD}$). The bottom edge of the parallelogram ($\overline{AB}$) coincides with compositions very near zero B. The top edge ($\overline{CD}$) is situated at ~0.9 B *apfu*. Are compositions of 0.9 → 1.0 B likely to be encountered ? Kornerupine *sensu stricto* (B < 0.5 *apfu*) occurs in silica undersaturated rocks (Grew *et al.*, 1996). Prismatine (B > 0.5 *apfu*) usually occurs with quartz, and will therefore have excess Si available during formation. Other B-bearing phases also commonly occur with prismatine (sapphirine, sillimanite, tourmaline). It has been shown that increased B-contents occur in sapphirine and sillimanite with increasing B in prismatine (Grew *et al.*, 1990a). Apparently excess B and Si are usually available during prismatine formation. It therefore appears that 0.9 B *apfu* may indeed represent an upper limit of B incorporation into the kornerupine structure during normal conditions of metamorphism.

*Fe (Fe^{2+} + Mn^{2+}) is plotted against Si *apfu* in Figure 25. Dashed boundary lines enclose the data within the triangle (*ACD*). Near (*D*), a maximum observed *Fe value of ~1.3 *apfu* occurs at ~3.7 Si *apfu*. With lesser or greater Si values, the maximum observed *Fe content falls rapidly.

The data points closest to the letters (*A,B,C,D*) correspond to the samples K40, K30, K13 and K11 (App. A), respectively, in Figures 24 and 25. In Figure 24, positions (*A*) and (*C*) represent two chemical extremes in terms of coupled B and Si values: low B and low Si characterize (*A*); high B and high Si characterize (*C*). In Figure 25, positions (*A*) and (*C*) are located at the vertices on the base of the dashed triangle situated above the minimum and maximum Si values, respectively. It can be inferred that conditions are not favorable for *Fe

substitution when B and Si values are both low, or both high. Located midway between (*A*) and (*C*) along the base of the triangle (Fig. 25) is position (*B*) at an intermediate Si composition. Neglible *Fe is also associated with position (*B*), and it can be said that at low B, conditions are not favorable for *Fe substitution, regardless of the Si content. The most favorable conditions for *Fe substitution seems to be coupled to moderate Si (~3.7 *apfu*) and high B; *i.e.*, position (*D*) on Figures 24 and 25.

B and *Fe are the two most variable major elements, that can be considered as non-essential elements in some samples (K40, near position (*A*), contains < 0.1 B + *Fe *apfu*); in other samples, they represent up to ~15% of the M-site + T-site atoms (K11, near position (*D*), contains > 2 B + *Fe *apfu*). In this respect, variations in B and *Fe can be used to indicate flexibility within the kornerupine structure. The maximum flexibility in regard to B substitution occurs at ~3.7 Si *apfu* ($\overline{BD}$, Fig. 24). At this same Si content, the greatest range in *Fe substitution also occurs($\overline{BD}$, Fig. 25). Therefore, kornerupine containing ~3.7 Si *apfu* represents a moderately flexible situation, whereby increased B content offers an additional degree of flexibility that enables increased *Fe substitution. To further illustrate this correlation between *Fe and B, Figure 26 shows *Fe / (Mg + *Fe) plotted against B *apfu*. The distribution of data widens across the diagram (left → right), indicating that, with increased B, conditions become increasingly favorable for *Fe substitution. If the distribution of data points in Figures 24 → 26 is viewed as strictly limiting, then a limit to *Fe ⇔ Mg substitution is implied at ~1.6 *Fe, where *Fe / (Mg + *Fe) < 0.5. All of the above statements regarding limits of observed *Fe substitution presume that excess *Fe and B were available during formation for samples near $\overline{AD}$ and $\overline{CD}$ in Figure 25.

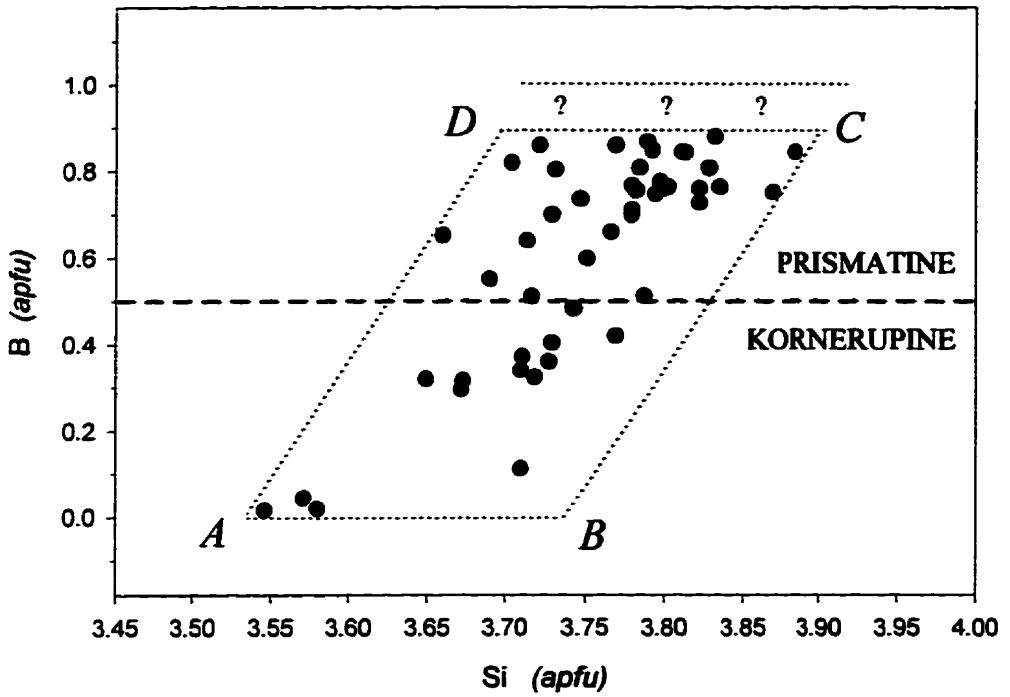


Figure 24: B *apfu* plotted against Si *apfu*. *A,B,C,D* nearest to samples K40, K30, K13, K11 respectively.

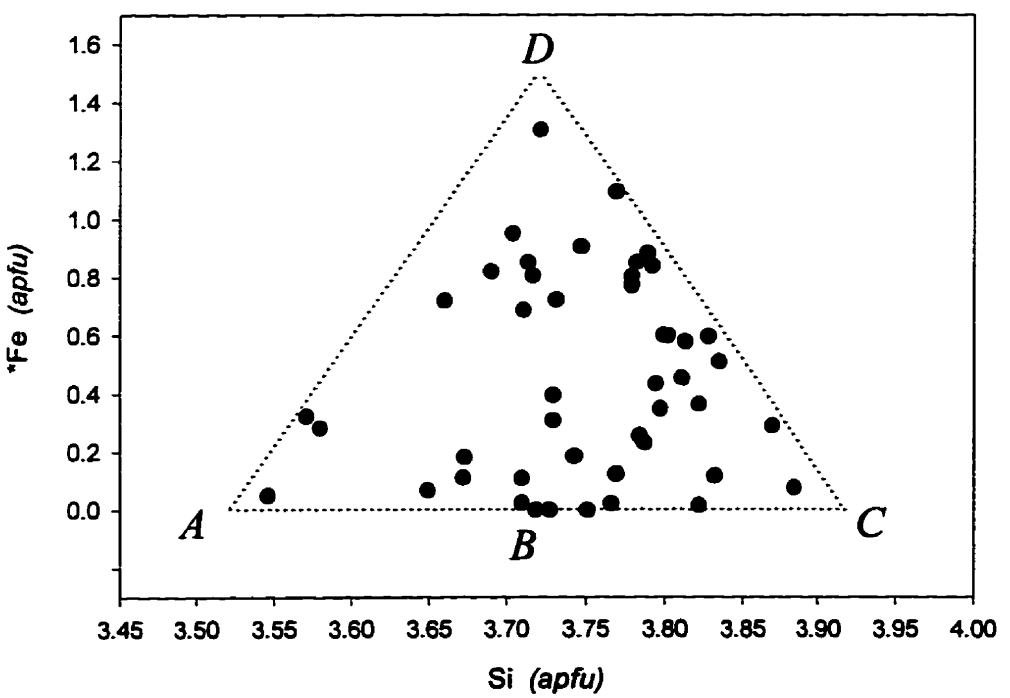


Figure 25: *Fe (Fe^{2+} + Mn^{2+}) *apfu* plotted against Si *apfu*. *A,B,C,D* nearest to samples K40, K30, K13, K11 respectively.

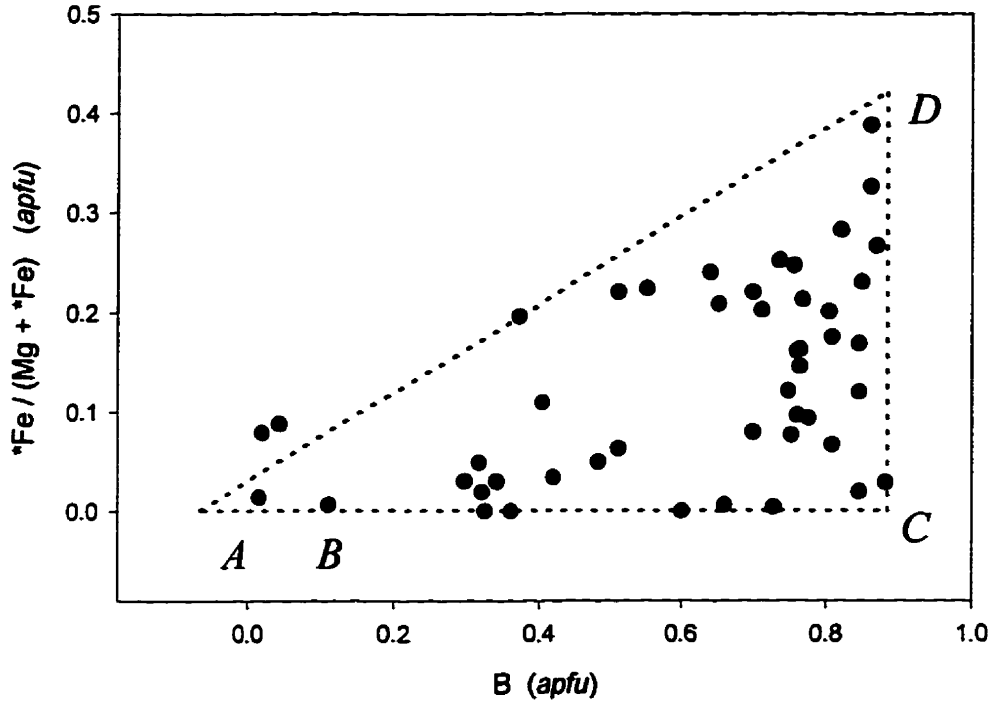


Figure 26: *Fe / (Mg + *Fe) *apfu* plotted against B *apfu*. *A,B,C,D* nearest to samples K40, K30, K13, K11 respectively.

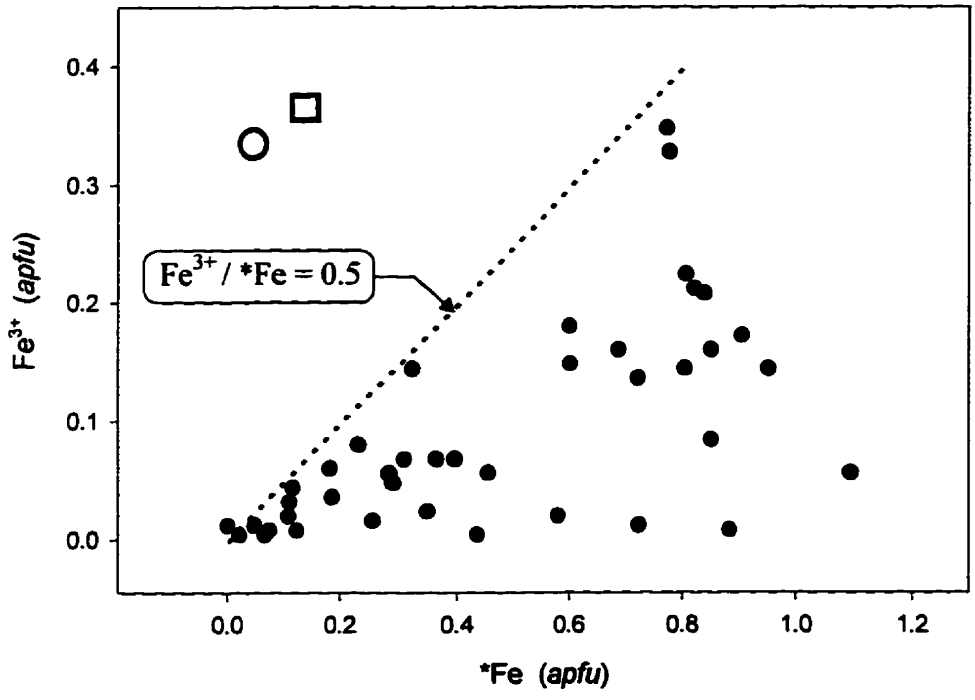


Figure 27: Fe^{3+} *apfu* plotted against *Fe *apfu*. Small filled circles : 47 ferrous kornerupines ; large square : (K4, K48, K51) ; large circle : (K44).

In Figure 27, Fe^{3+} is plotted against *Fe *apfu*; the Fe^{3+} values are from the site assignments [M(4) site (chapter 4; App. F)]. The dashed line has a slope of 0.5 and delineates compositions in which half of the Fe is ferric. All data for the ferrous kornerupines fall to the right of the dashed line, indicating that Fe^{3+} / Fe^{2+} ratios do not exceed 0.5. Also plotted on Figure 27 are the samples from Bamble, Norway [K4, K48, K51] (open square), and the sample from Mautia Hill, Tanganyika [K44] (open circle). These Fe^{3+} kornerupines clearly plot away from the other kornerupine data. When considering all data points on Figure 27, it seems inappropriate to consider the dashed line of slope 0.5 as a limiting feature. The Fe^{3+} / Fe^{2+} ratios represented in Figure 27 may suggest typical oxidizing conditions during kornerupine formation, and may not be indicative of structural limitations regarding Fe^{3+} / Fe^{2+} incorporation. As Fe^{3+} kornerupines (very rare) are not yet fully understood, details regarding the extent of Fe^{3+} substitution remain speculative.

Figures 28 through 32 show several chemical parameters plotted against B *apfu* ; namely divalent cations (Fig. 28), trivalent octahedral cations (Fig. 29), □ (Fig. 30), Na and Ca (Fig. 31), F (Fig. 32). All of these parameters plot over increasingly larger ranges with increasing B, supporting the idea of a more flexible kornerupine structure that permits more extensive substitution at higher B content.

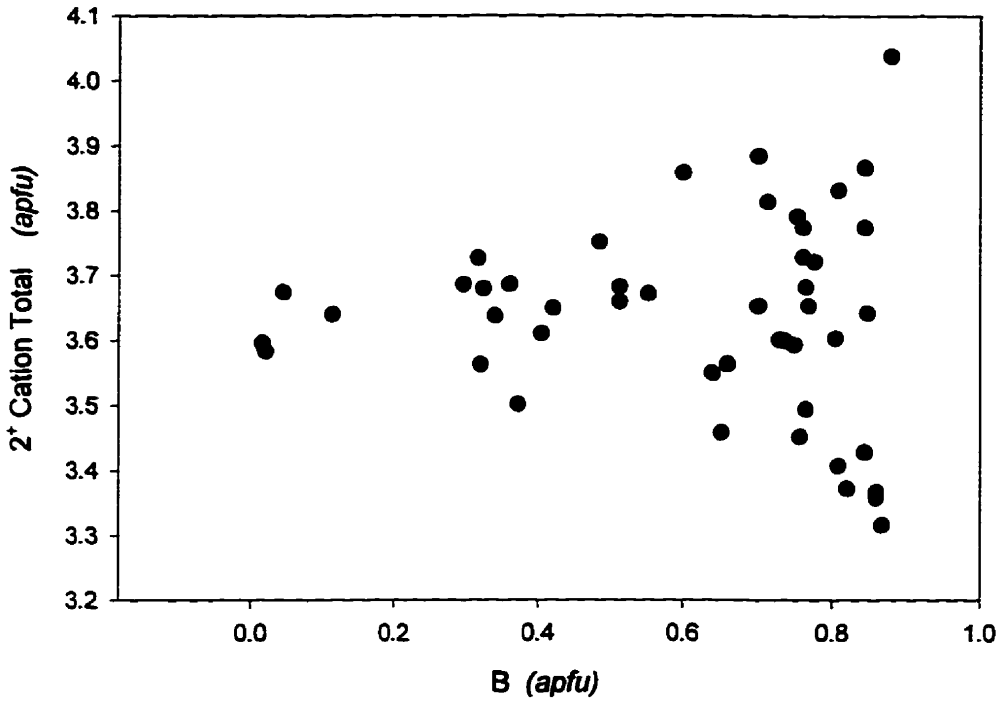


Figure 28: 2^+-cation total (Mg + Fe + Mn) *apfu* plotted against B *apfu*.

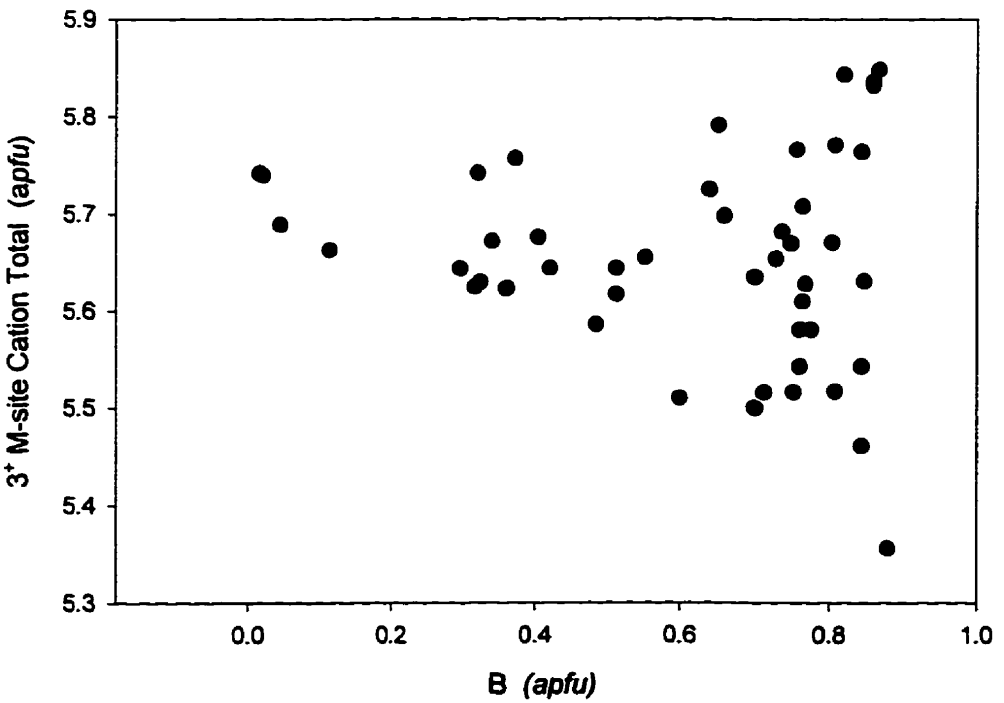


Figure 29: 3^+ M-site-cation total (Al + Fe + Cr + V + [Ti^{4+}]) *apfu* plotted against B *apfu*.

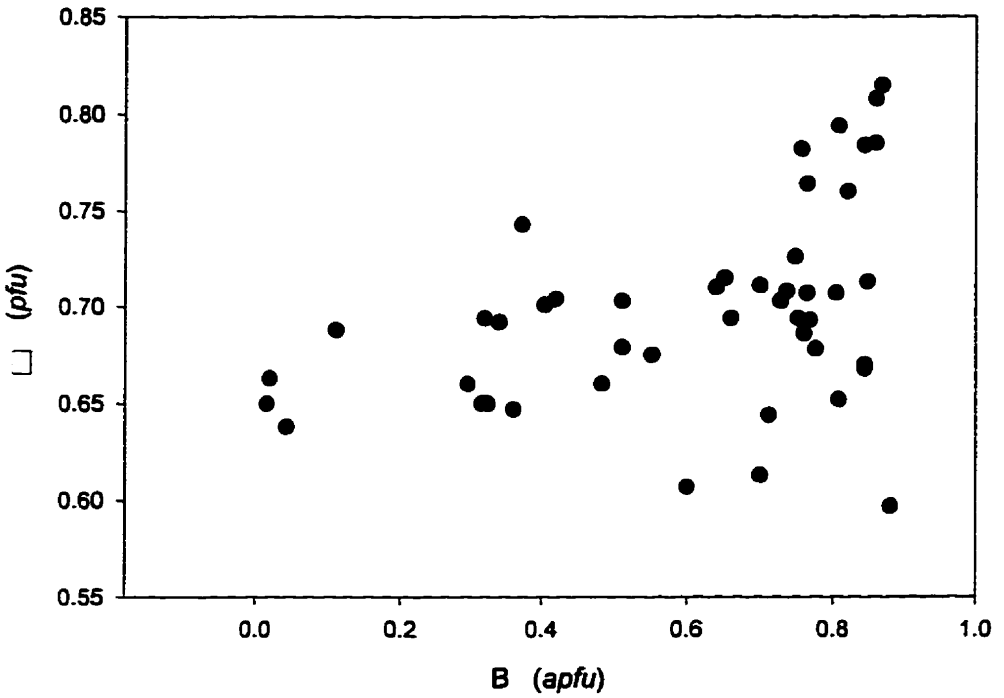


Figure 30: □ *pfu* plotted against B *apfu*.

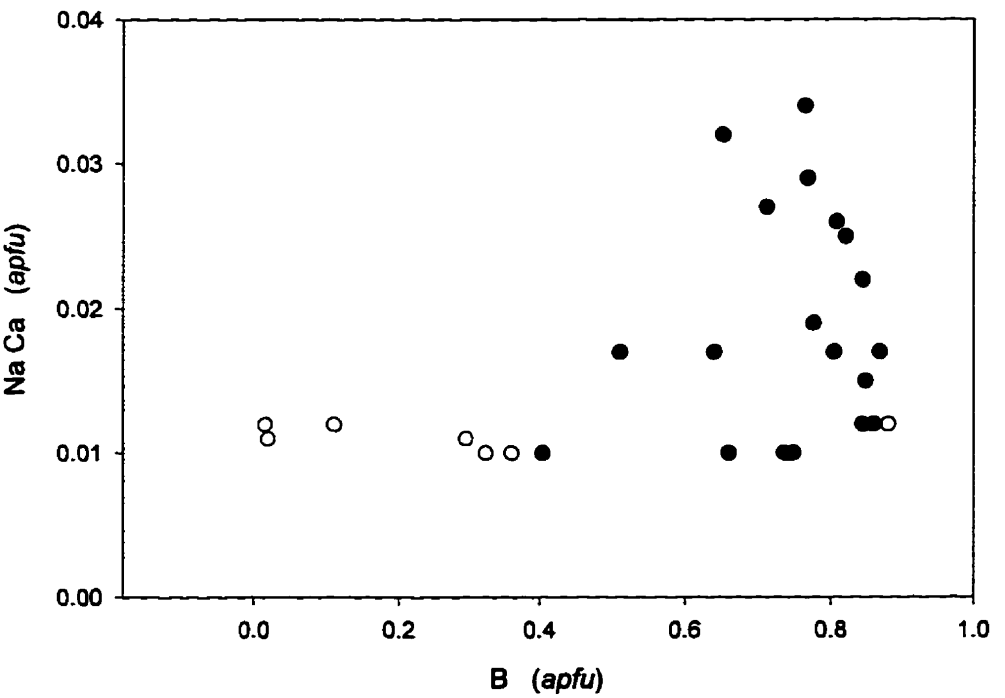


Figure 31: Na (filled circles) and Ca (open circles) *apfu* plotted against B *apfu*. Only significant data is plotted (≥ 0.01 *apfu*).

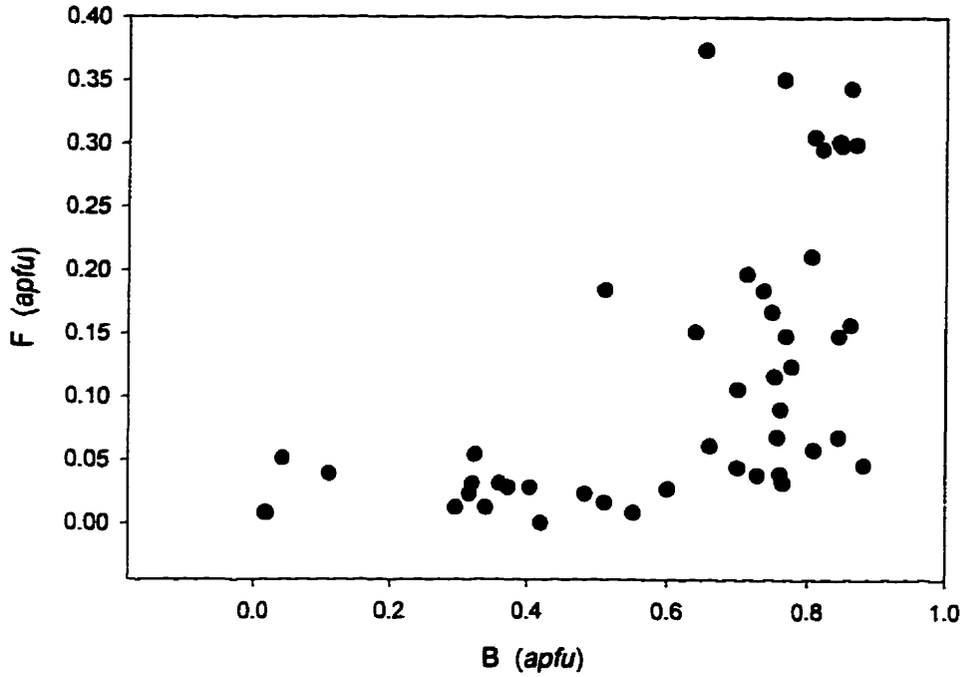


Figure 32: F *apfu* plotted against B *apfu*.

5.1.2 Major-element variation: summary

(1) a fixed anion charge $[O_{21} (F + OH)_1]^{43-}$ combined with a variable number of cations results in possible substitutions of the Tschermak type $[2(3^+) \Leftrightarrow (4^+) + (2^+)]$ in addition to those involving □.

(2) high B content (~0.8 - 0.9 *apfu*) occurs at moderate to high Si content (~3.7 - 3.9 *apfu*), and low B content (< 0.2 *apfu*) occurs at low-to-moderate Si content (~3.5 - 3.7 *apfu*). ~0.9 B *apfu* may represent an upper limit allowed by the kornerupine structure.

(3) maximum *Fe (~1.3 *apfu*) occurs at moderate Si content (~3.7 *apfu*) and high B content (~0.8 - 0.9 *apfu*). A structural limit involving *Fe substitution may be inferred at ~1.6 *Fe *apfu*.

(4) increased chemical variability in kornerupine is strongly correlated with increased B contents.

5.2 Tetrahedra

5.2.1 T(1)—T(1) dimer

The T(1) site (Figs. 2,3) is situated on the mirror at $z = {}^1/_4$, and is symmetrically related to another T(1) site [*i.e.*, T(1)′] across the mirror ($x = 0$). The O(9) site occurs on the mirror ($x = 0$) and links to T(1) and T(1)′, resulting in a T(1)—T(1) dimer. At the completion of the tetrahedral-site assignment, up to 0.100 Al (0.200 Al *apfu*) was assigned to the T(1) site (4.1; App. F). Two criteria supporting the assignment of Al to T(1) were: (1) a bond-length variation of 0.014 Å in ⟨T(1)-O⟩ (*i.e.*, 1.618 → 1.632 Å); (2) improved linearity at the T(2) and T(3) sites between ⟨T-O⟩ distances and respective constituent radii. It is well known that the average Al content of a tetrahedron has a pronounced effect on ⟨T-O⟩ distances (Smith, 1954; Smith & Bailey, 1963). However, estimating average-Al content based on a simple linear relation between ⟨T-O⟩ distances and constituent radii alone is not completely accurate (Geisinger *et al.*, 1985). Other bond-length perturbing factors resulting from the local environment also need to be considered. A useful parameter to examine in this regard is the T–O–T angle about the bridging O, or more specifically 1 / (1 - sec ∠ TOT) (Swanson *et al.*, 1980; Swanson, 1980). This quantity is referred to as f_s(O) or the fractional *s*-character of the bridging O. Slightly different minimum-energy angles exist for Si–O–Si and Si–O–Al configurations (Geisinger *et al.*, 1985). Therefore f_sO(9) values as calculated from T(1)–O(9)–T(1) angles should contain information regarding the probability of Al ordering at T(1). To test this hypothesis, ⟨T(1)-O⟩ distances are plotted against f_sO(9) values in Figure 33. The range in f_sO(9) values from 0.456 to 0.472 are calculated from T(1)–O(9)–T(1) angles in the range 147.04 to 153.19°, respectively (App. G.3). The solid line drawn through the data (slope = -0.229) is taken from the Geisinger *et al.* (1985) study that used accurate ⟨Si-O⟩ and Si–O–Si measurements taken from well-ordered framework silicates to develop the line *via* regression analysis. The line is shifted upwards (0.0141 Å)

relative to the Geisinger *et al.* (1985) study, so that it would pass through the lower data on Figure 33. The slope of the line is both shallow and negative (-0.229), indicating that as Si–O–Si angles increase, a subtle decrease in corresponding ⟨T-O⟩ distances is expected. A similiar trend (slope = -0.312) was found by Geisinger *et al.* (1985) for Al–O–Si angles (the trend is displaced vertically by ~+0.13 Å along the ⟨T-O⟩ axis and plots off Figure 33). The dashed line segments (Fig. 33) separate data according to assigned Al content reported in section 4.1. The labels on either side of the dashed lines indicate ranges of assigned Al *apfu*. The data plotting further above the solid line contain progressively more assigned Al (this reflects the fact that Al populations were extrapolated directly from ⟨T(1)-O⟩ distances). However, the data plotting near a T(1)–O(9)–T(1) angle of ~148.8° (f_sO(9) ≈ 0.461) span an appreciable range in ⟨T-O⟩, and a rather limited range in f_sO(9). The data points with greater assigned-Al deviate more substantially from the Greisinger *et al.* (1985) line for (Si–O–Si). This deviation toward greater ⟨T-O⟩ distances for a given T–O–T angle is consistent with Al at the T(1) site.

Another factor potentially influencing observed T(1)–O(9)–T(1) angles (to an unknown extent) is the variable H-bonding probably directed toward the O at the O(9) site. In an upcoming section (5.5) the H-bonding will be discussed in more detail. Variable coordination about O(9) is certainly capable of perturbing the T(1)–O(9)–T(1) geometry. Geisinger *et al.* (1985) observed decreased T–O–T angles when the coordination of the bridging O was increased from two to three. The degree to which the T–O–T angle is affected depends upon the chemical type of the coordinating cation, as well as its distance from the bridging O. Kornerupine bond-valence calculations (App. J) show that the O-atom at O(9) has its valence requirements completely satisfied [O(9) sums are in the range 2.022 → 2.118] by the two T(1)-site cation contributions. The strength of the H-bond must therefore be very weak in all cases, and its potential perturbing effect on the T–O–T angle can probably be disregarded.

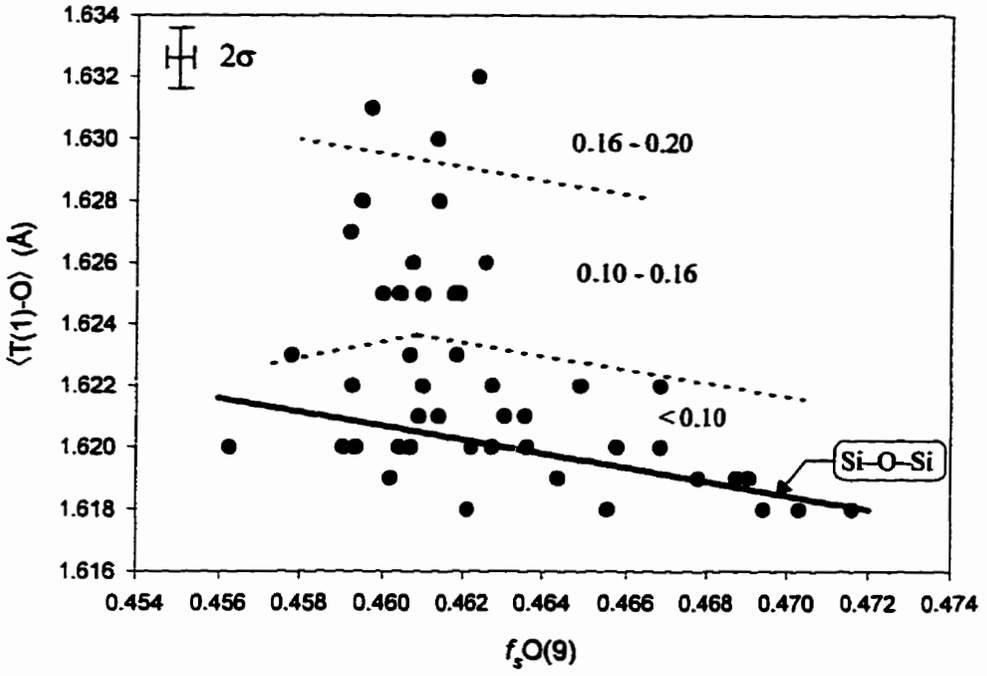


Figure 33: ⟨T(1)-O⟩ (Å) plotted against f_sO(9) [1 / (1 - sec ∠TOT)]. Si–O–Si line of Geisinger *et al.*, 1985 (solid line). Dashed lines divide fields according to $^{T(1)}$Al *apfu*.

In Figure 34, $^{T(1)}$Al *apfu* is plotted against B *apfu*. A well-defined inverse correlation between decreasing Al at T(1) and increasing B at T(3) is shown. This suggests the following coupled substitution:

$$^{T(3)}B + {}^{T(1)}Si \Leftrightarrow {}^{T(3)}(Si,Al) + {}^{T(1)}Al$$

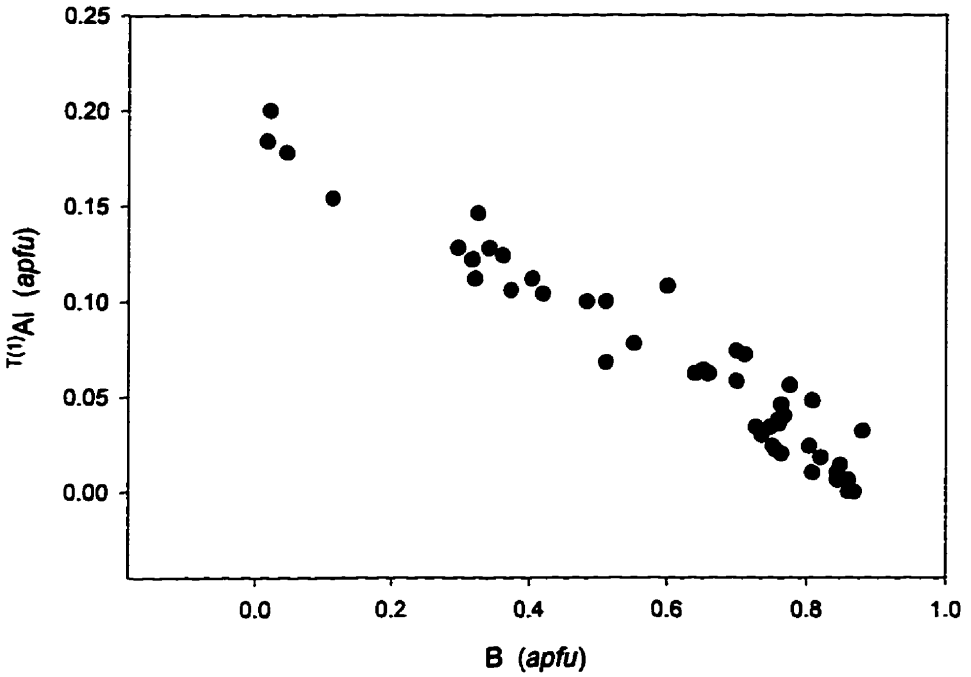


Figure 34: $^{T(1)}$Al (*apfu*) plotted against B (*apfu*).

5.2.2 T(2)—T(3)—T(2) trimer

The T(2) and T(3) sites (Figs. 2,3) reside on a mirror at $z = {}^1/_4$. The T(3) site is also on the mirror at $x = 0$, and the T(2) site is related to a symmetrically equivalent T(2)′ site across this mirror ($x = 0$). The O(7) site contains the bridging O common to T(2) and T(3), and the tetrahedral T(2)—T(3)—T(2) trimer results. At the completion of the tetrahedral assignments (Ch. 4), the following ranges in chemical substituents had been assigned to the T(2) and T(3) sites, respectively: $Si_{0.899}\ Al_{0.101}$ to $Si_{0.508}\ Al_{0.492}$; $B_{(0.016\rightarrow0.880)}$, $Si_{(0.057\rightarrow0.727)}$, $Al_{(0.053\rightarrow0.299)}$. ⟨T(2)-O⟩ distances (1.646 to 1.698 Å) and ⟨T(3)-O⟩ distances (1.505 to 1.665 Å) are consistent with B fully ordered at T(3) (4.1). How accurate are these B values calculated from site scattering refinement at T(3) (Ch. 3) ? An independent measure of the B content was attained for samples K1 to K32 *via* SIMS analysis (2.4). Table 5 lists the wt. % B_2O_3 contents for these samples measured by SIMS next to those arrived at by SREF. These B_2O_3 contents from SREF (Table 5) supersede similiar earlier values reported in Hawthorne *et al.* (1995). The data in Table 5 are compared graphically in Figure 35. The dashed line is drawn with a slope of unity for comparison purposes. The two methods used here for the analysis of B in kornerupine are physically independent. SREF involves X-ray scattering and SIMS involves ion ablation and mass spectrometry. The agreement between results of the two different methods is very good ($r^2 = 0.988$), and it can be concluded that both methods can give accurate B contents. Therefore, not only are the B populations at T(3) deemed accurate, but the possibility of additional B at the other tetrahedral sites has also been negated.

TABLE 5: B_2O_3 CONTENTS (wt. %) OF KORNERUPINE BY SIMS AND SREF

Sample	SIMS*	SREF		Sample	SIMS*	SREF
K1	1.98	1.88		K17	3.37	3.52
K2	2.52	2.41		K18	3.43	3.55
K3	3.84	3.76		K19	4.05	3.95
K4	2.35	N/A		K20	3.98	4.02
K5	3.62	3.52		K21	1.70	1.70
K6	3.15	3.37		K22	2.05	1.99
K7	3.66	3.56		K23	3.51	3.49
K8	2.45	2.51		K24	3.70	3.77
K9	3.98	3.96		K25	3.73	3.90
K10	3.06	3.22		K26	2.28	2.34
K11	3.86	3.89		K27	3.50	3.54
K12	1.35	1.39		K28	3.54	3.58
K13	4.36	4.08		K29	2.88	2.96
K14	3.38	3.47		K30	0.44	0.53
K15	3.15	3.24		K31	1.54	1.51
K16	3.81	3.93		K32	3.76	3.80

* from Hawthorne et al., 1995.

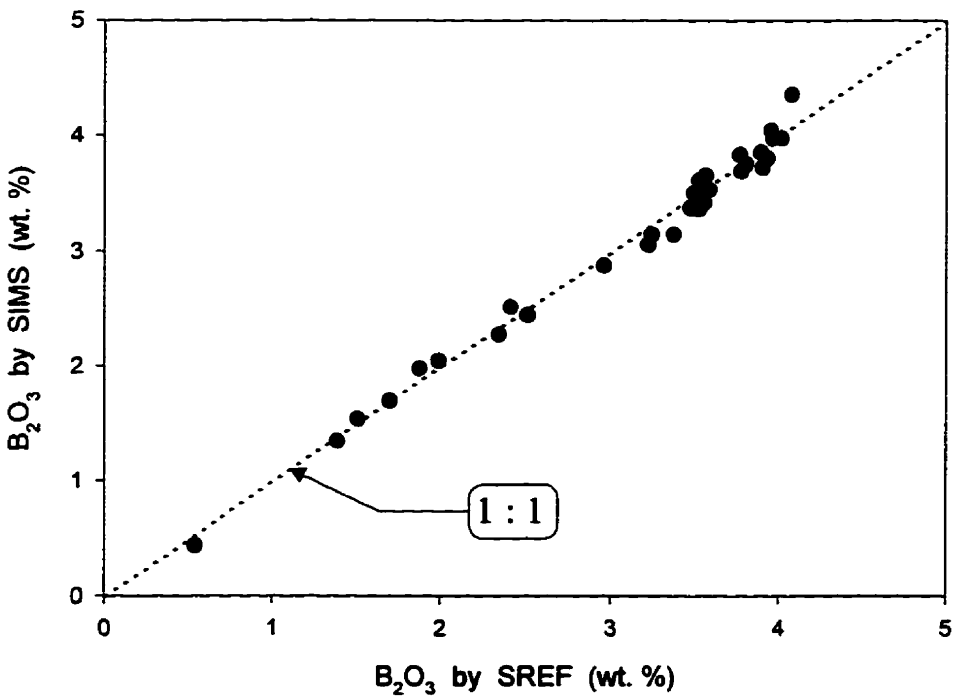


Figure 35: Comparison of B_2O_3 (wt. %) determined by SIMS and SREF. Dashed reference line has a slope = 1. Samples K1→K32 ; excluding K4.

The molecular orbital study of Geisinger *et al.* (1985) also involved calculation of minimum-energy angles for the Si–O–B configuration (minimum energy angle for a 2-coordinate bridging O = 125°). In kornerupine, the bridging O at the O(7) site is also linked to the M(1) site in addition to T(2) and T(3), and is therefore a 3-coordinate bridging O. A narrower and more restrictive T–O–T angle should then occur for this T(2)–O(7)–T(3) configuration in kornerupine (Geisinger *et al.*, 1985). In Figure 36, T(3)B (*apfu*) is plotted against the T(2)–O(7)–T(3) angle (°) (App. J). The range in observed T(2)–O(7)–T(3) angles is only 2.8°; 121.8° (at low B), 124.6° (at high B). This range of angles compares well with that predicted by Geisinger *et al.* (*i.e.*, < 125°). A striking feature of Figure 36 is the uniform positive correlation between increasing B contents and increasing T(2)–O(7)–T(3) angle from ~0 to 0.7 B *apfu*. As the B population increases at T(3), $^{T(2)}$Si–O–$^{T(3)}$B (and possibly $^{T(2)}$Al–O–$^{T(3)}$B) configurations must increase in frequency. The minimum-energy angle calculations of Geisinger *et al.* predict the opposite trend — *i.e.*, decreasing T(2)–O(7)–T(3) angles with increasing B. The local environment about the T(2)—T(3)—T(2) trimer is clearly exerting an influence on the observed T(2)–O(7)–T(3) angle that is greater than the driving force associated with attainment of the predicted minimum energy angle. The linkage of the T(2)—T(3)—T(2) trimer to the neighboring polyhedra (Figs. 3,37) shows that the O(6)–O(8) edge of the M(5) octahedron and the O(5)–O(7) edge of the M(1) octahedron likely impart geometrical constraints on the flexure of the tetrahedral trimer in the (001) plane. In fact, the M(5) octahedron could be considered the most rigid polyhedral element within the kornerupine structure, in terms of both site population and bond-length variation (Apps. F, G.2). The O(6)–O(8) edge of the M(5) octahedron shows a maximum variation of only 0.046 Å, 2.922 to 2.968 Å (App. G.3). The maximum variation in the length of the O(5)–O(7) polyhedral edge that is shared between T(2) and M(1) (Figs. 3,37) is only 0.029 Å, 2.504 to 2.533 Å (App. G.3).

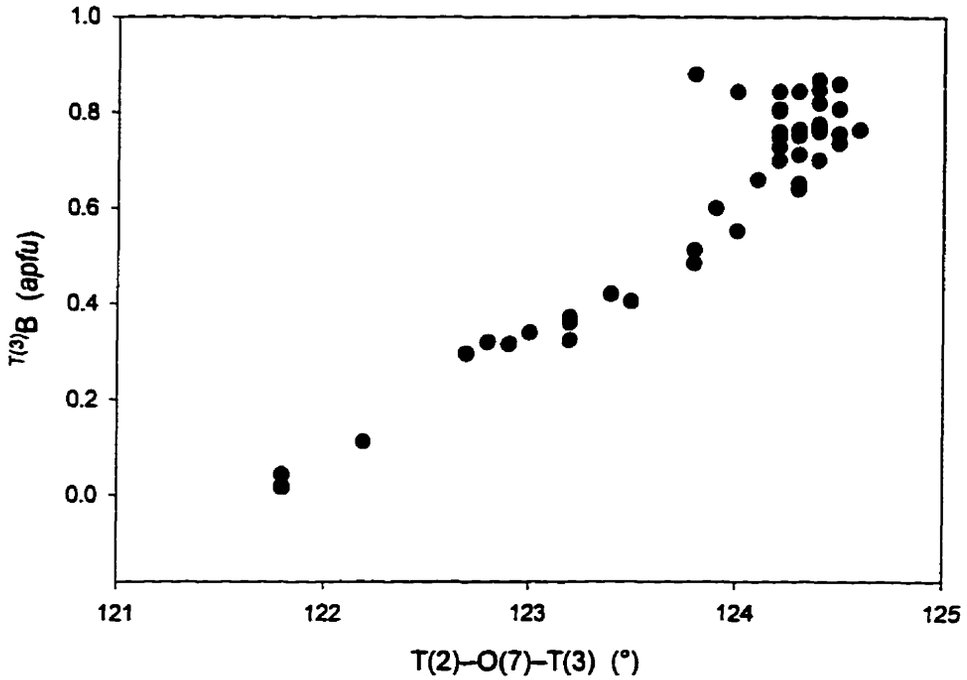


Figure 36: $^{T(3)}$B (*apfu*) plotted against the T(2)–O(7)–T(3) angle (°).

How are the ⟨T(3)-O⟩ distances able to span 0.16 Å in the presence of these relatively rigid neighboring constraints ? The answer lies in coupled shrinkage of the T(3) tetrahedron and rotation of the T(2) tetrahedron illustrated in Figure 37. The tetrahedra bounded by solid lines are drawn using coordinates from K35 (low B); corresponding T(2) and T(3) cation positions are shown as filled circles. The tetrahedra bounded by dashed lines are drawn using coordinates from K41 (high B); corresponding T(2) and T(3) cation positions are shown as open circles. Situated on the (001) mirror ($z = {}^{1}/_{4}$) [*i.e.*, plane of the page] are T(2), T(3), O(5), O(7), M(1), M(4), O(1), O(10) and their symmetry related sites across the (100) mirror ($x = 0$). The M(3), M(5), O(6) and O(8) sites lie above and below the mirror at (001). Visual inspection of the O(6)–O(8) and O(5)–O(7) edges at low and high B show only minor length adjustments. In this projection, the largest displacements involve the O(5), O(7), T(2) and T(3) positions; with

increasing B, O(8) remains essentially stationary and O(7) migrates toward the central T(3) cation. With the resulting shrinkage of the T(3) tetrahedron, the T(3) atom moves toward the O(8)–O(8)′ edge to maintain a central position within the tetrahedron. With neglible change in the O(6) position and O(5)–O(7) edge-length, the T(2) tetrahedron rotates about the O(6) position in tandem with the shrinking T(3) tetrahedron. Through this rotation, the size of the T(2) tetrahedron decreases slightly from 1.694 (K35) to 1.646 Å (K41) (App. G.2). Thin solid and dashed lines through the T(2), O(7) and T(3) positions mark out the T(2)–O(7)–T(3) angles at low and high B, respectively. The T(2)– O(7)–T(3) angle at high B (thin dashed) is the larger (by ~2°) of the two angles (*cf.* Fig. 36).

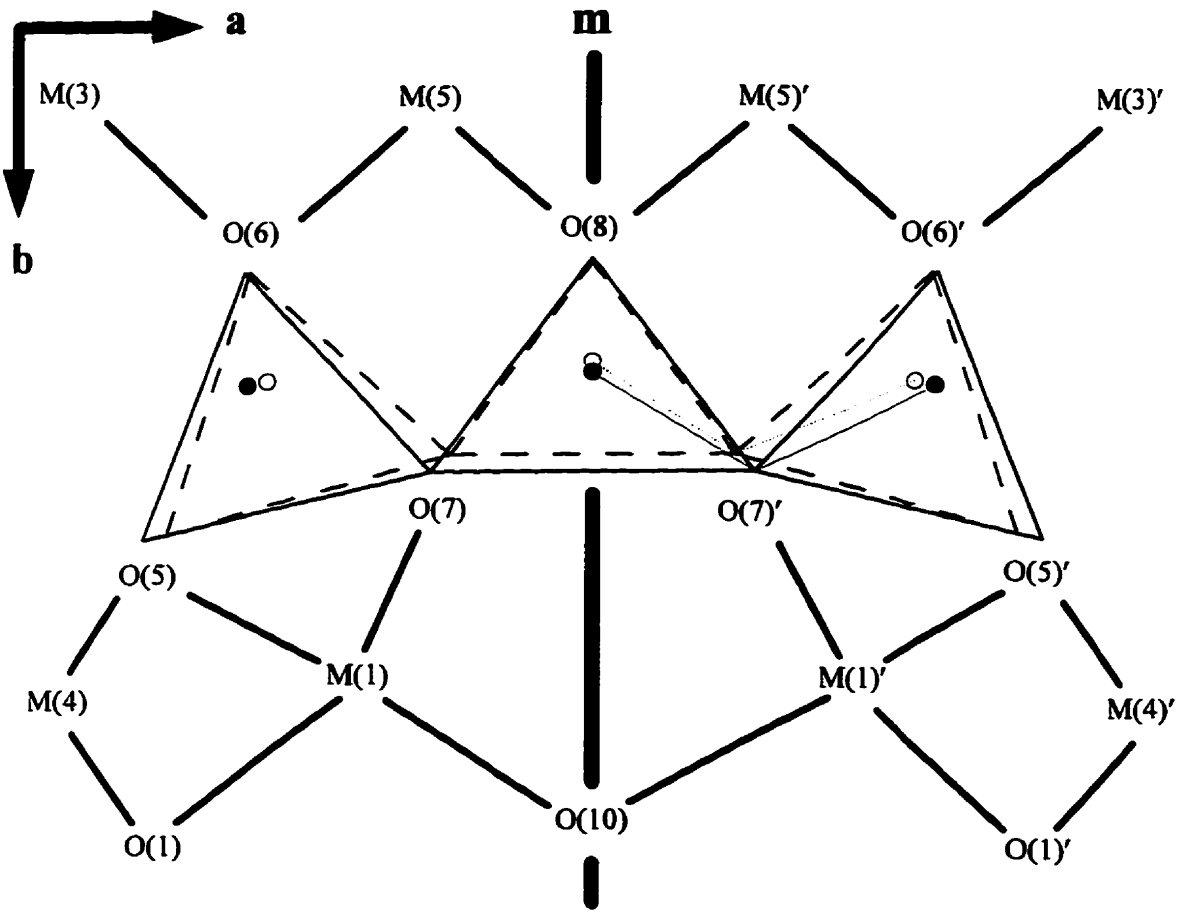


Figure 37: T(2)—T(3)—T(2) tetrahedral trimer and neighboring environment projected down [001]. K35 (low B) tetrahedra have solid outline, T-sites are filled circles; K41 (high B) tetrahedra have dashed outline, T-sites are open circles. T(2)–O(7)–T(3) angles are marked similarly.

The most important neighboring feature coupled to this flexure of the T(2)—T(3)—T(2) tetrahedral trimer is the rotation of the O(5)–O(7) edge. Tied to this rotation are significant geometric adjustments to the M(1) and M(4) octahedra (Fig. 37). With increasing B, the M(1) and M(1)′ polyhedra can easily adjust *via* bending at the corner-sharing O [O(10)]. Necessary adjustments along O(1)–O(5) are more constraining because this is a shared edge between the M(1) and M(4) octahedra. This accomodation by the M(1) and M(4) octahedra to the changing position of the O(5)–O(7) edge relates to two observations given in chapter 4: (1) proposed neighboring steric influences at M(1) as a function of B content at T(3) that perturb the ⟨M(1)-O⟩ *vs.*. *r*[M(1)] relation; (2) the low slope (0.78) for the ⟨M(4)-O⟩ *vs.* *r*[M(4)] relation. The first observation gains further credence from simple inspection of Figure 37. The low slope of the ⟨M(4)-O⟩ *vs.* *r*[M(4)] relation is complementary in helping to maintain the incident bond-valence at the 'migrating' O(5) position (App. J).

An interesting feature of Figure 36 is the wider distribution of T(2)–O(7)–T(3) angles at greater B content (B > 0.7 *apfu*). At ~0.8 to 0.9 B, angles from 123.8 to 124.5° are observed. These high-B samples (0.8 < B < 0.9) are shown in Figure 38 with $^{M(1)}Fe^{2+}$ plotted against T(2)–O(7)–T(3) angles. A good positive correlation exists between Fe^{2+} at M(1) and T(2)–O(7)–T(3) angles, in agreement with the Geisinger *et al.* (1985) findings that the chemical identity of a third cation bonded to the bridging O can impart a further influence upon T–O–T angles (*i.e.*, $^{M(1)}Mg$ *vs.* $^{M(1)}Fe^{2+}$). The perturbation in T(2)–O(7)–T(3) angles (Figure 36) is most obvious at high B (B > 0.8 *apfu*) because larger ranges in *Fe [Fe^{2+} at M(1)] only occur at high B (Fig. 26).

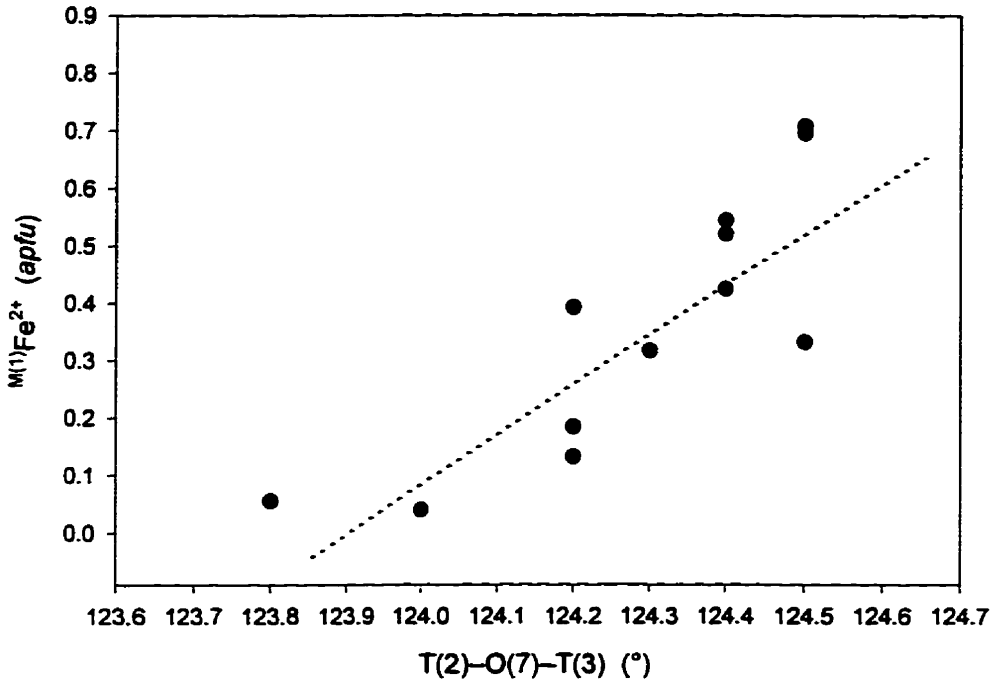


Figure 38: Relation between $^{M(1)}Fe^{2+}$ (*apfu*) and T(2)–O(7)–T(3) (°). The dashed line passing through the data points is estimated by eye.

5.2.3 Si – Al ordering among tetrahedral sites

The relative partitioning of Si at T(1), T(2) and T(3) with increasing B is shown in Figure 39. About half the Si is located at the T(1) site, the other half being partitioned between T(2) and T(3) in an increasingly disproportionate manner with increasing B. At very high B, nearly all Si is located at T(1) and T(2). The relative ordering of Si and Al between the T(1), T(2) and T(3) sites with increasing B is shown in Figure 40. Over all tetrahedral compositions, the T(1) site has the greatest affinity for Si relative to Al. At very low B values, up to 10% Al is present at T(1). The Si–Al ordering at T(2) and T(3) is somewhat variable for a given B value — *i.e.*, the data lie within broad fields [especially for T(3)]. A transition area occurs at moderate-B where Si and Al are approximately disordered over the T(2) and T(3) sites. At lower B values, T(3) is preferred over T(2) by Si, and at higher B values, the situation is reversed with T(2) becoming the the more favorable site for Si. The relations in Figures 39 and 40 indicate the following coupled substitution at the tetrahedra:

$$^{T(1)}Si + {}^{T(2)}Si + {}^{T(3)}B \Leftrightarrow {}^{T(1)}Al + {}^{T(2)}Al + {}^{T(3)}(Si,Al).$$

The relative Si contents for the tetrahedra are plotted against total *Fe *pfu* in Figure 41. Cooperative substitutions at the tetrahedral sites can promote increased *Fe → Mg substitution. A slight increase in the relative Si content at T(1), combined with high $^{T(2)}$Si content and low $^{T(3)}$Si content, is favorable for increased *Fe content. The labels (*C*) and (*D*) in Figure 41 are the same as those in Figures 24-26 (*i.e.*, K13 and K11 respectively), and data lying close to $\overline{CD}$ therefore contain high-B. Likewise, the labels (*A*) and (*B*) represent data points with low-B (*i.e.*, K40 and K30 respectively ; *cf.* Figs. 24-26). Therefore, high B at T(3) and high Si at T(1) and T(2) represent the most favorable compositional situation for maximum *Fe substitution. The variation in Si / (Al + Si) at T(3) is plotted against *Fe *pfu* in Figure 42. The wide scatter in the

distribution of data shows that Si – Al ordering at T(3) has little relation to observed *Fe content. Simple structural relaxation as a function of increased B at T(3) is the most important factor associated with increased Fe^{2+} → Mg substitution. Shrinkage of the T(3) (B → Si,Al) and T(2) (Si → Al) tetrahedra and rotation of the T(2) tetrahedron (Fig. 37), allow a geometrical relaxation that is conducive to Fe^{2+} → Mg substitution at M(1) and M(2). The larger (mostly vacant) X-site will not be affected in the same manner because the relative sizes of Fe^{2+} and Mg (0.78 and 0.72 Å) have little bearing on observed X-site populations in the presence of dominant □.

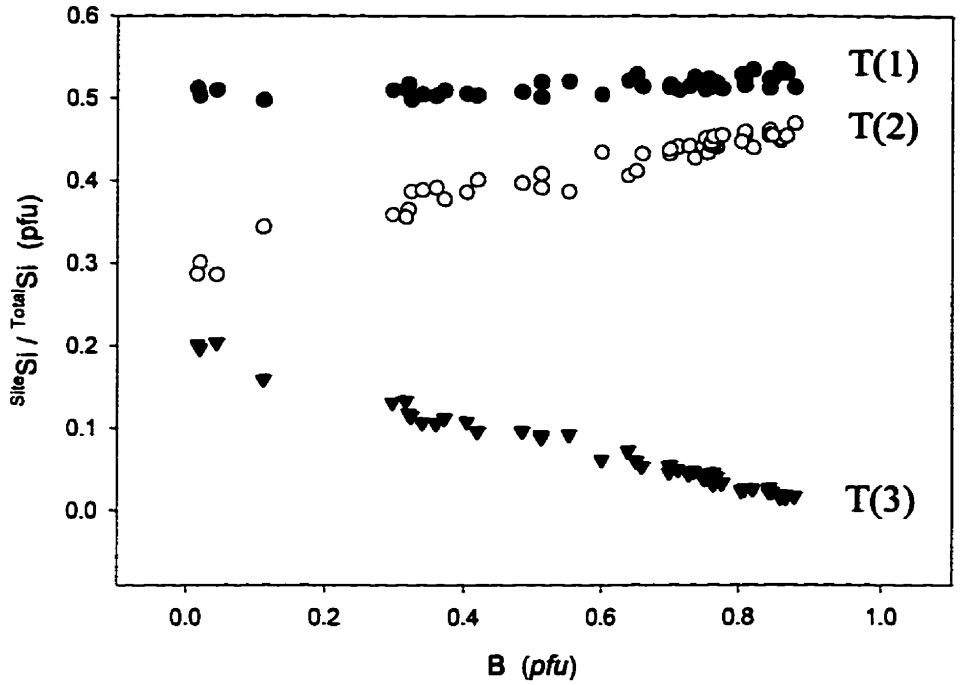


Figure 39: The relative Si contents (*pfu*) of the tetrahedra plotted against B (*pfu*). T(1) [filled circles]; T(2) [open circles]; T(3) [filled triangles].

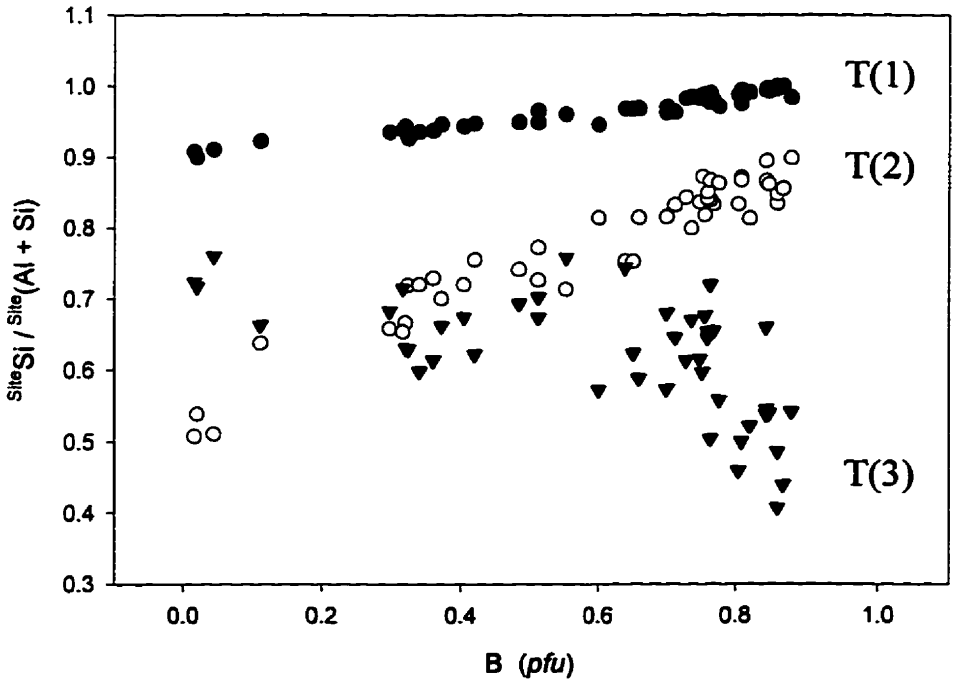


Figure 40: The Si / (Al + Si) distribution for the tetrahedra plotted against B (*pfu*). Symbols as in Fig. 39.

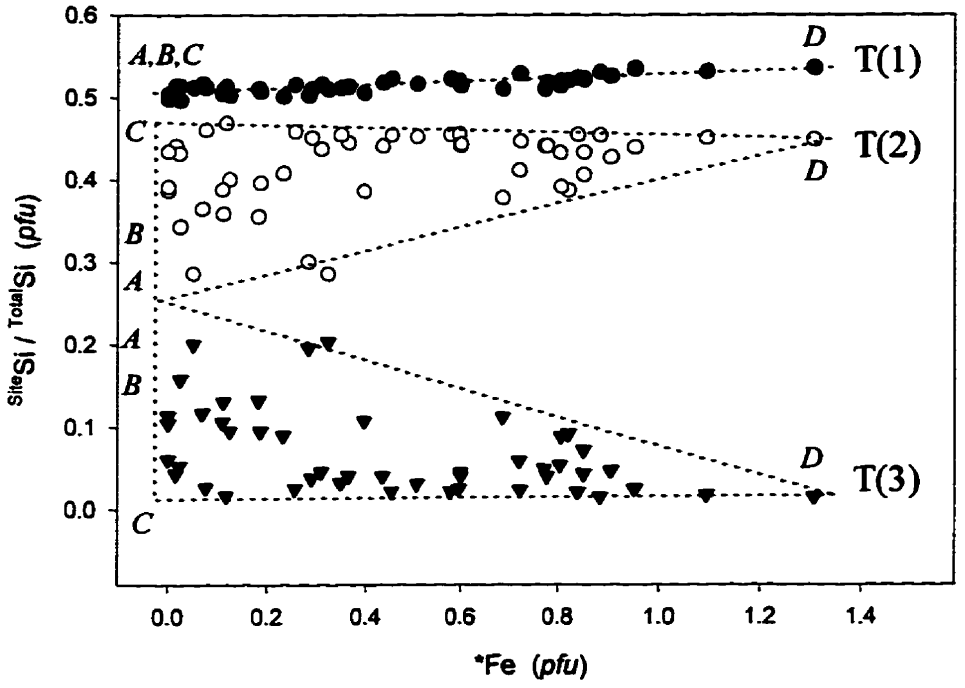


Figure 41: The relative Si contents (*pfu*) of the tetrahedra plotted against *Fe (*pfu*). Symbols as in Fig. 39. *A,B,C,D* near K40, K30, K13, K11 respectively.

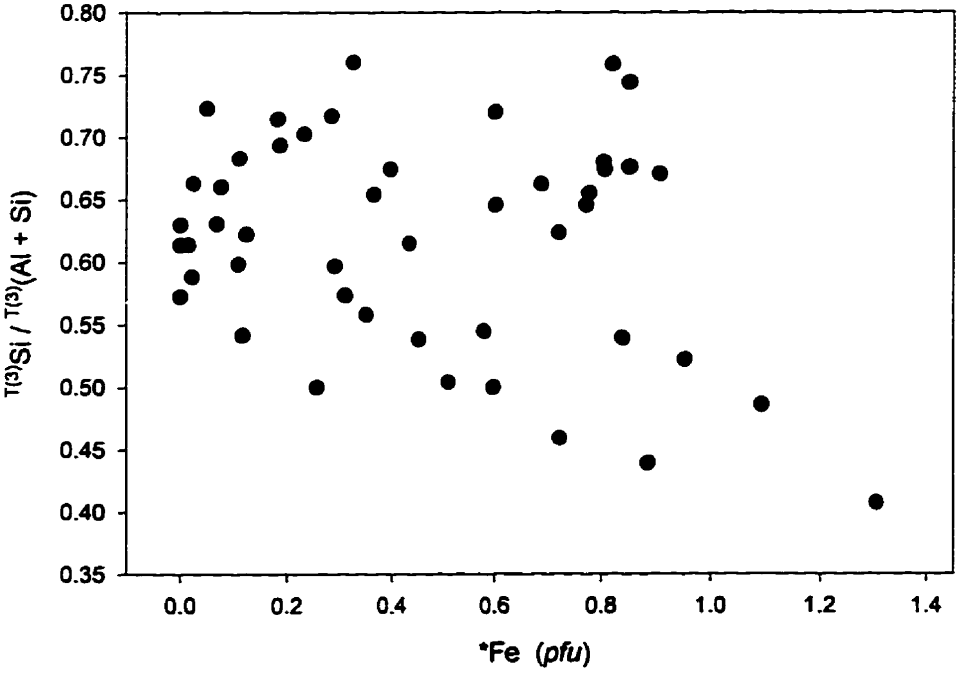


Figure 42: Si / (Al + Si) at T(3) plotted against *Fe (*pfu*).

5.3 Octahedra and X site

5.3.1 Fe – Mg ordering at X, M(1) and M(2)

The ordering of Fe^{2+} and Mg over the M(1) and M(2) sites is shown in Figure 43. The solid line passing through the origin has a slope of unity. Samples plotting on the solid line contain Fe^{2+} and Mg disordered over M(1) and M(2). Data falling to either side of the solid line is representative of a partly ordered Fe^{2+} – Mg distribution. At low Fe^{2+} content [Fe^{2+} / (Mg + Fe^{2+}) ≤ 0.10], two possible ordering schemes are shown: (1) Fe^{2+} and Mg disordered over M(1) and M(2); (2) a greater affinity for Fe^{2+} relative to Mg at M(1). At greater Fe^{2+} content [Fe^{2+} / (Mg + Fe^{2+}) > 0.10], the Fe^{2+} – Mg ordering is more varied: $^{M(1)}K_{Fe}$ / $^{M(2)}K_{Fe}$ ranges from ~2 to ~0.5 [where $K_{Fe} = Fe^{2+} / (Mg + Fe^{2+})$]. In Figures 44 and 45, $^{M(1)}K_{Fe}$ and $^{M(2)}K_{Fe}$ respectively, are plotted against B (*pfu*). The maximum $Fe^{2+} \rightarrow$ Mg substitution occurring at the M(1) and M(2) sites is coupled to the overall B content. Replacement of Mg by Fe^{2+} at M(1) and M(2) can be up to 35% and 50%, respectively (Figs. 44,45). A comparison of the ordering of $Fe^{2+}$and Mg between the X and M(1) site is shown in Figure 46, and between the X and M(2) site in Figure 47. Solid lines passing through the origin are drawn with a slope of unity for reference. In most cases, data lie appreciably above the reference line, suggesting that the X site usually possesses the greatest affinity for Fe^{2+}. In Figure 48, $^{X}K_{*Fe}$ is plotted against B (*pfu*) [K_{*Fe} = *Fe / (Mg + *Fe)]. For a given B content, there is no obvious restriction placed upon $^{X}K_{*Fe}$. Fe^{2+} and Mg are close in size (0.78 and 0.72 Å, respectively) and substitute freely for each other at X.

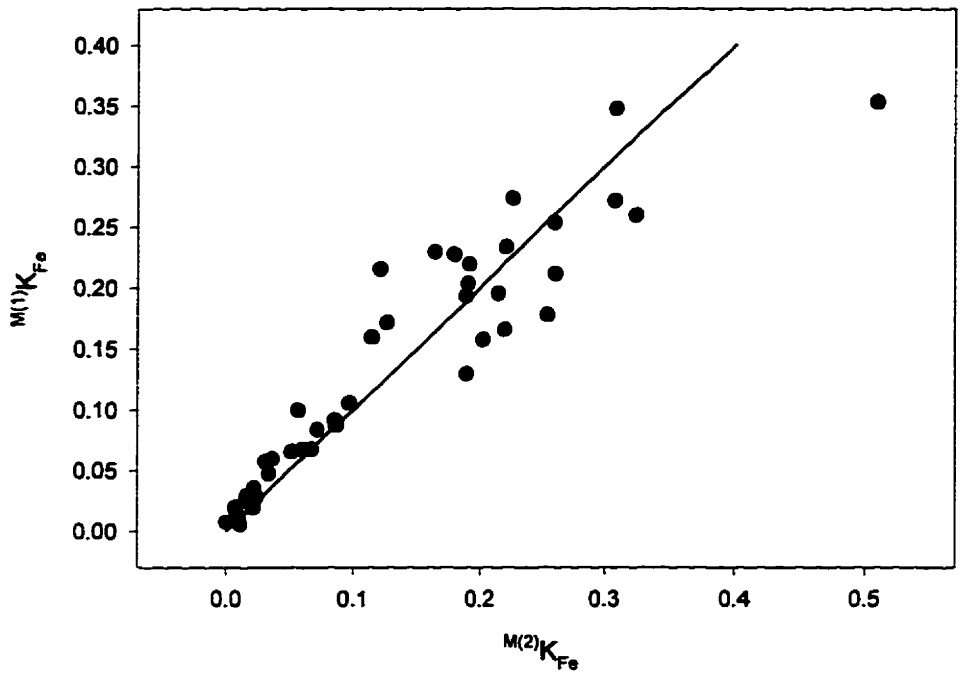


Figure 43: Relation between Fe^{2+} – Mg ordering at M(1) and M(2). [$K_{Fe} = Fe^{2+} / Mg + Fe^{2+}$)] Reference line through origin with slope = 1.

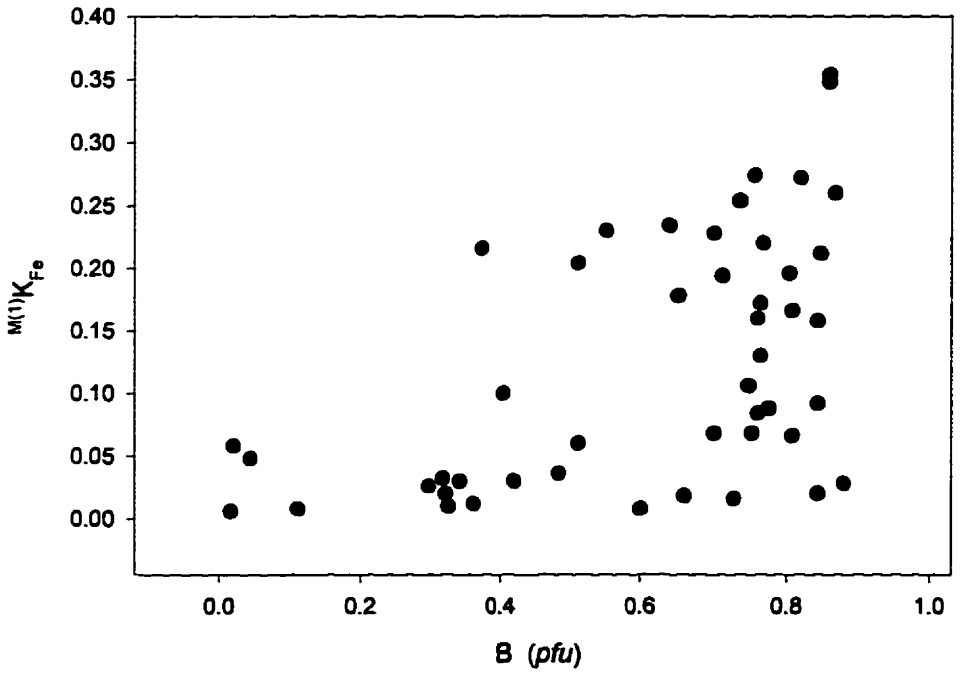


Figure 44: Relation between Fe^{2+} / (Mg + Fe^{2+}) ratio at M(1) and B content (*pfu*).

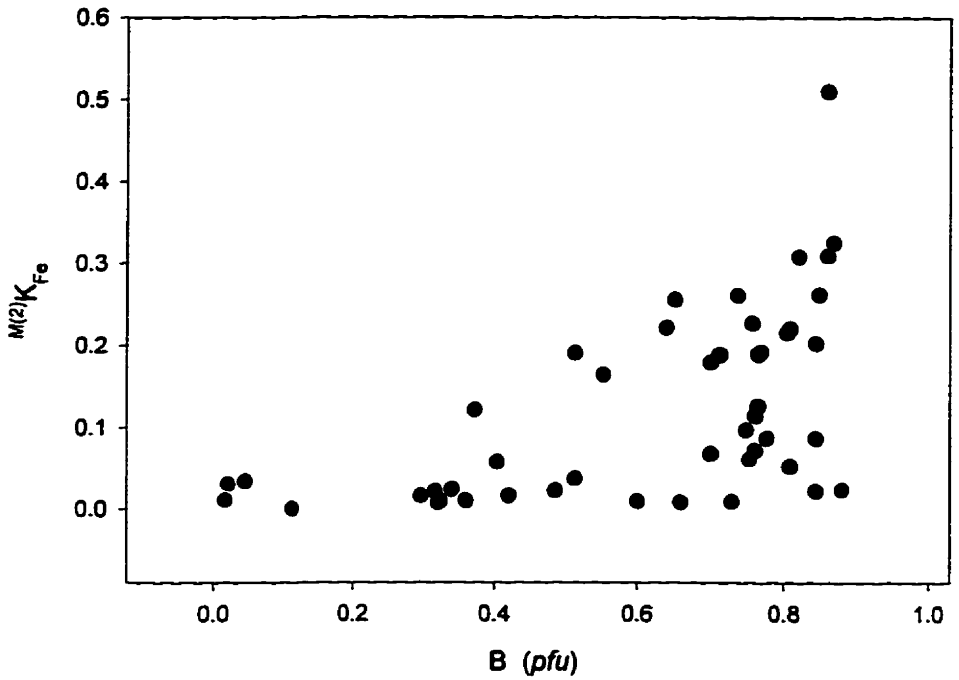


Figure 45: Relation between Fe^{2+} / (Mg + Fe^{2+}) ratio at M(2) and B content (*pfu*).

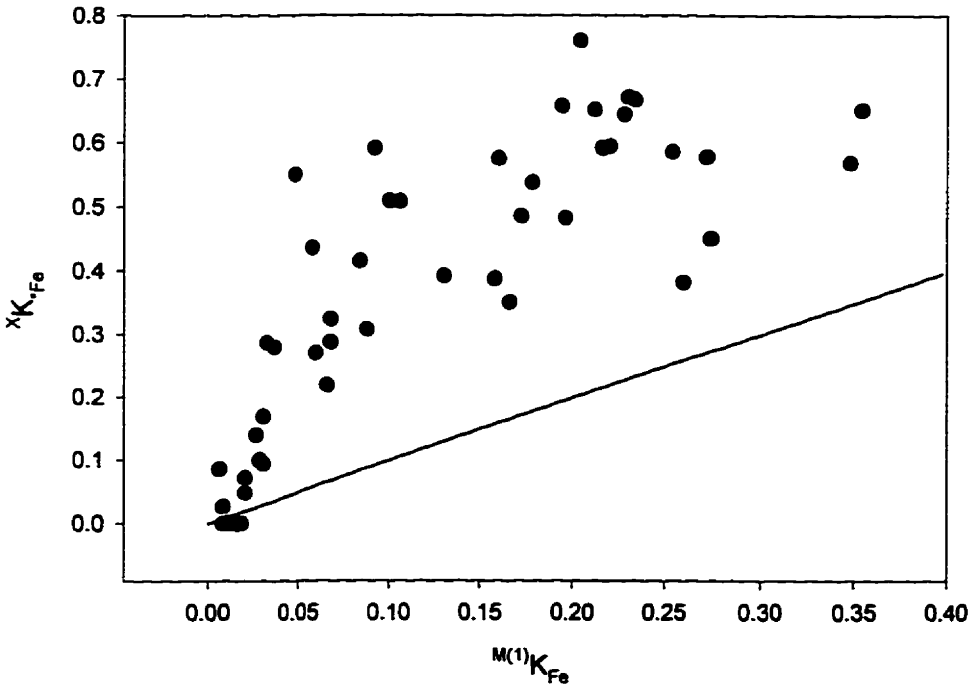


Figure 46: Relation between Fe^{2+} – Mg ordering at X and M(1).
Reference line through origin with slope = 1.

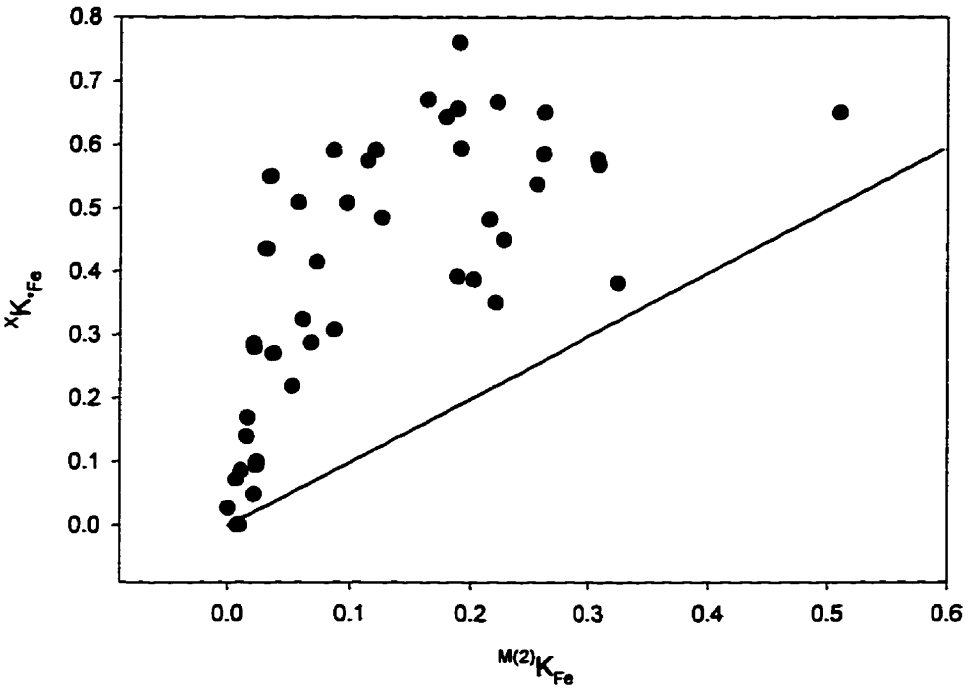


Figure 47: Relation between Fe^{2+} – Mg ordering at X and M(2).
Reference line through origin with slope = 1.

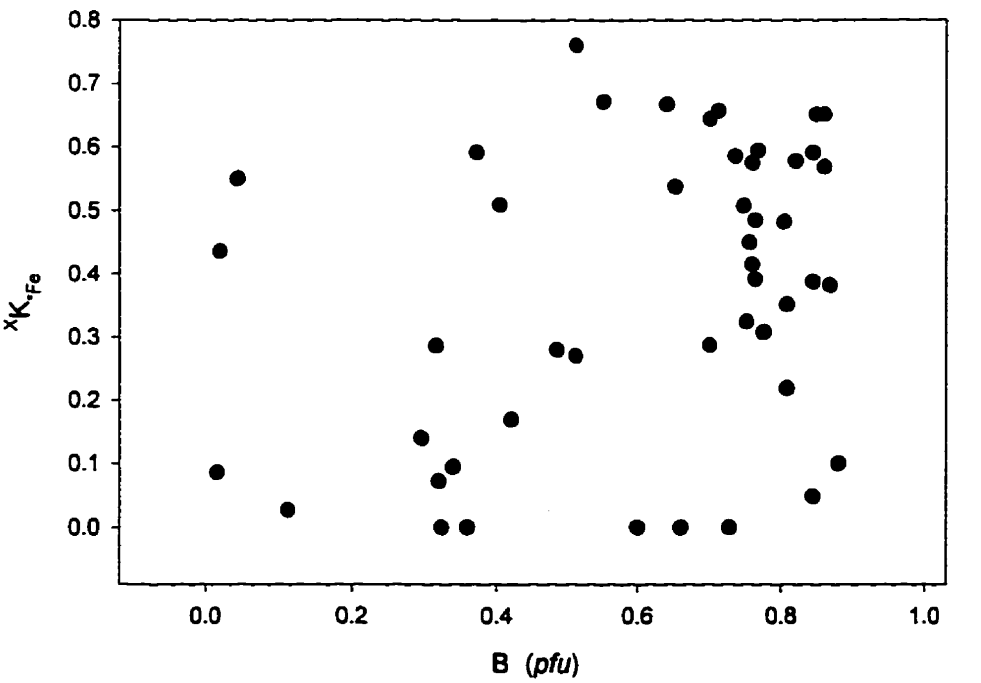


Figure 48: Relation between *Fe / (Mg + *Fe) ratio at X and B content (*pfu*).

5.3.2 Al distribution among M(2), M(3), M(4) and M(5)

In Figure 49, the $^{M(2)}$Al population (*pfu*) is plotted against B *pfu*. There is a well-defined linear relation between increasing $^{T(3)}$B and decreasing $^{M(2)}$Al. At high B values, the M(2) site is dominated by (Mg + Fe^{2+}) where the Fe^{2+} occupation may reach ~50%. Examination of the B layer in Figure 2a shows that one translation along *c* is comprised of an M(2) octahedron—T(3) tetrahedron pair that corner-share through O(8). With increased B at T(3), one might anticipate significant shortening along the *c* cell-parameter. However, over the entire range of B compositions, the range in *c* cell-parameter is only 0.07 Å (~6.69 to ~6.76 Å) (App. B). The O(8)–O(8) edge of the T(3) tetrahedron is parallel to [001] and varies in length from ~2.51 to ~2.73 Å (App. G.3), a difference of 0.22 Å. Therefore, a large component of the shortening along the O(8)–O(8) edge is compensated by a mutual lengthening of the M(2) octahedron along [001]. Coincident with the lengthening of the M(2) octahedron are M(2) cations of increased radii [*i.e.*, (Mg + Fe^{2+}) → Al].

In Figure 50, the $^{M(3)}$Al + $^{M(5)}$Al sum (*pfu*) is plotted against B *pfu*. There is a reasonable positive correlation between Al at M(3) + M(5) and B. The variation in Al population is coupled to ~5% substitution by Mg. The wall of edge-sharing and corner-sharing M(3) and M(5) octahedra in layer A (Fig. 1) must match dimensional changes occurring in the adjacent B layer (Figs. 2,3,37) at various B compositions. The size difference between Al (0.535 Å) and Mg (0.72 Å) is appreciable. At high B values, the B layer (Fig. 2) will be somewhat shortened along *a* and *c*. Matching of the A layer to this shortened B layer requires that M(3) and M(5) contain smaller cations (dominant Al). At low B, the B layer expands along *a* and *c*, and the A layer adjusts *via* Mg → Al substitution.

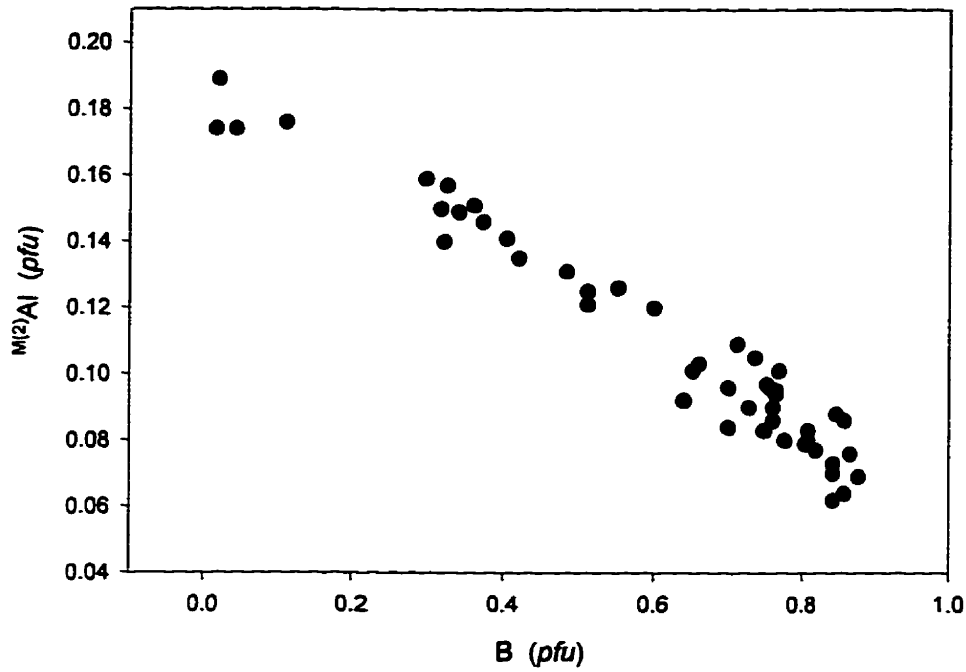


Figure 49: Relation between $^{M(2)}$Al *pfu* and B *pfu*.

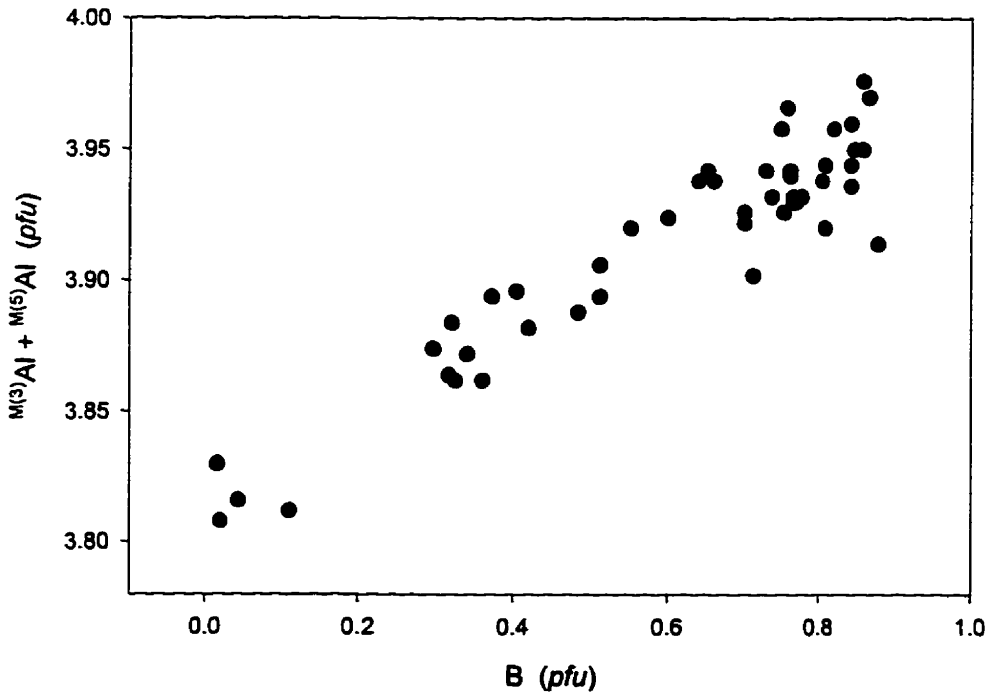


Figure 50: Relation between ($^{M(3)}$Al + $^{M(5)}$Al) *pfu* and B *pfu*.

In Figure 51, trivalent cations ($Al + Fe^{3+} + Cr + V + Ti^{4+}$) at M(4) *pfu* are plotted against B *pfu* (the $^{M(4)}Mg$ content is that which brings the M(4) cation-sum to 2 *apfu*). At very low B, the $^{3+}/_{2+}$ ratio at M(4) seems invariant. With increasing B content, the 3^+ cation total at M(4) may increase slightly, decrease appreciably (up to 0.4 *pfu* Mg $\rightarrow 3^+$), or adjust somewhere between these extremes. The M(4) site is populated mainly by Al (0.535 Å), but also contains up to ~0.4 Fe^{3+} (0.645 Å) and ~0.6 Mg (0.72 Å) *pfu* (Ch. 4). The ⟨M(4)–O⟩ distances span less than 0.04 Å (App. G.2) and the ⟨M(4)–O⟩ *vs.* *r*[M(4)] relation has a shallow slope (0.78) (Ch. 4). It was also shown in Figure 37 that M(4) octahedral distortions are induced through rotation of the T(2) tetrahedron during B sustitution at T(3). Within the B layer (Fig. 2), M(4) is situated between M(1) and M(2), and edge-shares to both. Variable $Fe^{2+} \rightarrow$ Mg substitution occurring on both sides of M(4) [at M(1) and M(2)] will introduce additional neighboring perturbations to the M(4) octahedron. All of these factors complicate the understanding of the M(4) role in kornerupine crystal-chemistry. The fact that the $^{3+}/_{2+}$ ratio at M(4) can either remain relatively invariant, or change significantly with changing B content, suggests that substitutions occurring at M(4) may be coupled to Tschermak-type substitutions in addition to those involving □. In Figure 52, M(4) trivalent cations *pfu* are plotted against □ *pfu*. An obvious correlation between increased 3^+ cations at M(4) and increased □ at X can be seen. Within the central region of the data, the relation is moderately perturbed. The dashed line has a slope of 2 and represents ideal charge-balance between changes in $^{3+}/_{2+}$ at M(4) and □ at X on a *pfu* basis. This can be expressed by the following equation for the dashed line:

$$^{M(4)}3^+[\times 2] + {}^{X}\square \Leftrightarrow {}^{X}2^+ + {}^{M(4)}2^+[\times 2]$$

Substitution paths can be envisioned that pass from the data plotting off the dashed line toward the dashed line. These paths, depending upon their orientation in Figure 52, may or may not involve coupled substitution with □, or adjustment in $^{3+}/_{2+}$ at M(4).

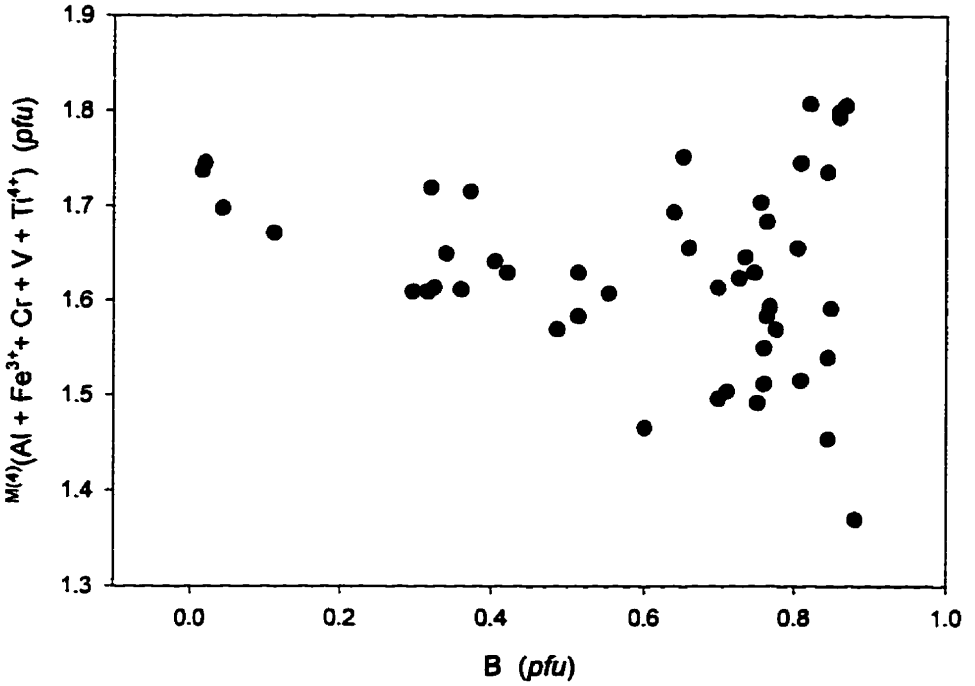


Figure 51: Relation between trivalent cations at M(4) *pfu* and B *pfu*.

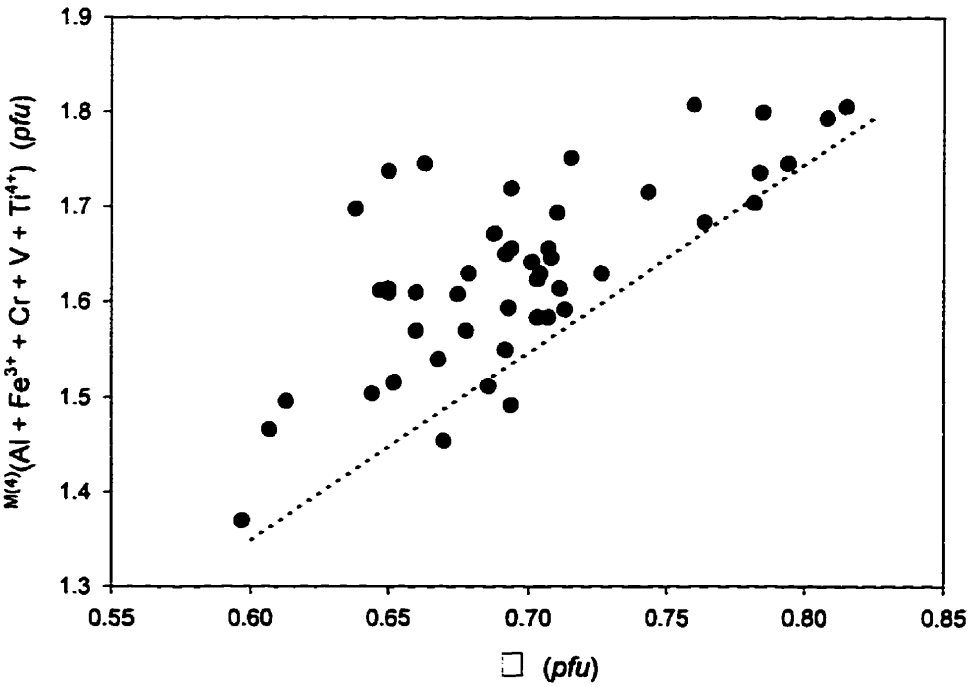


Figure 52: Relation between trivalent cations at M(4) *pfu* and □ *pfu*. The dashed line has a slope = 2.

If the M(4) site were involved in Tschermak-type substitution, one would anticipate correlation between $^{M(4)}3^{+}$ cations and Si content. Multiple-regression analysis using □ and Si *pfu* as independent variables gives an improved relation ($r^2 = 0.953$) with $^{M(4)}3^{+}$ content. This is illustrated in Figure 53 where the coefficients derived from multiple regression are multiplied by their respective independent-variable quantities, and the result is plotted against the trivalent cations at M(4). Substitutions ($2^{+} \Leftrightarrow 3^{+}$) occurring at M(4) therefore buffer geometric changes that occur with neighboring variable-B and $Fe^{2+} \Leftrightarrow Mg$ substitution, as well as charge differences associated with Tschermak-type and □-type substitutions.

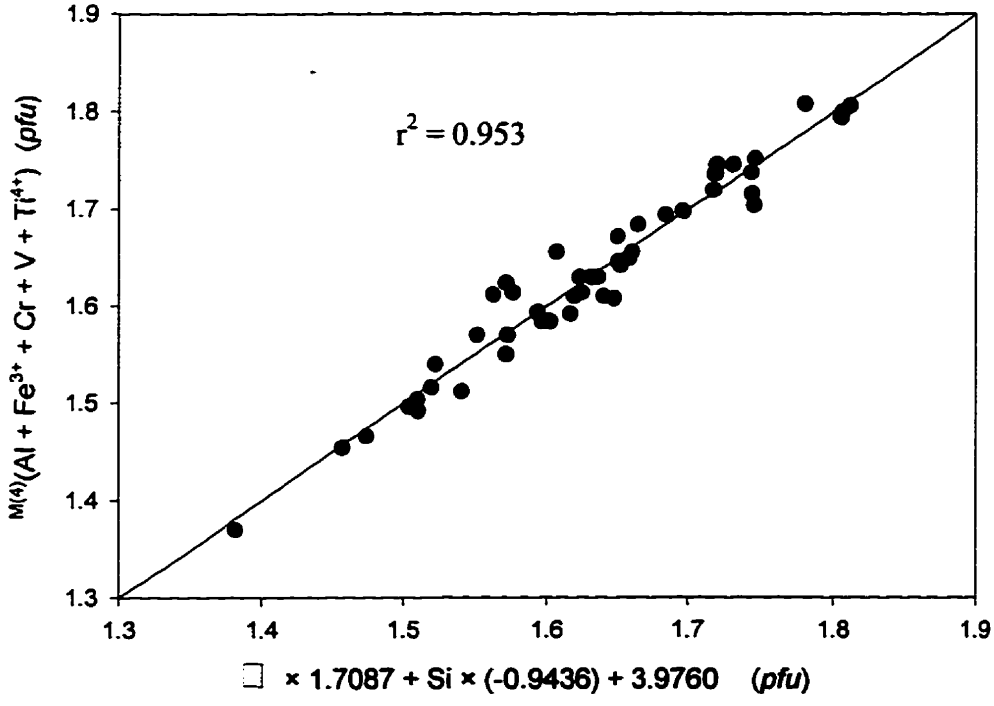


Figure 53: Relation between $^{M(4)}3^{+}$ cations and $^{M(4)}3^{+}_{predicted}$ cations from multiple regression using □ (*pfu*) and Si (*pfu*) as independent variables.

5.4 Substitution Pathways

Various plots within this chapter have shown the 47 ferrous kornerupines to occupy extensive fields. In these plots, there is no suggestion of possible substitutional gaps. Therefore, any two data points can be selected and compared in order to describe various substitutions. Table 6 contains six such data-pairs in which a path is characterized in terms of: (1) the type of substitution; (2) the relative changes in (B, Si, □, Fe^{2+}, Fe^{3+}); (3) a descriptive net equation containing coefficients (*apfu*). Figures 54 through 59 give further details regarding the substitutions for each of the paths 1 through 6, respectively. At the top of each figure, the net equation appears within a box. Directly below this equation, the net changes to the cations involved are given, and beneath the heavy dashed line are the details regarding atomic substitutions at the individual sites. All coefficients are expressed throughout as *apfu*. Algebraic signs (+/-) indicate relative changes to occupants in adherence to the path direction described in the net equation. Italicized site—occupant combinations (*e.g.*, *X Mg*, Fig.54) indicate that the site has remained unchanged with respect to its primary occupant. Horizontal and branched dashed-lines are site-specific linkages. Si components within thin outlines (*i.e.*, paths 3, 4, 6) algebraically sum to zero and therefore do not appear in the expressions above the heavy dashed horizontal line. Comparison between the relative magnitude of the coefficients associated with various site species helps to elucidate the more important substitutions.

TABLE 6: POSSIBLE SUBSTITUTION PATHS BETWEEN DATA PAIRS

Path	[1]Samples	[2]Type	[3]B	[3]Si	□	[3]Fe^{2+}	[3]Fe^{3+}	Net Equation
Path 1	K40→K13 *A* → *C*	T_S	L→H	L→H	$^2/_3$	L	L	$_{0.30}4^+ + _{0.30}2^+ \Rightarrow _{0.60}3^+$
Path 2	K13→K11 *C* → *D*	T_S, □	H	H→M	0.67→0.78	L→H	L	$_{0.11}□ + _{0.52}3^+ \Rightarrow _{0.15}4^+ + _{0.48}2^+$
Path 3	K30→K11 *B* → *D*	□	L→H	M	0.69→0.77	L→H	L	$_{0.08}□ + _{0.16}3^+ \Rightarrow _{0.24}2^+$
Path 4	K41→K24	□	H	M	0.60→0.81	L→M	L	$_{0.21}□ + _{0.42}3^+ \Rightarrow _{0.63}2^+$
Path 5	K40→K15	T_S	L→H	L→M	$^2/_3$	L→M	L→H	$_{0.23}4^+ + _{0.23}2^+ \Rightarrow _{0.46}3^+$
Path 6	K20→K15	□	H	M	0.82→0.65	M	L→H	$_{0.51}2^+ \Rightarrow _{0.17}□ + _{0.34}3^+$

[1] Letter labels (*A,B,C,D*) correspond to samples (K40,K30,K13,K11); see Figures 24-26

[2] T_S: Tschermak-type substitution; □: substitution involving coupled vacancies

[3] relative changes; L: low value, M: moderate value, H: high value

PATH 1

The path from sample K40 to K13 (*A* → *C*) represents the largest variation in Si content and therefore the most extensive Tschermak-type substitution. The vacancy at the X-site remains unchanged at ~$^2/_3$ □. Coincident with the increase in Si from lowest to highest value is the corresponding change in B (Fig. 24). This overall change in B and Si proceeds with coupled changes to Al and Mg. Inspection of Figure 54 reveals important substitutions involving $^{T(2)}$Si → $^{T(2)}$Al coupled to $^{T(3)}$B → $^{T(3)}$(Si, Al) in addition to $^{M(4)}$Mg → $^{M(4)}$Al.

PATH 2

The path from sample K13 to K11 (*C* → *D*) involves the greatest uptake of Fe^{2+} at a constant and high B-content. The net substitution involves both Tschermak- and □-type substitutions. Extensive Fe^{2+} → Mg substitution occurs at the M(1), M(2) and X sites. There is a charge deficit resulting from Al → Si substitution at T(2) and T(3) in combination with □ → Mg at X. Overall charge-balance is maintained by Al → Mg substitution at M(4).

PATH 3

The path from K30 to K11 (*B* → *D*) represents the □-type substitution occurring with no net change in Si content (Fig. 24). However, there is a significant redistribution of Si among the tetrahedral sites (Fig. 56). And in contrast to PATH 2, the increase in Fe^{2+} occurs with a corresponding increase in B content at T(3). The Al → Mg substitution at M(4) again contributes to maintain overall charge-balance.

PATH 4

The path from K41 to K24 involves extensive □-type substitution that occurs with only minor changes at the tetrahedral sites. Moderate Fe^{2+} → Mg substitution occurs at M(1) and M(2). □ → Mg substitution at X must be charge-balanced by Al → Mg substitution at M(4).

PATH 5

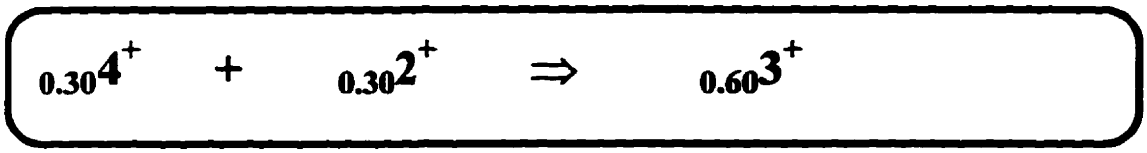
The path from K40 to K15 involves significant substitution of Fe^{3+} at M(4) during a Tschermak-type substitution. There is an excess of charge (+0.23) at the tetrahedra associated with (Si + B) → Al substitution. This is charge-balanced by the deficit in charge (-0.23) resulting from the (Mg + Fe^{3+}) → Al substitution at M(4).

PATH 6

The path from K20 to K15 involves significant substitution of Fe^{3+} at M(4) during a □-type substitution. In this case, there is an excess charge at the X-site associated with (Fe^{2+}, Mg) → □ substitution. Most of this charge-difference is balanced by the charge-deficit resulting from the (Mg + Fe^{3+}) → Al substitution at M(4).

Substitutions involving B → (Si, Al) at T(3) always involve a coupled Si → Al substitution at T(2). The most extensive Fe^{2+} → Mg substitution occurs at high B values where the M(1) and M(2) sites are dimensionally more receptive toward incorporation of the larger Fe^{2+} cation as a function of the neighboring dynamics involving the tetrahedral trimer. The M(4) site is actively involved in all net substitutions and provides necessary charge-balance *via* Mg ⇔ Al substitution. At higher B content, Fe^{3+} substitution at M(4) proceeds *via* (Mg + Fe^{3+}) → Al in relation to either Tschermak- or □-type substitutions.

Path 1



+0.30 Si **+0.30 Mg** ⇒ **+0.80 B**

-1.40 Al

$^{T(1)}$Si +0.15	.....	$^{T(1)}$Al -0.15
$^{T(2)}$Si +0.75	.....	$^{T(2)}$Al -0.75
$^{T(3)}$Si -0.60	.....	$^{T(3)}$Al -0.20
		$^{T(3)}$B +0.80

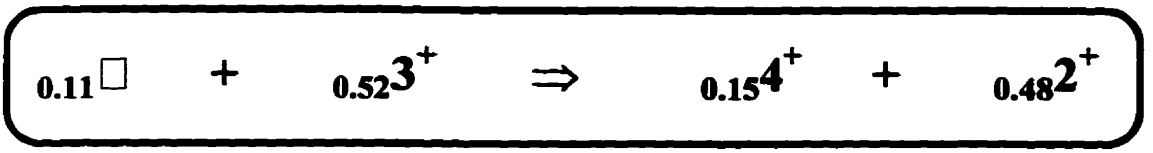
X Mg

M(1) Mg

$^{M(2)}$Mg +0.10	.....	$^{M(2)}$Al -0.10
$^{M(3)}$Mg -0.07	.....	$^{M(3)}$Al +0.07
$^{M(5)}$Mg -0.03	.....	$^{M(5)}$Al +0.03
$^{M(4)}$Mg +0.30	.....	$^{M(4)}$Al -0.30

Figure 54: Substitutional details associated with PATH 1; (K40 → K13).

Path 2



+0.11 □ **+0.52 Al** ⇒ **-0.15 Si** **+1.32 Fe^{2+}** **-1.80 Mg**

T(1) Si

$^{T(2)}$Al +0.11 ..... $^{T(2)}$Si -0.11

$^{T(3)}$Al +0.04 ..... $^{T(3)}$Si -0.04

T(3) B

^{X}□ +0.11 ..... $^{X}Fe^{2+}$ +0.12

^{X}Mg -0.23

$^{M(1)}Fe^{2+}$ +0.70

$^{M(1)}$Mg -0.70

M(2) Al ..... $^{M(2)}Fe^{2+}$ +0.50

$^{M(2)}$Mg -0.50

M(3) Al

M(5) Al

$^{M(4)}$Al +0.37 ..... $^{M(4)}$Mg -0.37

Figure 55: Substitutional details associated with PATH 2; (K13 → K11).

Path 3

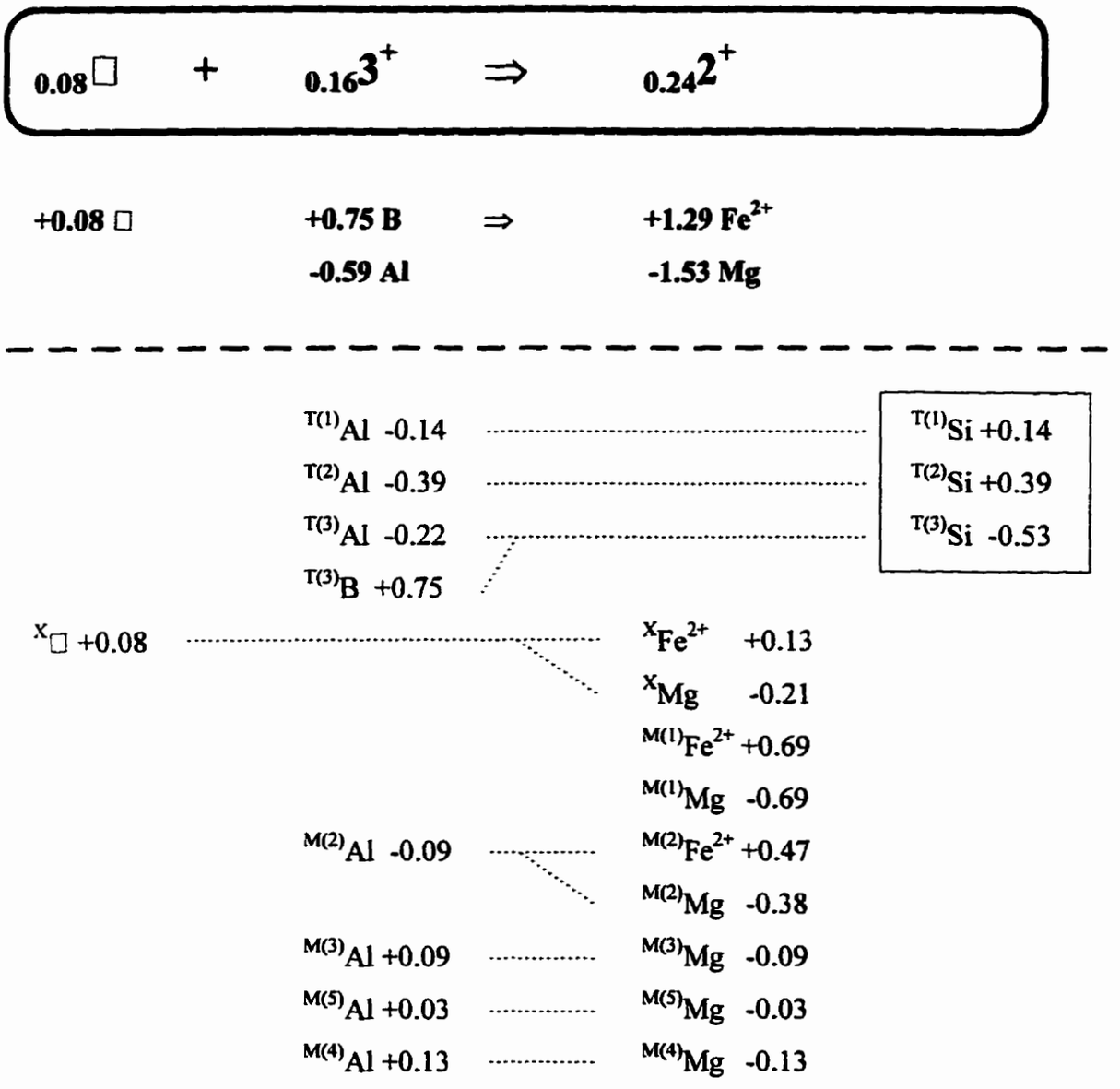


Figure 56: Substitutional details associated with PATH 3; (K30 → K11).

Path 4

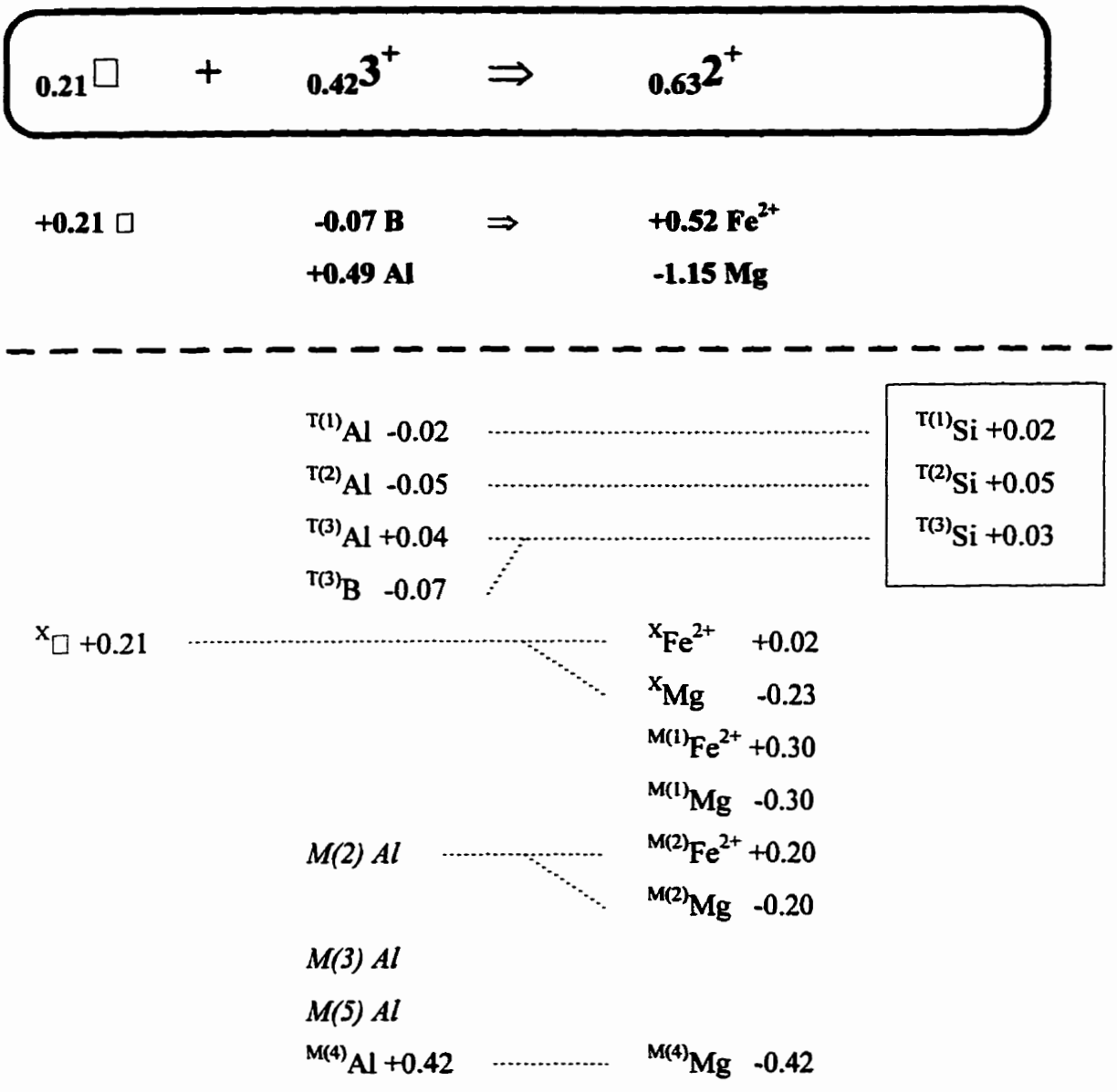
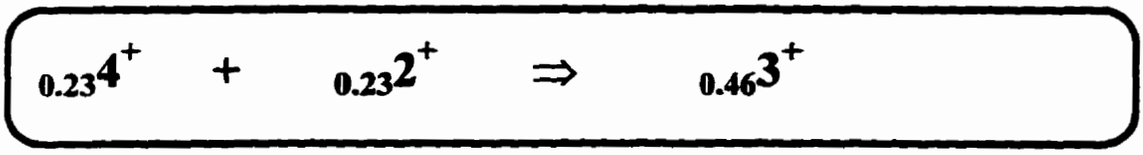


Figure 57: Substitutional details associated with PATH 4; (K41 → K24).

Path 5



+0.23 Si **+0.54 Fe^{2+}** ⇒ **+0.70 B**

-0.31 Mg **-1.50 Al**

+0.34 Fe^{3+}

$^{T(1)}Si$ +0.11 ..... $^{T(1)}Al$ -0.11

$^{T(2)}Si$ +0.65 ..... $^{T(2)}Al$ -0.65

$^{T(3)}Si$ -0.53 ..... $^{T(3)}Al$ -0.17

$^{T(3)}B$ +0.70

X Mg

$^{M(1)}Fe^{2+}$ +0.38

$^{M(1)}Mg$ -0.38

$^{M(2)}Fe^{2+}$ +0.16 ..... $^{M(2)}Al$ -0.07

$^{M(2)}Mg$ -0.09

$^{M(3)}Mg$ -0.03 ..... $^{M(3)}Al$ +0.03

$^{M(5)}Mg$ -0.04 ..... $^{M(5)}Al$ +0.04

$^{M(4)}Mg$ +0.23 ..... $^{M(4)}Al$ -0.57

$^{M(4)}Fe^{3+}$ +0.34

Figure 58: Substitutional details associated with PATH 5; (K40 → K15).

Path 6

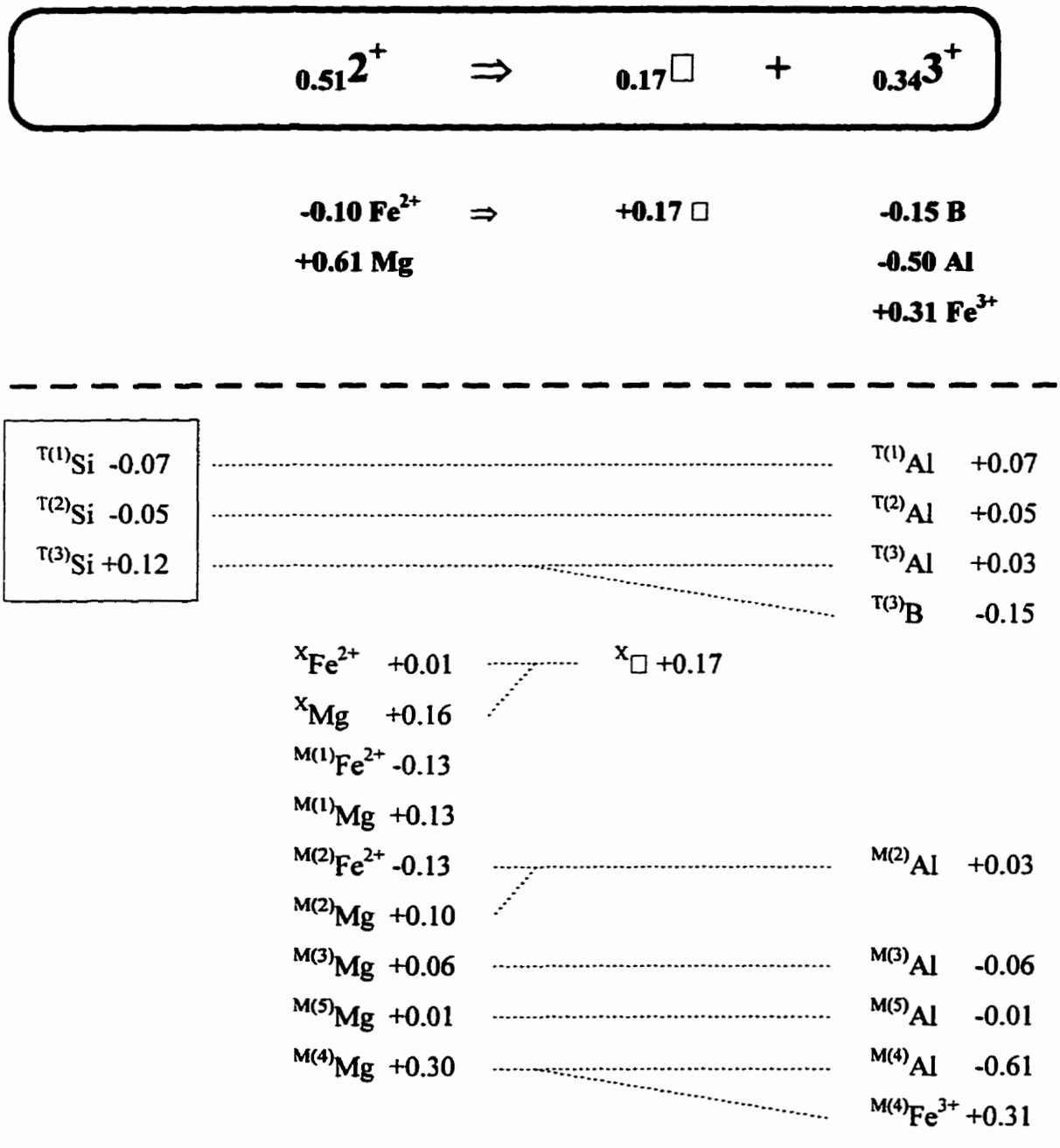


Figure 59: Substitutional details associated with PATH 6; (K20 → K15).

5.5 Anion Composition of the O(10) site

In previous studies, several possible occupants have been suggested for the O(10) site: O^{2-}, F, OH, H_2O (1.5.1). The site assignments in chapter 4 are consistent with cation totals developed from the EMP data using (F + OH) = 1. Support for a 1^- formal charge at the O(10) site was given using bond-valence criteria in section 3.1. In section 4.2.5, discussion involving the results of the ferric-iron kornerupines from Bamble, Norway, indicated that H_2O at the O(10) site would help rescale the cations from the formula calculation such that closer agreement with cations from SREF could be attained.

In Figure 60, F from EMPA is plotted against F from occupancy refinement at the O(10) site. For all refinements, scattering in excess of 8 electrons at the O(10) site was modelled with a combination of F^- and O^{2-} scattering factors. The dashed line drawn through the data (Fig. 60) has a slope of unity. There is a reasonably good agreement between F values arrived at by both methods. Therefore, residual electron-density in the vicinity of the O(10) site should better reflect the possible presence of an additional nearby scattering species, namely H.

At the final stages of refinement, the residual electron-density was investigated. The only significant density remaining in difference Fourier maps was always less than one electron, and occurred on the (100) plane at $x = 0$. For all refinements, the density was contoured and the different patterns of contours encountered are presented in Figure 61. In the upper left of each box, the kornerupine sample number is given. In a few instances, density maxima lie on the mirror (001) at $z = {}^1/_4$ [*i.e.*, H(1)]; samples K21, K40. For most samples, the density maxima are disordered off the mirror (001) at $z = {}^1/_4$ [*i.e.*, H(2)]; samples K22, K28, K38. A few samples show electron-density maxima at both H(1) and H(2) positions; sample K18. The majority of the samples show contouring that is most similar to that of K22–K28–K38, and therefore the H(2)

position should be regarded as the most prominent and therefore the most reliable. The H(1) contours are never circular on the mirror (001) at $z = {}^{1}/_{4}$ and should be considered as less reliable. Klaska & Grew, 1991 report a H atom at the 8f position (0*yz*), in agreement with the H(2) position reported here. Further discussion of the H content will be based only on the H(2) site. Results from polarized infrared spectroscopy suggest that OH bonds must lie within the (100) plane (A. Beran; reported in Klaska & Grew, 1991), in agreement with the O(10)—H(2) relation. The H at H(2) may H-bond to O(9) ~along *c* or to O(9)′ ~along *b* (Klaska & Grew, 1991). For K18, K38, K22 and K28, the geometry of the H-bonding is as follows: H(2)·····O(9) ranges from 2.67 to 2.78 Å; H(2)·····O(9)′ ranges from 2.30 to 2.42 Å; O(10)—H(2)·····O(9) ranges from 120 to 129°; O(10)—H(2)·····O(9)′ ranges from 102 to 110°. The acceptors are too distant and too skewed from the OH vector for there to be significant H-bonding. This is in agreement with the bond-valence calculations that show O(9) is already saturated with respect to its bonding requirements [incident bond-valence at O(9) ranges from 2.022 to 2.118 *vu* with no H-bond contribution; App. J].

The H(2) site is located ~1.1 Å from the X site, and the mutual occupation of X and an adjacent H(2) site is therefore not possible. Both the H content at H(2) [F + OH = 1] and H(2) ordering can limit the X-occupancy factor. Two end-member H(2)-ordering schemes are presented in Figure 62a and 62b. If the OH vector is progressively staggered along *c* such that each succeeding X-site is interfered with (Fig. 62a), then the X-occupancy must be zero. If successive pairs of OH vectors are directed toward each other along *c* such that every other X-site is interfered with (Fig. 62b), then the X-occupancy could reach 0.5 *apfu*. The X-site occupancies in this study range from 0.18 to 0.40 *apfu* (App. F) and fall between these two extremes.

Also illustrated in Figure 62c,d are two possible ordering schemes involving $^1/_3$ and $^2/_3$ H_2O *pfu*, respectively. Geometrically, these arrangements allow for up to $^1/_3$ and $^1/_4$ occupancy of X. H(2)—O(10)—H(2)' angles for K18, K38, K22 and K28 in Figure 61 range from 102 to 116° and are acceptable angles for an H_2O group. The greatest difficulty in placing H_2O at the O(10) site is related to the details regarding plausible H-bonding. The O of the H_2O group is bonded to two M(1) cations, and receives $\sim^1/_3$ *vu* from each M(1) cation. This O then has a total incident bond-valence of $\sim^2/_3$ *vu*. This requires that outgoing H-bonds are also strong (*i.e.*, $\sim^1/_3$ *vu* each). The problem arises from the fact that there are no suitable acceptors to receive these strong H-bonds [the O at O(9) is already saturated with respect to its bonding requirements]. The problem is also magnified when H-bonds are drawn in on Figure 62c,d, where it quickly becomes evident that $^1/_3$ of the O(9) sites must accept multiple H-bonds. So although the local geometry seems reasonable for an H_2O group, the lack of suitable H-bond acceptors provides compelling evidence against H_2O substitution at O(10).

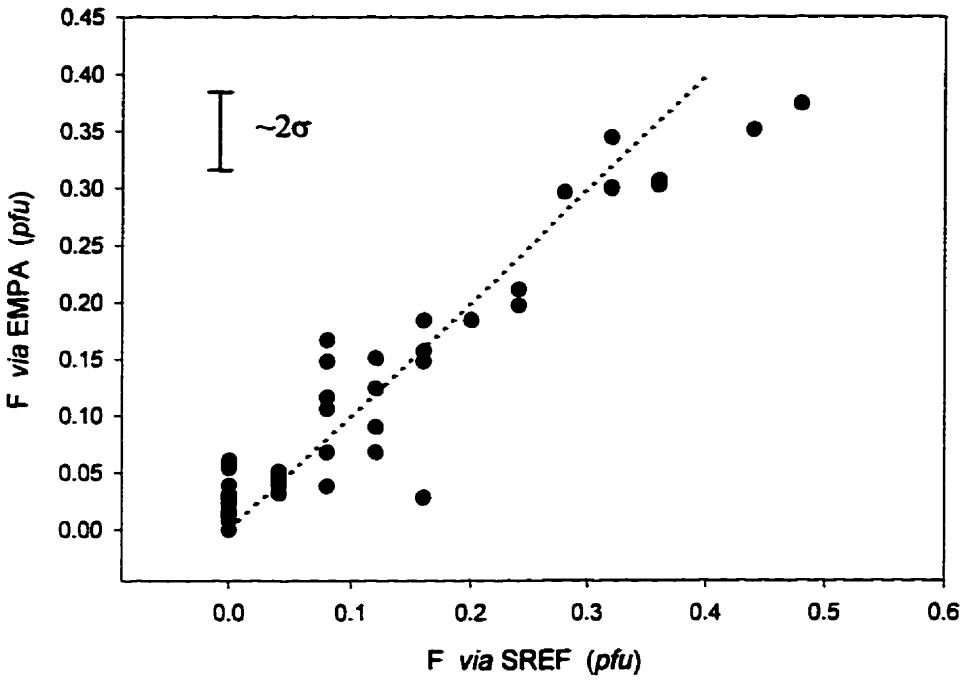


Figure 60: Comparison of F (*pfu*) from EMPA and SREF [47 ferrous-iron kornerupines]. Formula calculation based on O_{21} $(F + OH)_1$. Dashed reference line has a slope of unity.

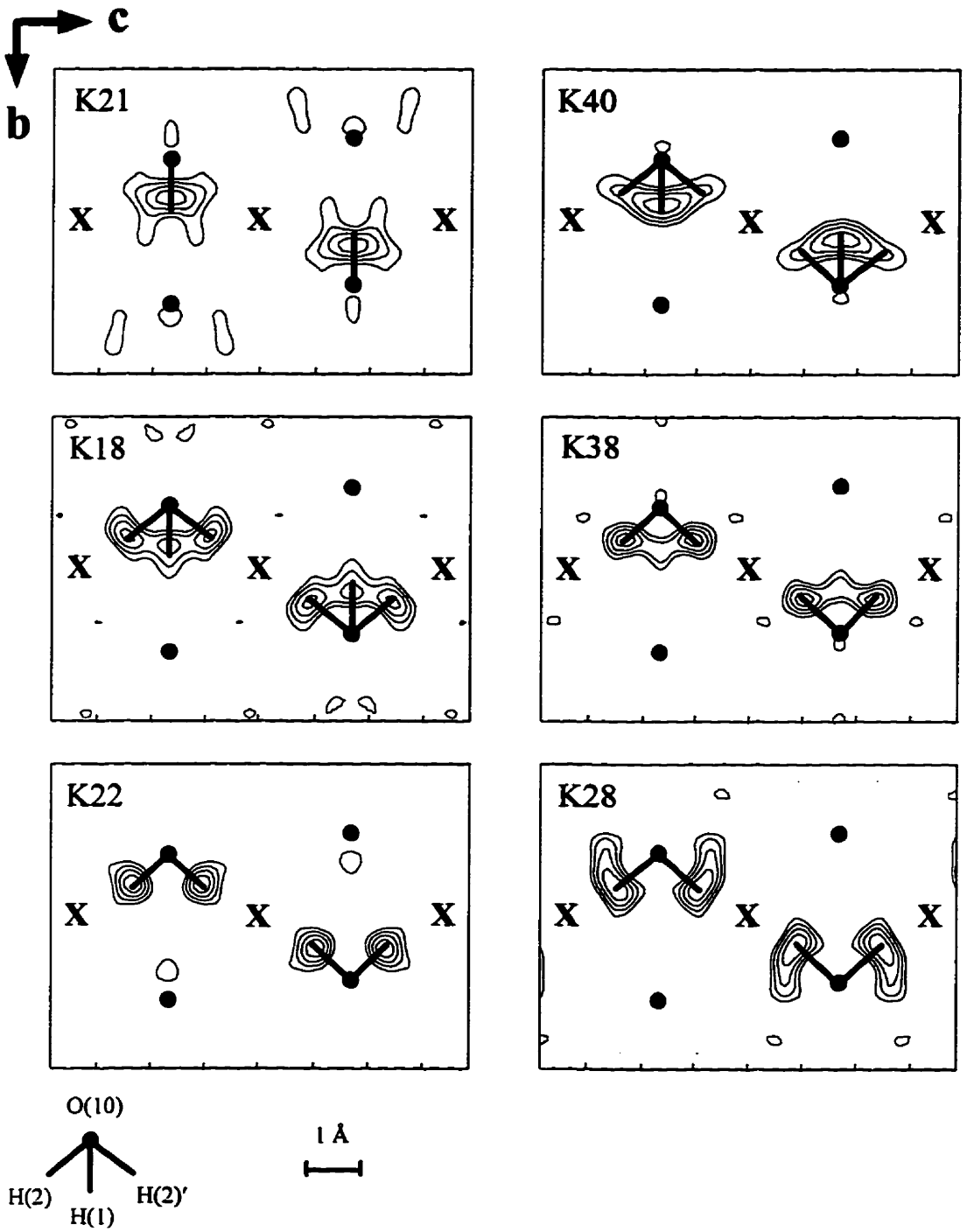
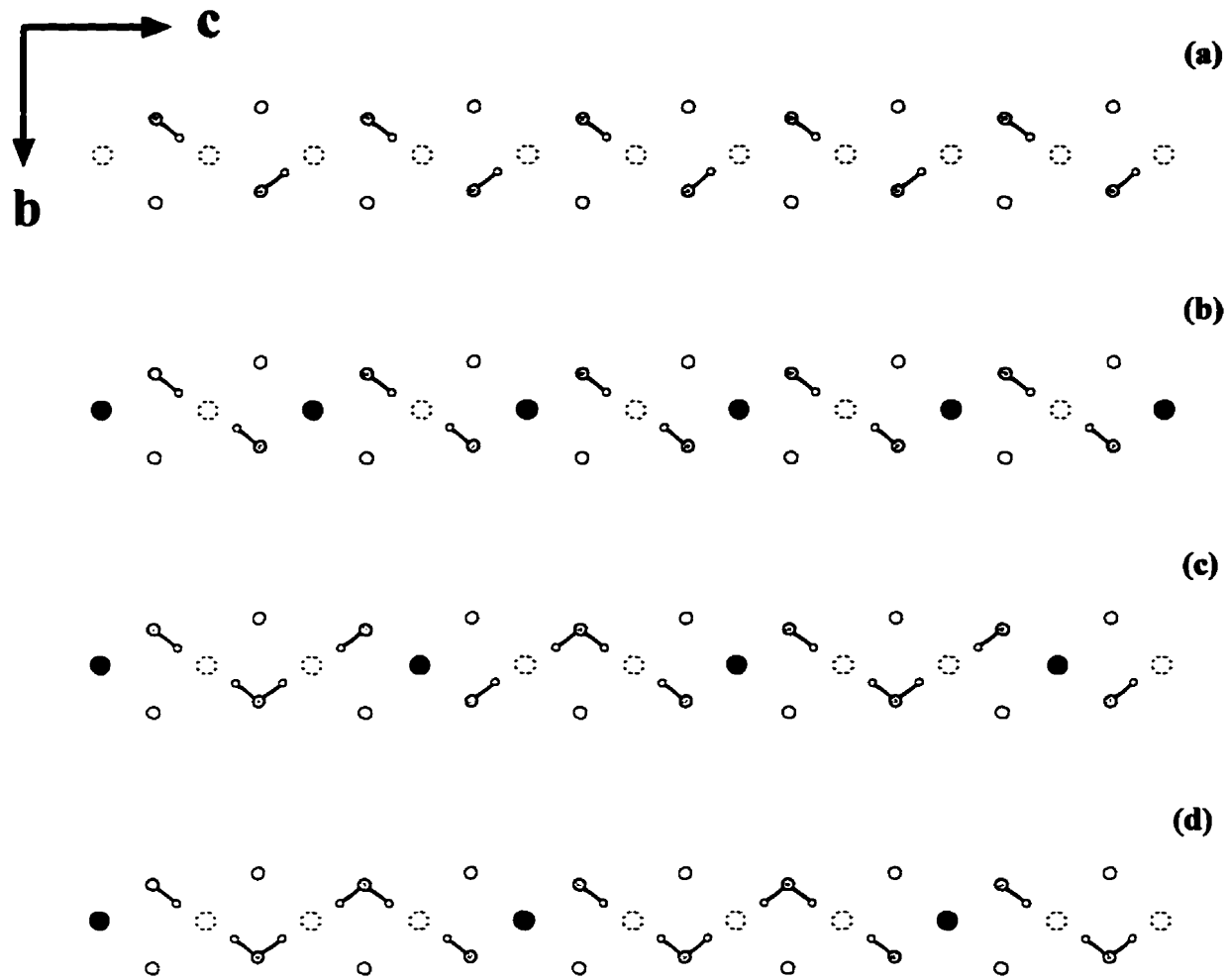
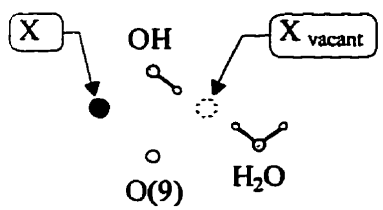


Figure 61: Contoured electron-density [(100) at $x = 0$] proximal to O(10). X-sites are labelled as X, O(9) and O(10) sites are filled circles. Inferred H positions are at the ends of the short heavy lines (~1.0 Å long). Contour values are 0.2, 0.3, 0.4, 0.5, 0.6 e/Å^3.





	X occupancy	(OH)	(H_2O)
(a)	0	1	0
(b)	1/2	1	0
(c)	1/3	2/3	1/3
(d)	1/4	1/2	2/3

Figure 62: Local ordering involving the H(2) site and X-site vacancies along [001]. Labelling as in legend.

CHAPTER 6

EMPIRICAL RELATIONS

6.1 Assessing B, Fe^{2+}, Fe^{3+}, F and H

This chapter gives a procedure for which the chemical parameters B, Fe^{2+}, Fe^{3+}, F, H can be derived for kornerupine using only the results from EMPA and powder X-ray diffraction (XRD). These two analytical methods provide sufficient information such that all of the above chemical parameters can be indirectly calculated using simple empirical relations.

F can be measured directly during regular EMPA, and the H can be calculated from the relation (OH + F) = 1 *pfu*. Extensive substitution of B at T(3) [0 → 0.9 B] is related to significant dimensional changes within the kornerupine structure. This is most obvious in Figure 37 which illustrates the adjustments of the T(2)—T(3)—T(2) trimer in response to various B contents at T(3). Variation in the *a* and *c* cell-parameters should correlate with B content, as the O(7)–O(7) and O(8)–O(8) edges of the T(3) tetrahedron lie along [100] and [001], respectively (Fig. 37). Many of the Figures in chapter 5 involved plotting various chemical parameters against B content. The major-element chemistry acquired from EMPA thus can provide additional constraint on the calculated B-content. Partitioning of Fe from EMPA into correct Fe^{2+} and Fe^{3+} values is more difficult. With both Tschermak- and □-type substitutions operating, there is no straightforward way to assess Fe^{2+} at M(1), M(2) and X. Another approach would involve assessing Fe^{3+} at the M(4) site. M(4) is occupied by appreciable Al (0.535 Å), Mg (0.72 Å) and Fe^{3+} (0.645 Å). The maximum Fe^{3+} at M(4) for the 47 ferrous kornerupines examined here is 0.348 *pfu* for K15 (App. F), which amounts to 17.4% Fe^{3+} at M(4). It therefore does not seem practical to attempt to develop a scheme of assessing Fe^{3+} content based on a dimensional arguement that would ultimately relate back to the 0.645 Å radius of Fe^{3+}. It was suggested in section 5.3.2 that the M(4) occupants are actively involved in both Tschermak- and □-type substitutions, and this was confirmed in section 5.4 which described the detailed site-

substitutions presumed to occur between various compositions. In Figure 53, the 3^+ cations at M(4) were plotted against the results of an expression involving □ and Si contents. □ and Si are key components in the □-type and Tschermak-type substitutions. The linearity of the plot indicated that $^{M(4)}(Al + Fe^{3+})$ could be estimated from □ and Si. The chemical parameters $^{M(4)}Al$, Si, and □ therefore offer a means to assess Fe^{3+} at M(4).

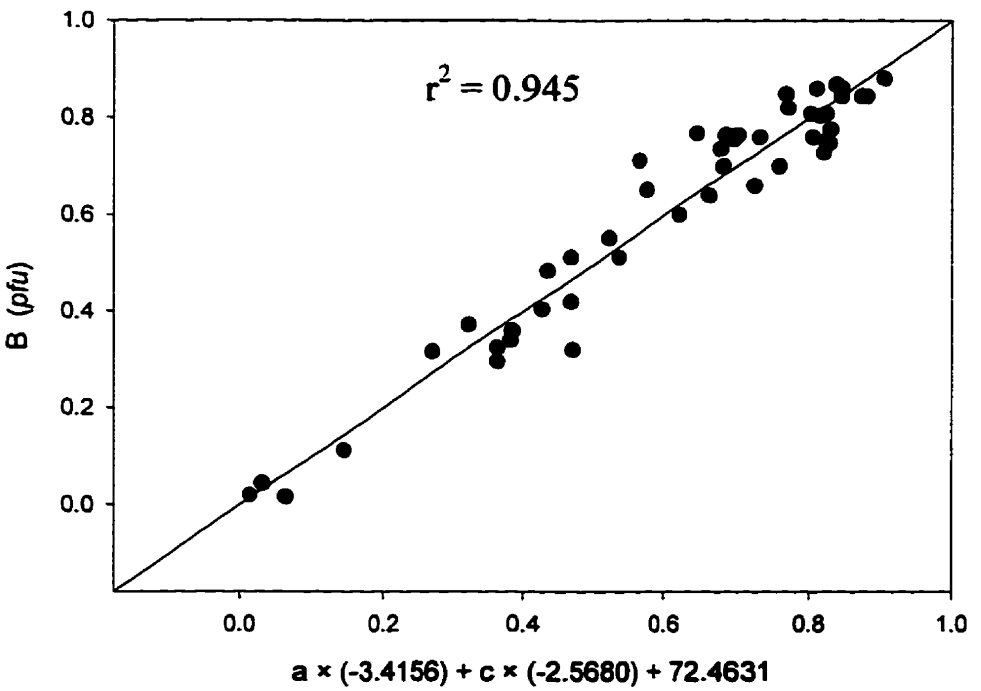


Figure 63: Relationship between B and $B_{predicted}$ from multiple regression using the *a* and *c* cell-parameters as independent variables.

6.2 Empirical relations

6.2.1 Assessing B content

Multiple-regression analysis using the *a* and *c* cell-parameters as independent variables produces a reasonably good correlation (r^2 = 0.945) when plotted against B values. This is illustrated in Figure 63, in which the coefficients derived from multiple-regression analysis are multiplied by their respective independent variables and the result is plotted against B *pfu*. Additional information in the form of Al *pfu* can be incorporated into the regression to give an improved relation (r^2 = 0.964) with B (Fig. 64). If the *Fe value is also added, the correlation improves to r^2 = 0.990 (Fig. 65). The precision to which the B content can be predicted is then dependent on the information available (*i.e.*, *a*, *c*, Al, *Fe).

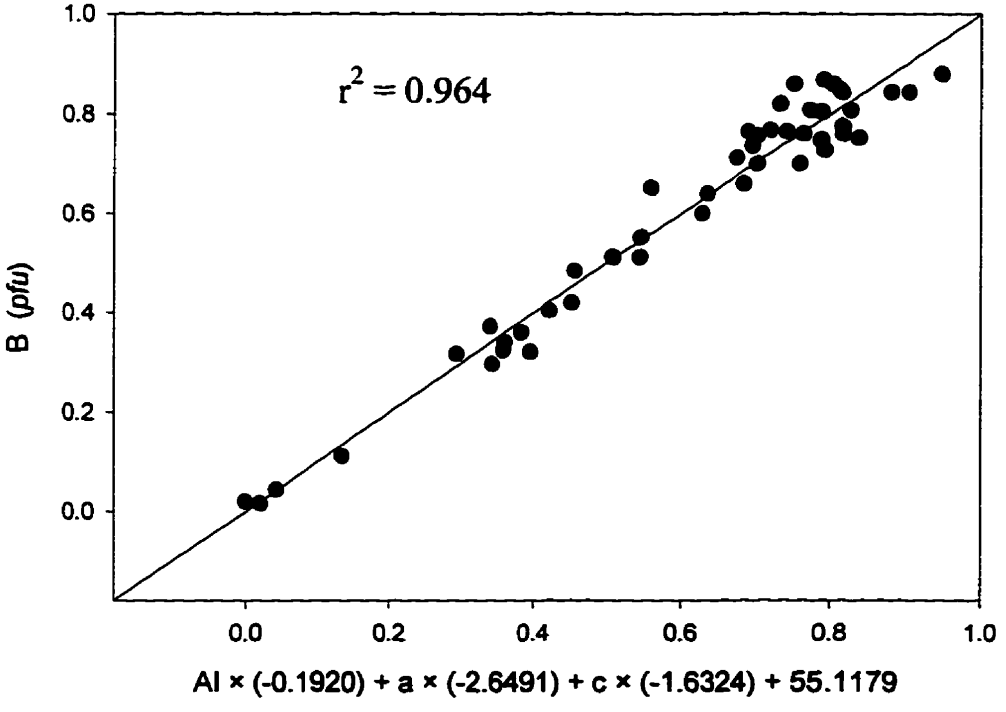


Figure 64: Relationship between B and $B_{predicted}$ from multiple-regression analysis using Al *pfu* and the *a* and *c* cell parameters as independent variables.

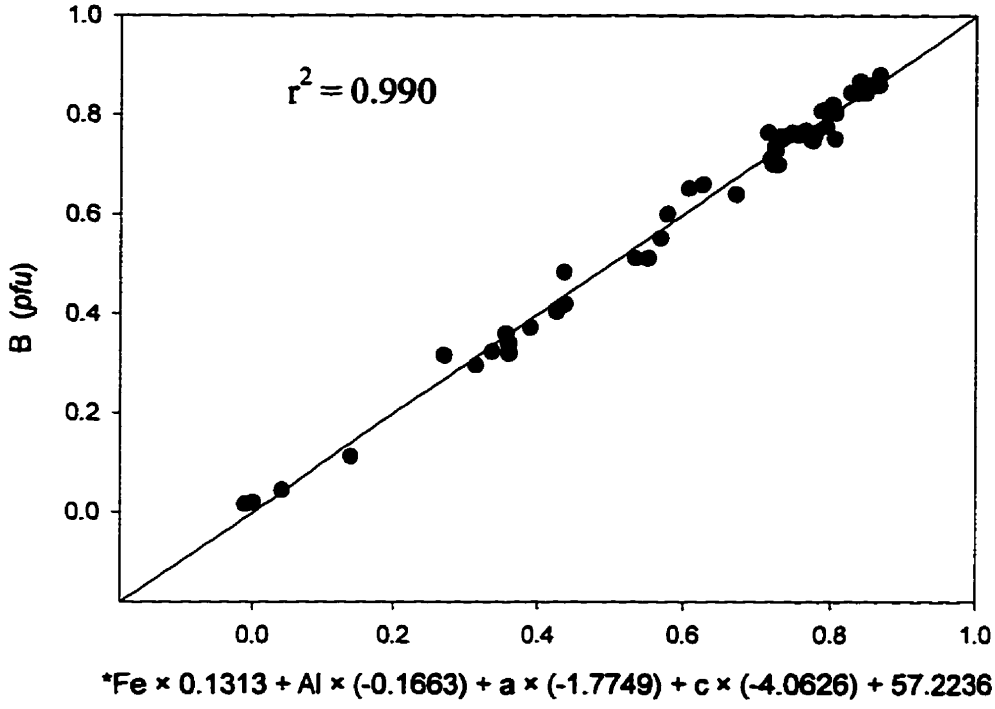


Figure 65: Relationship between B and $B_{predicted}$ from multiple-regression analysis using *Fe *pfu*, Al *pfu* and the *a* and *c* cell-parameters as independent variables.

6.2.2 Assessing $^{M(4)}$Al

The site populations in chapter 4 show that Al occurs at M(2), M(3), M(4) and M(5) in addition to all three tetrahdral sites. Indirectly determining Al at M(4) requires that Al populations be assessed at all other Al-bearing sites to a reasonable degree of accuracy. In Figure 66, the tetrahedral-Al sum *pfu* is plotted against B. In Figure 67, the Al sum for the M(3) and M(5) sites is plotted against B. Figure 68 illustrates the relation between $^{M(2)}$Al *pfu* and B. Equations for the regression lines in Figures 66 through 68 provide a mechanism by which all Al-bearing sites [other than M(4)] can assessed for Al content using only the B value as input. The quantity $^{M(4)}$Al can then be arrived at by difference from the equation $^{M(4)}Al = {}^{EMP}Al - [{}^{Tet}Al + {}^{M(2)}Al + {}^{M(3,5)}Al]$.

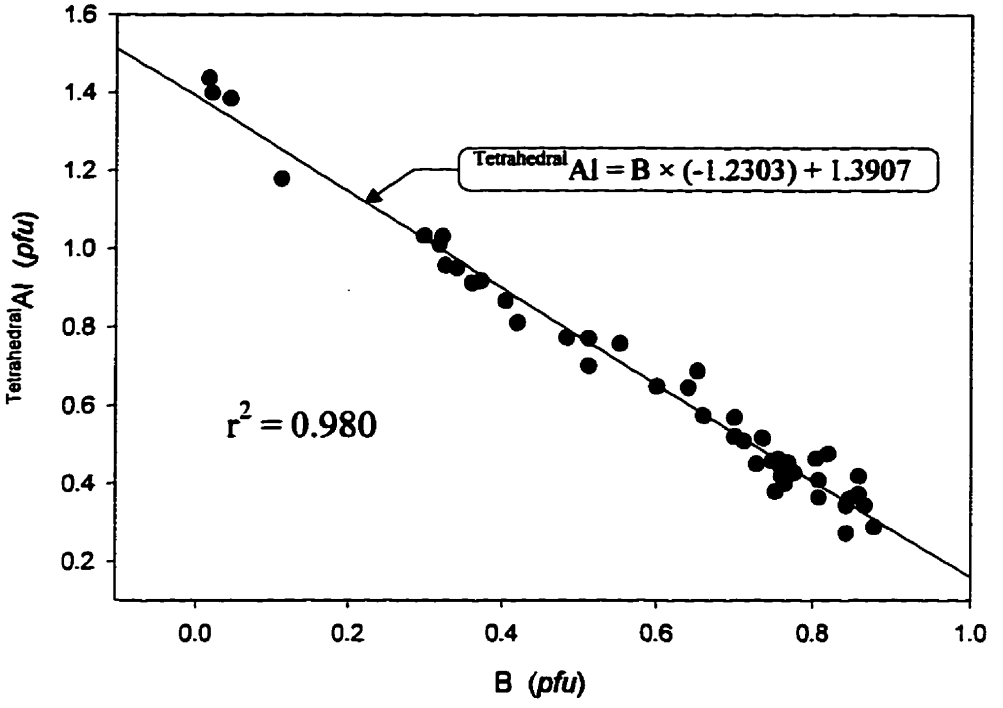


Figure 66: Relationship between the tetrahedal-Al sum *pfu* and B *pfu*.

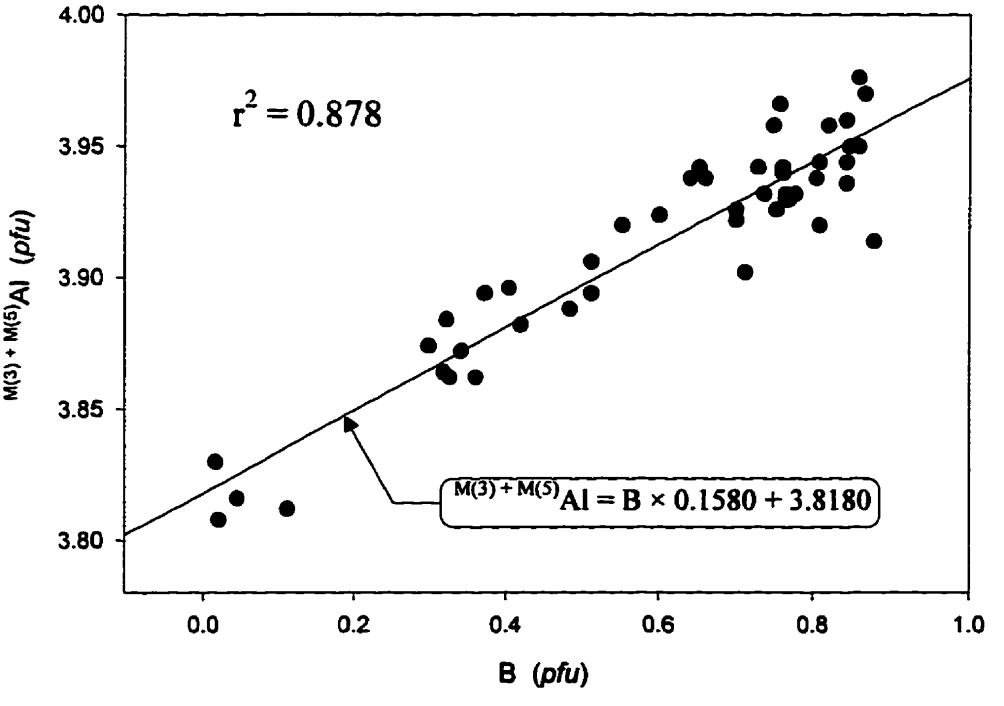


Figure 67: Relationship between the [M(3) + M(5)] Al sum *pfu* and B *pfu*.

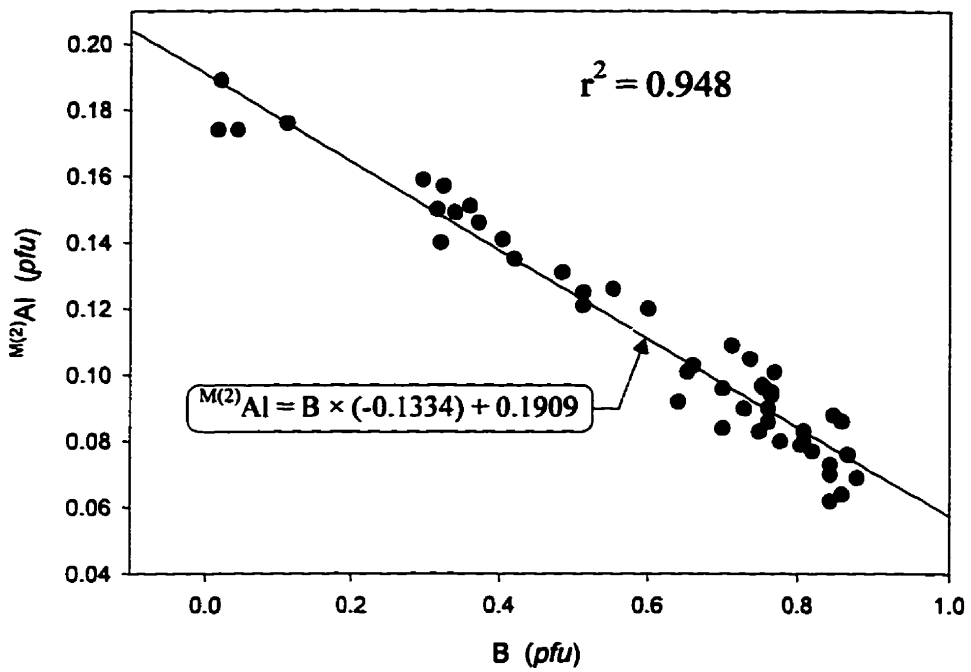


Figure 68: Relationship between Al at M(2) *pfu* and B *pfu*.

6.3 A worked example

To test the applicability of the equations in 6.2, one of the kornerupine samples that was known to contain appreciable Fe^{3+} (0.348 Fe^{3+} *pfu*) was selected (K15). For this test, cell dimensions were those from the single-crystal cell-refinement (App. B) and EMP results are taken from Appendix H. In practice, a kornerupine separate of a few tens of milligrams could be pulverized, and a diffractogram acquired with a powder XRD instrument. Least-squares software is available to process this diffraction data into refined cell-dimensions. EMPA could be done as in section 2.2. Processing the oxides into cations *pfu* is done using a current B-value estimated from the equations in combination with the anion-normalization scheme O_{21} $(OH + F)_1$. In the beginning, all Fe is assumed to be ferrous. This set of starting parameters, as well as the sequence of developed parameters and decision-making process, are illustrated in Figure 70. Progression through the flow chart involves obtaining a more accurate estimate of the B content and partitioning of Fe into Fe^{2+} and Fe^{3+}. Working with a current estimate of the B content (and possibly Fe^{3+}, Fe^{2+}), a position can be calculated in Figure 69. Figure 69 is reproduced from Figure 53, where the kornerupine data plotting about the ideal solid line lie within the enclosed dotted field. A current position calculated for Figure 69 will be in terms of **x** and **y** coordinates developed from the result of the expression along the abscissa using current □ and Si *pfu* values, and total $^{M(4)}3^+$ cations along the ordinate, respectively. Data points plotting below the ideal line indicate a current deficiency in 3^+ cations at M(4) in relation to the current Si and □ values. This is shown with the placement of the open circle in Figure 69, which is the plotted position for K15 using a B value estimated from the *a* and *c* cell-parameters alone, together with the assumption that all Fe is Fe^{2+}. The relative difference between the **x** and **y** coordinates can be used as gauge of the deficiency in $^{M(4)}3^+$ content as function of unaccounted Fe^{3+}. With increasing Fe^{3+} in the

formula calculation, improved estimates of B are attained and the [x, y] position moves progressively upward in Figure 69; the data point lies on the line when Fe^{3+} = 0.35 *apfu*. Estimated in this manner, the predicted chemical parameters B, Fe^{2+} and Fe^{3+} are compared to those arrived at from the structure refinement site assignments (Ch. 4; App. F) in Table 7. The ageement between the two sets of values is very good, and therefore supports the use of the empirical relations for calculating reasonably accurate B, Fe^{2+} and Fe^{3+} quantities.

TABLE 7: COMPARISON BETWEEN PREDICTED AND ASSIGNED B, Fe^{2+}, Fe^{3+} *apfu*

	B	Fe^{2+}	Fe^{3+}
Predicted values	0.72	0.77	0.35
SREF assignments	0.712	0.772	0.348

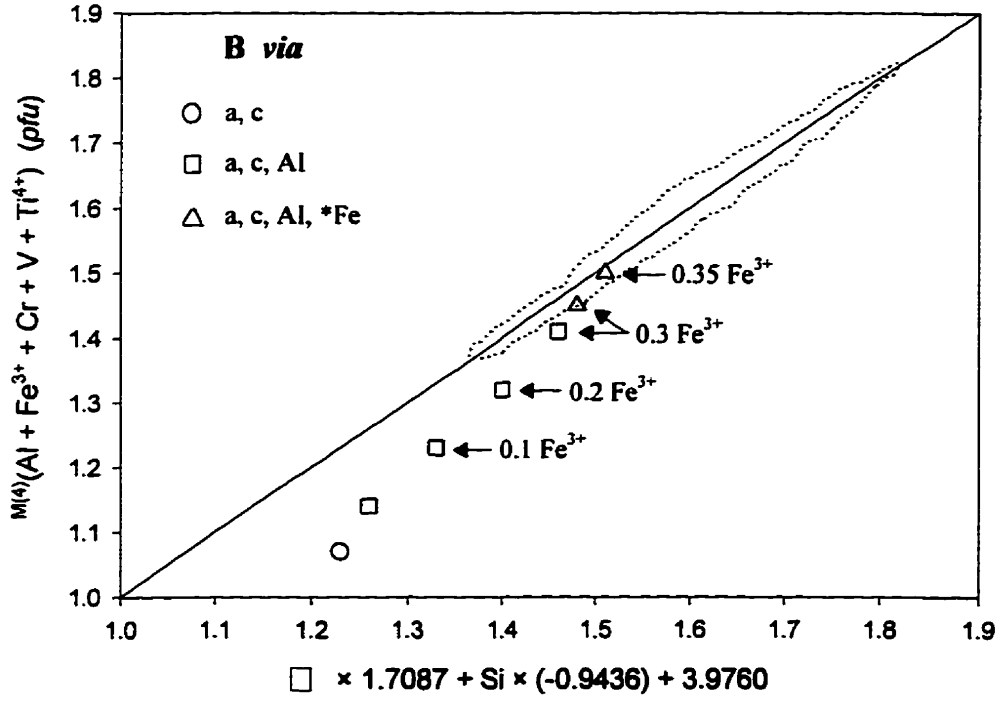


Figure 69: Relationship between $^{M(4)}3^{+}$ cations and $^{M(4)}3^{+}_{predicted}$ cations as in Figure 53. Data points in Figure 53 lie within the dotted field. The various symbol locations reflect the progressive plotting of sample K15 with increasing assigned Fe^{3+}.

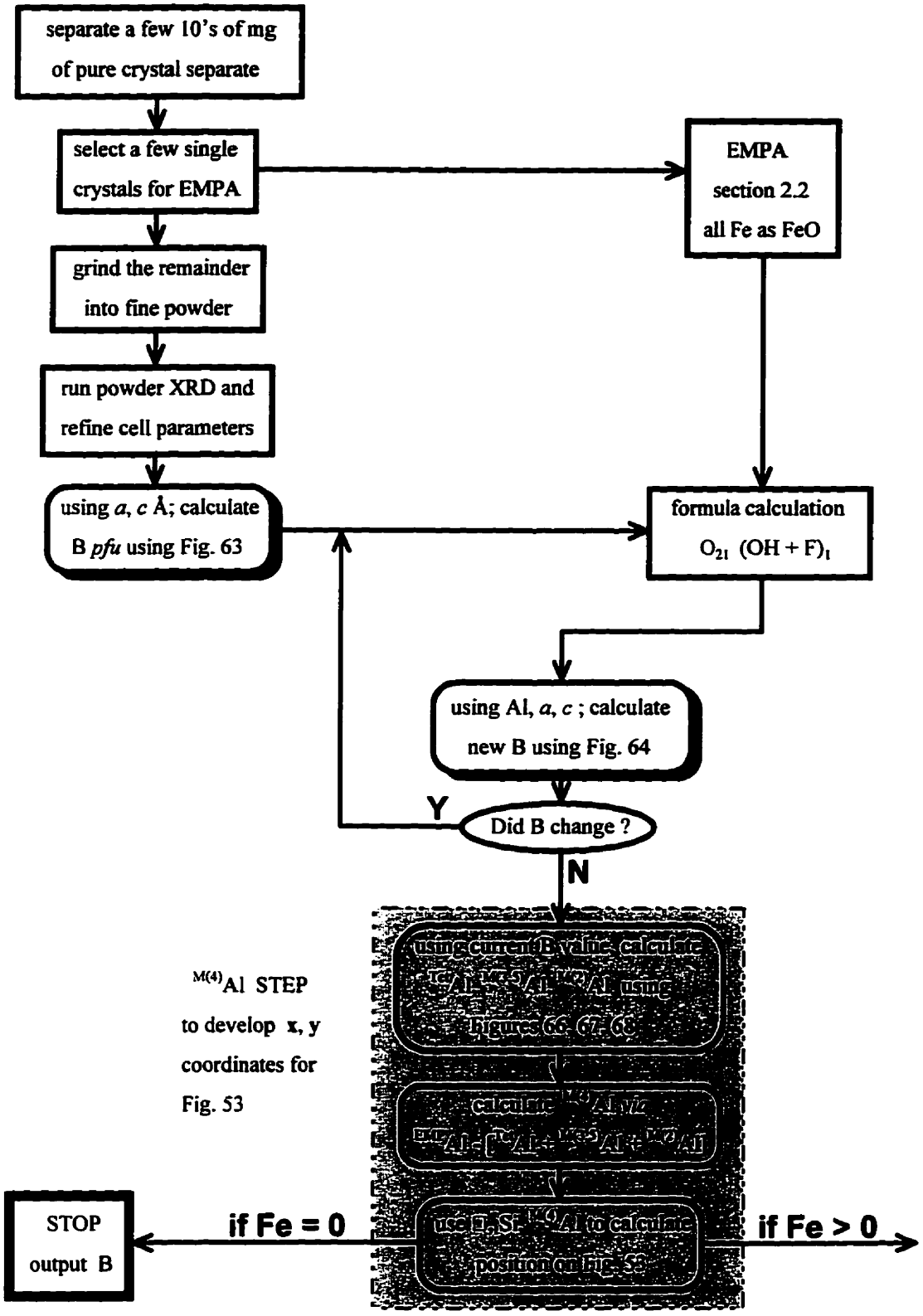


Figure 70: Flow chart illustrating the steps involved in assessing B, Fe^{2+} and Fe^{3+} from EMP and powder XRD data in combination with the empirical relations in the referenced figures.

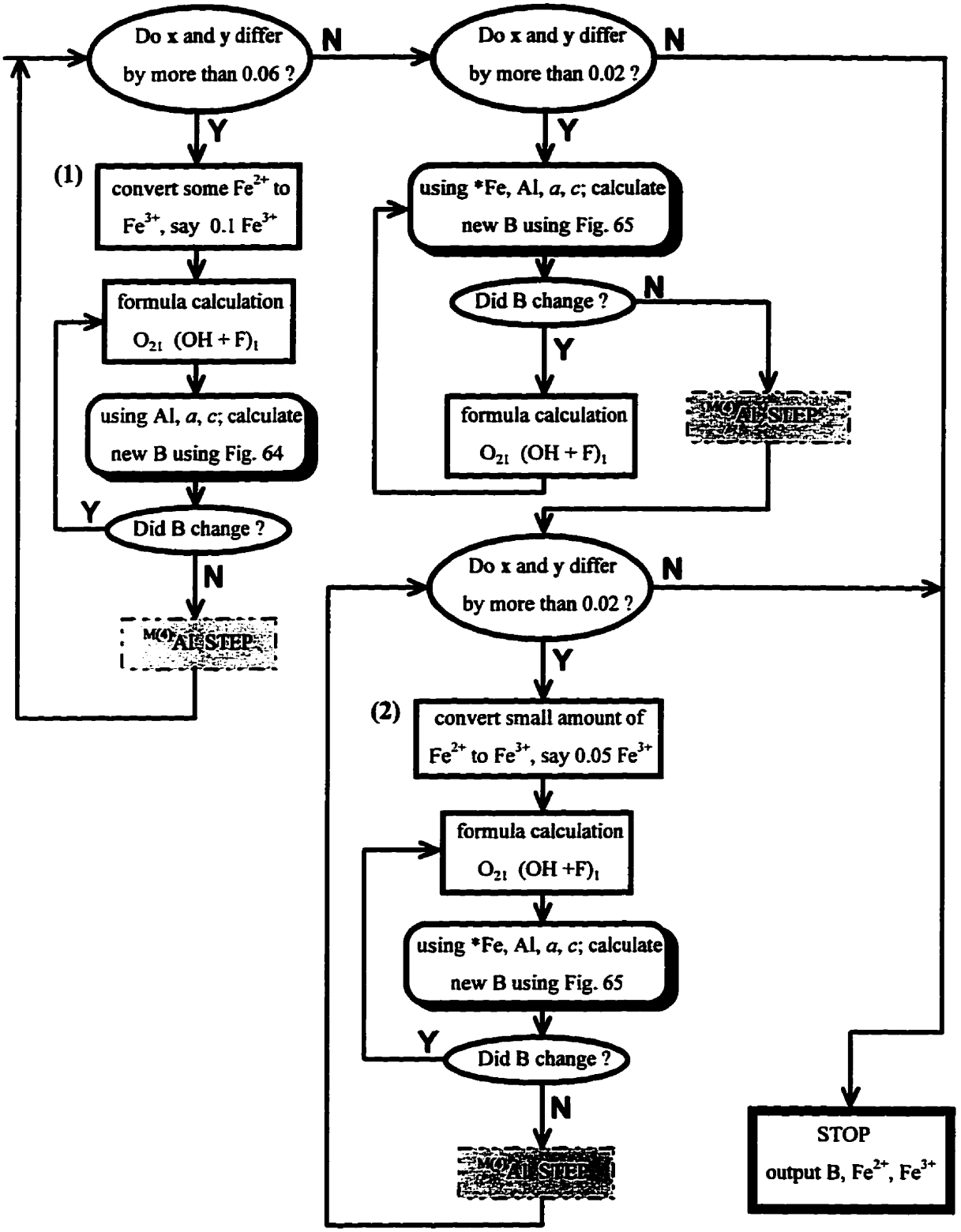


Figure 70: Flow chart continued. $Fe^{2+} \rightarrow Fe^{3+}$ conversions in (1) and (2) above are approximate recommendations and should be revised as required.

CHAPTER 7

GENERAL SUMMARY

Principal conclusions (and remaining questions) resulting from this study are as follows:

(1) The general formula for kornerupine can be written as

$$(\square, Mg, Fe)(Al, Mg, Fe)_9 (Si, Al, B)_5 O_{21} (OH, F)$$

The complete structural formula can be written as

$$^{X}(\square,Mg,Fe)\ ^{M(1)}(Mg,Fe)_2\ ^{M(2)}(Mg,Al,Fe)\ ^{M(3,5)}(Al,Mg)_4\ ^{M(4)}(Al,Mg,Fe^{3+})_2\ ^{T(1,2)}(Si,Al)_4\ ^{T(3)}(Si,B,Al)\ O_{21}\ (OH,F)$$

The best way to calculate the unit formula is based on O_{21} $(OH + F)_1$ and is supported by: (1) bond-valence arguements; (2) H-extraction line results; (3) the relative agreement between cations calculated from EMP and SREF data.

(2) The element B varies continuously from $0.0 \rightarrow 0.9$ B *pfu* and is completely ordered at the T(3) site. Overwhelming support for this statement is provided by the close agreement between SIMS and SREF results.

(3) The wide coverage in sample compositions provide a data distribution suggesting substitutional limits with regard to B and *Fe contents. An upper limit of ~0.9 B and ~1.6 *Fe *pfu* is inferred.

(4) Cation sums vary from 14.18 to 14.40 *apfu*. Tschermak-type and □-type substitutions can be used to explain variations in □, 2^+, 3^+ and 4^+ cations.

(5) Overall compositional variance is related to structural relaxation resulting from increased B → (Si, Al) substitution at T(3) coupled to Si → Al substitution at T(2). Dimensional kinking of the T(2)—T(3)—T(2) tetrahedral trimer, associated with size reduction of the T(3) tetrahedron and rotation of T(2) tetrahedra, provides the mechanism by which neighboring polyhedra are perturbed.

(6) Acute chemical and dimensional responses of the kornerupine structure at various B-contents allow accurate prediction of B from assessment of specific structural parameters. Empirical relations are given, from which accurate values for B, Fe^{2+}, Fe^{3+}, F and H can be calculated from powder XRD and EMP data.

(7) Although significant advances in the crystal chemistry of kornerupine have resulted from this study, the ferrian kornerupines from Bamble, Norway and Mautia Hill, Tanganyika require further study. Grew *et al.* (1990a) mention that kornerupine from Mautia Hill is stained pink by finely included hematite dust. Hematite is also present at the Bamble locality (Grew *et al.*, 1990a). If very fine hematite inclusions are evenly distributed through kornerupine, this could result in a Fe value from EMPA that is too high. It could also lead to Fe^{3+}/Fe^{2+} ratios that are too high as calculated from Mössbauer spectroscopy.

(8) Although the possibility of an H_2O group was dismissed, due to the unavailability of H-bond acceptors, polarized infrared spectroscopy should be done to confirm this contention. Samples from Bamble, Norway should be included in such a study, as greater H_2O activities are likely during more oxidizing conditions.

(9) Samples K38, K39 and K40 (App. A) are all from the same outcrop (pers. comm., Ole Petersen, 1995) and contain 0.316, 0.484 and 0.016 B *pfu*, respectively. Extremely subtle color differences between the crystals likely correspond to minor differences in Fe^{2+}, Fe^{3+} and Cr^{3+} content (App. H). Fe^{3+}/Fe^{2+} ratios for K38, K39 and K40 are 0.33, 0.19 and 0.24, respectively. These results suggest distinctive chemical heterogeneity in kornerupine at this occurrence (Walton's locality, Fiskenæsset, Greenland). Detailed spatial examination of chemical variations in kornerupine at a given locality is likely to provide the metamorphic petrologist with intriguing data concerning small-scale variation in such key parameters as fO_2, activity of B and activity of H.

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APPENDIX A

KORNERUPINE SAMPLES

Abbreviations used in APPENDIX A

Museum number or collection of:

a: Ed Grew; **b**: National Museum Natural History, Smithsonian Institution; **c**: J.K. Nanda; **d**: British Museum Natural History; **e**: American Museum of Natural History; **f**: P.H. Nixon; **g**: Royal Ontario Museum; **h**: Geologisk Museum (Copenhagen); **i**: Harvard University Mineralogical Museum; **j**: purchased from dealer; **k**: Duncan McKie; **l**: Muséum National d'Histoire Naturelle; **m**: Juergen Malley; **n**: R. G. Warren; **o**: Adelaide University; **p**: D.J. Waters; **q**: Institut fuer Mineralogie, Ruhr-Universitaet Bochum; **r**: Douglas E. Thost; **s**: N. N. Pertsev; **t**: Julie K. Vry; **u**: D. Young; **v**: Erik Jonsson; **w**: George Rossman

Donor:

Ed Grew : K1→K31, K33→K36, K42, K51, K52; Ole V. Petersen : K37→K40
Carl Francis : K41; George Rossman : K44→K50

Most recent reference:

1: Grew *et. al.*, 1990a; **2**: Grew *et. al.*, 1996; **3**: Vry, 1994; **4**: Young, 1995; **5**: Grew *et. al.*, 1991a,b; **6**: Waters & Moore, 1985; **7**: Grew *et. al.*, 1990b; **8**: Grew, 1996; **9**: Jonsson, 1996; **10**: Petersen & Secher, 1993

KORNERUPINE SAMPLES

This Study	Other Number		Locality	Reference
K 1	3083D	a	Ellammankovilpatti, India	1
K 2	133771	b	Bjørnesund, W.Greenland	8
K 3	J-21	c	Kondapalle, Andhra Pradesh, India	1
K 4	128415	b	Bjordam, Kragerø, Bamble, Norway	1
K 5	—	m	Elahera, Sri Lanka	8
K 6	134E	a	Aldan Shield, Yakutia, Russia	5
K 7	171.350	l	Madagascar	1
K 8	3053B	a	Ponakkadu, India	1
K 9	141255	b	Madagascar	1
K 10	24518	e	Lac Ste-Marie, Quebec, Canada	8
K 11	BM1940,39	d	Port Shepstone, S.Africa	1
K 12	31498	e	Fiskenæsset, Greenland	2
K 13	134H	a	Aldan Shield, Yakutia, Russia	5
K 14	5410	a	Wright locality, Lac Ste-Marie, Quebec	8
K 15	5032	n	Baldwin Locality,Hart's Range, Australia	8
K 16	5400C	a	Lac Ste-Marie, Quebec, Canada	8
K 17	24752	o	Harts Range, Australia	8
K 18	K2-F	p	Namaqualand, S.Africa	6
K 19	5126AA	a	Waldheim, Germany	2
K 20	12567	e	Waldheim, Germany	2
K 21	3083E2	a	Ellammankovilpatti, India	1
K 22	8497	q	Sinyoni Claims, Limpopo, Zimbabwe	8
K 23	BM1978,467	d	Kwale, Kenya	8
K 24	5105M	a	Waldheim, Germany	2
K 25	8812903	r	Larsemann Hills, East Antarctica	8
K 26	PHN984	f	Labwor Hills, Uganda	1

KORNERUPINE SAMPLES

This Study	Other Number		Locality	Reference
K 27	DWN138	p	Namaqualand, S.Africa	6
K 28	BM1972,170	d	Madagascar	1
K 29	142-1C	a	Aldan Shield, Yakutia, Russia	5
K 30	DC707H	a	Darai Stazh, SW Pamirs, Tajikistan	7
K 31	DC9141B	s	Darai Stazh, SW Pamirs, Tajikistan	7
K 32	—	j	Sri Lanka	8
K 33	E2724	g	Paderu, Andhra Pradesh, India	1
K 34	1892.1438	h	Waldheim, Germany	2
K 35	9365	q	Sinyoni Claims, Limpopo, Zimbabwe	1
K 36	XF-4	t	Reynolds Range, Australia	3
K 37	—	h	Walton's locality,Fiskenæsset, Greenland	10
K 38	—	h	Walton's locality,Fiskenæsset, Greenland	10
K 39	—	h	Walton's locality,Fiskenæsset, Greenland	10
K 40	—	h	Walton's locality,Fiskenæsset, Greenland	10
K 41	112233	i	near Itrongahy, Madagascar	1
K 42	T-8	u	Reading Prong, New Jersey, USA	4
K 43	—	j	Tanzania	8
K 44	D683	k	Mautia Hill, Tanzania	1
K 45	1774	w	—	—
K 46	729	w	Mindi Hills, Kenya	8
K 47	729	w	Mindi Hills, Kenya	8
K 48	1578	w	Kragerø, Bamble, Norway	8
K 49	263	w	Madagascar	8
K 50	1577	w	Sinyoni Claims, Limpopo, Zimbabwe	8
K 51	BJ-1	a	Bjordam, Kragerø, Bamble, Norway	8
K 52	—	v	Stakholmen, Hälsingland, Sweden	9

APPENDIX B

SREF MISCELLANEOUS INFORMATION

SREF MISCELLANEOUS INFORMATION

		K1	K2	K3	K5	K6
Cell Parameters	a (Å)	16.036(3)	16.014(4)	15.956(3)	15.940(3)	15.970(6)
	b	13.710(2)	13.728(2)	13.689(3)	13.701(2)	13.721(3)
	c	6.723(1)	6.710(1)	6.695(1)	6.694(1)	6.712(2)
	V (Å^3)	1478.2(4)	1475.1(5)	1462.4(5)	1461.9(4)	1470.7(7)
Crystal Dimensions	'X' (mm)	0.30	0.21	0.18	0.20	0.19
	'Y'	0.31	0.22	0.20	0.20	0.20
	'Z'	0.32	0.23	0.23	0.21	0.21
Total No. of Intensities		1248	1252	1243	1243	1249
No. of F_o^2		1203	1207	1198	1198	1204
No. of $F_o^2 > -3\sigma(F_o^2)$		1201	1207	1198	1198	1204
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1120	1078	1075	1059	1041
Scale factor (k)		0.4321(8)	0.2783(4)	0.2583(4)	0.2503(5)	0.2180(5)
Extinction (X)		0.0004(3)	0.0076(3)	—	0.0056(2)	0.0062(2)
Weight (a)		0.0238	0.0297	0.0223	0.0321	0.0265
Weight (b)		1.00	0.23	1.19	0.00	0.51
R(azimuthal)%		0.7 → 0.6	1.1 → 0.9	1.0 → 0.9	1.3 → 1.0	0.9 → 0.8
R_1 ($\|F_o\|>4\sigma$)%		1.7	1.9	1.9	2.0	2.0
wR_2 (F_o^2)%		4.6	4.9	4.9	5.1	5.2

		K7	K8	K9	K10	K11
Cell Parameters	a (Å)	15.943(3)	16.007(4)	15.926(4)	15.972(5)	15.946(4)
	b	13.716(2)	13.749(3)	13.704(4)	13.728(3)	13.679(3)
	c	6.692(1)	6.725(1)	6.695(2)	6.708(2)	6.693(2)
	V (Å^3)	1478.2(4)	1475.1(5)	1461.4(6)	1470.8(7)	1459.9(6)
Crystal Dimensions	'X' (mm)	0.20	0.21	0.24	0.21	0.24
	'Y'	0.21	0.22	0.24	0.22	0.25
	'Z'	0.22	0.23	0.25	0.23	0.26
Total No. of Intensities		1245	1256	1242	1251	1241
No. of F_o^2		1200	1212	1197	1206	1196
No. of $F_o^2 > -3\sigma(F_o^2)$		1200	1212	1197	1206	1196
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1048	1066	1073	1058	1080
Scale factor (k)		0.2497(5)	0.2427(5)	0.2815(6)	0.2408(5)	0.2697(6)
Extinction (X)		0.0034(2)	0.0037(2)	0.0070(3)	0.0048(2)	0.0045(2)
Weight (a)		0.0291	0.0344	0.0306	0.0293	0.0262
Weight (b)		0.17	0.00	0.30	0.00	0.76
R(azimuthal)%		0.9 → 0.9	1.0 → 0.9	0.9 → 0.8	1.0 → 0.8	1.0 → 0.9
R_1 ($\|F_o\|>4\sigma$)%		1.9	2.3	2.0	1.9	1.8
wR_2 (F_o^2)%		5.2	5.6	5.1	5.1	4.9

SREF MISCELLANEOUS INFORMATION

		K 12	K 13	K 14	K 15	K 16
Cell Parameters	a (Å)	16.050(6)	15.929(4)	15.968(8)	16.007(5)	15.931(5)
	b	13.742(4)	13.718(4)	13.704(4)	13.746(4)	13.660(5)
	c	6.728(2)	6.688(2)	6.708(2)	6.708(3)	6.699(2)
	V (Å^3)	1483.7(7)	1461.5(7)	1467.9(9)	1475.9(9)	1457.8(8)
Crystal Dimensions	'X' (mm)	0.16	0.24	0.22	0.24	0.25
	'Y'	0.18	0.25	0.24	0.25	0.26
	'Z'	0.20	0.26	0.26	0.26	0.27
Total No. of Intensities		1263	1240	1249	1253	1238
No. of F_o^2		1218	1196	1202	1208	1193
No. of $F_o^2 > -3\sigma(F_o^2)$		1216	1196	1202	1208	1193
No. of $\|F_o\| > 4\sigma(\|F_o\|)$		1011	1092	1078	1096	1077
Scale factor (k)		0.1783(3)	0.3148(7)	0.2755(6)	0.2870(7)	0.2733(5)
Extinction (X)		0.0003(1)	0.0050(3)	0.0046(2)	0.0065(3)	0.0054(2)
Weight (a)		0.0269	0.0292	0.0270	0.0297	0.0252
Weight (b)		0.00	0.84	0.78	0.98	0.92
R(azimuthal)%		1.2 → 1.0	0.9 → 0.9	0.9 → 0.8	1.0 → 1.0	0.9 → 0.8
R_1 ($\|F_o\| > 4\sigma$)%		2.1	2.0	1.7	1.9	1.8
wR_2 (F_o^2)%		5.1	5.3	5.0	5.6	4.7

		K 17	K 18	K 19	K 20	K 21
Cell Parameters	a (Å)	15.987(5)	15.970(2)	15.938(2)	15.938(3)	16.061(3)
	b	13.740(3)	13.720(2)	13.670(3)	13.673(3)	13.718(2)
	c	6.702(2)	6.703(1)	6.690(1)	6.693(1)	6.729(1)
	V (Å^3)	1472.2(7)	1475.1(5)	1457.6(4)	1470.8(7)	1482.7(4)
Crystal Dimensions	'X' (mm)	0.26	0.26	0.24	0.20	0.25
	'Y'	0.28	0.26	0.24	0.21	0.26
	'Z'	0.28	0.27	0.25	0.22	0.26
Total No. of Intensities		1249	1247	1240	1238	1261
No. of F_o^2		1204	1202	1195	1194	1216
No. of $F_o^2 > -3\sigma(F_o^2)$		1203	1202	1195	1193	1216
No. of $\|F_o\| > 4\sigma(\|F_o\|)$		1090	1082	1077	1048	1090
Scale factor (k)		0.2693(6)	0.2581(6)	0.2700(6)	0.2292(5)	0.2675(7)
Extinction (X)		0.0026(2)	0.0045(2)	0.0085(3)	0.0049(2)	0.0017(2)
Weight (a)		0.0259	0.0265	0.0241	0.0280	0.0226
Weight (b)		1.40	1.32	0.86	0.63	2.84
R(azimuthal)%		0.9 → 0.9	1.0 → 1.0	1.1 → 1.0	1.1 → 1.0	0.9 → 0.8
R_1 ($\|F_o\| > 4\sigma$)%		1.9	1.9	1.8	1.9	2.1
wR_2 (F_o^2)%		5.4	5.4	4.8	5.1	6.4

SREF MISCELLANEOUS INFORMATION

		K 22	K 23	K 24	K 25	K 26
Cell Parameters	a (Å)	16.031(3)	15.943(2)	15.949(2)	15.953(3)	16.025(3)
	b	13.704(2)	13.701(2)	13.669(2)	13.723(2)	13.742(2)
	c	6.714(1)	6.693(1)	6.692(1)	6.700(1)	6.722(1)
	V (Å^3)	1475.1(4)	1462.1(3)	1459.0(4)	1466.8(4)	1480.2(4)
Crystal Dimensions	'X' (mm)	0.24	0.24	0.24	0.24	0.20
	'Y'	0.24	0.25	0.24	0.25	0.24
	'Z'	0.25	0.26	0.26	0.26	0.24
Total No. of Intensities		1253	1243	1239	1247	1256
No. of F_o^2		1208	1198	1194	1202	1212
No. of $F_o^2 > -3\sigma(F_o^2)$		1207	1198	1193	1202	1211
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1059	1092	1062	1083	1028
Scale factor (k)		0.2607(5)	0.3048(6)	0.2570(6)	0.2767(6)	0.2256(6)
Extinction (X)		0.0042(2)	0.0111(3)	0.0028(2)	0.0110(4)	0.0004(2)
Weight (a)		0.0279	0.0268	0.0299	0.0308	0.0384
Weight (b)		0.75	0.66	0.86	0.70	0.54
R(azimuthal)%		1.0 → 0.9	1.0 → 1.0	1.1 → 1.0	1.0 → 0.8	2.1 → 1.1
R_1 ($\|F_o\|>4\sigma$)%		1.9	1.7	2.1	1.9	2.4
wR_2 (F_o^2)%		5.0	5.0	5.5	5.3	6.3

		K 27	K 28	K 29	K 30	K 31
Cell Parameters	a (Å)	15.960(2)	15.943(3)	15.976(2)	16.111(2)	16.025(5)
	b	13.725(2)	13.725(1)	13.710(2)	13.708(2)	13.703(3)
	c	6.705(1)	6.699(1)	6.710(1)	6.733(1)	6.721(2)
	V (Å^3)	1468.7(3)	1465.9(3)	1469.6(3)	1487.0(4)	1475.9(6)
Crystal Dimensions	'X' (mm)	0.16	0.24	0.26	0.25	0.26
	'Y'	0.18	0.25	0.28	0.26	0.27
	'Z'	0.20	0.26	0.30	0.26	0.28
Total No. of Intensities		1247	1246	1242	1264	1255
No. of F_o^2		1202	1201	1197	1219	1210
No. of $F_o^2 > -3\sigma(F_o^2)$		1202	1201	1196	1219	1208
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1012	1069	1096	1101	1092
Scale factor (k)		0.2008(4)	0.2589(5)	0.2898(8)	0.2699(7)	0.2636(7)
Extinction (X)		0.0047(2)	0.0031(2)	0.0030(3)	0.0016(2)	—
Weight (a)		0.0307	0.0335	0.0362	0.0248	0.0434
Weight (b)		0.00	0.00	1.50	1.82	1.07
R(azimuthal)%		1.2 → 1.1	1.1 → 1.1	1.4 → 1.3	1.1 → 1.1	3.6 → 1.0
R_1 ($\|F_o\|>4\sigma$)%		2.1	2.2	2.2	2.1	2.5
wR_2 (F_o^2)%		5.4	5.3	6.7	6.1	7.0

SREF MISCELLANEOUS INFORMATION

		K 32	K 33	K 34	K 35	K 36
Cell Parameters	a (Å)	15.942(2)	16.003(2)	15.980(3)	16.130(3)	16.125(2)
	b	13.708(2)	13.702(3)	13.697(2)	13.744(3)	13.761(2)
	c	6.693(1)	6.709(1)	6.696(2)	6.758(2)	6.758(1)
	V (Å^3)	1462.8(4)	1471.1(4)	1465.5(5)	1498.1(6)	1499.4(3)
Crystal Dimensions	'X' (mm)	0.24	0.32	0.24	0.23	0.24
	'Y'	0.26	0.34	0.25	0.24	0.25
	'Z'	0.28	0.34	0.26	0.24	0.26
Total No. of Intensities		1243	1245	1241	1275	1271
No. of F_o^2		1197	1200	1197	1230	1227
No. of $F_o^2 > -3\sigma(F_o^2)$		1197	1200	1197	1230	1227
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1097	1139	1107	1117	1121
Scale factor (k)		0.3087(7)	0.3872(9)	0.3388(8)	0.2963(6)	0.3335(7)
Extinction (X)		0.0135(4)	0.0118(4)	0.0041(3)	0.0080(3)	0.0024(2)
Weight (a)		0.0332	0.0224	0.0255	0.0292	0.0222
Weight (b)		0.67	1.84	1.62	0.72	1.22
R(azimuthal)%		1.4 → 1.2	1.0 → 0.8	0.8 → 0.8	1.0 → 0.9	0.9 → 0.9
R_1 ($\|F_o\|>4\sigma$)%		2.0	1.9	2.0	2.0	1.8
wR_2 (F_o^2)%		5.3	5.1	5.4	5.2	4.8

		K 38	K 39	K 40	K 41	K 42
Cell Parameters	a (Å)	16.071(2)	16.036(3)	16.118(2)	15.919(1)	15.941(1)
	b	13.746(2)	13.732(2)	13.732(2)	13.727(1)	13.696(1)
	c	6.736(1)	6.720(1)	6.755(1)	6.692(1)	6.697(1)
	V (Å^3)	1487.9(4)	1479.7(4)	1494.9(3)	1462.4(2)	1462.2(2)
Crystal Dimensions	'X' (mm)	0.24	0.20	0.27	0.28	0.15
	'Y'	0.25	0.21	0.28	0.28	0.17
	'Z'	0.26	0.22	0.28	0.28	0.21
Total No. of Intensities		1260	1253	1267	1242	1242
No. of F_o^2		1215	1210	1222	1197	1197
No. of $F_o^2 > -3\sigma(F_o^2)$		1215	1210	1222	1197	1197
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1107	1096	1135	1093	1021
Scale factor (k)		0.3441(6)	0.2680(6)	0.3802(7)	0.2644(7)	0.1443(3)
Extinction (X)		0.0019(2)	0.0038(2)	0.0030(2)	0.0141(5)	0.0025(2)
Weight (a)		0.0246	0.0195	0.0189	0.0331	0.0264
Weight (b)		0.60	1.67	1.27	0.75	0.08
R(azimuthal)%		1.1 → 0.9	0.9 → 0.9	0.8 → 0.8	1.6 → 1.0	1.1 → 0.9
R_1 ($\|F_o\|>4\sigma$)%		1.7	1.8	1.6	2.1	2.2
wR_2 (F_o^2)%		4.6	5.2	4.6	5.9	5.3

SREF MISCELLANEOUS INFORMATION

		K 43	K 45	K 46	K 47	K 49
Cell Parameters	a (Å)	15.965(2)	15.941(2)	16.056(2)	16.050(1)	15.955(1)
	b	13.697(1)	13.696(2)	13.717(2)	13.715(1)	13.721(1)
	c	6.701(1)	6.692(1)	6.720(1)	6.720(1)	6.701(1)
	V (Å^3)	1465.2(2)	1461.2(3)	1480.0(3)	1479.3(2)	1466.8(2)
Crystal Dimensions	'X' (mm)	0.20	0.21	0.24	0.18	0.22
	'Y'	0.21	0.22	0.25	0.19	0.23
	'Z'	0.22	0.23	0.26	0.20	0.24
Total No. of Intensities		1244	1242	1260	1257	1246
No. of F_o^2		1199	1197	1215	1212	1201
No. of $F_o^2 > -3\sigma(F_o^2)$		1199	1197	1215	1212	1201
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1078	1101	1128	1088	1120
Scale factor (k)		0.1920(4)	0.2102(5)	0.2598(6)	0.1684(4)	0.2370(6)
Extinction (X)		0.0088(3)	0.0036(3)	0.0071(3)	0.0026(2)	0.0062(3)
Weight (a)		0.0250	0.0367	0.0285	0.0244	0.0361
Weight (b)		0.61	0.58	0.89	0.73	0.47
R(azimuthal)%		1.4 → 1.0	1.0 → 0.9	1.0 → 1.0	1.2 → 0.9	1.0 → 0.9
R_1 ($\|F_o\|>4\sigma$)%		1.9	2.5	2.1	2.1	2.4
wR_2 (F_o^2)%		5.2	6.6	5.6	5.6	6.2

		K 50	K 52
Cell Parameters	a (Å)	16.053(2)	15.992(2)
	b	13.702(1)	13.721(2)
	c	6.717(1)	6.705(1)
	V (Å^3)	1477.4(3)	1471.2(3)
Crystal Dimensions	'X' (mm)	0.16	0.22
	'Y'	0.17	0.23
	'Z'	0.18	0.24
Total No. of Intensities		1256	1249
No. of F_o^2		1211	1204
No. of $F_o^2 > -3\sigma(F_o^2)$		1211	1204
No. of $\|F_o\|>4\sigma(\|F_o\|)$		1084	1104
Scale factor (k)		0.1620(4)	0.2151(5)
Extinction (X)		0.0032(2)	0.0017(2)
Weight (a)		0.0289	0.0275
Weight (b)		0.65	1.03
R(azimuthal)%		0.9 → 0.8	0.9 → 0.8
R_1 ($\|F_o\|>4\sigma$)%		2.3	2.1
wR_2 (F_o^2)%		5.8	5.5

APPENDIX C.1

CRYSTALLOGRAPHIC SITES

Abbreviations used in APPENDIX C.1

♣ : refining parameter
0.01° : fixed in refinement

CRYSTALLOGRAPHIC SITES

Crystallographic sites				Coordinates			Displacement parameters						
Name	Wyckoff	Mult.	Symm.	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{iso}
X	a	4	2/m . .	0	0	0	♣	♣	♣	♣	0	0	
M(1)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
M(2)	c	4	m 2 m	1/2	♣	1/4	♣	♣	♣	0	0	0	
M(3)	e	8	2 . .	♣	0	0	♣	♣	♣	♣	0	0	
M(4)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
M(5)	e	8	2 . .	♣	0	0	♣	♣	♣	♣	0	0	
T(1)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
T(2)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
T(3)	c	4	m 2 m	0	♣	1/4	♣	♣	♣	0	0	0	
O(1)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
O(2)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
O(3)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
O(4)	h	16	1	♣	♣	♣	♣	♣	♣	♣	♣	♣	
O(5)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
O(6)	h	16	1	♣	♣	♣	♣	♣	♣	♣	♣	♣	
O(7)	g	8	. . m	♣	♣	1/4	♣	♣	♣	0	0	♣	
O(8)	f	8	m . .	1/2	♣	♣	♣	♣	♣	♣	0	0	
O(9)	c	4	m 2 m	1/2	♣	1/4	♣	♣	♣	0	0	0	
O(10)	c	4	m 2 m	0	♣	1/4	♣	♣	♣	0	0	0	
H(1)	c	4	m 2 m	0	♣	1/4							0.01*
H(2)	f	8	m . .	0	♣	♣							0.01*

APPENDIX C.2

REFINED ATOMIC COORDINATES

Abbreviations used in APPENDIX C.2

Refined atomic fractional coordinates (x 10^5) ; (x 10^3) for **H(2)** y,z

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REFINED ATOMIC COORDINATES

Site		K1	K2	K3	K5	K6	K7
M(1)	x	12008(3)	12025(3)	11689(3)	11823(3)	11852(3)	11926(4)
	y	13805(3)	13941(4)	13874(3)	13962(4)	13978(4)	14081(4)
M(2)	y	14640(4)	14645(5)	14926(5)	14776(5)	14823(5)	14725(5)
M(3)	x	21560(2)	21544(3)	21503(3)	21516(3)	21533(3)	21519(3)
M(4)	x	31360(2)	31336(3)	31223(3)	31266(3)	31257(3)	31278(3)
	y	14130(3)	14160(3)	14187(3)	14169(3)	14199(4)	14215(4)
M(5)	x	40759(2)	40799(3)	40897(3)	40878(3)	40858(3)	40881(3)
T(1)	x	40151(2)	40158(2)	40124(3)	40124(3)	40130(3)	40146(3)
	y	35251(3)	35261(3)	35299(3)	35262(3)	35291(4)	35290(3)
T(2)	x	17866(3)	17753(3)	17495(3)	17549(3)	17563(3)	17532(3)
	y	33266(3)	33314(3)	33299(3)	33322(3)	33365(4)	33380(3)
T(3)	y	34189(5)	34280(7)	34579(13)	34491(10)	34497(11)	34523(11)
O(1)	x	22548(6)	22531(6)	22591(7)	22551(7)	22511(8)	22482(7)
	y	4498(7)	4507(7)	4531(9)	4534(8)	4517(9)	4536(8)
O(2)	x	40267(5)	40277(6)	40201(7)	40243(6)	40259(8)	40288(7)
	y	4634(7)	4661(8)	4788(9)	4739(8)	4749(9)	4744(9)
O(3)	x	40103(6)	40110(6)	39797(8)	39939(7)	39953(8)	40047(7)
	y	23427(7)	23441(8)	23442(9)	23444(8)	23483(10)	23500(9)
O(4)	x	13910(4)	13887(5)	13938(5)	13877(5)	13870(6)	13837(5)
	y	9995(5)	9983(5)	9993(6)	9979(5)	9952(6)	9970(6)
	z	- 5203(10)	- 5146(11)	- 5142(14)	- 5116(12)	- 5140(14)	- 5090(13)
O(5)	x	23410(7)	23274(8)	22996(8)	23061(8)	23046(9)	23013(8)
	y	23484(7)	23534(8)	23450(9)	23534(8)	23530(10)	23616(9)
O(6)	x	31661(4)	31666(4)	31669(5)	31657(5)	31655(5)	31655(5)
	y	9617(5)	9607(5)	9665(6)	9654(5)	9601(6)	9612(6)
	z	- 4604(11)	- 4685(12)	- 4677(14)	- 4763(12)	- 4712(15)	- 4832(13)
O(7)	x	8245(7)	8116(7)	7780(8)	7858(7)	7858(8)	7880(8)
	y	28147(8)	28309(8)	28639(9)	28570(8)	28622(10)	28632(9)
O(8)	y	8849(6)	8846(7)	8816(8)	8846(7)	8809(9)	8857(8)
	z	- 5396(15)	- 5589(16)	- 6150(19)	- 6025(17)	- 5980(20)	- 5982(18)
O(9)	y	38435(10)	38492(11)	38163(14)	38329(12)	38392(14)	38523(13)
O(10)	y	8801(11)	8815(12)	9017(14)	8872(13)	8894(15)	8963(13)
H(1)	y	1652(13)	—	1858(16)	1719(15)	—	—
H(2)	y	53 (3)	42 (2)	47 (3)	50 (3)	42 (2)	41 (2)
	z	123 (3)	138 (4)	134 (5)	127 (4)	140 (4)	142 (4)

REFINED ATOMIC COORDINATES

Site		K 8	K 9	K 10	K 11	K 12	K 13
M(1)	x	11979(3)	11864(3)	11860(3)	11643(3)	12178(5)	11948(4)
	y	13951(4)	14112(4)	13937(3)	13830(3)	13871(5)	14203(4)
M(2)	y	14717(5)	14785(5)	14774(5)	14992(4)	14564(7)	14721(5)
M(3)	x	21570(3)	21519(3)	21544(3)	21514(3)	21587(3)	21536(3)
M(4)	x	31307(3)	31248(3)	31282(3)	31182(3)	31391(4)	31259(3)
	y	14166(3)	14210(3)	14208(3)	14163(4)	14080(4)	14215(4)
M(5)	x	40783(3)	40916(3)	40859(3)	40903(3)	40706(3)	40917(3)
T(1)	x	40133(3)	40131(2)	40133(3)	40106(3)	40157(3)	40139(3)
	y	35258(3)	35289(3)	35288(3)	35288(3)	35219(4)	35280(3)
T(2)	x	17729(3)	17464(3)	17580(3)	17463(3)	17994(4)	17461(3)
	y	33373(4)	33384(3)	33358(3)	33277(3)	33250(4)	33411(3)
T(3)	y	34353(8)	34658(12)	34461(10)	34662(13)	34144(7)	34660(12)
O(1)	x	22490(8)	22492(6)	22535(7)	22644(7)	22523(8)	22456(7)
	y	4491(9)	4542(8)	4527(8)	4549(8)	4469(9)	4556(8)
O(2)	x	40317(7)	40273(6)	40265(7)	40125(7)	40271(8)	40303(7)
	y	4673(9)	4784(8)	4728(9)	4803(9)	4595(9)	4763(8)
O(3)	x	40084(7)	39972(7)	40003(7)	39693(7)	40170(8)	40026(7)
	y	23481(9)	23503(8)	23476(9)	23429(9)	23402(9)	23500(8)
O(4)	x	13880(5)	13849(5)	13907(5)	13924(5)	13851(6)	13798(5)
	y	9973(6)	9976(5)	9980(6)	9957(6)	9967(6)	9953(5)
	z	- 5204(13)	- 5067(12)	- 5159(13)	- 5166(13)	- 5205(14)	- 5022(12)
O(5)	x	23202(9)	22936(7)	23086(8)	22970(8)	23544(9)	22926(8)
	y	23489(10)	23594(8)	23555(9)	23456(9)	23449(10)	23631(8)
O(6)	x	31664(5)	31648(5)	31672(5)	31653(5)	31651(6)	31648(5)
	y	9548(6)	9603(5)	9599(6)	9703(6)	9581(6)	9606(5)
	z	- 4643(14)	- 4828(12)	- 4746(13)	- 4730(14)	- 4525(15)	- 4851(12)
O(7)	x	8032(8)	7766(7)	7910(8)	7734(8)	8375(9)	7778(7)
	y	28427(10)	28718(8)	28579(9)	28695(9)	27980(11)	28717(8)
O(8)	y	8823(8)	8840(7)	8818(8)	8794(8)	8856(9)	8866(8)
	z	- 5755(19)	- 6206(16)	- 5948(19)	- 6234(19)	- 5202(21)	- 6138(17)
O(9)	y	38481(13)	38446(12)	38421(13)	38037(13)	38502(14)	38557(13)
O(10)	y	8805(14)	8957(12)	8809(13)	8913(14)	8740(15)	8834(12)
H(1)	y	—	—	1671(15)	—	1608(17)	—
H(2)	y	40 (2)	50 (3)	51 (3)	43 (3)	52 (3)	49 (3)
	z	141 (4)	127 (4)	125 (3)	137 (4)	123 (4)	127 (4)

REFINED ATOMIC COORDINATES

Site		K 14	K 15	K 16	K 17	K 18	K 19
M(1)	x	11749(3)	11897(4)	11655(3)	11828(3)	11871(4)	11711(3)
	y	13885(3)	14054(4)	13802(3)	14018(4)	14022(4)	13911(4)
M(2)	y	14843(4)	14770(5)	14944(4)	14802(5)	14764(5)	14892(5)
M(3)	x	21518(3)	21501(3)	21510(3)	21505(3)	21525(3)	21486(3)
M(4)	x	31249(3)	31268(3)	31223(3)	31257(3)	31270(3)	31232(3)
	y	14207(3)	14278(3)	14186(3)	14259(3)	14223(4)	14188(3)
M(5)	x	40877(3)	40884(3)	40916(3)	40892(3)	40883(3)	40913(3)
T(1)	x	40123(3)	40177(3)	40105(3)	40165(3)	40138(3)	40135(3)
	y	35285(3)	35346(3)	35290(3)	35340(3)	35294(3)	35299(3)
T(2)	x	17528(3)	17513(3)	17454(3)	17499(3)	17517(3)	17473(3)
	y	33331(3)	33442(3)	33289(3)	33413(4)	33392(4)	33290(3)
T(3)	y	34521(11)	34515(11)	34646(13)	34532(12)	34521(11)	34596(12)
O(1)	x	22567(7)	22438(8)	22648(7)	22458(8)	22502(8)	22586(7)
	y	4536(8)	4513(9)	4553(8)	4530(9)	4530(9)	4549(8)
O(2)	x	40250(7)	40347(7)	40184(7)	40315(7)	40295(7)	40215(7)
	y	4761(8)	4718(9)	4806(8)	4752(9)	4742(9)	4797(8)
O(3)	x	39906(7)	40118(8)	39775(7)	40029(8)	40015(8)	39833(7)
	y	23473(9)	23580(9)	23421(8)	23549(9)	23493(9)	23436(9)
O(4)	x	13936(5)	13875(5)	13980(5)	13904(6)	13899(5)	13917(5)
	y	9977(5)	9977(6)	9996(5)	9987(6)	9986(6)	9990(6)
	z	- 5175(13)	- 5107(13)	- 5181(13)	- 5115(14)	- 5122(14)	- 5078(13)
O(5)	x	23026(8)	22991(9)	22979(7)	22966(9)	23017(9)	22966(8)
	y	23513(9)	23673(9)	23483(8)	23613(10)	23592(9)	23494(8)
O(6)	x	31678(5)	31681(5)	31685(5)	31674(5)	31673(5)	31671(5)
	y	9629(6)	9535(6)	9685(5)	9563(6)	9593(6)	9686(5)
	z	- 4724(13)	- 4822(14)	- 4720(13)	- 4789(14)	- 4795(14)	- 4756(13)
O(7)	x	7840(8)	7878(8)	7741(7)	7832(8)	7836(8)	7764(7)
	y	28624(9)	28651(9)	28687(8)	28675(10)	28635(9)	28637(9)
O(8)	y	8813(8)	8823(8)	8812(8)	8824(8)	8841(8)	8840(8)
	z	- 6028(18)	- 5947(19)	- 6224(18)	- 6048(20)	- 6045(19)	- 6177(18)
O(9)	y	38296(13)	38612(14)	38144(12)	38521(14)	38502(14)	38219(13)
O(10)	y	8735(13)	9139(14)	8773(13)	9043(15)	8853(14)	9071(13)
H(1)	y	—	—	1599(15)	—	1711(16)	1902(15)
H(2)	y	39 (2)	52 (3)	46 (3)	48 (3)	51 (3)	53 (3)
	z	143 (4)	128 (4)	132 (4)	132 (4)	126 (4)	125 (4)

REFINED ATOMIC COORDINATES

Site		K 20	K 21	K 22	K 23	K 24	K 25
M(1)	x	11639(3)	11957(5)	12033(4)	11887(4)	11691(4)	11804(3)
	y	13835(3)	13697(5)	13834(4)	14034(4)	13856(4)	14049(3)
M(2)	y	14947(5)	14655(7)	14606(6)	14719(5)	14895(5)	14867(4)
M(3)	x	21498(3)	21566(4)	21551(3)	21505(3)	21487(3)	21503(3)
M(4)	x	31204(3)	31368(4)	31368(3)	31283(3)	31239(3)	31231(3)
	y	14171(4)	14143(5)	14128(4)	14169(3)	14186(4)	14250(3)
M(5)	x	40913(3)	40751(4)	40777(3)	40875(3)	40903(3)	40918(3)
T(1)	x	40110(3)	40152(4)	40154(3)	40136(2)	40141(3)	40149(3)
	y	35283(3)	35260(4)	35243(3)	35260(3)	35299(3)	35339(3)
T(2)	x	17460(3)	17900(4)	17855(3)	17568(3)	17498(3)	17440(3)
	y	33279(3)	33253(5)	33249(3)	33318(3)	33270(3)	33394(3)
T(3)	y	34619(14)	34163(9)	34166(7)	34447(9)	34521(13)	34643(12)
O(1)	x	22638(7)	22563(10)	22581(7)	22536(7)	22610(8)	22487(7)
	y	4566(9)	4496(11)	4527(8)	4543(8)	4567(9)	4529(8)
O(2)	x	40177(7)	40251(9)	40246(7)	40261(6)	40191(7)	40272(7)
	y	4809(9)	4621(11)	4646(8)	4738(8)	4792(9)	4776(9)
O(3)	x	39744(7)	40096(10)	40105(7)	39989(7)	39831(8)	39950(7)
	y	23412(9)	23422(12)	23404(8)	23437(8)	23425(9)	23529(9)
O(4)	x	13945(5)	13940(7)	13896(5)	13879(5)	13923(5)	13878(5)
	y	9987(6)	9980(8)	9975(5)	9991(5)	10000(6)	9966(6)
	z	- 5158(14)	- 5266(17)	- 5167(12)	- 5097(12)	- 5099(14)	- 5074(13)
O(5)	x	22969(8)	23487(12)	23437(9)	23069(8)	23012(9)	22916(8)
	y	23447(9)	23462(13)	23530(9)	23539(8)	23514(9)	23593(9)
O(6)	x	31673(5)	31672(7)	31671(5)	31665(4)	31671(5)	31653(5)
	y	9704(6)	9606(8)	9640(6)	9653(5)	9707(6)	9593(6)
	z	- 4726(14)	- 4579(18)	- 4639(13)	- 4754(12)	- 4772(14)	- 4824(13)
O(7)	x	7752(8)	8298(11)	8262(8)	7897(7)	7817(8)	7766(8)
	y	28661(9)	28079(13)	28122(9)	28536(8)	28599(10)	28749(9)
O(8)	y	8834(8)	8835(11)	8850(8)	8862(7)	8840(8)	8824(8)
	z	- 6224(19)	- 5361(25)	- 5371(18)	- 5937(17)	- 6080(20)	- 6191(18)
O(9)	y	38092(14)	38415(17)	38429(13)	38392(12)	38175(14)	38428(13)
O(10)	y	8853(14)	8779(19)	8768(13)	8788(12)	9130(14)	9142(13)
H(1)	y	1686(16)	1635(20)	—	—	—	2000(15)
H(2)	y	—	—	43 (3)	37 (2)	43 (3)	48 (3)
	z	—	—	137 (4)	147 (5)	142 (5)	133 (5)

REFINED ATOMIC COORDINATES

Site		K 26	K 27	K 28	K 29	K 30	K 31
M(1)	x	11975(4)	11892(4)	11926(4)	11867(4)	12206(5)	12105(5)
	y	13923(4)	14033(4)	14098(4)	13910(4)	13721(5)	13815(5)
M(2)	y	14713(6)	14758(6)	14738(5)	14797(6)	14500(7)	14577(7)
M(3)	x	21557(4)	21532(3)	21533(3)	21553(4)	21595(4)	21587(4)
M(4)	x	31321(3)	31271(3)	31276(3)	31268(4)	31442(4)	31392(4)
	y	14175(4)	14213(4)	14199(3)	14137(4)	14052(4)	14073(4)
M(5)	x	40790(4)	40885(3)	40885(3)	40824(3)	40653(3)	40720(3)
T(1)	x	40163(3)	40135(3)	40137(3)	40121(3)	40173(3)	40153(3)
	y	35287(4)	35292(4)	35278(3)	35254(4)	35213(4)	35215(4)
T(2)	x	17765(4)	17532(4)	17526(3)	17661(4)	18155(4)	17979(4)
	y	33345(4)	33392(4)	33388(3)	33313(4)	33183(4)	33211(4)
T(3)	y	34287(10)	34507(12)	34546(11)	34400(10)	34032(6)	34107(7)
O(1)	x	22476(9)	22495(8)	22489(7)	22550(9)	22560(9)	22574(9)
	y	4486(10)	4523(9)	4525(8)	4505(10)	4479(10)	4485(10)
O(2)	x	40273(8)	40297(8)	40304(7)	40232(8)	40221(8)	40230(8)
	y	4669(11)	4741(9)	4742(8)	4723(10)	4571(10)	4620(10)
O(3)	x	40094(9)	40022(8)	40024(7)	39928(9)	40187(9)	40114(8)
	y	23492(11)	23501(10)	23505(9)	23430(11)	23367(10)	23364(10)
O(4)	x	13872(6)	13878(6)	13845(5)	13881(6)	13866(6)	13888(6)
	y	9953(7)	9979(6)	9972(6)	9961(7)	9962(7)	9978(7)
	z	- 5189(16)	- 5114(15)	- 5101(12)	- 5163(16)	- 5236(15)	- 5193(14)
O(5)	x	23268(11)	22998(9)	23014(8)	23149(10)	23765(10)	23554(10)
	y	23487(12)	23589(10)	23599(8)	23455(11)	23465(11)	23412(10)
O(6)	x	31662(6)	31667(6)	31658(5)	31653(6)	31636(6)	31664(6)
	y	9558(7)	9585(6)	9591(6)	9607(7)	9621(7)	9620(7)
	z	- 4638(16)	- 4793(15)	- 4808(12)	- 4633(16)	- 4470(16)	- 4464(15)
O(7)	x	8115(10)	7864(9)	7853(7)	7948(10)	8607(9)	8378(9)
	y	28336(12)	28634(10)	28644(9)	28482(11)	27739(11)	27954(11)
O(8)	y	8807(10)	8848(9)	8839(8)	8809(9)	8859(10)	8853(9)
	z	- 5603(23)	- 6049(21)	- 6039(17)	- 5899(22)	- 4844(21)	- 5214(21)
O(9)	y	38456(17)	38502(15)	38503(13)	38304(15)	38424(15)	38393(15)
O(10)	y	9028(17)	8852(15)	8909(13)	8845(16)	8761(16)	8728(16)
H(1)	y	—	1712(17)	—	—	—	1576(17)
H(2)	y	45 (3)	51 (3)	44 (2)	44 (3)	38 (3)	—
	z	137 (5)	125 (4)	137 (4)	136 (5)	145 (5)	—

REFINED ATOMIC COORDINATES

Site		K 32	K 33	K 34	K 35	K 36	K 38
M(1)	x	11907(3)	11832(3)	11728(4)	12229(4)	12282(3)	12163(3)
	y	14116(4)	13898(3)	13868(4)	13647(4)	13761(4)	13900(3)
M(2)	y	14734(5)	14849(4)	14864(5)	14475(5)	14480(5)	14565(5)
M(3)	x	21532(3)	21523(3)	21482(3)	21621(3)	21624(3)	21580(2)
M(4)	x	31263(3)	31271(3)	31256(3)	31450(3)	31437(3)	31378(2)
	y	14195(3)	14163(3)	14191(4)	14014(3)	14020(3)	14083(3)
M(5)	x	40902(3)	40844(3)	40898(3)	40590(3)	40578(3)	40703(2)
T(1)	x	40127(2)	40151(3)	40153(3)	40159(2)	40170(2)	40157(2)
	y	35270(3)	35290(3)	35303(3)	35188(3)	35200(3)	35223(3)
T(2)	x	17489(3)	17641(3)	17523(3)	18253(3)	18236(3)	17970(3)
	y	33386(3)	33286(3)	33279(3)	33173(3)	33228(3)	33280(3)
T(3)	y	34613(11)	34371(9)	34456(11)	34035(4)	34079(4)	34171(5)
O(1)	x	22493(6)	22544(7)	22582(7)	22572(7)	22498(6)	22499(6)
	y	4551(8)	4518(8)	4559(8)	4438(8)	4406(7)	4468(7)
O(2)	x	40281(6)	40219(7)	40201(7)	40214(6)	40261(6)	40275(5)
	y	4760(8)	4734(8)	4778(9)	4541(8)	4533(8)	4609(7)
O(3)	x	40001(7)	39908(7)	39883(8)	40188(6)	40209(6)	40162(6)
	y	23486(8)	23440(8)	23450(9)	23335(8)	23385(8)	23419(7)
O(4)	x	13842(5)	13897(5)	13908(5)	13887(5)	13844(5)	13850(4)
	y	9966(5)	9988(5)	9999(6)	9979(5)	9967(5)	9973(5)
	z	- 5075(11)	- 5128(12)	- 5095(13)	- 5276(11)	- 5254(11)	- 5198(10)
O(5)	x	22978(7)	23146(8)	23040(9)	23840(7)	23769(7)	23501(7)
	y	23622(8)	23449(9)	23546(9)	23350(8)	23319(9)	23425(7)
O(6)	x	31653(4)	31661(5)	31669(5)	31611(4)	31606(4)	31648(4)
	y	9622(5)	9622(6)	9693(6)	9594(5)	9528(5)	9561(5)
	z	- 4821(12)	- 4626(13)	- 4779(13)	- 4347(12)	- 4320(12)	- 4538(11)
O(7)	x	7815(7)	7957(8)	7874(8)	8656(7)	8592(7)	8336(6)
	y	28684(8)	28441(9)	28566(9)	27658(8)	27724(8)	28039(8)
O(8)	y	8860(7)	8820(7)	8840(8)	8858(7)	8845(7)	8836(6)
	z	- 6070(16)	- 5868(18)	- 5995(19)	- 4758(16)	- 4850(16)	- 5258(15)
O(9)	y	38490(12)	38253(13)	38262(14)	38356(11)	38470(11)	38499(10)
O(10)	y	8835(12)	9247(13)	9226(14)	8743(12)	8826(12)	8753(11)
H(1)	y	—	2095(15)	—	1613(14)	1704(15)	—
H(2)	y	43 (2)	57 (4)	52 (3)	49 (3)	50 (3)	45 (2)
	z	136 (4)	123 (4)	130 (5)	128 (4)	128 (4)	134 (3)

REFINED ATOMIC COORDINATES

Site		K 39	K 40	K 41	K 42	K 43	K 45
M(1)	x	12073(4)	12284(3)	12011(4)	11807(4)	11898(4)	11863(4)
	y	13955(4)	13721(4)	14295(4)	13993(4)	13985(4)	14048(4)
M(2)	y	14627(6)	14460(5)	14701(6)	14846(6)	14689(6)	14763(6)
M(3)	x	21555(3)	21632(3)	21546(3)	21525(3)	21520(3)	21516(3)
M(4)	x	31343(3)	31444(3)	31256(3)	31245(4)	31299(3)	31262(3)
	y	14139(4)	13984(3)	14239(4)	14178(4)	14146(4)	14198(4)
M(5)	x	40776(3)	40578(2)	40932(3)	40892(3)	40846(3)	40896(3)
T(1)	x	40152(3)	40157(2)	40143(3)	40126(3)	40137(3)	40132(3)
	y	35247(3)	35181(3)	35291(3)	35281(4)	35244(3)	35269(4)
T(2)	x	17794(3)	18268(2)	17419(3)	17513(4)	17638(3)	17517(3)
	y	33306(4)	33170(3)	33472(3)	33343(4)	33294(3)	33360(4)
T(3)	y	34246(8)	34032(4)	34757(14)	34604(14)	34381(9)	34550(12)
O(1)	x	22509(8)	22557(6)	22401(7)	22547(8)	22538(7)	22511(8)
	y	4492(9)	4421(7)	4566(8)	4546(10)	4529(8)	4563(9)
O(2)	x	40275(7)	40215(6)	40339(7)	40230(8)	40255(7)	40269(8)
	y	4665(9)	4540(7)	4783(9)	4786(10)	4723(8)	4761(10)
O(3)	x	40117(8)	40186(6)	40068(7)	39888(8)	39991(7)	39963(8)
	y	23451(9)	23339(7)	23547(9)	23456(10)	23418(8)	23465(10)
O(4)	x	13860(5)	13867(4)	13774(5)	13883(6)	13888(5)	13856(6)
	y	9975(6)	9974(5)	9931(6)	9972(7)	9997(6)	9973(6)
	z	- 5143(14)	- 5277(11)	- 5012(13)	- 5130(15)	- 5128(12)	- 5063(14)
O(5)	x	23305(9)	23839(7)	22879(8)	22994(9)	23147(8)	23001(9)
	y	23511(10)	23311(8)	23694(9)	23509(10)	23499(8)	23602(10)
O(6)	x	31656(5)	31610(4)	31637(5)	31649(6)	31665(5)	31661(5)
	y	9600(6)	9585(5)	9562(6)	9645(7)	9658(6)	9633(6)
	z	- 4642(14)	- 4294(11)	- 4897(13)	- 4764(15)	- 4726(13)	- 4785(14)
O(7)	x	8143(9)	8642(6)	7739(8)	7801(9)	7982(8)	7843(9)
	y	28272(10)	27647(7)	28797(8)	28653(10)	28441(9)	28649(10)
O(8)	y	8856(8)	8853(7)	8864(8)	8828(9)	8865(8)	8846(8)
	z	- 5536(20)	- 4790(15)	- 6224(18)	- 6112(21)	- 5846(18)	- 6067(20)
O(9)	y	38500(14)	38395(11)	38672(13)	38298(15)	38369(13)	38426(14)
O(10)	y	8784(14)	8680(11)	8862(13)	8950(16)	8764(13)	8956(14)
H(1)	y	—	1543(14)	—	—	—	—
H(2)	y	44 (3)	45 (3)	42 (3)	47 (3)	41 (3)	45 (3)
	z	135 (5)	132 (4)	140 (5)	132 (4)	139 (4)	136 (5)

REFINED ATOMIC COORDINATES

Site		K 46	K 47	K 49	K 50	K 52
M(1)	x	12085(4)	12078(4)	11992(4)	12069(4)	12055(4)
	y	13849(4)	13870(5)	14110(4)	13796(5)	14063(4)
M(2)	y	14572(5)	14584(6)	14704(5)	14583(6)	14636(6)
M(3)	x	21556(3)	21556(3)	21543(3)	21563(3)	21550(3)
M(4)	x	31387(3)	31371(3)	31290(3)	31383(3)	31325(3)
	y	14110(3)	14111(4)	14192(4)	14115(4)	14175(4)
M(5)	x	40743(3)	40749(3)	40865(3)	40747(3)	40836(3)
T(1)	x	40169(2)	40170(3)	40144(3)	40159(3)	40159(3)
	y	35236(3)	35239(3)	35274(3)	35242(3)	35266(3)
T(2)	x	17935(3)	17909(3)	17578(3)	17929(3)	17660(3)
	y	33242(3)	33257(4)	33387(3)	33237(4)	33352(3)
T(3)	y	34146(6)	34170(7)	34474(10)	34125(7)	34356(8)
O(1)	x	22532(7)	22525(7)	22458(7)	22565(8)	22468(7)
	y	4497(8)	4510(9)	4526(8)	4511(9)	4534(8)
O(2)	x	40243(6)	40259(7)	40302(7)	40232(7)	40302(7)
	y	4612(8)	4618(9)	4711(9)	4618(9)	4678(8)
O(3)	x	40159(7)	40137(7)	40050(7)	40128(8)	40116(7)
	y	23401(8)	23415(9)	23497(9)	23395(9)	23495(9)
O(4)	x	13855(5)	13841(5)	13816(5)	13885(6)	13820(5)
	y	9972(5)	9962(6)	9958(5)	9985(6)	9945(5)
	z	- 5170(12)	- 5184(13)	- 5079(12)	- 5190(13)	- 5092(12)
O(5)	x	23509(8)	23468(9)	23054(8)	23515(9)	23147(9)
	y	23504(8)	23501(9)	23589(8)	23496(10)	23608(9)
O(6)	x	31648(5)	31648(5)	31646(5)	31660(5)	31656(5)
	y	9623(6)	9618(6)	9580(6)	9634(6)	9602(6)
	z	- 4619(12)	- 4638(14)	- 4775(12)	- 4592(14)	- 4764(13)
O(7)	x	8373(8)	8339(8)	7910(8)	8357(8)	8043(8)
	y	28045(9)	28075(10)	28579(9)	28011(10)	28424(9)
O(8)	y	8853(7)	8853(8)	8847(7)	8848(8)	8861(8)
	z	- 5235(17)	- 5294(19)	- 5943(17)	- 5258(19)	- 5707(18)
O(9)	y	38462(12)	38476(13)	38542(12)	38464(13)	38598(13)
O(10)	y	8798(12)	8765(14)	8918(12)	8773(14)	8784(13)
H(1)	y	—	—	—	—	—
H(2)	y	66 (3)	49 (3)	50 (3)	38 (2)	52 (3)
	z	111 (2)	127 (4)	128 (4)	145 (5)	123 (4)

APPENDIX D

REFINED DISPLACEMENT PARAMETERS

Abbreviations used in APPENDIX D

Refined anisotropic displacement parameters (x 10^4)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K1	K2	K3	K5	K6	K7	K8	K9
X	U_{11}	316(11)	392(14)	305(17)	311(13)	295(12)	364(13)	295(9)	323(11)
	U_{22}	86(8)	100(9)	85(13)	106(10)	95(10)	82(9)	83(7)	81(8)
	U_{33}	64(8)	64(10)	78(14)	75(11)	53(10)	53(9)	60(8)	69(8)
	U_{23}	- 15(6)	- 11(7)	- 16(10)	- 9(7)	- 13(7)	- 13(6)	- 18(5)	- 11(6)
	U_{eq}	155(6)	185(7)	156(9)	164(7)	148(6)	166(6)	146(5)	158(5)
M(1)	U_{11}	163(3)	143(3)	122(2)	122(3)	130(3)	122(3)	148(3)	114(3)
	U_{22}	126(2)	119(3)	115(2)	115(3)	115(3)	105(3)	127(3)	102(3)
	U_{33}	88(2)	94(3)	96(3)	93(3)	103(3)	94(3)	104(3)	92(3)
	U_{12}	49(2)	35(2)	33(2)	29(2)	33(2)	25(2)	40(2)	27(2)
	U_{eq}	126(2)	119(2)	111(2)	110(2)	116(2)	107(2)	126(2)	103(2)
M(2)	U_{11}	60(3)	60(4)	54(3)	53(4)	66(4)	57(4)	57(4)	53(4)
	U_{22}	69(3)	75(4)	76(3)	78(4)	76(4)	63(4)	74(4)	63(3)
	U_{33}	134(4)	140(4)	157(4)	147(4)	116(4)	141(5)	168(4)	140(4)
	U_{eq}	88(2)	92(2)	95(2)	93(2)	103(2)	87(3)	100(2)	85(2)
M(3)	U_{11}	76(2)	74(2)	74(2)	75(2)	73(2)	66(2)	74(2)	71(2)
	U_{22}	74(2)	70(2)	64(2)	73(2)	69(3)	62(2)	69(2)	64(2)
	U_{33}	41(2)	42(2)	43(2)	43(2)	40(3)	39(2)	43(3)	43(2)
	U_{23}	- 6(1)	- 8(1)	- 5(2)	- 6(2)	- 6(2)	- 7(2)	- 4(2)	- 8(2)
	U_{eq}	64(1)	62(1)	60(1)	64(1)	60(1)	56(1)	62(1)	60(1)
M(4)	U_{11}	58(2)	56(2)	51(3)	54(3)	61(3)	53(3)	55(3)	45(2)
	U_{22}	60(2)	59(2)	53(2)	62(3)	59(3)	53(3)	63(2)	51(2)
	U_{33}	86(2)	87(2)	89(3)	91(3)	91(3)	83(3)	92(3)	87(3)
	U_{12}	- 4(1)	- 3(1)	- 0(2)	1(2)	- 3(2)	- 1(2)	- 1(2)	1(2)
	U_{eq}	68(2)	68(2)	64(2)	69(2)	71(2)	63(2)	70(2)	61(2)
M(5)	U_{11}	65(2)	64(2)	55(2)	62(2)	63(2)	53(2)	63(2)	58(2)
	U_{22}	66(2)	65(2)	62(2)	71(2)	66(2)	61(2)	61(2)	63(2)
	U_{33}	48(2)	47(2)	47(2)	49(2)	46(3)	42(2)	44(3)	47(2)
	U_{23}	- 6(1)	- 9(2)	- 8(2)	- 8(2)	- 5(2)	- 9(2)	- 7(2)	- 9(2)
	U_{eq}	60(1)	59(1)	55(1)	61(1)	58(1)	52(1)	56(1)	56(1)
T(1)	U_{11}	50(2)	48(2)	50(2)	51(2)	56(2)	49(2)	50(2)	50(2)
	U_{22}	54(2)	57(2)	53(2)	62(2)	58(2)	53(2)	60(2)	52(2)
	U_{33}	51(2)	50(2)	51(2)	54(2)	48(2)	51(2)	52(2)	54(2)
	U_{12}	8(1)	7(1)	9(2)	8(1)	9(2)	9(2)	9(2)	10(1)
	U_{eq}	52(1)	52(1)	51(1)	56(1)	54(1)	51(1)	54(1)	52(1)
T(2)	U_{11}	139(2)	139(2)	98(2)	110(2)	121(3)	105(2)	143(3)	93(2)
	U_{22}	61(2)	58(2)	54(2)	61(2)	58(2)	56(2)	59(2)	55(2)
	U_{33}	50(2)	51(2)	48(2)	53(2)	49(2)	48(2)	54(2)	49(2)
	U_{12}	- 9(1)	- 12(2)	2(2)	- 1(2)	- 5(2)	- 6(2)	- 10(2)	- 1(2)
	U_{eq}	83(1)	82(1)	67(1)	75(1)	76(1)	70(1)	86(1)	66(1)
T(3)	U_{11}	43(4)	46(4)	35(8)	53(7)	45(8)	42(7)	44(5)	39(8)
	U_{22}	81(4)	84(5)	83(9)	95(7)	78(8)	83(7)	67(6)	81(8)
	U_{33}	50(4)	46(5)	39(9)	41(7)	23(8)	29(7)	47(6)	46(8)
	U_{eq}	58(2)	59(3)	52(5)	63(4)	49(5)	52(5)	53(4)	55(5)
O(1)	U_{11}	84(4)	72(5)	64(5)	70(5)	79(6)	74(5)	86(6)	64(5)
	U_{22}	73(4)	71(4)	62(5)	74(5)	70(6)	65(5)	64(5)	71(5)
	U_{33}	39(4)	49(5)	42(5)	59(5)	48(6)	48(5)	51(6)	51(5)
	U_{12}	7(3)	6(4)	1(4)	5(4)	5(5)	7(4)	9(4)	7(4)
	U_{eq}	66(2)	64(2)	56(2)	68(2)	66(3)	62(2)	67(2)	62(2)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K1	K2	K3	K5	K6	K7	K8	K9
O(2)	U_{11}	67(4)	70(5)	61(5)	67(5)	69(6)	70(5)	63(5)	64(5)
	U_{22}	66(4)	67(5)	55(5)	67(5)	73(6)	68(5)	65(5)	65(5)
	U_{33}	43(4)	54(5)	51(6)	48(5)	35(6)	43(5)	56(6)	48(5)
	U_{12}	- 6(3)	- 10(4)	- 7(4)	- 14(4)	- 12(5)	- 10(4)	- 6(4)	- 11(4)
	U_{eq}	59(2)	63(2)	56(2)	61(2)	59(3)	60(2)	61(2)	59(2)
O(3)	U_{11}	94(4)	91(5)	101(6)	110(6)	113(7)	104(6)	89(6)	109(5)
	U_{22}	64(4)	63(4)	61(5)	65(5)	67(6)	65(5)	68(5)	64(5)
	U_{33}	105(5)	109(5)	112(6)	116(6)	108(7)	109(6)	111(6)	116(5)
	U_{12}	10(3)	12(4)	9(4)	11(4)	11(5)	18(4)	5(4)	18(4)
	U_{eq}	88(2)	88(2)	91(3)	97(2)	96(3)	93(3)	89(3)	96(2)
O(4)	U_{11}	112(3)	101(3)	98(4)	105(4)	107(4)	96(4)	101(4)	105(3)
	U_{22}	93(3)	93(3)	88(4)	92(3)	95(4)	97(4)	102(4)	94(3)
	U_{33}	64(3)	64(3)	64(4)	74(4)	67(4)	62(4)	71(4)	60(4)
	U_{23}	4(2)	2(3)	8(3)	7(3)	0(4)	3(3)	4(3)	4(3)
	U_{13}	- 13(3)	- 11(3)	- 16(3)	- 17(3)	- 17(4)	- 12(3)	- 15(3)	- 14(3)
	U_{12}	34(2)	35(3)	31(3)	36(3)	38(3)	34(3)	40(3)	40(3)
	U_{eq}	90(1)	86(2)	83(2)	90(2)	90(2)	85(2)	91(2)	87(2)
O(5)	U_{11}	218(5)	210(6)	128(6)	158(6)	156(7)	155(6)	181(7)	121(5)
	U_{22}	124(5)	113(5)	92(6)	101(5)	107(6)	89(5)	125(6)	89(5)
	U_{33}	101(5)	109(5)	107(6)	98(5)	91(6)	95(6)	101(6)	101(5)
	U_{12}	12(4)	- 1(5)	- 1(5)	- 1(4)	- 8(5)	- 4(5)	- 24(5)	- 2(4)
	U_{eq}	148(2)	144(2)	109(3)	119(2)	118(3)	113(3)	136(3)	104(2)
O(6)	U_{11}	74(3)	71(3)	66(4)	69(3)	70(4)	66(4)	70(4)	66(3)
	U_{22}	86(3)	84(3)	78(4)	89(3)	87(4)	83(4)	79(4)	81(3)
	U_{33}	82(3)	82(3)	74(4)	81(4)	73(4)	68(4)	87(4)	74(4)
	U_{23}	- 4(2)	0(3)	- 0(3)	3(3)	4(4)	12(3)	0(3)	5(3)
	U_{13}	- 6(2)	- 5(2)	- 7(3)	1(3)	- 0(3)	- 15(3)	- 6(3)	- 3(3)
	U_{12}	6(2)	4(3)	6(3)	4(3)	7(3)	7(3)	6(3)	5(3)
	U_{eq}	80(1)	79(2)	73(2)	80(2)	77(2)	72(2)	78(2)	74(2)
O(7)	U_{11}	162(5)	151(5)	84(5)	116(5)	111(6)	117(5)	133(6)	89(5)
	U_{22}	152(5)	153(5)	102(6)	125(5)	113(6)	111(6)	151(6)	90(5)
	U_{33}	87(5)	82(5)	84(6)	86(5)	95(7)	92(6)	82(6)	80(5)
	U_{12}	- 90(4)	- 87(4)	- 39(5)	- 61(5)	- 53(5)	- 50(5)	- 77(5)	- 30(4)
	U_{eq}	134(2)	128(2)	90(2)	109(2)	106(3)	107(3)	122(3)	86(2)
O(8)	U_{11}	53(4)	50(4)	52(5)	47(4)	54(5)	54(5)	52(5)	64(4)
	U_{22}	60(4)	57(4)	50(5)	64(4)	67(5)	60(5)	61(5)	56(4)
	U_{33}	104(4)	106(5)	75(6)	96(5)	85(6)	84(6)	97(6)	68(5)
	U_{23}	7(3)	4(4)	7(4)	3(4)	14(5)	10(4)	9(5)	4(4)
	U_{eq}	73(2)	71(2)	59(2)	69(2)	69(3)	66(2)	70(2)	63(2)
O(9)	U_{11}	54(6)	46(6)	45(8)	61(7)	61(8)	50(7)	48(8)	60(7)
	U_{22}	114(6)	127(7)	124(8)	124(8)	124(9)	137(8)	105(8)	125(7)
	U_{33}	217(8)	230(9)	194(10)	216(9)	207(11)	220(10)	215(10)	207(9)
	U_{eq}	128(3)	128(3)	121(4)	134(4)	131(4)	136(4)	123(4)	131(3)
O(10)	U_{11}	107(6)	134(3)	93(9)	73(8)	110(10)	84(9)	102(8)	71(8)
	U_{22}	133(6)	89(7)	181(10)	150(9)	153(11)	145(9)	120(8)	145(8)
	U_{33}	185(7)	120(7)	201(12)	170(10)	180(12)	145(10)	165(10)	155(9)
	U_{eq}	142(3)	172(8)	159(6)	131(5)	148(7)	125(6)	129(4)	124(5)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 10	K 11	K 12	K 13	K 14	K 15	K 16	K 17
X	U_{11}	287(11)	339(18)	438(20)	487(18)	313(17)	310(11)	302(18)	282(12)
	U_{22}	77(8)	111(13)	91(14)	100(11)	85(13)	73(8)	70(13)	77(10)
	U_{33}	50(9)	87(14)	88(16)	69(11)	58(14)	70(9)	70(14)	63(10)
	U_{23}	- 11(6)	- 19(10)	- 22(11)	- 13(8)	- 24(9)	- 8(6)	- 8(9)	- 16(7)
	U_{eq}	138(6)	179(9)	206(10)	219(8)	152(9)	151(6)	147(9)	141(6)
M(1)	U_{11}	144(3)	107(2)	144(4)	109(3)	126(2)	133(3)	126(2)	134(3)
	U_{22}	124(2)	113(2)	110(3)	89(3)	115(2)	114(3)	120(2)	112(3)
	U_{33}	96(3)	101(2)	95(4)	88(3)	94(2)	104(3)	96(2)	99(3)
	U_{12}	38(2)	30(1)	41(3)	14(2)	31(2)	31(2)	39(1)	30(2)
	U_{eq}	121(2)	107(1)	116(2)	95(2)	112(2)	117(2)	114(1)	115(2)
M(2)	U_{11}	64(3)	51(3)	62(4)	56(4)	56(3)	64(4)	58(3)	59(4)
	U_{22}	78(3)	77(3)	59(5)	64(4)	72(3)	71(4)	76(3)	73(4)
	U_{33}	164(4)	160(3)	119(5)	135(4)	155(4)	155(4)	154(3)	152(4)
	U_{eq}	102(2)	96(2)	80(3)	85(3)	94(2)	97(2)	96(2)	95(2)
M(3)	U_{11}	77(2)	71(2)	75(3)	70(2)	72(2)	74(2)	73(2)	75(2)
	U_{22}	70(2)	68(2)	66(2)	62(2)	66(2)	67(2)	66(2)	67(2)
	U_{33}	44(3)	45(2)	43(3)	38(2)	41(2)	46(3)	41(2)	45(3)
	U_{23}	- 7(2)	- 6(2)	- 9(2)	- 6(2)	- 7(2)	- 7(2)	- 8(2)	- 6(2)
	U_{eq}	64(1)	62(1)	61(1)	57(1)	60(1)	62(1)	60(1)	62(1)
M(4)	U_{11}	62(3)	50(2)	49(3)	49(3)	56(2)	58(2)	55(2)	57(2)
	U_{22}	61(2)	51(2)	55(3)	52(3)	57(2)	63(2)	52(2)	58(2)
	U_{33}	88(3)	93(3)	87(3)	84(3)	89(3)	88(3)	93(3)	86(3)
	U_{12}	- 3(2)	0(2)	- 2(2)	0(2)	0(2)	- 4(2)	- 0(2)	- 2(2)
	U_{eq}	71(2)	65(1)	64(2)	62(2)	67(2)	70(2)	67(2)	67(2)
M(5)	U_{11}	65(2)	53(2)	66(2)	56(2)	57(2)	60(2)	60(2)	61(2)
	U_{22}	65(2)	67(2)	60(2)	59(2)	64(2)	66(2)	62(2)	65(2)
	U_{33}	46(2)	48(2)	46(3)	43(2)	45(2)	51(3)	43(2)	45(3)
	U_{23}	- 8(2)	- 8(2)	- 8(2)	- 8(2)	- 10(2)	- 8(2)	- 8(2)	- 7(2)
	U_{eq}	59(1)	56(1)	58(1)	53(1)	55(1)	59(1)	55(1)	57(1)
T(1)	U_{11}	52(2)	50(2)	52(2)	49(2)	48(2)	56(2)	49(2)	53(2)
	U_{22}	57(2)	53(2)	45(2)	52(2)	57(2)	58(2)	51(2)	60(2)
	U_{33}	52(2)	54(2)	51(2)	48(2)	50(2)	59(2)	56(2)	55(2)
	U_{12}	8(2)	6(1)	5(2)	10(1)	7(1)	9(2)	8(1)	11(2)
	U_{eq}	54(1)	52(1)	49(1)	50(1)	52(1)	58(1)	52(1)	56(1)
T(2)	U_{11}	128(2)	90(2)	129(3)	90(2)	116(2)	123(2)	90(2)	118(2)
	U_{22}	61(2)	54(2)	54(2)	53(2)	54(2)	62(2)	51(2)	61(2)
	U_{33}	48(2)	49(2)	51(3)	46(2)	46(2)	54(2)	49(2)	52(2)
	U_{12}	- 7(2)	3(2)	- 12(2)	- 4(2)	- 1(2)	- 12(2)	3(2)	- 6(2)
	U_{eq}	79(1)	64(1)	78(1)	63(1)	72(1)	79(1)	64(1)	77(1)
T(3)	U_{11}	42(6)	42(9)	41(4)	31(8)	45(7)	50(7)	43(8)	42(8)
	U_{22}	83(7)	78(9)	60(5)	87(8)	87(7)	95(7)	77(8)	101(8)
	U_{33}	40(7)	49(9)	45(5)	47(8)	32(7)	43(7)	39(8)	48(8)
	U_{eq}	55(4)	56(6)	49(3)	55(5)	55(4)	63(5)	53(5)	64(5)
O(1)	U_{11}	75(5)	60(5)	76(6)	72(5)	73(5)	83(5)	64(5)	82(5)
	U_{22}	73(5)	64(5)	62(6)	67(5)	69(5)	70(5)	66(5)	71(5)
	U_{33}	47(5)	54(5)	53(6)	42(5)	43(5)	55(6)	46(5)	44(6)
	U_{12}	2(4)	1(4)	9(5)	12(4)	0(4)	3(4)	3(4)	2(4)
	U_{eq}	65(2)	59(2)	63(3)	60(2)	62(2)	69(2)	59(2)	66(2)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 10	K 11	K 12	K 13	K 14	K 15	K 16	K 17
O(2)	U_{11}	78(5)	64(5)	58(6)	64(5)	66(5)	71(5)	66(5)	68(5)
	U_{22}	65(5)	56(5)	47(6)	60(5)	59(5)	63(5)	54(5)	58(5)
	U_{33}	45(6)	54(5)	48(6)	36(5)	50(5)	48(6)	42(5)	52(6)
	U_{12}	- 6(4)	- 3(4)	- 8(5)	- 9(4)	- 5(4)	- 15(4)	- 2(4)	- 5(4)
	U_{eq}	63(2)	58(2)	51(3)	53(2)	58(2)	61(2)	54(2)	59(2)
O(3)	U_{11}	104(6)	101(6)	73(6)	108(5)	100(6)	103(6)	95(5)	104(6)
	U_{22}	68(5)	60(5)	62(6)	51(5)	63(5)	74(5)	57(5)	70(5)
	U_{33}	112(6)	122(6)	112(7)	112(6)	113(6)	111(6)	113(6)	117(6)
	U_{12}	10(4)	5(4)	6(5)	17(4)	8(4)	12(4)	5(4)	16(5)
	U_{eq}	95(3)	94(3)	82(3)	91(2)	92(2)	96(3)	88(2)	97(3)
O(4)	U_{11}	111(4)	100(4)	100(4)	101(4)	96(3)	110(4)	104(3)	110(4)
	U_{22}	94(4)	87(4)	82(4)	95(4)	88(4)	99(4)	87(3)	96(4)
	U_{33}	69(4)	73(4)	65(5)	56(4)	64(4)	68(4)	64(4)	64(4)
	U_{23}	2(3)	2(3)	3(4)	0(3)	- 0(3)	5(3)	1(3)	5(3)
	U_{13}	- 16(3)	- 20(3)	- 24(4)	- 10(3)	- 12(3)	- 21(3)	- 19(3)	- 18(3)
	U_{12}	36(3)	34(3)	35(3)	39(3)	36(3)	40(3)	32(3)	36(3)
	U_{eq}	91(2)	87(2)	82(2)	84(2)	83(2)	92(2)	85(2)	90(2)
O(5)	U_{11}	161(6)	121(6)	194(8)	129(6)	145(6)	188(7)	115(5)	161(7)
	U_{22}	110(6)	81(5)	122(7)	90(5)	94(5)	102(6)	84(5)	104(6)
	U_{33}	111(6)	102(6)	92(7)	99(5)	103(6)	101(6)	100(5)	108(6)
	U_{12}	- 12(5)	13(4)	21(6)	- 4(4)	- 8(5)	- 8(5)	4(4)	- 9(5)
	U_{eq}	127(3)	101(2)	136(3)	106(2)	114(2)	130(3)	100(2)	124(3)
O(6)	U_{11}	75(4)	64(4)	75(4)	61(3)	61(3)	74(4)	70(3)	75(4)
	U_{22}	89(4)	78(4)	79(4)	81(3)	82(3)	79(4)	76(3)	83(4)
	U_{33}	78(4)	71(4)	86(5)	70(4)	76(4)	81(4)	68(4)	74(4)
	U_{23}	2(3)	- 3(3)	- 2(4)	11(3)	- 1(3)	3(3)	2(3)	5(3)
	U_{13}	- 4(3)	2(3)	- 1(4)	- 3(3)	- 4(3)	- 6(3)	- 5(3)	- 3(3)
	U_{12}	6(3)	8(3)	- 2(3)	3(3)	5(3)	4(3)	6(3)	8(3)
	U_{eq}	80(2)	71(2)	80(2)	71(2)	73(2)	78(2)	71(2)	77(2)
O(7)	U_{11}	115(6)	82(5)	140(7)	87(5)	99(5)	126(6)	83(5)	100(6)
	U_{22}	141(6)	93(5)	134(7)	89(5)	119(6)	130(6)	89(5)	120(6)
	U_{33}	87(6)	92(6)	93(7)	83(5)	88(6)	81(6)	89(5)	93(6)
	U_{12}	- 60(5)	- 31(4)	- 71(6)	- 31(4)	- 52(4)	- 64(5)	- 34(4)	- 46(5)
	U_{eq}	114(3)	89(2)	122(3)	87(2)	102(2)	112(3)	87(2)	105(3)
O(8)	U_{11}	51(5)	49(5)	52(5)	53(4)	46(4)	59(5)	55(4)	56(5)
	U_{22}	70(5)	60(5)	55(5)	62(4)	60(4)	56(5)	59(4)	55(5)
	U_{33}	99(6)	84(5)	94(7)	74(5)	86(5)	100(6)	72(5)	92(6)
	U_{23}	9(4)	9(4)	- 0(5)	7(4)	3(4)	7(4)	9(4)	8(4)
	U_{eq}	73(2)	64(2)	67(3)	63(2)	64(2)	72(2)	62(2)	68(2)
O(9)	U_{11}	72(8)	48(8)	46(8)	47(7)	64(7)	57(8)	49(7)	55(8)
	U_{22}	133(8)	119(8)	93(9)	134(8)	116(8)	123(8)	110(8)	144(9)
	U_{33}	229(10)	188(9)	238(12)	234(9)	218(10)	216(10)	203(9)	202(10)
	U_{eq}	145(4)	118(4)	126(4)	138(4)	133(4)	132(4)	121(3)	134(4)
O(10)	U_{11}	104(9)	101(9)	90(9)	77(8)	100(9)	110(9)	100(9)	98(9)
	U_{22}	138(9)	184(10)	105(9)	144(9)	137(9)	194(10)	167(10)	177(10)
	U_{33}	159(11)	226(11)	181(11)	138(9)	178(10)	176(11)	236(11)	179(11)
	U_{eq}	134(6)	170(6)	125(4)	120(5)	138(6)	160(6)	168(6)	151(6)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 18	K 19	K 20	K 21	K 22	K 23	K 24	K 25
X	U_{11}	292(12)	308(18)	313(23)	299(17)	454(20)	486(26)	293(20)	305(11)
	U_{22}	84(10)	110(15)	114(18)	101(13)	109(13)	112(16)	71(15)	74(9)
	U_{33}	63(10)	77(15)	68(19)	66(13)	66(13)	88(17)	63(16)	63(9)
	U_{23}	- 17(7)	- 5(10)	- 12(13)	- 25(10)	- 16(10)	- 17(11)	- 21(11)	- 13(6)
	U_{eq}	146(7)	165(9)	165(12)	156(9)	210(10)	229(12)	142(10)	147(6)
M(1)	U_{11}	134(3)	117(3)	119(3)	183(4)	144(3)	122(3)	121(3)	128(3)
	U_{22}	113(3)	109(3)	111(3)	146(4)	121(3)	94(3)	121(3)	112(2)
	U_{33}	98(3)	97(3)	94(3)	102(3)	96(3)	89(3)	97(3)	100(3)
	U_{12}	36(2)	29(2)	30(2)	72(3)	40(2)	17(2)	31(2)	31(2)
	U_{eq}	115(2)	107(2)	108(2)	144(2)	120(2)	102(2)	113(2)	113(2)
M(2)	U_{11}	63(4)	55(3)	60(3)	59(5)	58(4)	62(4)	55(4)	57(3)
	U_{22}	67(4)	75(3)	77(3)	70(5)	75(4)	65(4)	80(4)	73(3)
	U_{33}	150(5)	148(4)	152(4)	145(6)	130(5)	141(4)	148(4)	147(4)
	U_{eq}	93(3)	93(2)	96(2)	91(3)	88(3)	90(3)	94(2)	92(2)
M(3)	U_{11}	72(2)	71(2)	74(2)	78(3)	75(2)	70(2)	68(2)	75(2)
	U_{22}	65(2)	63(2)	65(2)	72(3)	72(2)	63(2)	66(2)	66(2)
	U_{33}	40(3)	41(2)	39(2)	45(3)	40(2)	39(2)	39(2)	42(2)
	U_{23}	- 5(2)	- 6(2)	- 7(2)	- 5(2)	- 6(2)	- 5(2)	- 5(2)	- 8(2)
	U_{eq}	59(1)	58(1)	59(1)	65(2)	62(1)	57(1)	58(1)	61(1)
M(4)	U_{11}	56(3)	53(3)	62(3)	59(3)	56(3)	58(2)	56(2)	54(2)
	U_{22}	57(3)	54(2)	55(3)	61(3)	62(3)	56(2)	57(2)	56(2)
	U_{33}	84(3)	93(3)	87(3)	93(3)	93(3)	90(2)	96(3)	87(3)
	U_{12}	0(2)	2(2)	- 2(2)	- 2(2)	- 1(2)	- 2(2)	- 1(2)	1(1)
	U_{eq}	66(2)	67(2)	68(2)	71(2)	70(2)	68(1)	70(1)	66(2)
M(5)	U_{11}	59(2)	54(2)	58(2)	67(3)	63(2)	61(2)	55(2)	60(2)
	U_{22}	60(2)	61(2)	61(2)	65(3)	67(2)	60(2)	61(2)	64(2)
	U_{33}	42(2)	44(2)	40(2)	50(3)	47(2)	46(2)	43(2)	43(2)
	U_{23}	- 9(2)	- 8(2)	- 7(2)	- 9(2)	- 9(2)	- 9(2)	- 6(2)	- 8(2)
	U_{eq}	54(1)	53(1)	53(1)	61(2)	59(1)	56(1)	53(1)	56(1)
T(1)	U_{11}	46(2)	46(2)	52(2)	52(3)	47(2)	48(2)	47(2)	53(2)
	U_{22}	57(2)	51(2)	52(2)	55(3)	55(2)	47(2)	50(2)	58(2)
	U_{33}	51(2)	55(2)	50(2)	52(3)	53(2)	50(2)	54(2)	54(2)
	U_{12}	7(2)	8(1)	7(2)	6(2)	7(1)	8(1)	6(2)	10(1)
	U_{eq}	52(1)	51(1)	51(1)	53(1)	52(1)	48(1)	50(1)	55(1)
T(2)	U_{11}	112(2)	91(2)	86(2)	142(3)	130(2)	111(2)	97(2)	99(2)
	U_{22}	58(2)	52(2)	53(2)	63(3)	62(2)	53(2)	53(2)	58(2)
	U_{33}	45(2)	47(2)	43(2)	51(3)	55(2)	47(2)	49(2)	48(2)
	U_{12}	- 6(2)	- 1(2)	2(2)	- 10(2)	- 10(2)	- 7(1)	- 1(2)	- 4(2)
	U_{eq}	72(1)	63(1)	61(1)	85(2)	82(1)	70(1)	67(1)	68(1)
T(3)	U_{11}	46(7)	34(8)	37(9)	50(6)	38(4)	41(6)	32(8)	45(8)
	U_{22}	75(8)	74(8)	66(9)	75(6)	74(5)	79(6)	80(8)	77(8)
	U_{33}	28(8)	28(8)	26(9)	48(6)	49(5)	41(6)	45(8)	41(8)
	U_{eq}	50(5)	45(5)	43(6)	58(4)	54(3)	54(4)	53(5)	54(5)
O(1)	U_{11}	75(5)	67(5)	68(5)	78(7)	81(5)	66(5)	63(5)	77(5)
	U_{22}	64(5)	66(5)	69(5)	72(7)	73(5)	68(5)	61(5)	71(5)
	U_{33}	44(6)	47(5)	49(5)	46(7)	48(5)	47(5)	53(5)	47(5)
	U_{12}	1(4)	- 0(4)	- 1(4)	6(6)	- 4(4)	1(4)	- 3(4)	2(4)
	U_{eq}	61(2)	60(2)	62(2)	65(3)	67(2)	61(2)	59(2)	65(2)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 18	K 19	K 20	K 21	K 22	K 23	K 24	K 25
O(2)	U_{11}	60(5)	57(5)	59(5)	67(7)	69(5)	66(5)	61(5)	66(5)
	U_{22}	68(5)	58(5)	54(5)	62(7)	69(5)	59(5)	60(5)	63(5)
	U_{33}	52(6)	46(5)	45(6)	48(7)	47(5)	44(5)	52(6)	49(5)
	U_{12}	- 7(4)	- 3(4)	3(4)	- 9(5)	- 6(4)	- 9(4)	- 2(4)	- 10(4)
	U_{eq}	60(2)	54(2)	52(2)	59(3)	62(2)	57(2)	58(2)	59(2)
O(3)	U_{11}	111(6)	98(5)	95(6)	81(7)	88(5)	96(5)	98(6)	119(6)
	U_{22}	58(5)	60(5)	48(5)	70(7)	63(5)	56(5)	61(5)	66(5)
	U_{33}	120(6)	117(6)	117(6)	113(8)	113(6)	114(5)	115(6)	113(6)
	U_{12}	15(4)	9(4)	8(4)	5(6)	8(4)	11(4)	13(4)	13(4)
	U_{eq}	97(3)	92(2)	86(3)	88(3)	88(2)	89(2)	91(3)	100(2)
O(4)	U_{11}	102(4)	98(4)	98(4)	105(5)	106(4)	97(3)	96(4)	105(4)
	U_{22}	91(4)	89(4)	85(4)	92(5)	91(4)	85(3)	86(4)	92(4)
	U_{33}	64(4)	61(4)	65(4)	65(5)	58(4)	59(3)	64(4)	64(4)
	U_{23}	5(3)	7(3)	7(3)	3(4)	7(3)	5(3)	4(3)	6(3)
	U_{13}	- 10(3)	- 16(3)	- 15(3)	- 10(4)	- 12(3)	- 12(3)	- 15(3)	- 9(3)
	U_{12}	36(3)	32(3)	30(3)	35(4)	37(3)	35(3)	32(3)	35(3)
	U_{eq}	86(2)	83(2)	83(2)	87(2)	85(2)	80(2)	82(2)	87(2)
O(5)	U_{11}	153(7)	130(6)	120(6)	223(9)	226(7)	164(6)	144(6)	134(6)
	U_{22}	103(6)	82(5)	78(6)	131(8)	116(6)	92(5)	83(6)	98(5)
	U_{33}	100(6)	107(5)	101(6)	104(8)	101(6)	104(5)	99(6)	107(6)
	U_{12}	- 13(5)	4(4)	7(5)	21(7)	19(5)	0(4)	11(5)	- 7(4)
	U_{eq}	118(3)	106(2)	100(3)	153(4)	148(3)	120(2)	109(3)	113(2)
O(6)	U_{11}	70(4)	67(3)	68(4)	72(5)	74(3)	66(3)	65(4)	70(3)
	U_{22}	80(4)	77(3)	76(4)	89(5)	84(3)	79(3)	75(4)	86(4)
	U_{33}	76(4)	70(4)	60(4)	79(5)	77(4)	72(4)	76(4)	70(4)
	U_{23}	3(3)	12(3)	2(3)	- 7(4)	4(3)	3(3)	6(3)	7(3)
	U_{13}	- 3(3)	- 4(3)	4(3)	- 3(4)	- 6(3)	- 4(3)	- 1(3)	- 7(3)
	U_{12}	5(3)	4(3)	8(3)	6(4)	9(3)	4(3)	6(3)	6(3)
	U_{eq}	75(2)	71(2)	68(2)	80(2)	78(2)	72(2)	72(2)	75(2)
O(7)	U_{11}	106(6)	90(5)	78(5)	155(8)	158(6)	114(5)	95(5)	90(5)
	U_{22}	111(6)	94(5)	94(6)	152(8)	144(6)	116(5)	112(6)	109(5)
	U_{33}	84(6)	88(5)	82(6)	91(8)	87(6)	74(5)	87(6)	81(6)
	U_{12}	- 49(5)	- 35(4)	- 30(5)	- 89(7)	- 86(5)	- 57(4)	- 44(5)	- 33(4)
	U_{eq}	100(3)	91(2)	85(2)	133(4)	129(3)	101(2)	98(3)	93(2)
O(8)	U_{11}	59(5)	47(4)	57(5)	53(6)	52(5)	56(4)	52(5)	55(5)
	U_{22}	60(5)	58(4)	58(5)	61(6)	67(5)	50(4)	56(5)	62(4)
	U_{33}	73(6)	74(5)	78(6)	99(7)	105(5)	92(5)	89(6)	77(5)
	U_{23}	8(4)	16(4)	2(4)	7(6)	5(4)	6(4)	8(4)	12(4)
	U_{eq}	64(2)	60(2)	64(2)	71(3)	75(2)	66(2)	66(2)	65(2)
O(9)	U_{11}	69(8)	53(7)	51(8)	57(10)	44(7)	55(7)	61(8)	57(7)
	U_{22}	123(9)	130(8)	119(8)	108(11)	121(8)	117(7)	122(9)	151(8)
	U_{33}	198(10)	206(9)	186(10)	214(13)	230(10)	223(9)	194(10)	211(10)
	U_{eq}	130(4)	129(4)	119(4)	126(5)	132(4)	132(3)	126(4)	140(4)
O(10)	U_{11}	98(9)	103(9)	101(9)	116(12)	84(8)	83(8)	95(9)	98(9)
	U_{22}	143(10)	178(9)	184(11)	155(13)	122(8)	139(8)	185(10)	202(10)
	U_{33}	165(11)	205(10)	238(12)	232(15)	178(9)	152(9)	205(11)	185(10)
	U_{eq}	135(6)	162(6)	174(6)	168(8)	128(4)	124(5)	162(6)	162(6)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 26	K 27	K 28	K 29	K 30	K 31	K 32	K 33
X	U_{11}	306(12)	293(12)	328(11)	295(13)	584(35)	538(29)	376(12)	285(12)
	U_{22}	78(9)	74(10)	83(8)	89(10)	110(20)	109(17)	76(9)	76(10)
	U_{33}	53(10)	74(11)	63(8)	74(11)	100(21)	85(18)	47(9)	59(10)
	U_{23}	- 5(7)	- 9(7)	- 4(6)	- 16(7)	- 10(15)	3(12)	- 12(6)	- 5(7)
	U_{eq}	146(6)	147(7)	158(6)	153(7)	265(15)	244(13)	166(6)	140(6)
M(1)	U_{11}	154(3)	133(3)	122(3)	144(3)	152(4)	164(4)	115(3)	140(3)
	U_{22}	133(3)	109(3)	108(3)	118(3)	109(4)	130(4)	98(3)	118(3)
	U_{33}	94(3)	102(3)	95(3)	101(3)	90(4)	70(4)	91(3)	100(3)
	U_{12}	41(2)	32(2)	30(2)	36(2)	59(3)	41(3)	25(2)	37(2)
	U_{eq}	127(2)	115(2)	108(2)	121(2)	117(3)	121(2)	101(2)	119(2)
M(2)	U_{11}	67(4)	59(4)	55(4)	65(4)	55(5)	67(5)	56(4)	59(3)
	U_{22}	88(4)	61(4)	66(4)	76(4)	59(5)	74(5)	62(4)	75(3)
	U_{33}	149(5)	145(5)	139(4)	167(5)	82(5)	104(5)	137(4)	161(4)
	U_{eq}	102(3)	88(3)	87(2)	103(3)	65(3)	82(3)	85(2)	99(2)
M(3)	U_{11}	81(3)	73(2)	70(2)	82(3)	78(3)	89(3)	74(2)	76(2)
	U_{22}	73(3)	65(3)	61(2)	69(3)	61(3)	81(3)	61(2)	67(2)
	U_{33}	33(3)	42(3)	41(2)	42(3)	39(3)	15(3)	36(2)	39(2)
	U_{23}	- 4(2)	- 6(2)	- 5(2)	- 4(2)	- 6(2)	- 6(2)	- 7(1)	- 4(2)
	U_{eq}	62(1)	60(1)	57(1)	64(1)	59(1)	62(1)	57(1)	61(1)
M(4)	U_{11}	62(3)	56(3)	54(3)	67(3)	50(3)	66(3)	58(3)	56(2)
	U_{22}	64(3)	53(3)	57(2)	59(3)	53(3)	74(3)	54(2)	56(2)
	U_{33}	80(3)	84(3)	85(3)	98(3)	89(3)	73(3)	84(3)	87(3)
	U_{12}	- 1(2)	- 4(2)	- 1(2)	- 3(2)	3(2)	- 0(2)	- 2(2)	- 2(1)
	U_{eq}	69(2)	64(2)	65(2)	75(2)	64(1)	71(2)	65(2)	66(2)
M(5)	U_{11}	65(3)	59(2)	58(2)	69(3)	68(3)	73(3)	59(2)	58(2)
	U_{22}	70(3)	59(2)	59(2)	67(3)	62(3)	77(3)	57(2)	63(2)
	U_{33}	40(3)	46(3)	46(2)	46(3)	42(3)	26(3)	40(2)	44(2)
	U_{23}	- 9(2)	- 9(2)	- 6(2)	- 8(2)	- 10(2)	- 10(2)	- 6(2)	- 8(2)
	U_{eq}	58(1)	54(1)	54(1)	61(1)	57(1)	59(1)	52(1)	55(1)
T(1)	U_{11}	50(2)	52(2)	49(2)	57(2)	46(2)	60(2)	49(2)	48(2)
	U_{22}	69(3)	55(2)	50(2)	51(2)	44(2)	65(2)	47(2)	53(2)
	U_{33}	44(3)	54(3)	54(2)	58(3)	47(3)	25(2)	45(2)	51(2)
	U_{12}	11(2)	7(2)	10(1)	10(2)	7(2)	6(2)	10(1)	7(1)
	U_{eq}	54(1)	53(1)	51(1)	55(1)	46(1)	50(1)	47(1)	50(1)
T(2)	U_{11}	139(3)	120(3)	107(2)	134(3)	87(3)	137(3)	96(2)	126(2)
	U_{22}	74(3)	53(2)	56(2)	59(2)	54(2)	71(2)	52(2)	55(2)
	U_{33}	43(3)	49(2)	50(2)	50(3)	48(3)	30(2)	42(2)	46(2)
	U_{12}	- 9(2)	- 5(2)	- 8(2)	- 4(2)	- 1(2)	- 2(2)	- 5(1)	- 6(2)
	U_{eq}	86(1)	74(1)	71(1)	81(1)	63(1)	79(1)	63(1)	76(1)
T(3)	U_{11}	39(6)	36(8)	45(7)	57(7)	44(4)	52(5)	34(7)	45(6)
	U_{22}	77(7)	68(8)	81(7)	71(7)	63(4)	76(5)	78(7)	82(6)
	U_{33}	44(7)	20(8)	40(7)	45(7)	43(4)	26(5)	36(7)	42(6)
	U_{eq}	53(4)	41(5)	56(4)	58(5)	50(3)	51(3)	50(5)	56(4)
O(1)	U_{11}	75(6)	75(6)	77(5)	79(6)	74(6)	86(6)	77(5)	70(5)
	U_{22}	72(6)	58(6)	64(5)	73(6)	63(6)	86(6)	65(4)	68(5)
	U_{33}	43(7)	46(6)	47(5)	48(6)	40(6)	24(6)	41(5)	46(5)
	U_{12}	4(5)	- 3(5)	- 1(4)	6(5)	6(5)	- 3(5)	7(4)	4(4)
	U_{eq}	63(3)	60(3)	62(2)	67(3)	59(3)	65(3)	61(2)	61(2)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 26	K 27	K 28	K 29	K 30	K 31	K 32	K 33
O(2)	U_{11}	75(6)	69(6)	67(5)	76(6)	65(6)	75(6)	71(5)	59(5)
	U_{22}	74(7)	54(6)	61(5)	63(6)	56(6)	82(6)	58(5)	60(5)
	U_{33}	48(7)	58(6)	48(5)	47(6)	45(6)	21(6)	41(5)	49(5)
	U_{12}	- 8(5)	- 13(5)	- 6(4)	1(5)	- 4(5)	- 8(5)	- 14(3)	- 0(4)
	U_{eq}	66(3)	60(3)	59(2)	62(3)	55(3)	59(3)	57(2)	56(2)
O(3)	U_{11}	99(7)	111(7)	105(6)	111(7)	79(6)	88(6)	109(5)	110(5)
	U_{22}	85(7)	60(6)	62(5)	70(6)	61(6)	69(6)	56(5)	58(5)
	U_{33}	111(7)	113(7)	104(6)	116(7)	99(7)	79(6)	100(5)	107(6)
	U_{12}	11(5)	17(5)	16(4)	7(5)	4(5)	3(5)	20(4)	6(4)
	U_{eq}	98(3)	95(3)	90(2)	99(3)	80(3)	78(3)	88(2)	91(2)
O(4)	U_{11}	113(4)	105(4)	101(4)	110(4)	104(4)	112(4)	109(3)	100(3)
	U_{22}	101(5)	91(4)	90(4)	95(4)	83(4)	103(4)	92(3)	88(3)
	U_{33}	54(5)	72(5)	64(4)	72(5)	53(5)	33(4)	60(3)	61(4)
	U_{23}	1(4)	4(4)	6(3)	1(4)	2(4)	3(3)	4(3)	7(3)
	U_{13}	- 13(4)	- 9(4)	- 15(3)	- 17(4)	- 9(4)	- 14(4)	- 15(3)	- 12(3)
	U_{12}	36(4)	41(3)	42(3)	37(3)	33(4)	43(4)	41(3)	33(3)
	U_{eq}	89(2)	89(2)	85(2)	92(2)	80(2)	83(2)	87(2)	83(2)
O(5)	U_{11}	211(8)	144(7)	159(6)	175(7)	159(7)	200(7)	146(5)	179(6)
	U_{22}	121(7)	97(6)	91(5)	111(7)	147(7)	130(7)	89(5)	103(5)
	U_{33}	99(7)	97(7)	94(5)	111(7)	94(7)	87(6)	90(5)	103(5)
	U_{12}	- 1(6)	- 8(5)	- 16(5)	- 12(6)	48(6)	40(6)	- 7(4)	6(5)
	U_{eq}	144(3)	113(3)	114(2)	132(3)	133(3)	139(3)	108(2)	128(2)
O(6)	U_{11}	77(4)	67(4)	63(3)	76(4)	80(4)	87(4)	67(3)	70(3)
	U_{22}	83(4)	79(4)	81(4)	84(4)	78(4)	97(4)	77(3)	83(3)
	U_{33}	78(5)	80(5)	76(4)	83(5)	78(5)	54(4)	70(3)	82(4)
	U_{23}	3(4)	6(4)	13(3)	1(4)	- 8(4)	- 3(4)	13(3)	- 4(3)
	U_{13}	- 9(4)	- 5(4)	- 3(3)	- 2(4)	- 5(4)	- 6(3)	- 2(3)	- 4(3)
	U_{12}	6(4)	10(3)	7(3)	9(3)	7(4)	7(3)	6(3)	4(3)
	U_{eq}	79(2)	75(2)	73(2)	81(2)	79(2)	80(2)	71(2)	78(2)
O(7)	U_{11}	159(7)	111(6)	104(5)	131(7)	119(7)	158(7)	95(5)	127(5)
	U_{22}	154(8)	106(6)	114(6)	126(7)	95(6)	148(7)	97(5)	126(5)
	U_{33}	76(7)	83(7)	83(6)	111(7)	86(7)	57(6)	78(5)	89(5)
	U_{12}	- 89(6)	- 53(5)	- 51(5)	- 65(6)	- 37(5)	- 76(6)	- 45(4)	- 71(5)
	U_{eq}	130(3)	100(3)	101(2)	123(3)	100(3)	121(3)	90(2)	114(2)
O(8)	U_{11}	64(6)	48(5)	51(5)	64(6)	62(6)	54(5)	55(4)	54(4)
	U_{22}	69(6)	62(5)	60(5)	59(5)	56(5)	78(5)	57(4)	50(4)
	U_{33}	93(7)	82(6)	83(5)	95(6)	77(6)	77(6)	76(5)	100(5)
	U_{23}	10(5)	7(5)	18(4)	5(5)	- 5(5)	2(5)	8(4)	6(4)
	U_{eq}	75(3)	64(3)	65(2)	72(3)	65(3)	69(3)	63(2)	68(2)
O(9)	U_{11}	55(9)	64(9)	63(7)	62(9)	46(9)	64(8)	59(7)	52(7)
	U_{22}	149(11)	116(9)	126(8)	114(9)	93(9)	116(9)	123(7)	129(8)
	U_{33}	209(12)	209(11)	226(10)	215(11)	223(12)	202(11)	206(8)	201(9)
	U_{eq}	138(5)	129(4)	138(4)	130(4)	120(4)	127(4)	129(3)	127(3)
O(10)	U_{11}	108(11)	108(11)	79(8)	96(10)	94(9)	101(9)	74(7)	106(8)
	U_{22}	185(12)	131(11)	145(9)	162(11)	114(10)	126(9)	121(7)	222(10)
	U_{33}	160(13)	157(12)	153(10)	166(12)	192(11)	181(10)	125(7)	212(10)
	U_{eq}	151(7)	132(7)	126(5)	142(7)	134(4)	136(4)	107(3)	180(6)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 34	K 35	K 36	K 38	K 39	K 40	K 41	K 42
X	U_{11}	289(18)	321(12)	347(10)	408(12)	381(16)	546(21)	427(15)	298(13)
	U_{22}	79(14)	87(8)	74(7)	87(8)	97(12)	101(12)	91(10)	70(11)
	U_{33}	63(14)	78(9)	69(7)	69(8)	77(12)	89(13)	70(10)	52(11)
	U_{23}	- 4(10)	- 14(6)	- 11(5)	- 12(6)	- 13(9)	- 21(9)	- 23(7)	- 10(8)
	U_{eq}	144(9)	162(6)	163(5)	188(6)	185(8)	245(9)	196(7)	140(7)
M(1)	U_{11}	124(3)	166(3)	147(3)	144(3)	144(3)	151(3)	96(3)	124(3)
	U_{22}	114(3)	131(3)	117(3)	114(2)	107(3)	105(3)	87(3)	113(3)
	U_{33}	93(3)	98(3)	90(3)	90(2)	95(3)	93(3)	102(3)	101(3)
	U_{12}	31(2)	83(2)	70(2)	40(2)	31(2)	64(2)	16(2)	32(2)
	U_{eq}	110(2)	132(2)	118(2)	116(2)	115(2)	116(2)	95(2)	113(2)
M(2)	U_{11}	61(4)	52(4)	52(4)	64(3)	59(4)	57(3)	43(4)	62(4)
	U_{22}	73(4)	64(4)	66(4)	70(3)	63(4)	61(3)	61(4)	74(4)
	U_{33}	144(4)	83(4)	81(4)	128(4)	144(5)	82(4)	135(5)	155(5)
	U_{eq}	93(2)	67(2)	66(2)	87(2)	89(3)	67(2)	80(3)	97(3)
M(3)	U_{11}	75(2)	69(2)	69(2)	80(2)	74(2)	72(2)	64(2)	72(3)
	U_{22}	62(2)	71(2)	68(2)	72(2)	65(2)	64(2)	60(2)	66(3)
	U_{33}	38(2)	45(2)	39(2)	36(2)	44(2)	40(2)	44(2)	40(3)
	U_{23}	- 6(2)	- 6(2)	- 5(2)	- 6(1)	- 5(2)	- 7(1)	- 7(2)	- 7(2)
	U_{eq}	58(1)	62(1)	58(1)	63(1)	61(1)	59(1)	56(1)	59(1)
M(4)	U_{11}	58(2)	43(2)	42(2)	57(2)	54(3)	45(2)	46(3)	61(3)
	U_{22}	55(2)	56(2)	59(2)	64(2)	53(3)	54(2)	55(3)	55(3)
	U_{33}	91(3)	97(3)	88(2)	85(2)	87(3)	91(2)	90(3)	86(3)
	U_{12}	- 1(2)	6(1)	7(1)	- 1(1)	- 4(2)	5(1)	2(2)	2(2)
	U_{eq}	68(1)	65(2)	63(2)	69(1)	65(2)	63(2)	64(2)	67(2)
M(5)	U_{11}	57(2)	61(2)	58(2)	68(2)	65(2)	64(2)	50(2)	54(3)
	U_{22}	61(2)	67(2)	65(2)	65(2)	61(2)	61(2)	59(2)	59(3)
	U_{33}	39(2)	45(2)	42(2)	44(2)	52(2)	41(2)	46(3)	46(3)
	U_{23}	- 8(2)	- 7(2)	- 7(2)	- 6(1)	- 8(2)	- 7(1)	- 9(2)	- 5(2)
	U_{eq}	52(1)	58(1)	55(1)	59(1)	59(1)	56(1)	52(1)	53(1)
T(1)	U_{11}	51(2)	41(2)	42(2)	49(2)	48(2)	45(2)	43(2)	44(2)
	U_{22}	48(2)	50(2)	51(2)	55(2)	50(2)	44(2)	50(2)	55(2)
	U_{33}	51(2)	50(2)	46(2)	48(2)	53(2)	45(2)	54(2)	52(3)
	U_{12}	9(1)	8(1)	9(1)	8(1)	7(2)	6(1)	8(1)	11(2)
	U_{eq}	50(1)	47(1)	46(1)	51(1)	50(1)	45(1)	49(1)	50(1)
T(2)	U_{11}	103(2)	61(2)	67(2)	134(2)	140(2)	64(2)	75(2)	97(3)
	U_{22}	52(2)	62(2)	61(2)	64(2)	56(2)	56(2)	54(2)	57(2)
	U_{33}	43(2)	55(2)	53(2)	48(2)	51(2)	50(2)	51(2)	46(3)
	U_{12}	- 7(2)	9(1)	5(1)	- 9(1)	- 15(2)	9(1)	- 4(2)	1(2)
	U_{eq}	66(1)	59(1)	60(1)	82(1)	82(1)	57(1)	60(1)	67(1)
T(3)	U_{11}	39(7)	45(3)	43(3)	42(3)	43(5)	47(3)	38(9)	32(9)
	U_{22}	73(7)	55(3)	57(3)	76(3)	71(5)	55(3)	80(9)	80(10)
	U_{33}	45(8)	54(3)	46(3)	48(3)	49(5)	48(3)	38(9)	37(10)
	U_{eq}	52(5)	51(2)	49(2)	55(2)	54(3)	50(2)	52(6)	50(6)
O(1)	U_{11}	70(5)	58(4)	63(4)	78(4)	78(5)	60(4)	67(5)	54(6)
	U_{22}	61(5)	76(5)	71(4)	77(4)	65(5)	73(4)	66(5)	74(6)
	U_{33}	41(5)	50(5)	45(5)	48(4)	48(6)	45(4)	50(5)	55(7)
	U_{12}	2(4)	2(4)	9(4)	4(3)	- 1(4)	6(3)	10(4)	- 5(5)
	U_{eq}	57(2)	61(2)	60(2)	68(2)	64(2)	59(2)	61(2)	61(3)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 34	K 35	K 36	K 38	K 39	K 40	K 41	K 42
O(2)	U_{11}	66(5)	62(5)	70(4)	68(4)	70(5)	67(4)	57(5)	70(6)
	U_{22}	67(5)	66(5)	59(5)	70(4)	58(5)	55(4)	64(5)	54(6)
	U_{33}	36(5)	52(5)	41(5)	46(4)	48(5)	40(4)	50(5)	36(6)
	U_{12}	- 1(4)	- 2(4)	- 6(4)	- 9(3)	- 8(4)	- 2(3)	- 16(4)	- 7(5)
	U_{eq}	56(2)	60(2)	59(2)	61(2)	58(2)	54(2)	57(2)	53(3)
O(3)	U_{11}	108(6)	71(5)	71(5)	82(4)	94(6)	75(4)	105(6)	118(7)
	U_{22}	61(5)	62(5)	61(5)	70(4)	58(5)	50(4)	56(5)	53(6)
	U_{33}	99(6)	105(5)	109(5)	106(5)	111(6)	104(5)	115(6)	110(7)
	U_{12}	10(4)	12(4)	11(4)	8(3)	10(4)	11(3)	24(4)	24(5)
	U_{eq}	89(3)	79(2)	81(2)	86(2)	88(3)	76(2)	92(3)	94(3)
O(4)	U_{11}	98(4)	98(3)	101(3)	105(3)	106(4)	98(3)	96(4)	104(4)
	U_{22}	89(4)	91(3)	91(3)	97(3)	88(4)	82(3)	93(4)	84(4)
	U_{33}	60(4)	68(4)	61(3)	63(3)	64(4)	60(3)	68(4)	65(5)
	U_{23}	8(3)	2(3)	3(3)	4(2)	3(3)	- 0(3)	4(3)	2(4)
	U_{13}	- 9(3)	- 17(3)	- 16(3)	- 9(3)	- 17(3)	- 16(3)	- 11(3)	- 18(4)
	U_{12}	31(3)	34(3)	40(3)	35(2)	38(3)	36(2)	44(3)	41(4)
	U_{eq}	82(2)	86(2)	84(2)	88(1)	86(2)	80(2)	86(2)	84(2)
O(5)	U_{11}	168(6)	115(5)	119(5)	209(5)	207(7)	117(5)	112(6)	127(7)
	U_{22}	89(6)	162(6)	173(6)	133(5)	110(6)	154(5)	91(5)	92(7)
	U_{33}	97(6)	111(5)	109(5)	100(5)	102(6)	103(5)	100(6)	96(7)
	U_{12}	14(5)	69(5)	60(5)	11(4)	- 0(5)	60(4)	- 10(4)	- 5(6)
	U_{eq}	118(3)	129(2)	134(2)	147(2)	140(3)	125(2)	101(3)	105(3)
O(6)	U_{11}	66(4)	68(3)	62(3)	74(3)	71(4)	68(3)	55(4)	67(4)
	U_{22}	77(4)	96(3)	95(3)	88(3)	81(4)	87(3)	82(4)	84(4)
	U_{33}	68(4)	88(4)	82(4)	82(3)	82(4)	85(3)	74(4)	73(5)
	U_{23}	4(3)	- 13(3)	- 11(3)	- 4(3)	2(3)	- 18(3)	13(3)	3(4)
	U_{13}	- 3(3)	- 9(3)	- 8(3)	- 6(2)	- 6(3)	- 3(3)	- 3(3)	- 2(4)
	U_{12}	6(3)	8(3)	12(3)	9(2)	4(3)	9(2)	5(3)	10(4)
	U_{eq}	70(2)	84(2)	80(2)	81(1)	78(2)	80(2)	70(2)	75(2)
O(7)	U_{11}	115(5)	88(5)	87(5)	147(5)	149(6)	95(5)	70(5)	93(6)
	U_{22}	114(6)	78(5)	80(5)	133(5)	148(6)	62(4)	83(5)	102(7)
	U_{33}	84(6)	96(5)	95(5)	89(5)	83(6)	99(5)	85(6)	82(7)
	U_{12}	- 57(5)	- 20(4)	- 24(4)	- 72(4)	- 75(5)	- 14(3)	- 22(4)	- 42(6)
	U_{eq}	105(3)	87(2)	87(2)	123(2)	126(3)	85(2)	80(2)	92(3)
O(8)	U_{11}	52(5)	61(4)	56(4)	60(4)	57(5)	63(4)	47(5)	55(6)
	U_{22}	59(5)	63(4)	64(4)	63(4)	58(5)	58(4)	61(5)	56(6)
	U_{33}	94(6)	70(5)	71(5)	94(4)	99(6)	68(4)	76(5)	74(7)
	U_{23}	5(4)	5(4)	2(4)	3(3)	6(5)	- 2(4)	10(4)	2(5)
	U_{eq}	68(2)	64(2)	64(2)	72(2)	71(2)	63(2)	61(2)	62(3)
O(9)	U_{11}	55(7)	53(7)	48(6)	57(6)	54(8)	53(6)	45(7)	42(9)
	U_{22}	127(8)	101(7)	104(7)	113(6)	114(9)	92(7)	137(8)	140(10)
	U_{33}	188(10)	210(9)	217(9)	229(8)	232(11)	228(8)	233(10)	216(12)
	U_{eq}	124(4)	121(3)	123(3)	133(3)	133(4)	124(3)	138(4)	132(5)
O(10)	U_{11}	100(9)	105(7)	84(8)	100(6)	81(8)	95(7)	68(8)	95(11)
	U_{22}	207(10)	112(7)	151(9)	122(6)	125(9)	115(7)	127(9)	188(12)
	U_{33}	195(11)	196(9)	160(9)	156(7)	171(10)	180(8)	137(9)	153(13)
	U_{eq}	167(6)	138(3)	132(5)	126(3)	125(4)	130(3)	111(5)	145(7)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 43	K 45	K 46	K 47	K 49	K 50	K 52
X	U_{11}	469(29)	325(14)	537(27)	562(30)	357(11)	464(22)	627(26)
	U_{22}	117(19)	77(10)	117(16)	124(18)	83(8)	88(13)	123(14)
	U_{33}	77(19)	65(11)	110(17)	89(19)	66(8)	90(15)	99(15)
	U_{23}	- 25(13)	- 9(7)	- 18(12)	- 23(14)	- 10(5)	- 20(10)	- 15(10)
	U_{eq}	221(14)	156(7)	255(12)	258(13)	169(6)	214(10)	283(12)
M(1)	U_{11}	125(3)	120(3)	137(3)	129(3)	124(3)	150(3)	125(3)
	U_{22}	99(3)	110(3)	113(3)	116(3)	103(3)	120(3)	102(3)
	U_{33}	89(3)	94(3)	94(3)	95(3)	99(3)	96(3)	91(3)
	U_{12}	21(2)	28(2)	33(2)	34(2)	23(2)	45(2)	20(2)
	U_{eq}	104(2)	108(2)	115(2)	113(2)	109(2)	122(2)	106(2)
M(2)	U_{11}	59(4)	58(4)	62(4)	55(4)	63(4)	65(4)	59(4)
	U_{22}	63(4)	76(4)	68(4)	69(4)	67(4)	69(4)	69(4)
	U_{33}	140(5)	141(5)	128(4)	126(5)	154(4)	128(5)	145(5)
	U_{eq}	87(3)	92(3)	86(3)	83(3)	94(3)	88(3)	91(3)
M(3)	U_{11}	76(2)	67(3)	75(2)	74(2)	75(2)	77(2)	76(2)
	U_{22}	64(2)	67(3)	67(2)	69(2)	64(2)	67(2)	67(2)
	U_{33}	42(2)	41(3)	44(2)	42(2)	41(2)	43(3)	40(2)
	U_{23}	- 5(2)	- 4(2)	- 5(2)	- 7(2)	- 5(2)	- 8(2)	- 6(2)
	U_{eq}	60(1)	58(1)	62(1)	61(1)	60(1)	63(1)	61(1)
M(4)	U_{11}	58(3)	53(3)	60(2)	55(2)	60(3)	58(3)	59(3)
	U_{22}	53(3)	57(3)	60(2)	62(2)	61(3)	61(3)	63(3)
	U_{33}	88(3)	89(3)	97(2)	92(3)	90(3)	93(3)	91(3)
	U_{12}	- 2(2)	- 3(2)	- 1(2)	2(2)	- 3(2)	- 2(2)	- 2(2)
	U_{eq}	66(2)	66(2)	72(1)	69(1)	70(2)	71(2)	71(2)
M(5)	U_{11}	62(2)	52(3)	68(2)	63(2)	63(2)	68(2)	66(2)
	U_{22}	60(2)	66(3)	59(2)	63(2)	63(2)	58(2)	64(2)
	U_{33}	45(2)	46(3)	45(2)	44(3)	47(2)	52(3)	47(2)
	U_{23}	- 5(2)	- 7(2)	- 6(2)	- 7(2)	- 6(2)	- 9(2)	- 7(2)
	U_{eq}	56(1)	55(1)	58(1)	57(1)	58(1)	59(1)	59(1)
T(1)	U_{11}	46(2)	50(2)	49(2)	47(2)	51(2)	49(2)	54(2)
	U_{22}	48(2)	52(2)	50(2)	52(2)	51(2)	50(2)	52(2)
	U_{33}	51(2)	51(2)	49(2)	50(2)	55(2)	50(2)	47(2)
	U_{12}	8(1)	7(2)	7(1)	5(2)	10(1)	8(2)	8(1)
	U_{eq}	49(1)	51(1)	49(1)	50(1)	52(1)	50(1)	51(1)
T(2)	U_{11}	114(3)	100(3)	126(2)	128(2)	119(2)	129(3)	131(2)
	U_{22}	50(3)	61(2)	59(2)	58(2)	56(2)	59(2)	57(2)
	U_{33}	44(3)	45(2)	53(2)	53(2)	53(2)	53(2)	45(2)
	U_{12}	- 3(2)	- 3(2)	- 9(2)	- 8(2)	- 8(2)	- 10(2)	- 10(2)
	U_{eq}	69(1)	69(1)	79(1)	80(1)	76(1)	81(1)	78(1)
T(3)	U_{11}	43(6)	45(8)	48(4)	37(4)	37(6)	46(4)	45(5)
	U_{22}	68(6)	82(8)	75(4)	68(5)	85(6)	69(5)	83(6)
	U_{33}	36(6)	49(8)	54(4)	47(5)	45(6)	45(5)	36(6)
	U_{eq}	49(4)	59(5)	59(3)	50(3)	56(4)	53(3)	55(4)
O(1)	U_{11}	65(5)	61(5)	74(5)	70(5)	78(5)	87(5)	77(5)
	U_{22}	59(5)	74(5)	73(5)	71(5)	65(5)	67(5)	72(5)
	U_{33}	47(5)	40(5)	48(5)	46(5)	51(5)	46(5)	43(5)
	U_{12}	1(4)	4(4)	1(4)	8(4)	5(4)	1(5)	9(4)
	U_{eq}	57(2)	58(2)	65(2)	62(2)	65(2)	67(2)	64(2)

REFINED DISPLACEMENT PARAMETERS

Site	U_{ij}	K 43	K 45	K 46	K 47	K 49	K 50	K 52
O(2)	U_{11}	61(5)	64(6)	60(5)	63(5)	63(5)	63(5)	69(5)
	U_{22}	56(5)	63(6)	64(5)	67(5)	69(5)	59(5)	70(5)
	U_{33}	55(5)	45(6)	51(5)	52(6)	52(5)	56(6)	46(5)
	U_{12}	- 9(4)	- 3(4)	- 4(4)	- 12(4)	- 15(4)	- 8(4)	- 9(4)
	U_{eq}	57(2)	58(3)	59(2)	60(2)	62(2)	59(2)	62(2)
O(3)	U_{11}	92(5)	95(6)	89(5)	76(6)	109(6)	84(6)	104(5)
	U_{22}	55(5)	66(6)	56(5)	64(5)	66(5)	64(6)	69(5)
	U_{33}	109(6)	110(6)	104(5)	103(6)	113(6)	105(6)	100(6)
	U_{12}	15(4)	16(4)	8(4)	11(4)	18(4)	3(4)	16(4)
	U_{eq}	85(2)	90(3)	83(2)	81(3)	96(2)	84(3)	91(2)
O(4)	U_{11}	91(4)	101(4)	101(3)	100(4)	111(4)	103(4)	103(4)
	U_{22}	90(4)	96(4)	89(3)	91(4)	93(4)	88(4)	96(3)
	U_{33}	58(4)	65(4)	61(3)	62(4)	66(4)	68(4)	65(4)
	U_{23}	4(3)	3(3)	3(3)	2(3)	0(3)	1(3)	4(3)
	U_{13}	- 8(3)	- 15(3)	- 9(3)	- 8(3)	- 11(3)	- 14(3)	- 10(3)
	U_{12}	36(3)	39(3)	31(3)	34(3)	41(3)	31(3)	36(3)
	U_{eq}	80(2)	88(2)	84(2)	84(2)	90(2)	86(2)	88(2)
O(5)	U_{11}	181(6)	142(7)	216(6)	219(7)	163(6)	218(7)	208(6)
	U_{22}	87(5)	96(6)	121(5)	123(6)	106(5)	125(6)	105(5)
	U_{33}	94(5)	104(6)	104(5)	103(6)	101(5)	95(6)	94(6)
	U_{12}	1(5)	- 3(5)	28(5)	16(6)	- 15(5)	16(6)	- 7(5)
	U_{eq}	121(3)	114(3)	147(3)	148(3)	123(2)	146(3)	136(3)
O(6)	U_{11}	66(3)	64(4)	70(3)	69(4)	65(4)	68(4)	70(3)
	U_{22}	80(4)	82(4)	88(3)	86(4)	81(4)	82(4)	86(4)
	U_{33}	73(4)	76(4)	82(4)	82(4)	78(4)	85(4)	80(4)
	U_{23}	4(3)	3(3)	1(3)	- 6(3)	9(3)	- 2(3)	4(3)
	U_{13}	- 3(3)	- 4(3)	- 2(3)	- 4(3)	- 1(3)	- 5(3)	- 6(3)
	U_{12}	8(3)	1(3)	6(3)	3(3)	5(3)	5(3)	3(3)
	U_{eq}	73(2)	74(2)	80(2)	79(2)	75(2)	78(2)	79(2)
O(7)	U_{11}	132(6)	95(6)	160(6)	159(7)	120(5)	160(7)	137(6)
	U_{22}	122(6)	111(6)	144(6)	144(6)	123(5)	139(6)	146(6)
	U_{33}	81(6)	88(6)	88(5)	90(6)	80(5)	83(6)	81(6)
	U_{12}	- 68(5)	- 37(5)	- 85(4)	- 86(5)	- 58(5)	- 79(5)	- 78(5)
	U_{eq}	111(3)	98(3)	130(3)	131(3)	108(2)	127(3)	122(3)
O(8)	U_{11}	48(5)	58(5)	55(4)	48(5)	53(5)	56(5)	61(5)
	U_{22}	59(4)	57(5)	56(4)	59(5)	61(4)	55(5)	64(4)
	U_{33}	88(5)	83(6)	108(5)	107(6)	96(5)	100(6)	104(5)
	U_{23}	5(4)	9(4)	5(4)	0(5)	11(4)	5(5)	3(4)
	U_{eq}	65(2)	66(2)	73(2)	71(2)	70(2)	70(2)	76(2)
O(9)	U_{11}	46(7)	48(8)	53(7)	46(8)	56(7)	59(8)	66(7)
	U_{22}	129(8)	137(9)	109(7)	111(8)	118(8)	111(9)	124(8)
	U_{33}	222(9)	205(10)	222(9)	227(10)	238(9)	232(11)	232(9)
	U_{eq}	132(4)	130(4)	128(3)	128(4)	137(4)	134(4)	140(4)
O(10)	U_{11}	88(8)	84(9)	87(7)	83(8)	86(8)	95(9)	82(7)
	U_{22}	118(8)	148(10)	131(7)	120(8)	139(9)	126(9)	124(8)
	U_{33}	153(9)	164(11)	152(8)	164(10)	140(9)	187(10)	148(8)
	U_{eq}	119(4)	132(6)	123(3)	122(4)	122(5)	136(4)	118(3)

APPENDIX E

SREF SCATTERING FACTOR ASSIGNMENT

Abbreviations used in APPENDIX E

✓: only X-site vacancies are considered
R: refining occupancy factor
F: fixed occupancy factor
AR: alternatively refined occupancy factors
EX: minor site occupant excluded in refinements

SREF SCATTERING FACTOR ASSIGNMENT

Site	□	B	O^{2-}	F^-	Na	Mg	Al	Si	Ca	Ti	V	Cr	Fe
X	✓				F	AR			F				AR
M(1)						R							R
M(2)						R	EX						R
M(3)						EX	F						
M(4)						R	F			F	F	F	R
M(5)						EX	F						
T(1)							F	F					
T(2)							F	F					
T(3)		R					F	R					
O(10)			R	R									

APPENDIX F

SITE SCATTERING & SITE POPULATIONS

Abbreviations used in APPENDIX F

Site-scattering values as (*epfu*); e.s.d are ~0.1 electrons
Site populations as (*apfu*)
*Fe = (Fe^{2+} + Mn^{2+})

SITE SCATTERING & SITE POPULATIONS

	K1	K2	K3	K5	K6	K7	K8	K9	K10	K11
X {*epfu*} [Mg]	5.25	4.99	4.45	5.01	6.11	5.81	7.54	6.18	6.14	4.26
X {*epfu*} [Fe]	5.10	4.81	4.31	4.84	5.91	5.62	7.23	5.96	5.90	4.14
Mg	0.142	0.217	0.091	0.130	0.117	0.207	0.107	0.131	0.103	0.071
*Fe	0.147	0.080	0.124	0.134	0.165	0.099	0.218	0.189	0.186	0.132
Na	0.010	0.000	0.025	0.010	0.010	0.000	0.000	0.012	0.000	0.012
Ca	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
□	0.701	0.703	0.760	0.726	0.708	0.694	0.675	0.668	0.711	0.785
M(1) {*epfu*}	26.80	25.68	31.62	26.97	31.11	25.90	30.44	26.58	30.38	33.91
Mg	1.800	1.880	1.456	1.788	1.492	1.864	1.540	1.816	1.544	1.292
Fe	0.200	0.120	0.544	0.212	0.508	0.136	0.460	0.184	0.456	0.708
M(2) {*epfu*}	12.83	12.57	16.05	13.33	15.37	12.87	14.13	13.20	14.36	18.61
Mg	0.810	0.843	0.639	0.828	0.662	0.848	0.731	0.857	0.742	0.448
Al	0.141	0.125	0.077	0.083	0.105	0.097	0.126	0.062	0.096	0.086
Fe	0.049	0.032	0.284	0.089	0.233	0.055	0.143	0.081	0.162	0.466
M(3) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.926	1.932	1.984	1.974	1.960	1.958	1.944	1.972	1.952	1.986
Mg	0.074	0.068	0.016	0.026	0.040	0.042	0.056	0.028	0.048	0.014
M(4) {*epfu*}	26.63	26.62	27.68	25.68	27.88	26.12	28.36	26.27	27.59	25.98
Al	1.562	1.504	1.664	1.626	1.474	1.444	1.396	1.484	1.458	1.780
Mg	0.358	0.416	0.192	0.370	0.354	0.508	0.392	0.460	0.386	0.200
Fe	0.068	0.080	0.144	0.004	0.172	0.048	0.212	0.056	0.144	0.000
Ti	0.012	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.012	0.020
Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
V	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
M(5) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.970	1.974	1.974	1.984	1.972	1.968	1.976	1.972	1.974	1.964
Mg	0.030	0.026	0.026	0.016	0.028	0.032	0.024	0.028	0.026	0.036
T(1) {*epfu*}	27.89	27.90	27.98	27.97	27.97	27.98	27.92	27.99	27.94	27.99
Si	1.888	1.900	1.982	1.966	1.970	1.976	1.922	1.994	1.942	1.994
Al	0.112	0.100	0.018	0.034	0.030	0.024	0.078	0.006	0.058	0.006
T(2) {*epfu*}	27.44	27.55	27.63	27.67	27.60	27.75	27.43	27.73	27.63	27.67
Si	1.442	1.546	1.628	1.674	1.600	1.746	1.428	1.732	1.634	1.670
Al	0.558	0.454	0.372	0.326	0.400	0.254	0.572	0.268	0.366	0.330
T(3) {*epfu*}	10.17	9.25	6.53	7.17	7.29	7.13	8.92	6.33	7.60	6.18
Si	0.402	0.343	0.094	0.155	0.177	0.148	0.340	0.084	0.204	0.057
Al	0.194	0.145	0.086	0.097	0.087	0.100	0.108	0.072	0.096	0.083
B	0.404	0.512	0.820	0.748	0.736	0.752	0.552	0.844	0.700	0.860
O(10) {*epfu*}	8.00	8.00	8.28	8.08	8.20	8.08	8.00	8.08	8.04	8.32
O	1.00	1.00	0.72	0.92	0.80	0.92	1.00	0.92	0.96	0.68
F	0.00	0.00	0.28	0.08	0.20	0.08	0.00	0.08	0.04	0.32

SITE SCATTERING & SITE POPULATIONS

	K 12	K 13	K 14	K 15	K 16	K 17	K 18	K 19	K 20	K 21
X {*epfu*} [Mg]	4.68	4.85	3.89	6.78	3.65	5.79	5.62	3.84	3.31	5.38
X {*epfu*} [Fe]	4.51	4.68	3.74	6.54	3.54	5.60	5.43	3.73	3.18	5.20
Mg	0.283	0.314	0.120	0.113	0.083	0.113	0.151	0.119	0.104	0.105
*Fe	0.046	0.016	0.098	0.216	0.109	0.165	0.142	0.075	0.064	0.152
Na	0.000	0.000	0.000	0.027	0.000	0.029	0.000	0.022	0.017	0.000
Ca	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
□	0.660	0.670	0.782	0.644	0.808	0.693	0.707	0.784	0.815	0.743
M(1) {*epfu*}	24.73	24.56	31.67	29.43	33.74	30.16	28.82	28.42	31.28	30.05
Mg	1.948	1.960	1.452	1.612	1.304	1.560	1.656	1.684	1.480	1.568
Fe	0.052	0.040	0.548	0.388	0.696	0.440	0.344	0.316	0.520	0.432
M(2) {*epfu*}	12.34	12.35	14.97	14.46	16.11	14.51	13.69	14.70	16.28	13.59
Mg	0.828	0.907	0.699	0.723	0.647	0.727	0.791	0.742	0.624	0.751
Al	0.159	0.073	0.096	0.109	0.064	0.101	0.095	0.070	0.076	0.146
Fe	0.013	0.020	0.205	0.168	0.289	0.172	0.114	0.188	0.300	0.103
M(3) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.910	1.968	1.978	1.930	1.988	1.954	1.960	1.980	1.990	1.920
Mg	0.090	0.032	0.022	0.070	0.012	0.046	0.040	0.020	0.010	0.080
M(4) {*epfu*}	26.03	25.56	27.89	30.15	26.68	29.86	27.92	26.41	26.32	27.94
Al	1.578	1.446	1.532	1.142	1.720	1.266	1.404	1.674	1.756	1.540
Mg	0.390	0.546	0.296	0.496	0.206	0.406	0.416	0.264	0.194	0.284
Fe	0.032	0.008	0.160	0.348	0.056	0.328	0.180	0.020	0.008	0.160
Ti	0.000	0.000	0.012	0.014	0.018	0.000	0.000	0.018	0.020	0.016
Cr	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.014	0.012	0.000
V	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.010	0.010	0.000
M(5) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.964	1.968	1.988	1.972	1.988	1.976	1.972	1.980	1.980	1.974
Mg	0.036	0.032	0.012	0.028	0.012	0.024	0.028	0.020	0.020	0.026
T(1) {*epfu*}	27.87	27.99	27.98	27.93	28.00	27.96	27.95	27.99	28.00	27.89
Si	1.872	1.990	1.978	1.928	2.000	1.960	1.954	1.994	2.000	1.894
Al	0.128	0.010	0.022	0.072	0.000	0.040	0.046	0.006	0.000	0.106
T(2) {*epfu*}	27.32	27.79	27.64	27.67	27.70	27.67	27.68	27.73	27.71	27.40
Si	1.318	1.790	1.638	1.666	1.696	1.668	1.678	1.734	1.712	1.402
Al	0.682	0.210	0.362	0.334	0.304	0.332	0.322	0.266	0.288	0.598
T(3) {*epfu*}	11.11	6.35	7.12	7.49	6.19	7.01	7.06	6.33	6.11	10.44
Si	0.481	0.103	0.165	0.186	0.068	0.152	0.170	0.085	0.058	0.416
Al	0.223	0.053	0.079	0.102	0.072	0.080	0.066	0.071	0.074	0.212
B	0.296	0.844	0.756	0.712	0.860	0.768	0.764	0.844	0.868	0.372
O(10) {*epfu*}	8.00	8.12	8.08	8.24	8.16	8.16	8.04	8.36	8.32	8.16
O	1.00	0.88	0.92	0.76	0.84	0.84	0.96	0.64	0.68	0.84
F	0.00	0.12	0.08	0.24	0.16	0.16	0.04	0.36	0.32	0.16

SITE SCATTERING & SITE POPULATIONS

	K22	K23	K24	K25	K26	K27	K28	K29	K30	K31
X {*epfu*} [Mg]	4.13	3.22	3.74	5.97	7.10	6.05	6.29	6.28	3.70	3.89
X {*epfu*} [Fe]	3.98	3.12	3.61	5.78	6.84	5.82	6.06	6.06	3.57	3.74
Mg	0.246	0.282	0.117	0.095	0.073	0.131	0.184	0.091	0.292	0.284
*Fe	0.050	0.000	0.063	0.177	0.231	0.177	0.130	0.182	0.008	0.022
Na	0.000	0.000	0.026	0.015	0.017	0.000	0.000	0.017	0.000	0.000
Ca	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.012	0.000
□	0.704	0.718	0.794	0.713	0.679	0.692	0.686	0.710	0.688	0.694
M(1) {*epfu*}	24.84	24.45	28.65	29.94	29.71	28.48	26.35	30.55	24.22	24.56
Mg	1.940	1.968	1.668	1.576	1.592	1.680	1.832	1.532	1.984	1.960
Fe	0.060	0.032	0.332	0.424	0.408	0.320	0.168	0.468	0.016	0.040
M(2) {*epfu*}	12.33	12.20	14.91	15.42	14.46	13.55	13.01	14.91	12.18	12.22
Mg	0.851	0.902	0.715	0.674	0.712	0.806	0.848	0.707	0.824	0.854
Al	0.135	0.090	0.083	0.088	0.121	0.090	0.086	0.092	0.176	0.140
Fe	0.014	0.008	0.202	0.238	0.167	0.104	0.066	0.201	0.000	0.006
M(3) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.914	1.966	1.966	1.980	1.926	1.970	1.966	1.964	1.884	1.910
Mg	0.086	0.034	0.034	0.020	0.074	0.030	0.034	0.036	0.116	0.090
M(4) {*epfu*}	25.73	25.97	26.20	28.46	28.72	27.47	26.40	26.79	25.67	25.77
Al	1.622	1.588	1.700	1.366	1.386	1.402	1.444	1.610	1.672	1.716
Mg	0.370	0.376	0.254	0.408	0.370	0.450	0.488	0.306	0.328	0.280
Fe	0.008	0.000	0.000	0.208	0.224	0.148	0.068	0.084	0.000	0.004
Ti	0.000	0.016	0.020	0.018	0.020	0.000	0.000	0.000	0.000	0.000
Cr	0.000	0.000	0.014	0.000	0.000	0.000	0.000	0.000	0.000	0.000
V	0.000	0.020	0.012	0.000	0.000	0.000	0.000	0.000	0.000	0.000
M(5) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.968	1.976	1.978	1.970	1.968	1.970	1.976	1.974	1.928	1.974
Mg	0.032	0.024	0.022	0.030	0.032	0.030	0.024	0.026	0.072	0.026
T(1) {*epfu*}	27.90	27.97	27.99	27.99	27.93	27.96	27.96	27.94	27.85	27.89
Si	1.896	1.966	1.990	1.986	1.932	1.962	1.964	1.938	1.846	1.888
Al	0.104	0.034	0.010	0.014	0.068	0.038	0.036	0.062	0.154	0.112
T(2) {*epfu*}	27.51	27.69	27.74	27.72	27.45	27.68	27.70	27.51	27.28	27.33
Si	1.512	1.688	1.744	1.724	1.454	1.684	1.702	1.508	1.276	1.334
Al	0.488	0.312	0.256	0.276	0.546	0.316	0.298	0.492	0.724	0.666
T(3) {*epfu*}	10.00	7.34	6.63	6.30	9.23	7.08	7.08	8.15	12.69	10.87
Si	0.361	0.167	0.096	0.082	0.329	0.155	0.157	0.268	0.589	0.429
Al	0.219	0.105	0.096	0.070	0.159	0.085	0.083	0.092	0.299	0.251
B	0.420	0.728	0.808	0.848	0.512	0.760	0.760	0.640	0.112	0.320
O(10) {*epfu*}	8.00	8.08	8.36	8.32	8.16	8.04	8.12	8.12	8.00	8.00
O	1.00	0.92	0.64	0.68	0.84	0.96	0.88	0.88	1.00	1.00
F	0.00	0.08	0.36	0.32	0.16	0.04	0.12	0.12	0.00	0.00

SITE SCATTERING & SITE POPULATIONS

	K 32	K 33	K 34	K 35	K 36	K 38	K 39	K 40	K 41	K 42
X {*epfu*} [Mg]	5.57	5.34	4.17	5.79	6.67	5.28	4.90	4.22	5.71	5.95
X {*epfu*} [Fe]	5.38	5.19	4.04	5.58	6.45	5.10	4.71	4.06	5.54	5.73
Mg	0.272	0.117	0.123	0.184	0.163	0.250	0.245	0.309	0.352	0.143
*Fe	0.076	0.136	0.079	0.142	0.199	0.100	0.095	0.029	0.039	0.133
Na	0.000	0.032	0.034	0.000	0.000	0.000	0.000	0.000	0.000	0.017
Ca	0.000	0.000	0.000	0.011	0.000	0.000	0.000	0.012	0.012	0.000
□	0.652	0.715	0.764	0.663	0.638	0.650	0.660	0.650	0.597	0.707
M(1) {*epfu*}	25.85	28.98	27.64	25.62	25.34	24.90	25.01	24.17	24.78	29.49
Mg	1.868	1.644	1.740	1.884	1.904	1.936	1.928	1.988	1.944	1.608
Fe	0.132	0.356	0.260	0.116	0.096	0.064	0.072	0.012	0.056	0.392
M(2) {*epfu*}	12.75	15.31	14.49	12.54	12.57	12.40	12.40	12.30	12.38	14.85
Mg	0.872	0.670	0.735	0.786	0.798	0.832	0.850	0.817	0.909	0.723
Al	0.080	0.101	0.094	0.189	0.174	0.150	0.131	0.174	0.069	0.079
Fe	0.048	0.229	0.171	0.025	0.028	0.018	0.019	0.009	0.022	0.198
M(3) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.960	1.960	1.960	1.888	1.892	1.900	1.928	1.898	1.968	1.974
Mg	0.040	0.040	0.040	0.112	0.108	0.100	0.072	0.102	0.032	0.026
M(4) {*epfu*}	25.72	27.74	26.24	26.58	27.68	26.70	26.21	26.00	25.94	26.18
Al	1.500	1.592	1.628	1.678	1.542	1.522	1.518	1.714	1.326	1.604
Mg	0.484	0.248	0.316	0.254	0.302	0.390	0.430	0.262	0.630	0.344
Fe	0.016	0.136	0.000	0.056	0.144	0.060	0.036	0.012	0.044	0.012
Ti	0.000	0.024	0.020	0.012	0.012	0.000	0.000	0.012	0.000	0.028
Cr	0.000	0.000	0.020	0.000	0.000	0.028	0.016	0.000	0.000	0.000
V	0.000	0.000	0.016	0.000	0.000	0.000	0.000	0.000	0.000	0.012
M(5) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.960	1.982	1.970	1.920	1.924	1.964	1.960	1.932	1.946	1.964
Mg	0.040	0.018	0.030	0.080	0.076	0.036	0.040	0.068	0.054	0.036
T(1) {*epfu*}	27.95	27.94	27.98	27.80	27.82	27.88	27.90	27.82	27.97	27.98
Si	1.952	1.936	1.980	1.800	1.822	1.878	1.900	1.816	1.968	1.976
Al	0.048	0.064	0.020	0.200	0.178	0.122	0.100	0.184	0.032	0.024
T(2) {*epfu*}	27.74	27.51	27.73	27.08	27.02	27.31	27.48	27.02	27.80	27.67
Si	1.736	1.506	1.734	1.078	1.022	1.308	1.484	1.016	1.798	1.668
Al	0.264	0.494	0.266	0.922	0.978	0.692	0.516	0.984	0.202	0.332
T(3) {*epfu*}	6.63	8.00	7.01	13.54	13.38	10.96	9.49	13.58	6.03	6.66
Si	0.096	0.217	0.119	0.703	0.727	0.489	0.358	0.712	0.065	0.090
Al	0.096	0.131	0.117	0.277	0.229	0.195	0.158	0.272	0.055	0.106
B	0.808	0.652	0.764	0.020	0.044	0.316	0.484	0.016	0.880	0.804
O(10) {*epfu*}	8.00	8.48	8.44	8.00	8.04	8.00	8.00	8.00	8.04	8.24
O	1.00	0.52	0.56	1.00	0.96	1.00	1.00	1.00	0.96	0.76
F	0.00	0.48	0.44	0.00	0.04	0.00	0.00	0.00	0.04	0.24

SITE SCATTERING & SITE POPULATIONS

	K 43	K 45	K 46	K 47	K 49	K 50	K 52
X {*epfu*} [Mg]	3.02	5.73	3.61	3.56	6.58	4.22	4.03
X {*epfu*} [Fe]	2.89	5.51	3.48	3.45	6.37	4.06	3.87
Mg	0.281	0.210	0.340	0.343	0.276	0.279	0.393
*Fe	0.000	0.093	0.000	0.000	0.111	0.029	0.000
Na	0.010	0.019	0.000	0.000	0.000	0.000	0.000
Ca	0.000	0.000	0.010	0.010	0.000	0.000	0.000
□	0.719	0.678	0.650	0.647	0.613	0.692	0.607
M(1) {*epfu*}	24.50	26.46	24.28	24.34	25.90	24.84	24.22
Mg	1.964	1.824	1.980	1.976	1.864	1.940	1.984
Fe	0.036	0.176	0.020	0.024	0.136	0.060	0.016
M(2) {*epfu*}	12.20	13.20	12.27	12.26	12.95	12.43	12.23
Mg	0.890	0.840	0.835	0.841	0.854	0.831	0.872
Al	0.103	0.080	0.157	0.151	0.084	0.149	0.120
Fe	0.007	0.080	0.008	0.008	0.062	0.020	0.008
M(3) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.958	1.966	1.904	1.904	1.950	1.904	1.946
Mg	0.042	0.034	0.096	0.096	0.050	0.096	0.054
M(4) {*epfu*}	25.85	25.88	26.03	25.98	26.38	25.91	25.62
Al	1.636	1.546	1.574	1.576	1.428	1.630	1.454
Mg	0.344	0.430	0.386	0.388	0.504	0.350	0.534
Fe	0.004	0.024	0.000	0.000	0.068	0.020	0.012
Ti	0.016	0.000	0.014	0.012	0.000	0.000	0.000
Cr	0.000	0.000	0.026	0.024	0.000	0.000	0.000
V	0.000	0.000	0.000	0.000	0.000	0.000	0.000
M(5) {*epfu*}	26.00	26.00	26.00	26.00	26.00	26.00	26.00
Al	1.980	1.966	1.958	1.958	1.972	1.968	1.978
Mg	0.020	0.034	0.042	0.042	0.028	0.032	0.022
T(1) {*epfu*}	27.94	27.94	27.85	27.88	27.93	27.87	27.89
Si	1.938	1.944	1.854	1.876	1.926	1.872	1.892
Al	0.062	0.056	0.146	0.124	0.074	0.128	0.108
T(2) {*epfu*}	27.63	27.73	27.44	27.46	27.63	27.44	27.63
Si	1.630	1.728	1.440	1.460	1.632	1.442	1.630
Al	0.370	0.272	0.560	0.540	0.368	0.558	0.370
T(3) {*epfu*}	7.92	6.92	10.83	10.51	7.57	10.68	8.43
Si	0.200	0.125	0.426	0.393	0.172	0.395	0.229
Al	0.140	0.099	0.250	0.247	0.128	0.265	0.171
B	0.660	0.776	0.324	0.360	0.700	0.340	0.600
O(10) {*epfu*}	8.00	8.12	8.00	8.00	8.08	8.00	8.00
O	1.00	0.88	1.00	1.00	0.92	1.00	1.00
F	0.00	0.12	0.00	0.00	0.08	0.00	0.00

APPENDIX G.1

THE COORDINATION POLYHEDRA

Abbreviations used in APPENDIX G.1

symmetry operators :

a: x, -y, -z	b: -x, -y, -z	c: -x, y, z	d: x-½, y-½, z
e: -x+½, -y+½, -z	f: x, y, -z+½	g: -x+1, y, -z+½	h: x, -y, z-½
i: -x+1, -y, -z	j: -x+½, -y+½, z+½	k: -x, y, -z+½	

THE COORDINATION POLYHEDRA

Eight-coordinate site

X - O(4),a,b,c (x4)
X - O(9)d,e (x2)
X - O(10),b (x2)

Octahedral sites

M(1) - O(1)
M(1) - O(4),f (x2)
M(1) - O(5)
M(1) - O(7)
M(1) - O(10)

M(2) - O(2),g (x2)
M(2) - O(3),g (x2)
M(2) - O(8),f (x2)

M(3) - O(1),h (x2)
M(3) - O(4),a (x2)
M(3) - O(6),a (x2)

M(4) - O(1)
M(4) - O(2)
M(4) - O(3)
M(4) - O(5)
M(4) - O(6),f (x2)

M(5) - O(2),h (x2)
M(5) - O(6),a (x2)
M(5) - O(8),i (x2)

Tetrahedral sites

T(1) - O(3)
T(1) - O(4)e,j (x2)
T(1) - O(9)

T(2) - O(5)
T(2) - O(6)e,j (x2)
T(2) - O(7)

T(3) - O(7),k (x2)
T(3) - O(8)e,j (x2)

APPENDIX G.2

POLYHEDRAL BOND LENGTHS

Abbreviations used in APPENDIX G.2

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e.s.d. are ≤ 0.002 Å for individual distances

POLYHEDRAL BOND LENGTHS

	K1	K2	K3	K5	K6	K7	K8	K9	K10	K11
X-O(4)	2.641	2.635	2.633	2.623	2.625	2.618	2.634	2.617	2.633	2.628
-O(9)	2.311	2.304	2.330	2.315	2.314	2.297	2.310	2.304	2.311	2.340
-O(10)	2.069	2.068	2.080	2.068	2.075	2.076	2.072	2.076	2.068	2.070
<X-O>	2.416	2.411	2.419	2.407	2.410	2.402	2.413	2.404	2.411	2.417
M(1)-O(1)	2.118	2.123	2.159	2.143	2.141	2.132	2.127	2.141	2.139	2.165
-O(4)	2.119	2.116	2.117	2.114	2.122	2.113	2.125	2.115	2.120	2.119
-O(5)	2.259	2.231	2.230	2.220	2.217	2.199	2.224	2.190	2.227	2.235
-O(7)	2.057	2.069	2.115	2.099	2.108	2.098	2.088	2.105	2.107	2.127
-O(10)	2.044	2.050	1.980	2.009	2.017	2.027	2.044	2.017	2.021	1.975
<M(1)-O>	2.119	2.118	2.120	2.117	2.121	2.114	2.122	2.114	2.122	2.123
M(2)-O(2)	2.078	2.074	2.091	2.076	2.081	2.067	2.076	2.068	2.078	2.103
-O(3)	1.993	1.992	2.002	1.995	1.997	1.992	1.993	1.994	1.994	2.008
-O(8)	2.192	2.201	2.247	2.230	2.237	2.224	2.221	2.243	2.231	2.256
<M(2)-O>	2.088	2.089	2.113	2.101	2.105	2.094	2.097	2.102	2.101	2.122
M(3)-O(1)	1.797	1.795	1.793	1.793	1.796	1.792	1.797	1.792	1.795	1.794
-O(4)	1.872	1.871	1.857	1.863	1.866	1.867	1.876	1.864	1.867	1.855
-O(6)	2.111	2.113	2.117	2.113	2.109	2.110	2.105	2.107	2.111	2.116
<M(3)-O>	1.927	1.926	1.922	1.923	1.924	1.923	1.926	1.922	1.924	1.922
M(4)-O(1)	1.934	1.935	1.909	1.916	1.928	1.931	1.939	1.924	1.928	1.893
-O(2)	1.933	1.937	1.925	1.928	1.936	1.937	1.945	1.932	1.937	1.917
-O(3)	1.895	1.897	1.865	1.878	1.885	1.891	1.901	1.885	1.886	1.857
-O(5)	1.808	1.823	1.825	1.832	1.833	1.844	1.824	1.846	1.833	1.825
-O(6)	2.085	2.088	2.082	2.087	2.093	2.095	2.093	2.095	2.094	2.083
<M(4)-O>	1.957	1.961	1.948	1.955	1.961	1.966	1.966	1.963	1.962	1.943
M(5)-O(2)	1.799	1.797	1.801	1.798	1.803	1.798	1.801	1.800	1.801	1.802
-O(6)	1.991	1.994	2.004	2.003	1.999	2.002	1.988	2.004	1.998	2.009
-O(8)	1.949	1.946	1.933	1.935	1.937	1.936	1.949	1.932	1.938	1.930
<M(5)-O>	1.913	1.912	1.913	1.912	1.913	1.912	1.913	1.912	1.912	1.914
T(1)-O(3)	1.621	1.623	1.624	1.620	1.620	1.617	1.619	1.615	1.622	1.624
-O(4)	1.619	1.619	1.613	1.613	1.616	1.613	1.617	1.614	1.616	1.612
-O(9)	1.639	1.637	1.624	1.629	1.633	1.632	1.640	1.630	1.634	1.622
<T(1)-O>	1.625	1.625	1.619	1.619	1.621	1.619	1.623	1.618	1.622	1.618
T(2)-O(5)	1.609	1.608	1.609	1.603	1.609	1.599	1.617	1.600	1.608	1.605
-O(6)	1.685	1.677	1.672	1.667	1.674	1.662	1.682	1.664	1.672	1.668
-O(7)	1.695	1.689	1.676	1.676	1.681	1.671	1.695	1.672	1.678	1.673
<T(2)-O>	1.669	1.663	1.657	1.653	1.660	1.649	1.670	1.650	1.657	1.654
T(3)-O(7)	1.560	1.537	1.484	1.492	1.491	1.494	1.522	1.481	1.499	1.479
-O(8)	1.627	1.608	1.552	1.564	1.573	1.563	1.599	1.542	1.576	1.542
<T(3)-O>	1.594	1.573	1.518	1.528	1.533	1.529	1.561	1.512	1.538	1.511

POLYHEDRAL BOND LENGTHS

	K12	K13	K14	K15	K16	K17	K18	K19	K20	K21
X-O(4)	2.635	2.609	2.635	2.633	2.635	2.635	2.631	2.627	2.631	2.648
-O(9)	2.308	2.293	2.321	2.294	2.330	2.301	2.301	2.322	2.335	2.314
-O(10)	2.067	2.065	2.060	2.095	2.059	2.086	2.070	2.082	2.065	2.069
<X-O>	2.411	2.394	2.413	2.414	2.415	2.414	2.408	2.415	2.416	2.420
M(1)-O(1)	2.104	2.134	2.151	2.137	2.160	2.142	2.140	2.155	2.163	2.120
-O(4)	2.119	2.111	2.123	2.120	2.120	2.119	2.118	2.112	2.118	2.124
-O(5)	2.249	2.175	2.232	2.214	2.237	2.216	2.212	2.221	2.233	2.286
-O(7)	2.033	2.099	2.114	2.107	2.127	2.113	2.106	2.109	2.120	2.059
-O(10)	2.078	2.041	2.004	2.021	1.980	2.011	2.024	1.980	1.976	2.035
<M(1)-O>	2.117	2.112	2.125	2.120	2.124	2.120	2.120	2.115	2.121	2.124
M(2)-O(2)	2.077	2.062	2.081	2.073	2.089	2.075	2.072	2.082	2.091	2.085
-O(3)	1.991	1.994	1.999	1.992	1.999	1.996	1.994	1.997	2.003	1.994
-O(8)	2.178	2.232	2.239	2.231	2.253	2.237	2.234	2.244	2.251	2.193
<M(2)-O>	2.082	2.096	2.106	2.099	2.114	2.103	2.100	2.108	2.115	2.091
M(3)-O(1)	1.797	1.791	1.796	1.794	1.796	1.794	1.794	1.793	1.795	1.799
-O(4)	1.882	1.870	1.859	1.868	1.850	1.865	1.865	1.854	1.853	1.871
-O(6)	2.106	2.106	2.115	2.116	2.116	2.115	2.112	2.119	2.119	2.113
<M(3)-O>	1.928	1.922	1.923	1.926	1.921	1.925	1.924	1.922	1.922	1.928
M(4)-O(1)	1.942	1.929	1.918	1.949	1.897	1.941	1.931	1.907	1.894	1.937
-O(2)	1.931	1.938	1.934	1.959	1.918	1.950	1.942	1.923	1.919	1.934
-O(3)	1.904	1.890	1.877	1.908	1.857	1.896	1.889	1.865	1.857	1.893
-O(5)	1.801	1.852	1.830	1.850	1.827	1.846	1.841	1.831	1.825	1.799
-O(6)	2.081	2.095	2.091	2.105	2.085	2.099	2.097	2.085	2.083	2.086
<M(4)-O>	1.957	1.967	1.957	1.979	1.945	1.972	1.966	1.949	1.944	1.956
M(5)-O(2)	1.798	1.798	1.802	1.800	1.803	1.801	1.800	1.800	1.802	1.800
-O(6)	1.985	2.005	2.000	1.998	2.003	2.000	2.000	2.006	2.007	1.989
-O(8)	1.957	1.934	1.935	1.939	1.928	1.938	1.938	1.931	1.931	1.951
<M(5)-O>	1.913	1.912	1.912	1.912	1.911	1.913	1.913	1.912	1.913	1.913
T(1)-O(3)	1.624	1.616	1.619	1.617	1.622	1.620	1.619	1.622	1.624	1.624
-O(4)	1.620	1.614	1.616	1.617	1.613	1.616	1.616	1.615	1.612	1.619
-O(9)	1.643	1.634	1.630	1.635	1.624	1.632	1.635	1.622	1.622	1.640
<T(1)-O>	1.627	1.620	1.620	1.622	1.618	1.621	1.622	1.619	1.618	1.626
T(2)-O(5)	1.615	1.599	1.607	1.604	1.603	1.605	1.606	1.600	1.606	1.615
-O(6)	1.695	1.659	1.672	1.668	1.669	1.668	1.666	1.666	1.668	1.689
-O(7)	1.705	1.671	1.676	1.677	1.670	1.677	1.678	1.673	1.671	1.698
<T(2)-O>	1.678	1.648	1.657	1.654	1.653	1.655	1.655	1.651	1.653	1.673
T(3)-O(7)	1.589	1.483	1.490	1.497	1.478	1.488	1.489	1.481	1.480	1.573
-O(8)	1.643	1.543	1.567	1.572	1.543	1.564	1.563	1.546	1.543	1.634
<T(3)-O>	1.616	1.513	1.528	1.535	1.511	1.526	1.526	1.514	1.512	1.604

POLYHEDRAL BOND LENGTHS

	K22	K23	K24	K25	K26	K27	K28	K29	K30	K31
X-O(4)	2.637	2.624	2.630	2.624	2.633	2.627	2.620	2.627	2.642	2.635
-O(9)	2.309	2.308	2.326	2.308	2.311	2.302	2.301	2.321	2.313	2.314
-O(10)	2.064	2.061	2.087	2.093	2.089	2.070	2.074	2.070	2.068	2.062
<X-O>	2.412	2.404	2.418	2.412	2.417	2.407	2.404	2.411	2.416	2.412
M(1)-O(1)	2.118	2.139	2.155	2.147	2.124	2.137	2.136	2.139	2.095	2.109
-O(4)	2.115	2.113	2.112	2.117	2.123	2.118	2.117	2.120	2.117	2.116
-O(5)	2.260	2.208	2.237	2.204	2.237	2.205	2.197	2.227	2.292	2.257
-O(7)	2.049	2.086	2.108	2.118	2.075	2.105	2.099	2.094	2.007	2.027
-O(10)	2.050	2.027	1.973	2.000	2.034	2.027	2.030	2.019	2.081	2.061
<M(1)-O>	2.118	2.114	2.116	2.117	2.119	2.118	2.116	2.120	2.118	2.114
M(2)-O(2)	2.076	2.069	2.087	2.080	2.082	2.071	2.067	2.084	2.082	2.077
-O(3)	1.992	1.993	1.997	1.996	1.994	1.994	1.994	1.998	1.994	1.990
-O(8)	2.186	2.221	2.239	2.248	2.211	2.234	2.231	2.230	2.153	2.177
<M(2)-O>	2.085	2.094	2.108	2.108	2.096	2.100	2.098	2.104	2.076	2.081
M(3)-O(1)	1.797	1.793	1.795	1.793	1.796	1.794	1.793	1.795	1.798	1.796
-O(4)	1.869	1.862	1.855	1.862	1.873	1.867	1.869	1.867	1.881	1.874
-O(6)	2.115	2.115	2.121	2.112	2.108	2.110	2.108	2.106	2.109	2.106
<M(3)-O>	1.927	1.923	1.924	1.922	1.926	1.923	1.923	1.923	1.929	1.926
M(4)-O(1)	1.928	1.919	1.903	1.930	1.945	1.931	1.930	1.919	1.942	1.929
-O(2)	1.927	1.928	1.920	1.942	1.940	1.940	1.938	1.928	1.921	1.919
-O(3)	1.891	1.881	1.864	1.886	1.902	1.891	1.891	1.881	1.902	1.891
-O(5)	1.810	1.834	1.829	1.845	1.817	1.844	1.844	1.821	1.787	1.793
-O(6)	2.083	2.086	2.085	2.099	2.092	2.097	2.095	2.084	2.075	2.073
<M(4)-O>	1.954	1.956	1.948	1.967	1.964	1.967	1.966	1.953	1.950	1.946
M(5)-O(2)	1.797	1.797	1.800	1.802	1.801	1.801	1.799	1.801	1.797	1.797
-O(6)	1.993	2.002	2.008	2.005	1.991	2.000	2.000	1.995	1.985	1.983
-O(8)	1.946	1.936	1.931	1.933	1.945	1.938	1.936	1.940	1.962	1.951
<M(5)-O>	1.912	1.912	1.913	1.913	1.912	1.913	1.912	1.912	1.915	1.910
T(1)-O(3)	1.623	1.620	1.624	1.621	1.621	1.618	1.616	1.621	1.624	1.624
-O(4)	1.620	1.615	1.615	1.616	1.618	1.615	1.614	1.616	1.622	1.620
-O(9)	1.638	1.630	1.621	1.628	1.635	1.635	1.634	1.633	1.643	1.637
<T(1)-O>	1.625	1.620	1.619	1.620	1.623	1.621	1.620	1.622	1.628	1.625
T(2)-O(5)	1.605	1.601	1.598	1.604	1.616	1.603	1.603	1.611	1.610	1.613
-O(6)	1.681	1.667	1.665	1.666	1.683	1.668	1.666	1.680	1.698	1.695
-O(7)	1.691	1.675	1.671	1.670	1.693	1.675	1.674	1.687	1.710	1.699
<T(2)-O>	1.665	1.653	1.650	1.652	1.669	1.654	1.652	1.665	1.680	1.676
T(3)-O(7)	1.562	1.497	1.486	1.480	1.536	1.492	1.491	1.507	1.633	1.585
-O(8)	1.629	1.571	1.558	1.547	1.613	1.564	1.561	1.584	1.671	1.643
<T(3)-O>	1.596	1.534	1.522	1.514	1.575	1.528	1.526	1.546	1.652	1.614

POLYHEDRAL BOND LENGTHS

	K 32	K 33	K 34	K 35	K 36	K 38	K 39	K 40	K 41	K 42
X-O(4)	2.617	2.634	2.633	2.651	2.644	2.638	2.634	2.646	2.604	2.623
-O(9)	2.300	2.325	2.321	2.327	2.318	2.310	2.306	2.322	2.284	2.318
-O(10)	2.066	2.102	2.097	2.073	2.081	2.070	2.068	2.067	2.069	2.075
<X-O>	2.400	2.424	2.421	2.426	2.422	2.414	2.411	2.420	2.390	2.410
M(1)-O(1)	2.137	2.143	2.153	2.094	2.091	2.107	2.119	2.091	2.126	2.146
-O(4)	2.114	2.117	2.113	2.124	2.125	2.122	2.118	2.124	2.115	2.118
-O(5)	2.194	2.234	2.242	2.299	2.272	2.244	2.229	2.281	2.158	2.209
-O(7)	2.101	2.087	2.105	2.010	2.011	2.038	2.065	2.000	2.104	2.107
-O(10)	2.031	1.998	1.979	2.084	2.094	2.079	2.062	2.097	2.052	2.005
<M(1)-O>	2.115	2.116	2.118	2.123	2.120	2.119	2.118	2.120	2.111	2.117
M(2)-O(2)	2.066	2.091	2.088	2.087	2.083	2.077	2.074	2.084	2.054	2.079
-O(3)	1.995	1.999	1.999	1.997	1.998	1.995	1.995	1.997	1.994	1.997
-O(8)	2.230	2.230	2.233	2.154	2.161	2.185	2.200	2.155	2.238	2.241
<M(2)-O>	2.097	2.107	2.107	2.079	2.081	2.086	2.090	2.079	2.095	2.106
M(3)-O(1)	1.792	1.795	1.795	1.803	1.801	1.799	1.796	1.801	1.792	1.794
-O(4)	1.867	1.866	1.859	1.888	1.892	1.883	1.876	1.889	1.871	1.862
-O(6)	2.109	2.113	2.125	2.103	2.096	2.107	2.112	2.098	2.100	2.110
<M(3)-O>	1.923	1.925	1.926	1.931	1.930	1.930	1.928	1.929	1.921	1.922
M(4)-O(1)	1.924	1.923	1.914	1.945	1.957	1.945	1.939	1.943	1.937	1.914
-O(2)	1.934	1.929	1.925	1.922	1.931	1.934	1.935	1.918	1.943	1.925
-O(3)	1.887	1.878	1.873	1.905	1.914	1.908	1.901	1.907	1.897	1.874
-O(5)	1.848	1.819	1.835	1.776	1.779	1.803	1.821	1.773	1.861	1.834
-O(6)	2.093	2.084	2.088	2.074	2.076	2.085	2.088	2.069	2.102	2.089
<M(4)-O>	1.963	1.953	1.954	1.949	1.956	1.960	1.962	1.947	1.974	1.954
M(5)-O(2)	1.799	1.801	1.801	1.802	1.802	1.801	1.800	1.801	1.800	1.801
-O(6)	2.004	1.998	2.010	1.981	1.974	1.985	1.993	1.976	2.005	2.004
-O(8)	1.935	1.940	1.935	1.972	1.974	1.958	1.951	1.972	1.933	1.933
<M(5)-O>	1.913	1.913	1.915	1.918	1.917	1.914	1.915	1.916	1.913	1.913
T(1)-O(3)	1.615	1.624	1.624	1.629	1.626	1.623	1.620	1.626	1.612	1.620
-O(4)	1.614	1.617	1.616	1.626	1.625	1.622	1.620	1.624	1.615	1.613
-O(9)	1.635	1.628	1.625	1.646	1.648	1.645	1.641	1.647	1.636	1.627
<T(1)-O>	1.620	1.622	1.620	1.632	1.631	1.628	1.625	1.630	1.620	1.618
T(2)-O(5)	1.599	1.610	1.598	1.623	1.629	1.620	1.609	1.625	1.599	1.606
-O(6)	1.662	1.681	1.666	1.714	1.717	1.695	1.682	1.717	1.657	1.666
-O(7)	1.672	1.686	1.672	1.724	1.730	1.708	1.695	1.727	1.669	1.676
<T(2)-O>	1.649	1.665	1.651	1.694	1.698	1.680	1.667	1.697	1.646	1.653
T(3)-O(7)	1.487	1.511	1.495	1.648	1.638	1.583	1.542	1.646	1.479	1.487
-O(8)	1.551	1.587	1.569	1.681	1.674	1.641	1.615	1.679	1.532	1.552
<T(3)-O>	1.519	1.549	1.532	1.665	1.656	1.612	1.579	1.663	1.505	1.520

POLYHEDRAL BOND LENGTHS

	K 43	K 45	K 46	K 47	K 49	K 50	K 52
X-O(4)	2.629	2.619	2.634	2.631	2.616	2.639	2.620
-O(9)	2.312	2.305	2.308	2.307	2.297	2.306	2.293
-O(10)	2.061	2.074	2.069	2.066	2.075	2.065	2.065
<X-O>	2.408	2.404	2.411	2.409	2.401	2.412	2.400
M(1)-O(1)	2.136	2.137	2.112	2.112	2.125	2.111	2.117
-O(4)	2.115	2.112	2.115	2.117	2.115	2.114	2.114
-O(5)	2.219	2.206	2.262	2.255	2.192	2.268	2.205
-O(7)	2.076	2.100	2.036	2.039	2.089	2.037	2.072
-O(10)	2.030	2.016	2.060	2.061	2.042	2.056	2.059
<M(1)-O>	2.115	2.114	2.117	2.117	2.113	2.117	2.114
M(2)-O(2)	2.070	2.069	2.079	2.077	2.067	2.079	2.067
-O(3)	1.996	1.995	1.991	1.993	1.994	1.992	1.994
-O(8)	2.216	2.231	2.178	2.182	2.224	2.179	2.206
<M(2)-O>	2.094	2.098	2.083	2.084	2.095	2.083	2.089
M(3)-O(1)	1.794	1.793	1.797	1.797	1.793	1.797	1.794
-O(4)	1.865	1.863	1.876	1.877	1.872	1.874	1.873
-O(6)	2.115	2.112	2.113	2.112	2.104	2.113	2.109
<M(3)-O>	1.925	1.922	1.929	1.929	1.923	1.928	1.925
M(4)-O(1)	1.921	1.920	1.939	1.936	1.935	1.933	1.938
-O(2)	1.926	1.932	1.928	1.931	1.939	1.927	1.939
-O(3)	1.881	1.880	1.899	1.899	1.893	1.894	1.901
-O(5)	1.826	1.842	1.806	1.808	1.841	1.802	1.840
-O(6)	2.085	2.090	2.084	2.085	2.094	2.081	2.093
<M(4)-O>	1.954	1.959	1.957	1.957	1.966	1.953	1.967
M(5)-O(2)	1.798	1.798	1.797	1.797	1.798	1.796	1.797
-O(6)	2.000	2.003	1.993	1.993	1.998	1.991	1.998
-O(8)	1.940	1.934	1.951	1.951	1.938	1.950	1.942
<M(5)-O>	1.913	1.912	1.914	1.914	1.911	1.912	1.912
T(1)-O(3)	1.620	1.617	1.624	1.622	1.616	1.623	1.615
-O(4)	1.616	1.615	1.620	1.619	1.615	1.619	1.618
-O(9)	1.632	1.631	1.639	1.639	1.635	1.640	1.639
<T(1)-O>	1.621	1.620	1.626	1.625	1.620	1.625	1.623
T(2)-O(5)	1.604	1.597	1.608	1.608	1.603	1.608	1.599
-O(6)	1.670	1.664	1.685	1.683	1.668	1.685	1.670
-O(7)	1.679	1.672	1.693	1.692	1.678	1.695	1.680
<T(2)-O>	1.656	1.649	1.668	1.667	1.654	1.668	1.655
T(3)-O(7)	1.512	1.489	1.584	1.578	1.499	1.582	1.522
-O(8)	1.582	1.557	1.639	1.634	1.572	1.639	1.594
<T(3)-O>	1.547	1.523	1.611	1.606	1.536	1.611	1.558

APPENDIX G.3

SELECTED BOND LENGTHS (Å) & ANGLES (°)

Abbreviations used in APPENDIX G.3

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e.s.d are ≤ 0.002 Å for distances and 0.1° for angles

SELECTED BOND LENGTHS (Å) & ANGLES (°)

	K 1	K 2	K 3	K 5	K 6	K 7	K 8	K 9	K 10	K 11
O(6)-O(8)	2.943	2.938	2.929	2.927	2.933	2.928	2.938	2.926	2.930	2.930
O(5)-O(7)	2.514	2.514	2.530	2.520	2.524	2.509	2.521	2.516	2.520	2.533
O(8)-O(8)	2.636	2.605	2.524	2.540	2.553	2.545	2.588	2.517	2.556	2.512
T(1)-O(9)-T(1)	149.1	148.6	152.1	150.1	149.8	148.5	148.7	149.2	149.5	153.2
T(2)-O(7)-T(3)	123.5	123.8	124.4	124.2	124.5	124.3	124.0	124.2	124.4	124.5

	K 12	K 13	K 14	K 15	K 16	K 17	K 18	K 19	K 20	K 21
O(6)-O(8)	2.947	2.926	2.929	2.935	2.922	2.933	2.930	2.925	2.925	2.946
O(5)-O(7)	2.513	2.512	2.524	2.514	2.530	2.517	2.521	2.523	2.528	2.520
O(8)-O(8)	2.664	2.523	2.545	2.556	2.516	2.540	2.541	2.519	2.513	2.643
T(1)-O(9)-T(1)	148.1	148.1	150.7	148.1	152.2	148.9	148.8	151.5	152.6	149.4
T(2)-O(7)-T(3)	122.7	124.0	124.5	124.3	124.5	124.4	124.3	124.3	124.4	123.2

	K 22	K 23	K 24	K 25	K 26	K 27	K 28	K 29	K 30	K 31
O(6)-O(8)	2.941	2.926	2.927	2.930	2.941	2.929	2.927	2.934	2.961	2.941
O(5)-O(7)	2.513	2.514	2.521	2.518	2.518	2.513	2.514	2.524	2.511	2.510
O(8)-O(8)	2.636	2.552	2.532	2.520	2.608	2.541	2.540	2.563	2.714	2.660
T(1)-O(9)-T(1)	149.1	149.5	151.9	149.8	149.1	148.7	148.6	150.3	148.9	149.1
T(2)-O(7)-T(3)	123.4	124.2	124.5	124.4	123.8	124.4	124.2	124.3	122.2	122.8

	K 32	K 33	K 34	K 35	K 36	K 38	K 39	K 40	K 41	K 42
O(6)-O(8)	2.928	2.938	2.933	2.968	2.968	2.951	2.944	2.966	2.926	2.929
O(5)-O(7)	2.515	2.525	2.519	2.520	2.521	2.518	2.518	2.521	2.510	2.522
O(8)-O(8)	2.534	2.567	2.545	2.736	2.723	2.660	2.612	2.730	2.513	2.530
T(1)-O(9)-T(1)	148.7	151.1	151.1	149.3	148.3	148.2	148.4	148.9	147.0	150.6
T(2)-O(7)-T(3)	124.2	124.3	124.6	121.8	121.8	122.9	123.8	121.8	123.8	124.2

	K 43	K 45	K 46	K 47	K 49	K 50	K 52
O(6)-O(8)	2.930	2.927	2.949	2.948	2.931	2.946	2.936
O(5)-O(7)	2.514	2.513	2.509	2.508	2.511	2.511	2.504
O(8)-O(8)	2.567	2.534	2.656	2.648	2.554	2.652	2.587
T(1)-O(9)-T(1)	149.6	149.3	148.7	148.6	148.2	148.8	147.6
T(2)-O(7)-T(3)	124.1	124.4	123.2	123.2	124.2	123.0	123.9

APPENDIX H

EMPA & FORMULA CALCULATION

Abbreviations used in APPENDIX H

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average of 10 points and standard deviation (σ)
σ ($x10^2$) for oxides ; σ ($x10^3$) for atoms per formula unit (*apfu*)
* B *via* SREF at T(3)
** Fe^{3+} *via* SREF at M(4)
*** anion normalization based on O_{21} $(OH + F)_1$
— near detection limits and less than 0.01 (*apfu*)

EMPA & FORMULA CALCULATION

	K1	σ	K2	σ	K3	σ	K5	σ	K6	σ	K7	σ	K8	σ
SiO_2	29.97	26	30.75	15	29.30	30	30.82	33	29.60	20	31.63	35	29.01	20
Al_2O_3	44.06	18	42.98	27	41.45	50	42.21	21	40.40	21	40.56	30	41.36	19
B_2O_3*	1.88		2.41		3.76		3.52		3.37		3.56		2.51	
MgO	17.32	17	18.79	16	12.84	16	17.21	12	14.27	13	19.20	39	15.03	13
FeO	3.80	6	2.25	5	9.01	22	4.09	10	8.20	8	2.83	9	7.41	15
Fe_2O_3**	0.73		0.86		1.51		0.04		1.81		0.52		2.21	
MnO	—		—		—		0.13	3	0.35	3	—		0.31	3
V_2O_3	—		—		—		—		—		—		—	
Cr_2O_3	—		—		—		—		—		—		—	
TiO_2	0.12	5	—		—		—		—		—		—	
Na_2O	0.04	2	—		0.10	1	0.04	1	0.04	2	—		—	
CaO	—		—		—		—		—		—		—	
F	0.07	6	0.04	5	0.74	7	0.43	7	0.46	7	0.30	9	0.02	3
H_2O***	1.17		1.20		0.84		1.01		0.97		1.08		1.17	
O=F	- 0.03		- 0.02		- 0.31		- 0.18		- 0.19		- 0.13		- 0.01	
TOTAL	99.13		99.26		99.24		99.33		99.27		99.56		99.03	
Si	3.730	25	3.787	23	3.704	43	3.794	27	3.747	22	3.869	37	3.690	22
Al	0.866	17	0.701	22	0.476	62	0.458	27	0.517	24	0.379	41	0.758	24
B	0.404		0.512		0.820		0.748		0.736		0.752		0.552	
ΣTet.	5.000		5.000		5.000		5.000		5.000		5.000		5.000	
Al	5.597		5.537		5.699		5.666		5.510		5.468		5.443	
Mg	3.214	33	3.450	21	2.420	27	3.158	21	2.693	21	3.501	71	2.850	22
Fe^{2+}	0.396	6	0.396	6	0.952	24	0.421	12	0.868	7	0.290	9	0.788	14
Fe^{3+}	0.068		0.080		0.144		0.004		0.172		0.048		0.212	
Mn^{2+}	—		—		—		0.014	3	0.038	4	—		0.033	3
V^{3+}	—		—		—		—		—		—		—	
Cr^{3+}	—		—		—		—		—		—		—	
Ti	0.011	4	—		—		—		—		—		—	
Na	0.010	4	—		0.025	3	0.010	3	0.010	4	—		—	
Ca	—		—		—		—		—		—		—	
CATSUM	14.296		14.298		14.239		14.273		14.290		14.307		14.327	
F	0.028	24	0.016	21	0.296	28	0.167	25	0.184	29	0.116	34	0.008	14
OH	0.972		0.984		0.704		0.833		0.816		0.884		0.992	

EMPA & FORMULA CALCULATION

	K 9	σ	K 10	σ	K 11	σ	K 12	σ	K 13	σ	K 14	σ	K 15	σ
SiO_2	30.89	33	29.96	31	29.10	33	29.78	28	32.38	25	29.98	19	29.69	39
Al_2O_3	40.11	22	40.36	11	41.35	24	45.72	37	40.50	22	40.73	18	37.75	37
B_2O_3*	3.96		3.22		3.89		1.39		4.08		3.47		3.24	
MgO	18.05	11	15.15	6	10.81	13	19.45	18	21.20	14	18.83	11	16.03	16
FeO	4.26	7	7.62	10	12.09	10	1.08	6	0.76	4	8.07	9	7.25	10
Fe_2O_3**	0.60		1.52		—		0.34		0.09		1.69		3.63	
MnO	0.13	3	—		0.12	3	—		—		—		—	
V_2O_3	—		—		—		—		—		—		—	
Cr_2O_3	—		—		—		—		—		—		—	
TiO_2	—		0.13	4	0.21	6	—		—		0.13	4	0.15	4
Na_2O	0.05	1	—		0.05	1	—		—		—		0.11	2
CaO	—		—		—		0.08	1	—		—		—	
F	0.38	5	0.11	8	0.85	10	0.03	5	0.18	8	0.17	5	0.49	10
H_2O***	1.03		1.14		0.77		1.20		1.16		1.11		0.95	
O=F	-0.16		-0.05		-0.36		-0.01		-0.08		-0.07		-0.21	
TOTAL	99.31		99.15		98.89		99.06		100.27		99.10		99.08	
Si	3.811	32	3.779	25	3.722	36	3.672	31	3.884	21	3.782	17	3.779	40
Al	0.345	30	0.521	23	0.418	34	1.032	36	0.272	24	0.462	24	0.509	34
B	0.844		0.700		0.860		0.296		0.844		0.756		0.712	
ΣTet.	5.000		5.000		5.000		5.000		5.000		5.000		5.000	
Al	5.487		5.479		5.816		5.612		5.453		5.594		5.154	
Mg	3.320	20	2.849	18	2.061	19	3.575	22	3.791	20	2.601	14	3.042	28
Fe^{2+}	0.440	8	0.804	12	1.293	10	0.111	6	0.076	4	0.851	11	0.772	11
Fe^{3+}	0.056		0.144		—		0.032		0.008		0.160		0.348	
Mn^{2+}	0.014	3	—		0.013	3	—		—		—		—	
V^{3+}	—		—		—		—		—		—		—	
Cr^{3+}	—		—		—		—		—		—		—	
Ti	—		0.012	4	0.020	6	—		—		0.012	4	0.014	4
Na	0.012	3	—		0.012	3	—		—		—		0.027	4
Ca	—		—		—		0.011	2	—		—		—	
CATSUM	14.329		14.287		14.217		14.342		14.328		14.219		14.358	
F	0.148	20	0.044	30	0.344	41	0.012	18	0.068	30	0.068	22	0.197	41
OH	0.852		0.956		0.656		0.988		0.932		0.932		0.803	

EMPA & FORMULA CALCULATION

	K 16	σ	K 17	σ	K 18	σ	K 19	σ	K 20	σ	K 21	σ	K 22	σ
SiO_2	29.70	30	29.86	28	30.46	27	30.79	35	30.31	17	29.27	19	30.84	22
Al_2O_3	40.98	23	38.57	16	39.86	29	41.42	23	41.69	21	43.49	30	44.76	18
B_2O_3*	3.93		3.52		3.55		3.95		4.02		1.70		1.99	
MgO	11.97	8	15.24	18	16.56	18	15.43	11	13.05	11	14.89	9	19.35	5
FeO	10.31	10	7.34	17	5.51	13	5.59	10	8.35	12	6.48	11	1.21	3
Fe_2O_3**	0.59		3.44		1.92		0.21		0.09		1.68		0.09	
MnO	—		—		0.24	2	—		0.10	2	—		—	
V_2O_3	—		—		—		0.10	4	0.10	4	—		—	
Cr_2O_3	—		—		—		0.13	3	0.11	1	—		—	
TiO_2	0.19	7	—		—		0.19	5	0.21	5	0.17	3	—	
Na_2O	—		0.12	2	—		0.09	2	0.07	1	—		—	
CaO	—		—		—		—		—		—		—	
F	0.39	6	0.37	7	0.08	6	0.77	11	0.76	12	0.07	5	0.00	0
H_2O***	1.00		1.01		1.16		0.85		0.84		1.15		1.23	
O=F	- 0.16		- 0.16		- 0.03		- 0.32		- 0.32		- 0.03		- 0.00	
TOTAL	98.88		99.31		99.30		99.19		99.38		98.87		99.46	
Si	3.769	33	3.779	28	3.802	30	3.813	38	3.789	16	3.711	24	3.769	22
Al	0.371	32	0.453	38	0.434	27	0.343	39	0.343	23	0.917	29	0.811	27
B	0.860		0.768		0.764		0.844		0.868		0.372		0.420	
∑Tet.	5.000		5.000		5.000		5.000		5.000		5.000		5.000	
Al	5.758		5.300		5.430		5.703		5.799		5.581		5.636	
Mg	2.264	14	2.876	29	3.082	22	2.849	21	2.432	15	2.814	9	3.525	9
Fe^{2+}	1.094	13	0.777	16	0.575	10	0.579	10	0.873	12	0.687	12	0.124	3
Fe^{3+}	0.056		0.328		0.180		0.020		0.008		0.160		0.008	
Mn^{2+}	—		—		0.025	2	—		0.011	2	—		—	
V^{3+}	—		—		—		0.010	4	0.010	4	—		—	
Cr^{3+}	—		—		—		0.013	3	0.011	1	—		—	
Ti	0.018	6	—		—		0.018	4	0.020	5	0.016	3	—	
Na	—		0.029	5	—		0.022	6	0.017	2	—		—	
Ca	—		—		—		—		—		—		—	
CATSUM	14.191		14.311		14.293		14.213		14.180		14.258		14.293	
F	0.157	25	0.148	28	0.032	23	0.302	41	0.300	45	0.028	21	0.000	0
OH	0.843		0.852		0.968		0.698		0.700		0.972		1.000	

EMPA & FORMULA CALCULATION

	K 23	σ	K 24	σ	K 25	σ	K 26	σ	K 27	σ	K 28	σ	K 29	σ
SiO_2	31.63	28	30.85	33	30.07	16	29.31	20	30.56	30	31.06	26	29.63	29
Al_2O_3	42.63	25	41.65	22	38.79	16	41.29	36	40.09	28	40.63	25	42.56	21
B_2O_3*	3.49		3.77		3.90		2.34		3.54		3.58		2.96	
MgO	19.91	15	15.19	11	14.91	6	15.09	14	16.87	17	18.59	14	14.44	9
FeO	—		5.75	10	7.96	17	7.25	13	5.57	5	3.54	4	7.80	12
Fe_2O_3**	—		—		2.19		—		1.58		0.73		0.89	
MnO	0.15	2	—		—		0.34	2	0.21	3	—		0.31	3
V_2O_3	0.20	3	0.12	3	—		—		—		—		—	
Cr_2O_3	—		0.13	2	—		—		—		—		—	
TiO_2	0.16	5	0.20	5	0.19	6	0.21	3	—		—		—	
Na_2O	—		0.11	1	0.06	1	0.07	1	—		—		0.07	1
CaO	—		—		—		—		—		—		—	
F	0.10	7	0.78	12	0.75	6	0.46	5	0.10	6	0.23	8	0.38	11
H_2O***	1.19		0.84		0.83		0.96		1.16		1.11		1.02	
O=F	- 0.04		- 0.33		- 0.32		- 0.19		- 0.04		- 0.10		- 0.16	
TOTAL	99.42		99.06		99.34		99.48		99.64		99.37		99.89	
Si	3.822	30	3.828	30	3.792	21	3.717	29	3.799	34	3.822	29	3.714	24
Al	0.450	33	0.364	30	0.360	19	0.771	38	0.441	32	0.418	28	0.646	24
B	0.728		0.808		0.848		0.512		0.760		0.760		0.640	
ΣTet.	5.000		5.000		5.000		5.000		5.000		5.000		5.000	
Al	5.620		5.727		5.405		5.400		5.433		5.475		5.641	
Mg	3.586	24	2.810	24	2.803	13	2.853	25	3.127	27	3.410	17	2.698	12
Fe^{2+}	—		0.597	10	0.839	18	0.769	15	0.579	8	0.364	5	0.818	12
Fe^{3+}	—		—		0.208		0.224		0.148		0.068		0.084	
Mn^{2+}	0.015	2	—		—		0.037	2	0.022	3	—		0.033	3
V^{3+}	0.019	3	0.012	3	—		—		—		—		—	
Cr^{3+}	—		0.013	2	—		—		—		—		—	
Ti	0.015	4	0.019	4	0.018	6	0.020	3	—		—		—	
Na	—		0.026	3	0.015	3	0.017	3	—		—		0.017	3
Ca	—		—		—		—		—		—		—	
CATSUM	14.255		14.204		14.287		14.319		14.310		14.317		14.290	
F	0.038	27	0.306	48	0.299	26	0.184	20	0.039	23	0.090	33	0.151	41
OH	0.962		0.694		0.701		0.816		0.961		0.910		0.849	

EMPA & FORMULA CALCULATION

	K 30	σ	K 31	σ	K 32	σ	K 33	σ	K 34	σ	K 35	σ	K 36	σ
SiO_2	30.18	17	29.77	30	30.69	51	29.08	15	31.07	15	28.66	15	28.53	10
Al_2O_3	47.22	32	46.85	51	40.66	52	42.61	20	41.62	10	48.04	10	46.90	12
B_2O_3*	0.53		1.51		3.80		3.00		3.59		0.09		0.20	
MgO	19.73	12	19.12	26	19.45	25	14.59	5	16.22	12	17.72	7	17.96	8
FeO	0.23	2	0.66	5	2.48	3	6.85	11	4.94	10	2.71	6	3.09	12
Fe_2O_3**	—		0.04		0.17		1.44		—		0.60		1.53	
MnO	—		—		—		—		—		—		—	
V_2O_3	—		—		—		—		0.16	3	—		—	
Cr_2O_3	—		—		—		—		0.20	2	—		—	
TiO_2	—		—		—		0.24	2	0.21	2	0.12	2	0.13	2
Na_2O	—		—		—		0.13	2	0.14	1	—		—	
CaO	0.09	1	—		—		—		—		0.08	1	—	
F	0.10	6	0.08	6	0.15	5	0.94	9	0.90	11	0.02	4	0.13	7
H_2O***	1.17		1.18		1.14		0.75		0.79		1.19		1.14	
O=F	- 0.04		- 0.03		- 0.06		- 0.40		- 0.38		- 0.01		- 0.05	
TOTAL	99.21		99.19		98.48		99.23		99.46		99.22		99.55	
Si	3.710	29	3.649	28	3.784	66	3.660	14	3.835	14	3.580	14	3.571	10
Al	1.178	32	1.031	61	0.408	60	0.688	18	0.401	14	1.400	12	1.385	14
B	0.112		0.320		0.808		0.652		0.764		0.020		0.044	
ΣTet.	5.000		5.000		5.000		5.000		5.000		5.000		5.000	
Al	5.663		5.738		5.501		5.632		5.653		5.673		5.533	
Mg	3.616	16	3.494	50	3.576	38	2.737	12	2.984	16	3.300	17	3.351	15
Fe^{2+}	0.024	2	0.068	5	0.256	4	0.721	12	0.510	10	0.283	6	0.323	12
Fe^{3+}	—		0.004		0.016		0.136		—		0.056		0.144	
Mn^{2+}	—		—		—		—		—		—		—	
V^{3+}	—		—		—		—		0.016	3	—		—	
Cr^{3+}	—		—		—		—		0.020	2	—		—	
Ti	—		—		—		0.023	2	0.019	1	0.011	2	0.012	2
Na	—		—		—		0.032	4	0.034	3	—		—	
Ca	0.012	2	—		—		—		—		0.011	1	—	
CATSUM	14.314		14.304		14.349		14.280		14.236		14.334		14.364	
F	0.039	24	0.031	22	0.058	19	0.374	38	0.351	44	0.008	16	0.051	27
OH	0.961		0.969		0.942		0.626		0.649		0.992		0.949	

EMPA & FORMULA CALCULATION

	K 38	σ	K 39	σ	K 40	σ	K 41	σ	K 42	σ	K 43	σ	K 45	σ
SiO_2	29.68	18	30.60	14	28.95	8	31.67	19	29.63	27	31.05	19	30.91	16
Al_2O_3	44.91	20	43.76	10	49.57	11	39.27	11	40.98	31	43.73	22	41.33	12
B_2O_3*	1.48		2.29		0.08		4.21		3.70		3.15		3.66	
MgO	19.21	9	19.55	8	19.42	10	21.74	15	15.34	18	19.58	8	18.41	7
FeO	1.76	4	1.82	6	0.49	3	1.16	6	6.86	14	0.07	3	3.26	6
Fe_2O_3**	0.64		0.39		0.13		0.48		0.13		0.04		0.26	
MnO	—		—		—		—		—		0.15	3	0.13	3
V_2O_3	—		—		—		—		0.12	3	—		—	
Cr_2O_3	0.28	3	0.15	2	—		—		—		—		—	
TiO_2	—		—		0.13	2	—		0.30	7	0.17	4	—	
Na_2O	—		—		—		—		0.07	1	—		0.08	2
CaO	—		—		0.09	1	0.09	1	—		—		—	
F	0.06	3	0.06	5	0.02	6	0.12	7	0.53	9	0.16	7	0.32	9
H_2O***	1.18		1.20		1.21		1.18		0.94		1.16		1.07	
O=F	- 0.03		- 0.03		- 0.01		- 0.05		- 0.22		- 0.07		- 0.13	
TOTAL	99.18		99.80		100.08		99.88		98.37		99.20		99.29	
Si	3.673	13	3.743	11	3.546	7	3.832	18	3.732	30	3.766	23	3.797	12
Al	1.011	26	0.773	13	1.438	12	0.288	13	0.464	29	0.574	25	0.427	19
B	0.316		0.484		0.016		0.880		0.804		0.660		0.776	
ΣTet.	5.000		5.000		5.000		5.000		5.000		5.000		5.000	
Al	5.538		5.535		5.718		5.312		5.619		5.678		5.557	
Mg	3.544	12	3.565	8	3.546	14	3.921	21	2.880	23	3.541	14	3.372	13
Fe^{2+}	0.182	4	0.186	6	0.050	3	0.117	6	0.723	15	0.007	3	0.335	7
Fe^{3+}	0.060		0.036		0.012		0.044		0.012		0.004		0.024	
Mn^{2+}	—		—		—		—		—		0.015	3	0.014	3
V^{3+}	—		—		—		—		0.012	3	—		—	
Cr^{3+}	0.027	3	0.015	1	—		—		—		—		—	
Ti	—		—		0.012	2	—		0.028	6	0.016	4	—	
Na	—		—		—		—		0.017	3	—		0.019	4
Ca	—		—		0.012	2	0.012	1	—		—		—	
CATSUM	14.351		14.336		14.350		14.406		14.292		14.260		14.320	
F	0.023	13	0.023	21	0.008	23	0.046	26	0.211	35	0.061	28	0.124	34
OH	0.977		0.977		0.992		0.954		0.789		0.939		0.876	

EMPA & FORMULA CALCULATION

	K 46	σ	K 47	σ	K 49	σ	K 50	σ	K 52	σ
SiO_2	30.71	21	30.51	16	30.18	22	30.20	26	30.78	22
Al_2O_3	45.88	14	45.14	14	41.20	22	45.59	11	42.79	14
B_2O_3*	1.55		1.71		3.28		1.60		2.85	
MgO	20.38	6	20.24	7	19.41	16	19.26	5	21.24	10
FeO	—		—		2.99	11	1.06	5	—	
Fe_2O_3**	—		—		0.73		0.22		0.13	3
MnO	—		—		—		—		—	
V_2O_3	—		—		—		—		—	
Cr_2O_3	0.26	3	0.25	2	—		—		—	
TiO_2	0.15	6	0.12	5	—		—		—	
Na_2O	—		—		—		—		—	
CaO	0.08	1	0.08	1	—		—		—	
F	0.14	10	0.08	5	0.27	10	0.03	4	0.07	6
H_2O***	1.17		1.19		1.08		1.21		1.20	
O=F	- 0.06		- 0.03		- 0.11		- 0.01		- 0.03	
TOTAL	100.26		99.28		99.03		99.15		99.03	
Si	3.719	18	3.728	13	3.730	26	3.710	21	3.751	22
Al	0.957	19	0.912	20	0.570	22	0.950	23	0.649	22
B	0.324		0.360		0.700		0.340		0.600	
ΣTet.	5.000		5.000		5.000		5.000		5.000	
Al	5.591		5.588		5.432		5.652		5.498	
Mg	3.679	16	3.686	11	3.576	22	3.528	10	3.859	21
Fe^{2+}	—		—		0.309	11	0.109	5	—	
Fe^{3+}	—		—		0.068		0.020		0.012	3
Mn^{2+}	—		—		—		—		—	
V^{3+}	—		—		—		—		—	
Cr^{3+}	0.025	3	0.024	2	—		—		—	
Ti	0.014	5	0.011	4	—		—		—	
Na	—		—		—		—		—	
Ca	0.010	2	0.010	2	—		—		—	
CATSUM	14.319		14.319		14.385		14.309		14.369	
F	0.054	38	0.031	21	0.106	38	0.012	16	0.027	25
OH	0.946		0.969		0.894		0.988		0.973	

APPENDIX I

LIGHT ELEMENT ANALYSES

Abbreviations used in APPENDIX I

F as (*apfu*), H_2O & B_2O_3 as (wt.%)
[1] : from occupancy refinement of O(10) site, e.s.d. ≈0.04 F *apfu*
[2] : calculated using O_{21} $(OH + F)_1$, σ ≈0.04 F *apfu*
[3] : from H-extraction line analysis
[4] : calculated using O_{21} $(OH + F)_1$ and F from EMPA
[5] : calibrated using Si from EMPA

LIGHT ELEMENT ANALYSES

	F (SREF)[1]	F (EMPA)[2]	H_2O (H.E.L.)[3]	H_2O (EMPA)[4]	B_2O_3 (SIMS)[5]	B_2O_3 (SREF)
K 1	0.00	0.03		1.2	1.98	1.88
K 2	0.00	0.02	1.4	1.2	2.52	2.41
K 3	0.28	0.30		0.8	3.84	3.76
K 5	0.08	0.17	1.2	1.0	3.62	3.52
K 6	0.20	0.18	1.1	1.0	3.15	3.37
K 7	0.08	0.12		1.1	3.66	3.56
K 8	0.00	0.01		1.2	2.45	2.51
K 9	0.08	0.15		1.0	3.98	3.96
K 10	0.04	0.04		1.1	3.06	3.22
K 11	0.32	0.34		0.8	3.86	3.89
K 12	0.00	0.01		1.2	1.35	1.39
K 13	0.12	0.07		1.2	4.36	4.08
K 14	0.08	0.07		1.1	3.38	3.47
K 15	0.24	0.20		1.0	3.15	3.24
K 16	0.16	0.16		1.0	3.81	3.93
K 17	0.16	0.15		1.0	3.37	3.52
K 18	0.04	0.03		1.2	3.43	3.55
K 19	0.36	0.30		0.9	4.05	3.95
K 20	0.32	0.30		0.8	3.98	4.02
K 21	0.16	0.03		1.2	1.70	1.70
K 22	0.00	0.00	1.3	1.2	2.05	1.99
K 23	0.08	0.04	1.1	1.2	3.51	3.49
K 24	0.36	0.31		0.8	3.70	3.77
K 25	0.32	0.30	0.9	0.8	3.73	3.90
K 26	0.16	0.18		1.0	2.28	2.34
K 27	0.04	0.04		1.2	3.50	3.54
K 28	0.12	0.09		1.1	3.54	3.58
K 29	0.12	0.15		1.0	2.88	2.96
K 30	0.00	0.04		1.2	0.44	0.53
K 31	0.00	0.03		1.2	1.54	1.51
K 32	0.00	0.06	1.2	1.1	3.76	3.80
K 33	0.48	0.37		0.8		3.00
K 34	0.44	0.35		0.8		3.59
K 35	0.00	0.01		1.2		0.09
K 36	0.04	0.05		1.1		0.20
K 38	0.00	0.02		1.2		1.48
K 39	0.00	0.02		1.2		2.29
K 40	0.00	0.01		1.2		0.08
K 41	0.04	0.05		1.2		4.21
K 42	0.24	0.21		0.9		3.70
K 43	0.00	0.06		1.2		3.15
K 45	0.12	0.12		1.1		3.66
K 46	0.00	0.05		1.2		1.55
K 47	0.00	0.03		1.2		1.71
K 49	0.08	0.11		1.1		3.28
K 50	0.00	0.01		1.2		1.60
K 52	0.00	0.03		1.2		2.85

APPENDIX J

BOND-VALENCE CALCULATIONS

Abbreviations used in APPENDIX J

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calculated using the curves of Brown, 1981
using valence units (*vu*)

BOND-VALENCE CALCULATIONS

Multiplicative factors

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)				↓×2 ×2→						
O(2)			↓×2			↓×2 ×2→				
O(3)			↓×2							
O(4)	↓×4	↓×2		↓×2			↓×2			
O(5)										
O(6)				↓×2	↓×2	↓×2		↓×2		
O(7)									↓×2	
O(8)			↓×2			↓×2 ×2→			↓×2	
O(9)	↓×2 ×2→						×2→			
O(10)	↓×2 ×2→	×2→								
Σ										

K11

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.302		0.649	0.518					2.118
O(2)			0.352		0.491	0.637				2.117
O(3)			0.442		0.563		0.995			2.000
O(4)	0.025	0.334		0.562			1.027			1.948
O(5)		0.260			0.606			1.046		1.912
O(6)				0.320	0.343	0.399		0.887		1.949
O(7)		0.328						0.876	0.842	2.046
O(8)			0.250			0.474			0.708	1.906
O(9)	0.045						1.000			2.090
O(10)	0.078	0.434								1.024
Σ	0.346	1.992	2.088	3.062	2.864	3.020	4.049	3.696	3.100	

K13

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.309		0.654	0.476					2.093
O(2)			0.358		0.467	0.643				2.111
O(3)			0.414		0.520		1.016			1.950
O(4)	0.043	0.324		0.543			1.021			1.931
O(5)		0.285			0.567			1.063		1.915
O(6)				0.326	0.334	0.403		0.908		1.971
O(7)		0.332						0.880	0.844	2.056
O(8)			0.255			0.470			0.716	1.911
O(9)	0.075						0.969			2.088
O(10)	0.116	0.369								0.970
Σ	0.554	1.943	2.054	3.046	2.698	3.032	4.027	3.759	3.120	

BOND-VALENCE CALCULATIONS

K15

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.314		0.649	0.481					2.093
O(2)			0.360		0.470	0.640				2.110
O(3)			0.431		0.530		1.013			1.974
O(4)	0.041	0.326		0.546			1.013			1.926
O(5)		0.268			0.612			1.049		1.929
O(6)				0.320	0.338	0.409		0.887		1.954
O(7)		0.335						0.867	0.906	2.108
O(8)			0.258			0.465			0.737	1.925
O(9)	0.083						0.966			2.098
O(10)	0.125	0.388								1.026
Σ	0.580	1.957	2.098	3.030	2.769	3.028	4.005	3.690	3.286	

K20

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.300		0.647	0.520					2.114
O(2)			0.353		0.491	0.637				2.118
O(3)			0.432		0.566		0.995			1.993
O(4)	0.022	0.331		0.565			1.027			1.945
O(5)		0.259			0.610			1.043		1.912
O(6)				0.318	0.344	0.401		0.887		1.950
O(7)		0.329						0.880	0.833	2.042
O(8)			0.250			0.473			0.702	1.898
O(9)	0.039						1.000			2.078
O(10)	0.065	0.428								0.986
Σ	0.296	1.978	2.070	3.060	2.875	3.022	4.049	3.697	3.070	

K24

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.302		0.647	0.509					2.105
O(2)			0.351		0.490	0.640				2.121
O(3)			0.429		0.556		0.995			1.980
O(4)	0.025	0.330		0.562			1.019			1.936
O(5)		0.255			0.604			1.066		1.925
O(6)				0.316	0.342	0.400		0.894		1.952
O(7)		0.333						0.880	0.864	2.077
O(8)			0.255			0.473			0.709	1.910
O(9)	0.044						1.003			2.094
O(10)	0.069	0.422								0.982
Σ	0.326	1.972	2.070	3.050	2.843	3.026	4.036	3.734	3.146	

BOND-VALENCE CALCULATIONS

K30

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.334		0.643	0.462					2.082
O(2)			0.343		0.484	0.644				2.115
O(3)			0.412		0.505		0.995			1.912
O(4)	0.039	0.319		0.530			1.000			1.888
O(5)		0.227			0.660			1.032		1.919
O(6)				0.324	0.348	0.420		0.822		1.914
O(7)		0.402						0.797	0.917	2.116
O(8)			0.297			0.442			0.831	2.012
O(9)	0.070						0.946			2.032
O(10)	0.113	0.341								0.908
Σ	0.522	1.942	2.104	2.994	2.807	3.012	3.941	3.473	3.496	

K35

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.337		0.635	0.464					2.071
O(2)			0.341		0.489	0.637				2.104
O(3)			0.412		0.508		0.982			1.902
O(4)	0.039	0.317		0.521			0.989			1.866
O(5)		0.224			0.690			0.997		1.911
O(6)				0.328	0.351	0.424		0.789		1.892
O(7)		0.404						0.770	0.925	2.099
O(8)			0.297			0.432			0.849	2.010
O(9)	0.074						0.939			2.026
O(10)	0.129	0.344								0.946
Σ	0.562	1.943	2.100	2.968	2.853	2.986	3.899	3.345	3.548	

K40

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.337		0.638	0.463					2.076
O(2)			0.342		0.490	0.638				2.108
O(3)			0.411		0.502		0.989			1.902
O(4)	0.043	0.315		0.520			0.995			1.873
O(5)		0.232			0.687			0.992		1.911
O(6)				0.332	0.353	0.429		0.783		1.897
O(7)		0.408						0.764	0.931	2.103
O(8)			0.296			0.432			0.855	2.015
O(9)	0.077						0.936			2.026
O(10)	0.129	0.332								0.922
Σ	0.548	1.939	2.098	2.980	2.848	2.998	3.915	3.322	3.572	

BOND-VALENCE CALCULATIONS

K41

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.314		0.652	0.470					2.088
O(2)			0.365		0.464	0.640				2.109
O(3)			0.415		0.515		1.027			1.957
O(4)	0.053	0.322		0.542			1.019			1.936
O(5)		0.295			0.559			1.063		1.917
O(6)				0.330	0.330	0.403		0.912		1.975
O(7)		0.329						0.885	0.827	2.041
O(8)			0.252			0.471			0.715	1.909
O(9)	0.095						0.964			2.118
O(10)	0.146	0.363								1.018
Σ	0.694	1.945	2.064	3.048	2.668	3.028	4.029	3.772	3.084	

minimum and maximum values for all 47 ferrous-iron kornerupines

	X	M(1)	M(2)	M(3)	M(4)	M(5)	T(1)	T(2)	T(3)	Σ
O(1)		0.30 0.34		0.64 0.65	0.46 0.52					2.07 2.12
O(2)			0.34 0.37		0.46 0.49	0.64 0.65				2.10 2.12
O(3)			0.41 0.44		0.50 0.57		0.98 1.03			1.90 2.00
O(4)	0.02 0.05	0.32 0.33		0.52 0.57			0.99 1.03			1.87 1.95
O(5)		0.22 0.30			0.56 0.70			0.98 1.07		1.90 1.93
O(6)				0.31 0.33	0.33 0.35	0.40 0.43		0.78 0.91		1.89 1.98
O(7)		0.33 0.41						0.76 0.89	0.83 0.95	2.04 2.14
O(8)			0.25 0.30			0.43 0.48			0.70 0.86	1.90 2.02
O(9)	0.04 0.10						0.93 1.00			2.02 2.12
O(10)	0.07 0.15	0.33 0.45								0.91 1.04
Σ	0.30 0.69	1.93 2.00	2.05 2.10	2.97 3.07	2.67 2.88	2.99 3.04	3.90 4.05	3.31 3.77	3.07 3.58	

BOND-VALENCE CALCULATIONS

bond-valence incident at O(9) and O(10) [excluding H contribution]

	K 1	K 2	K 3	K 5	K 6	K 7	K 8	K 9
O(9)	2.046	2.056	2.092	2.084	2.072	2.088	2.054	2.108
O(10)	0.980	0.956	1.020	0.990	1.010	0.978	1.028	1.022

	K 10	K 11	K 12	K 13	K 14	K 15	K 16	K 17
O(9)	2.068	2.090	2.046	2.088	2.052	2.098	2.072	2.088
O(10)	1.034	1.024	0.944	0.970	1.012	1.026	1.040	1.028

	K 18	K 19	K 20	K 21	K 22	K 23	K 24	K 25
O(9)	2.066	2.094	2.078	2.022	2.048	2.082	2.094	2.098
O(10)	1.018	0.974	0.986	0.984	0.954	0.964	0.982	0.998

	K 26	K 27	K 28	K 29	K 30	K 31	K 32	K 33
O(9)	2.076	2.072	2.080	2.068	2.032	2.056	2.088	2.092
O(10)	0.990	1.024	0.992	1.014	0.908	0.934	1.014	0.970

	K 34	K 35	K 36	K 38	K 39	K 40	K 41	K 42
O(9)	2.086	2.026	2.028	2.038	2.054	2.026	2.118	2.102
O(10)	0.968	0.946	0.936	0.948	0.966	0.922	1.018	1.014

	K 43	K 45	K 46	K 47	K 49	K 50	K 52
O(9)	2.070	2.098	2.068	2.070	2.108	2.044	2.090
O(10)	0.954	1.010	0.960	0.966	1.012	0.948	0.994

APPENDIX K

STRUCTURE FACTORS

Observed and calculated structure factors for K1

h	k	l	10Fo	10Fc	10s
2	0	0	644	665	2
4	0	0	1140	1139	3
6	0	0	629	644	4
8	0	0	1062	1044	5
12	0	0	1458	1465	6
14	0	0	282	271	3
16	0	0	376	359	3
18	0	0	460	464	4
20	0	0	439	441	4
22	0	0	1840	1811	9
1	1	0	730	772	2
3	1	0	239	231	2
5	1	0	538	537	4
7	1	0	437	442	3
9	1	0	1569	1538	5
11	1	0	3034	2959	6
13	1	0	438	438	3
15	1	0	240	253	3
17	1	0	354	362	3
19	1	0	547	542	4
21	1	0	823	836	6
0	2	0	1268	1304	2
2	2	0	286	302	2
4	2	0	598	616	3
6	2	0	160	168	2
8	2	0	271	273	2
10	2	0	599	605	4
12	2	0	411	404	3
14	2	0	863	857	6
16	2	0	783	783	5
18	2	0	143	136	4
20	2	0	96	89	7
22	2	0	260	249	4
1	3	0	289	288	2
3	3	0	447	461	3
7	3	0	524	507	4
9	3	0	847	837	5
11	3	0	454	455	3
13	3	0	318	314	3
15	3	0	946	952	6
17	3	0	1000	1009	6
19	3	0	275	283	3
21	3	0	283	284	4
0	4	0	2121	2136	3
2	4	0	630	625	4
4	4	0	1013	1007	4
8	4	0	421	412	3
10	4	0	471	473	4
12	4	0	216	223	3
14	4	0	707	705	5
16	4	0	2099	2076	8
18	4	0	67	59	8
20	4	0	170	164	4
22	4	0	497	489	4
1	5	0	1469	1465	4
3	5	0	110	106	2
7	5	0	882	876	5
9	5	0	23	1	22
11	5	0	368	388	3
13	5	0	199	202	3
15	5	0	255	266	3
17	5	0	508	508	4
19	5	0	146	157	5
21	5	0	414	420	4
0	6	0	874	878	4
2	6	0	156	158	2
4	6	0	237	244	2
6	6	0	440	430	1
8	6	0	623	612	5
10	6	0	1513	1501	6
12	6	0	173	181	3
14	6	0	382	380	3
16	6	0	445	449	4
18	6	0	384	385	3
20	6	0	32	24	31
1	7	0	640	629	5
3	7	0	230	229	2
5	7	0	1424	1402	5
7	7	0	487	478	4
9	7	0	1171	1162	6
11	7	0	639	609	5
13	7	0	292	289	3
15	7	0	286	287	3
17	7	0	353	349	4
19	7	0	651	655	5
21	7	0	604	604	5
0	8	0	2674	2651	5
2	8	0	142	140	3
4	8	0	554	551	4
6	8	0	622	636	5
8	8	0	512	521	4
10	8	0	1243	1235	7
12	8	0	116	123	4
14	8	0	87	88	6
16	8	0	312	315	3
18	8	0	0	3	1
20	8	0	321	299	4
1	9	0	156	135	3
3	9	0	324	330	3
5	9	0	1871	1903	6
7	9	0	878	881	6
9	9	0	132	119	4
11	9	0	626	610	5
13	9	0	234	228	3
15	9	0	719	742	5
17	9	0	556	555	4
19	9	0	181	188	4
0	10	0	305	317	3
2	10	0	79	90	5
4	10	0	328	336	3
6	10	0	273	280	3
8	10	0	258	266	3
10	10	0	516	522	4
12	10	0	246	251	3
14	10	0	1047	1061	8
16	10	0	312	311	3
18	10	0	371	377	4
1	11	0	277	271	3
3	11	0	277	283	3
5	11	0	811	822	6
7	11	0	93	101	5
9	11	0	119	106	4
11	11	0	419	436	4
13	11	0	249	263	3
15	11	0	748	750	5
17	11	0	448	449	4
0	12	0	1483	1490	7
2	12	0	167	166	3
4	12	0	376	377	3
6	12	0	599	596	5
8	12	0	181	187	3
10	12	0	761	727	6
12	12	0	530	532	4
14	12	0	150	150	5
16	12	0	61	27	11
1	13	0	565	561	4
3	13	0	188	192	3
5	13	0	327	330	3
7	13	0	481	479	4
9	13	0	326	325	3
11	13	0	916	919	7
13	13	0	252	258	4
15	13	0	260	264	4
0	14	0	1361	1370	8
2	14	0	376	379	3
4	14	0	202	198	3
6	14	0	680	677	5
8	14	0	187	168	4
10	14	0	1208	1250	9
12	14	0	82	94	9
14	14	0	40	19	21
1	15	0	351	342	3
3	15	0	351	344	3
5	15	0	495	499	4
7	15	0	58	75	10
9	15	0	233	235	4
11	15	0	414	415	4
13	15	0	171	177	4
0	16	0	557	550	4
2	16	0	221	223	4
4	16	0	143	128	5
6	16	0	779	781	5
8	16	0	66	55	10
10	16	0	125	86	6
12	16	0	459	463	4
1	17	0	282	276	3
3	17	0	298	299	3
5	17	0	1710	1734	9
7	17	0	53	56	13
9	17	0	24	27	21
0	18	0	362	354	4
2	18	0	254	262	4
4	18	0	87	92	8
6	18	0	291	281	4
8	18	0	273	269	4
1	19	0	173	182	5
3	19	0	125	125	6
1	1	1	132	124	2
3	1	1	363	353	3
5	1	1	899	911	4
7	1	1	20	13	19
9	1	1	274	267	2
11	1	1	730	750	5
13	1	1	269	270	3
15	1	1	224	218	3
17	1	1	686	690	5
19	1	1	488	491	4
21	1	1	650	654	5
0	2	1	240	60	-2
2	2	1	546	561	3
4	2	1	332	335	2
6	2	1	278	266	2
8	2	1	544	556	3
10	2	1	40	38	10
12	2	1	876	892	6
14	2	1	88	86	5
16	2	1	588	599	4
18	2	1	29	1	29
20	2	1	316	313	3
22	2	1	258	251	4
1	3	1	338	349	2
3	3	1	246	242	2
5	3	1	330	328	2
7	3	1	420	415	3
9	3	1	264	265	2
11	3	1	341	354	3
13	3	1	235	241	3
15	3	1	89	91	5
17	3	1	299	298	3
19	3	1	185	184	4
21	3	1	375	373	4
0	4	1	1156	1166	4
2	4	1	136	143	2
4	4	1	154	147	2
6	4	1	710	673	5
8	4	1	375	382	3
10	4	1	524	511	4
12	4	1	649	655	5
14	4	1	258	260	3
16	4	1	511	516	4
18	4	1	231	234	3
20	4	1	31	19	31
1	5	1	94	95	3
3	5	1	418	425	3
5	5	1	1292	1259	5
7	5	1	866	851	5
9	5	1	415	411	3
11	5	1	300	319	3
13	5	1	577	571	4
15	5	1	116	115	4
17	5	1	206	199	3
19	5	1	0	15	1
21	5	1	607	609	5
0	6	1	454	440	3
2	6	1	117	114	2
4	6	1	319	312	2
6	6	1	965	962	5
8	6	1	510	499	4
10	6	1	92	85	4
12	6	1	371	374	3
14	6	1	31	33	21
16	6	1	1003	1009	6
18	6	1	253	253	3
20	6	1	474	467	4
1	7	1	122	120	3
3	7	1	474	478	4
5	7	1	741	752	5
7	7	1	200	195	3
9	7	1	380	390	3
11	7	1	98	82	5
13	7	1	79	82	6
15	7	1	118	116	5
17	7	1	242	233	3
19	7	1	170	155	4
0	8	1	533	498	4
2	8	1	107	94	3
4	8	1	40	29	10
6	8	1	296	308	3
8	8	1	52	59	8
10	8	1	92	108	5
12	8	1	468	474	4
14	8	1	503	504	4
16	8	1	514	514	4
18	8	1	290	289	3
20	8	1	327	327	4
1	9	1	913	891	6
3	9	1	75	63	5
5	9	1	436	449	4
7	9	1	326	337	3
9	9	1	58	59	8
11	9	1	1658	1692	7
13	9	1	121	106	4
15	9	1	183	174	4
17	9	1	113	123	6
19	9	1	195	197	4
0	10	1	1404	1415	6
2	10	1	750	746	5
4	10	1	226	227	3
6	10	1	470	476	3
8	10	1	110	113	4
10	10	1	359	359	3
12	10	1	17	1	16
14	10	1	612	619	5
16	10	1	459	461	4
18	10	1	210	209	4
1	11	1	124	135	4
3	11	1	89	82	5
5	11	1	796	805	6
7	11	1	506	508	4
9	11	1	294	294	3
11	11	1	225	232	3
13	11	1	167	174	4
15	11	1	287	277	3
17	11	1	410	417	4
0	12	1	1019	1024	7
2	12	1	554	551	4
4	12	1	137	140	4
6	12	1	717	717	5
8	12	1	96	96	5
10	12	1	53	60	10
12	12	1	222	230	4
14	12	1	52	68	12
16	12	1	770	753	6
1	13	1	428	418	3
3	13	1	298	300	3
5	13	1	1023	1042	8
7	13	1	108	105	5
9	13	1	304	312	3
11	13	1	1199	1195	8
13	13	1	164	158	4
15	13	1	158	157	5
0	14	1	854	870	6
2	14	1	185	182	3
4	14	1	409	418	4
6	14	1	256	256	3
8	14	1	233	229	3
10	14	1	372	374	4
12	14	1	129	137	6
14	14	1	317	324	4
1	15	1	31	29	10
3	15	1	363	370	3
5	15	1	150	149	4
7	15	1	347	344	3
9	15	1	19	41	18
11	15	1	160	150	5
13	15	1	219	213	4
0	16	1	383	390	4
2	16	1	208	202	4
4	16	1	49	37	13
6	16	1	1287	1283	9
8	16	1	340	339	4
10	16	1	0	38	1
12	16	1	68	56	10
1	17	1	102	96	6
3	17	1	207	209	4
5	17	1	804	823	6
7	17	1	239	240	4
9	17	1	317	326	4
0	18	1	307	310	4
2	18	1	115	109	6
4	18	1	319	341	4
6	18	1	300	304	4
1	19	1	415	415	4
3	19	1	398	410	4
2	0	2	626	642	4
4	0	2	308	299	2
6	0	2	764	727	5
8	0	2	634	624	4
10	0	2	1513	1466	6
12	0	2	1000	1001	7
14	0	2	1330	1318	7
16	0	2	851	856	6
18	0	2	580	575	4
20	0	2	178	168	4
22	0	2	386	388	4
1	1	2	518	528	4
3	1	2	716	713	4
5	1	2	1111	1120	4
7	1	2	120	111	2
9	1	2	627	620	4
11	1	2	580	575	4
13	1	2	84	79	5
15	1	2	689	702	5
17	1	2	54	54	10
19	1	2	0	16	1
21	1	2	281	279	4
2	2	2	346	340	2
4	2	2	438	439	3
6	2	2	448	437	3
8	2	2	174	167	2
10	2	2	1383	1386	6
12	2	2	578	595	4
14	2	2	44	31	11
16	2	2	300	296	3
18	2	2	17	12	16
20	2	2	117	123	6
1	3	2	451	446	3
3	3	2	211	211	2
5	3	2	1164	1158	5
7	3	2	190	187	2
9	3	2	1415	1403	6
11	3	2	1497	1511	6
13	3	2	316	313	3
15	3	2	231	223	3
17	3	2	406	387	3
19	3	2	768	773	5
21	3	2	680	679	5
0	4	2	1924	1887	4
2	4	2	648	647	4
4	4	2	68	54	4
6	4	2	394	377	3
8	4	2	157	164	3
10	4	2	2051	2081	6
12	4	2	161	168	3
14	4	2	183	176	3
16	4	2	70	62	8
18	4	2	548	536	4
20	4	2	280	280	4
1	5	2	1050	1020	4
3	5	2	82	80	3
5	5	2	1849	1818	5
7	5	2	205	197	2
9	5	2	527	532	4
11	5	2	664	670	5
13	5	2	66	61	7
15	5	2	358	326	3
17	5	2	713	720	5
19	5	2	367	360	4
21	5	2	380	368	4
0	6	2	1123	1113	5
2	6	2	81	85	4
4	6	2	840	840	5
6	6	2	2500	2455	6
8	6	2	313	311	3
10	6	2	118	127	4
12	6	2	347	353	3
14	6	2	807	806	5
16	6	2	1539	1548	8
18	6	2	28	27	28
20	6	2	71	62	9
1	7	2	655	638	4
3	7	2	122	121	3
7	7	2	189	190	3
9	7	2	454	463	3
11	7	2	52	47	9
13	7	2	375	371	3
15	7	2	1010	1028	7
17	7	2	1044	1036	7
19	7	2	113	113	6
0	8	2	371	382	3
2	8	2	501	495	4
4	8	2	282	291	3
6	8	2	354	349	3
8	8	2	554	568	4
10	8	2	63	55	8
12	8	2	85	78	6
14	8	2	532	540	4
16	8	2	866	877	6
18	8	2	21	10	21
20	8	2	180	172	5
1	9	2	508	509	4
3	9	2	103	99	4
5	9	2	497	501	4
7	9	2	464	462	4
9	9	2	563	564	4
11	9	2	1568	1574	7
13	9	2	228	233	3
15	9	2	157	145	4
17	9	2	725	720	5
19	9	2	284	283	4

Observed and calculated structure factors for K1

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	10	2	582	570	4	7	1	1	721	713	5	6	12	3	211	209	3	18	4	4	134	129	5	5	15	4	235	237	4
4	10	2	647	654	5	9	1	1	217	207	3	8	12	3	30	23	29	1	5	4	972	960	6	7	15	4	71	67	9
6	10	2	68	64	6	11	1	1	1368	1388	7	10	12	3	84	78	7	3	5	4	119	109	3	9	15	4	214	218	4
8	10	2	287	295	3	13	1	1	23	20	23	12	12	3	241	228	4	5	5	4	1559	1587	6	0	16	4	148	148	5
10	10	2	1831	1859	8	15	1	1	157	168	4	14	12	3	155	162	5	7	5	4	393	393	3	2	16	4	221	216	4
12	10	2	416	414	4	17	1	1	241	253	3	16	12	3	474	466	4	9	5	4	39	39	13	4	16	4	90	61	7
14	10	2	296	303	3	19	1	1	115	119	6	1	13	3	123	120	3	11	5	4	903	907	6	6	16	4	439	436	4
16	10	2	166	160	5	21	1	1	418	421	4	3	13	3	392	408	4	13	5	4	50	48	11	8	16	4	0	3	1
18	10	2	211	204	4	0	4	1	2242	2159	5	5	13	3	448	452	4	15	5	4	285	283	3	1	17	4	339	331	4
1	11	2	400	398	3	2	4	3	26	19	14	7	13	3	104	110	5	17	5	4	132	133	5	3	17	4	210	199	4
3	11	2	679	681	5	4	4	3	310	303	3	9	13	3	252	250	3	19	5	4	120	101	6	1	1	5	72	28	5
5	11	2	33	18	17	6	4	3	277	266	2	11	13	3	501	490	4	0	6	4	2079	2110	6	3	1	5	153	159	3
7	11	2	30	10	24	8	4	3	173	186	3	13	13	3	41	14	19	2	6	4	183	183	3	5	1	5	720	720	5
9	11	2	599	602	4	10	4	3	578	584	4	15	13	3	68	69	10	4	6	4	301	300	3	7	1	5	31	28	19
11	11	2	1788	1796	8	12	4	3	696	713	5	0	14	3	214	211	3	6	6	4	398	404	-3	9	1	5	227	231	3
13	11	2	48	43	12	14	4	3	99	104	5	2	14	3	152	145	4	8	6	4	334	322	3	11	1	5	187	183	3
15	11	2	87	92	7	16	4	3	139	136	4	4	14	3	345	347	3	10	6	4	1328	1340	7	13	1	5	116	128	5
17	11	2	83	75	8	18	4	3	131	135	5	6	14	3	162	164	4	12	6	4	267	271	3	15	1	5	141	150	5
0	12	2	1365	1355	7	20	4	3	67	71	10	8	14	3	293	285	3	14	6	4	196	195	4	17	1	5	719	712	5
2	12	2	87	88	5	1	5	3	85	87	4	10	14	3	204	209	4	16	6	4	157	156	4	19	1	5	384	387	4
4	12	2	165	162	3	3	5	3	260	260	2	12	14	3	51	26	14	18	6	4	278	269	4	0	2	5	755	745	5
6	12	2	810	810	6	5	5	3	702	699	5	1	15	3	202	196	4	1	7	4	248	244	3	2	2	5	156	146	3
8	12	2	221	226	3	7	5	3	845	842	6	3	15	3	288	291	3	3	7	4	272	266	3	4	2	5	328	334	3
10	12	2	707	717	5	9	5	3	306	307	3	5	15	3	335	339	3	5	7	4	1248	1272	7	6	2	5	480	480	4
12	12	2	269	265	3	11	5	3	154	149	3	7	15	3	209	211	4	7	7	4	371	372	3	8	2	5	279	275	3
14	12	2	418	420	4	13	5	3	439	433	4	9	15	3	85	94	8	9	7	4	899	914	6	10	2	5	104	100	5
16	12	2	467	468	4	15	5	3	176	176	4	11	15	3	147	130	4	11	7	4	744	751	5	12	2	5	728	721	5
1	13	2	97	109	5	17	5	3	253	258	3	0	16	3	225	216	4	13	7	4	240	236	3	14	2	5	10	12	10
3	13	2	51	31	10	19	5	3	55	51	12	2	16	3	52	45	12	15	7	4	250	261	3	16	2	5	186	185	4
5	13	2	1750	1746	8	0	6	3	567	556	4	4	16	3	254	250	4	17	7	4	426	431	4	18	2	5	110	102	6
7	13	2	43	1	13	2	6	3	164	155	2	6	16	3	1114	1118	7	0	8	4	1899	1931	7	1	3	5	121	116	3
9	13	2	37	35	18	4	6	3	538	523	4	8	16	3	294	290	4	2	8	4	0	13	1	3	3	5	216	219	3
11	13	2	103	104	6	6	6	3	1243	1265	6	10	16	3	177	186	5	4	8	4	279	291	3	5	3	5	519	530	4
13	13	2	134	135	5	8	6	3	353	359	3	1	17	3	160	165	5	6	8	4	580	577	4	7	3	5	122	85	4
15	13	2	569	556	5	10	6	3	141	147	3	3	17	3	241	235	4	8	8	4	397	408	3	9	3	5	132	129	4
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4	14	2	697	701	5	16	6	3	1090	1075	7	0	18	3	193	191	4	14	8	4	73	71	8	15	3	5	33	29	30
6	14	2	486	483	4	18	6	3	375	380	4	2	18	3	209	212	4	16	8	4	267	263	4	17	3	5	515	513	4
8	14	2	196	186	4	20	6	3	426	421	4	4	18	3	158	159	5	18	8	4	54	55	13	0	4	5	164	164	3
10	14	2	61	66	10	1	7	3	145	143	3	2	0	4	339	343	3	1	9	4	77	63	6	2	4	5	89	77	5
12	14	2	49	22	13	3	7	3	183	188	3	4	0	4	574	579	4	3	9	4	210	208	3	4	4	5	59	61	7
14	14	2	319	333	4	5	7	3	1421	1412	6	6	0	4	320	308	3	5	9	4	1762	1780	7	6	4	5	638	621	4
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5	15	2	1475	1466	8	11	7	3	853	862	6	12	0	4	1011	1011	7	11	9	4	209	204	3	12	4	5	426	435	4
7	15	2	461	449	4	13	7	3	126	126	4	14	0	4	418	417	3	13	9	4	72	75	8	14	4	5	261	261	3
9	15	2	50	15	13	15	7	3	55	10	10	16	0	4	31	27	30	15	9	4	536	544	4	16	4	5	570	568	4
11	15	2	406	409	4	17	7	3	652	644	5	18	0	4	476	476	4	17	9	4	640	631	5	18	4	5	242	246	4
13	15	2	150	149	5	19	7	3	138	126	5	20	0	4	313	310	4	0	10	4	847	846	6	1	5	5	140	128	3
0	16	2	929	922	7	0	8	3	978	952	6	1	1	4	345	331	3	2	10	4	0	19	1	3	5	5	223	221	3
2	16	2	170	161	4	2	8	3	46	46	9	3	1	4	60	45	5	4	10	4	430	417	3	5	5	5	585	579	4
4	16	2	109	117	6	4	8	3	243	250	3	5	1	4	163	152	3	6	10	4	189	186	3	7	5	5	583	579	4
6	16	2	531	530	4	6	8	3	551	549	4	7	1	4	36	18	12	8	10	4	283	286	3	9	5	5	304	305	3
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3	17	2	379	370	4	14	8	3	301	297	3	15	1	4	153	154	4	16	10	4	428	424	4	17	5	5	141	140	5
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7	17	2	125	125	6	18	8	3	113	115	6	19	1	4	497	490	4	3	11	4	342	340	3	2	6	5	65	63	6
9	17	2	329	332	4	1	9	3	559	562	4	0	2	4	339	356	3	5	11	4	1004	1027	8	4	6	5	13	10	12
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2	18	2	82	72	8	5	9	3	227	223	3	4	2	4	191	186	3	9	11	4	98	69	6	8	6	5	329	334	3
4	18	2	279	286	4	7	9	3	232	229	3	6	2	4	433	454	3	11	11	4	0	17	1	10	6	5	43	47	12
6	18	2	359	364	4	9	9	3	93	88	5	8	2	4	103	109	4	13	11	4	167	169	4	12	6	5	277	271	3
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3	1	3	566	561	4	13	9	3	57	61	10	12	2	4	375	376	3	0	12	4	995	961	6	16	6	5	684	684	5
5	1	3	113	110	3	15	9	3	190	178	4	14	2	4	635	638	4	2	12	4	181	176	3	1	7	5	78	72	6
7	1	3	360	363	3	17	9	3	445	458	4	16	2	4	755	770	5	4	12	4	261	265	3	3	7	5	400	413	4
9	1	3	232	235	3	0	10	3	996	1010	7	18	2	4	138	135	5	6	12	4	291	291	3	5	7	5	239	234	3
11	1	3	1268	1279	7	2	10	3	730	737	5	20	2	4	51	49	14	8	12	4	227	225	3	7	7	5	299	297	3
13	1	3	364	368	3	4	10	3	318	321	3	1	3	4	176	177	2	10	12	4	516	517	4	9	7	5	260	263	3
15	1	3	270	273	3	6	10	3	255	252	3	3	3	4	386	378	3	12	12	4	379	375	4	11	7	5	322	318	3
17	1	3	320	321	3	8	10	3	169	174	3	5	3	4	3450	3459	6	14	12	4	64	66	10	13	7	5	184	176	4
19	1	3	469	475	4	10	10	3	158	167	4	7	3	4	177	178	3	1	13	4	330	338	4	15	7	5	152	154	5
21	1	3	635	629	5	12	10	3	89	96	6	9	3	4	645	648	5	3	13	4	131	135	5	17	7	5	37	36	26
0	2	3	2216	2162	4	14	10	3	604	601	5	11	3	4	169	170	3	5	13	4	218	221	4	0	8	5	690	707	5
2	2	3	657	644	5	16	10	3	247	253	4	13	3	4	291	293	3	7	13	4	280	283	3	2	8	5	192	184	3
4	2	3	211	208	2	1	11	3	251	250	3	15	3	4	821	825	6	9	13	4	333	330	3	4	8	5	87	95	6
6	2	3	1081	1051	5	3	11	3	52	39	9	17	3	4	799	777	5	11	13	4	752	744	6	6	8	5	554	556	4
8	2	3	660	651	5	5	11	3	854	850	6	19	3	4	245	245	4	13	13	4	138	141	5	8	8	5	71	75	7
10	2	3	76	75	6	7	11	3	204	200	3	0	4	4	569	586	4	0	14	4	1317	1342	9	10	8	5	82	85	7
12	2	3	663	676	5	9	11	3	355	354	3	2	4	4	458	441	3	2	14	4	221	221	4	12	8	5	324	327	3
14	2	3	292	293	3	11	11	3	37	31	18	4	4	4	555	576	4	4	14	4	318	315	3	14	8	5	451	447	4
16	2	3	954	968	7	13	11	3	0	7	1	6	4	4	1962	1959	6	6	14	4	452	451	4	16	8	5	607	600	5
18	2	3	184	187	4	15	11	3	129	118	5	8	4	4	171	175	3	8	14	4	150	144	5	1	9	5	665	664	5
20	2	3	223	227	4	17	11	3	520	522	4	10	4	4	355	362	3	10	14	4	974	976	7	3	9	5	33	20	19
1	3	3	496	491	3	0	12	3	167	164	3	12	4	4	152	151	4	12	14	4	58	53	12	5	9	5	530	536	4
3	3	3	254	255	2	2	12	3	333	330	3	14	4	4	714	713	5	1	15	4	296	301	3	7	9	5	330	330	3
5	3	3	1035	1007	5	4	12	3	388	392	3	16	4	4	1498	1520	9	3	15	4	361	353	4	9	9	5	41	45	15

Observed and calculated structure factors for K1

h	k	l	10Fo	10Fc	10s
11	9	5	1509	1534	9
13	9	5	146	146	5
15	9	5	161	158	5
0	10	5	1120	1111	8
2	10	5	466	474	4
4	10	5	87	85	6
6	10	5	494	483	4
8	10	5	77	78	7
10	10	5	352	348	3
12	10	5	78	65	8
14	10	5	463	463	4
1	11	5	41	38	14
3	11	5	79	86	7
5	11	5	565	551	4
7	11	5	505	505	4
9	11	5	194	190	4
11	11	5	300	302	3
13	11	5	225	223	4
0	12	5	1028	1034	7
2	12	5	525	524	4
4	12	5	34	29	22
6	12	5	751	748	5
8	12	5	59	58	10
10	12	5	0	2	1
12	12	5	198	187	4
1	13	5	360	358	4
3	13	5	208	209	4
5	13	5	996	1005	7
7	13	5	197	195	4
9	13	5	283	273	4
11	13	5	1282	1262	8
0	14	5	1027	1006	7
2	14	5	154	155	5
4	14	5	333	326	4
6	14	5	412	414	4
8	14	5	149	147	5
10	14	5	393	390	4
1	15	5	68	68	10
3	15	5	299	303	4
5	15	5	0	4	1
7	15	5	325	323	4
0	16	5	329	326	4
2	16	5	231	235	4
4	16	5	91	88	8
0	0	6	2589	2589	7
2	0	6	113	110	4
4	0	6	599	602	4
6	0	6	669	680	5
8	0	6	398	400	3
10	0	6	907	914	7
12	0	6	746	756	5
14	0	6	760	757	6
16	0	6	895	896	7
1	1	6	175	170	3
3	1	6	111	106	4
5	1	6	1691	1705	7
7	1	6	115	122	4
9	1	6	132	141	3
11	1	6	235	243	3
13	1	6	43	52	16
15	1	6	451	447	4
17	1	6	321	313	4
0	2	6	1734	1729	7
2	2	6	187	188	3
4	2	6	150	141	3
6	2	6	472	472	4
8	2	6	183	186	3
10	2	6	858	868	6
12	2	6	336	335	3
14	2	6	24	41	23
16	2	6	344	345	3
1	3	6	244	235	3
3	3	6	55	48	8
5	3	6	869	878	6
7	3	6	77	76	6
9	3	6	938	947	7
11	3	6	1170	1174	8
13	3	6	128	137	5
15	3	6	106	113	6
17	3	6	394	390	4
0	4	6	2395	2406	7
2	4	6	51	56	9
4	4	6	330	339	3
6	4	6	531	540	4
8	4	6	140	146	4
10	4	6	1358	1373	8
12	4	6	168	170	4
14	4	6	36	19	23
16	4	6	230	234	4
1	5	6	329	327	3
3	5	6	304	305	3
5	5	6	515	515	4
7	5	6	102	99	5
9	5	6	296	305	3
11	5	6	299	303	3
13	5	6	84	81	7
15	5	6	290	293	4
0	6	6	110	108	5
2	6	6	53	48	9
4	6	6	366	365	3
6	6	6	933	941	6
8	6	6	319	315	3
10	6	6	14	22	13
12	6	6	172	175	4
14	6	6	711	717	5
16	6	6	797	795	6
1	7	6	509	517	4
3	7	6	92	82	5
5	7	6	2456	2497	8
7	7	6	127	111	4
9	7	6	352	364	4
11	7	6	386	391	4
13	7	6	242	236	4
15	7	6	706	700	5
0	8	6	254	248	3
2	8	6	225	222	3
4	8	6	357	359	3
6	8	6	254	257	3
8	8	6	140	142	3
10	8	6	174	173	4
12	8	6	109	107	6
14	8	6	174	175	4
1	9	6	387	384	3
3	9	6	67	72	8
5	9	6	28	8	28
7	9	6	525	530	4
9	9	6	379	380	3
11	9	6	728	724	5
13	9	6	21	42	21
0	10	6	2171	2181	8
2	10	6	256	250	3
4	10	6	243	243	3
6	10	6	521	528	4
8	10	6	105	105	6
10	10	6	1296	1295	9
12	10	6	247	250	4
1	11	6	136	134	5
3	11	6	326	321	3
5	11	6	442	451	4
7	11	6	119	116	5
9	11	6	445	440	4
11	11	6	771	770	5
0	12	6	562	552	4
2	12	6	101	104	6
4	12	6	141	140	5
6	12	6	855	852	6
8	12	6	92	85	7
10	12	6	400	385	4
1	13	6	0	23	1
3	13	6	30	23	30
5	13	6	1103	1296	9
7	13	6	144	131	5
0	14	6	90	85	7
2	14	6	349	355	4
4	14	6	311	308	4
6	14	6	150	153	5
1	1	7	67	70	7
3	1	7	205	199	3
5	1	7	81	83	6
7	1	7	277	273	3
9	1	7	139	136	5
11	1	7	697	700	5
13	1	7	272	270	4
15	1	7	210	212	4
0	2	7	659	677	4
2	2	7	144	138	3
4	2	7	55	47	9
6	2	7	479	478	4
8	2	7	271	264	3
10	2	7	44	23	15
12	2	7	454	457	4
14	2	7	156	155	5
1	3	7	224	224	3
3	3	7	31	11	22
5	3	7	425	421	4
7	3	7	382	390	3
9	3	7	153	159	4
11	3	7	837	828	6
13	3	7	51	45	14
0	4	7	1077	1049	6
2	4	7	50	53	11
4	4	7	181	178	4
6	4	7	154	138	4
8	4	7	147	151	4
10	4	7	395	396	4
12	4	7	455	455	4
14	4	7	106	112	6
1	5	7	21	18	21
3	5	7	123	122	5
5	5	7	269	216	3
7	5	7	512	511	4
9	5	7	213	218	4
11	5	7	40	43	20
13	5	7	254	267	4
0	6	7	254	251	3
2	6	7	133	135	4
4	6	7	227	231	3
6	6	7	729	723	5
8	6	7	236	247	4
10	6	7	123	121	5
12	6	7	214	216	4
1	7	7	89	98	6
3	7	7	199	198	4
5	7	7	843	855	6
7	7	7	125	112	5
9	7	7	288	281	3
11	7	7	542	542	4
0	8	7	608	591	4
2	8	7	35	32	20
4	8	7	181	176	4
6	8	7	345	340	3
8	8	7	0	7	1
10	8	7	181	178	4
12	8	7	368	366	4
1	9	7	323	333	4
3	9	7	92	88	7
5	9	7	222	212	4
7	9	7	147	150	5
9	9	7	39	25	20
11	9	7	557	571	5
0	10	7	636	644	5
2	10	7	411	417	4
4	10	7	159	156	5
6	10	7	202	192	4
8	10	7	91	89	7
1	11	7	132	136	5
3	11	7	44	33	17
5	11	7	581	579	5
7	11	7	139	143	5
0	12	7	27	20	26
2	12	7	216	213	4
4	12	7	263	255	4
1	13	7	203	205	4
0	0	8	2538	2569	8
2	0	8	131	133	5
4	0	8	188	190	4
6	0	8	663	662	5
8	0	8	65	54	10
10	0	8	1549	1541	9
12	0	8	530	522	4
1	1	8	141	137	5
3	1	8	99	100	6
5	1	8	426	431	4
7	1	8	224	214	4
9	1	8	646	631	5
11	1	8	555	554	4
0	2	8	21	0	20
2	2	8	96	99	6
4	2	8	237	229	4
6	2	8	495	492	4
8	2	8	34	17	33
10	2	8	225	213	4
1	3	8	91	96	6
3	3	8	263	264	3
5	3	8	1819	1831	9
7	3	8	11	4	11
9	3	8	146	154	4
11	3	8	90	85	7
0	4	8	187	205	4
2	4	8	292	296	3
4	4	8	215	204	4
6	4	8	643	661	5
8	4	8	0	13	1
10	4	8	174	173	5
1	5	8	530	524	4
3	5	8	142	144	5
5	5	8	456	453	4
7	5	8	33	22	32
9	5	8	73	78	9
0	6	8	1829	1828	9
2	6	8	174	178	4
4	6	8	277	273	4
6	6	8	478	476	4
8	6	8	118	129	6
1	7	8	49	51	15
3	7	8	192	186	4
5	7	8	882	887	6
7	7	8	211	217	4
0	8	8	950	951	7
2	8	8	30	45	10
4	8	8	87	75	7
6	8	8	399	405	4
1	9	8	0	11	1
3	9	8	102	95	7
5	9	8	1226	1242	8
0	10	8	1024	1021	7
2	10	8	83	74	8
1	1	9	0	11	1
3	1	9	143	144	5
5	1	9	328	325	4
0	2	9	128	119	6
2	2	9	100	104	7
4	2	9	108	111	6
6	2	9	62	42	10
1	3	9	106	100	6
3	3	9	40	15	20
5	3	9	110	101	6
0	4	9	424	416	4
2	4	9	32	46	32
4	4	9	67	64	10
1	5	9	0	10	1
3	5	9	72	59	9
0	6	9	120	108	6

Observed and calculated structure factors for K2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	679	699	4	0	8	0	2618	2585	9	3	19	0	126	107	11	3	9	1	73	68	12	1	1	2	505	513	4
4	0	0	1177	1165	5	2	8	0	175	169	4	1	1	1	151	145	3	5	9	1	383	399	4	3	1	2	763	763	5
6	0	0	613	625	5	4	8	0	489	487	4	3	1	1	372	365	3	7	9	1	331	346	4	5	1	2	1074	1068	7
8	0	0	957	932	6	6	8	0	619	617	5	5	1	1	935	931	6	9	9	1	60	54	17	7	1	2	124	116	5
10	0	0	3735	3742	10	8	8	0	461	465	4	7	1	1	0	23	1	11	9	1	1729	1696	12	9	1	2	628	628	5
12	0	0	1432	1442	10	10	8	0	1247	1238	9	9	1	1	328	327	4	13	9	1	114	108	10	11	1	2	606	608	5
14	0	0	232	229	5	12	8	0	131	140	8	11	1	1	777	793	6	15	9	1	157	156	8	13	1	2	45	40	32
16	0	0	306	300	5	14	8	0	118	118	9	13	1	1	317	315	4	17	9	1	144	141	9	15	1	2	669	673	6
18	0	0	458	458	5	16	8	0	319	323	5	15	1	1	189	184	6	19	9	1	180	194	8	17	1	2	61	67	21
20	0	0	376	368	6	18	8	0	11	39	10	17	1	1	707	703	6	0	10	1	1316	1342	10	19	1	2	32	11	31
22	0	0	1775	1792	13	20	8	0	328	299	6	19	1	1	466	483	5	2	10	1	768	751	6	21	1	2	311	308	6
1	1	0	783	798	3	1	9	0	104	86	7	21	1	1	716	720	7	4	10	1	219	216	5	0	2	2	4041	4103	8
3	1	0	214	211	3	3	9	0	368	371	4	0	2	1	90	115	5	6	10	1	468	475	4	2	2	2	355	351	3
5	1	0	495	501	4	5	9	0	1852	1893	10	2	2	1	550	565	4	8	10	1	147	147	7	4	2	2	477	473	4
7	1	0	436	438	4	7	9	0	879	860	6	4	2	1	408	404	3	10	10	1	307	312	5	6	2	2	460	451	4
9	1	0	1589	1564	8	9	9	0	60	58	17	6	2	1	257	246	3	12	10	1	31	17	30	8	2	2	232	220	4
11	1	0	2967	2948	10	11	9	0	646	626	5	8	2	1	528	541	4	14	10	1	598	600	6	10	2	2	1338	1344	10
13	1	0	407	409	4	13	9	0	231	227	6	10	2	1	62	87	14	16	10	1	384	398	6	12	2	2	563	569	5
15	1	0	263	273	5	15	9	0	653	679	6	12	2	1	913	916	6	18	10	1	210	211	7	14	2	2	76	51	13
17	1	0	360	364	5	17	9	0	512	520	5	14	2	1	120	113	9	1	11	1	134	137	7	16	2	2	327	325	5
19	1	0	544	549	6	19	9	0	193	199	8	16	2	1	620	627	5	3	11	1	140	137	7	18	2	2	0	17	1
21	1	0	800	807	7	0	10	0	308	320	4	18	2	1	0	28	1	5	11	1	757	765	6	20	2	2	72	74	21
0	2	0	1278	1311	4	2	10	0	44	43	24	20	2	1	290	282	6	7	11	1	531	530	5	1	3	2	458	454	4
2	2	0	279	101	3	4	10	0	362	366	4	22	2	1	240	233	7	9	11	1	287	284	5	3	3	2	244	249	3
4	2	0	617	630	5	6	10	0	265	266	5	1	3	1	354	360	3	11	11	1	281	272	5	5	3	2	1124	1101	7
6	2	0	149	158	4	8	10	0	250	265	5	3	3	1	257	254	3	13	11	1	151	158	8	7	3	2	184	176	4
8	2	0	274	279	3	10	10	0	513	515	5	5	3	1	357	348	3	15	11	1	210	223	7	9	3	2	1436	1449	9
10	2	0	613	622	5	12	10	0	229	229	6	7	3	1	432	434	4	17	11	1	435	442	6	11	3	2	1469	1477	10
12	2	0	389	389	4	14	10	0	1085	1099	7	9	3	1	239	237	4	0	12	1	1029	1040	8	13	3	2	151	147	4
14	2	0	875	852	7	16	10	0	269	277	6	11	3	1	313	318	4	2	12	1	535	538	5	15	3	2	201	191	6
16	2	0	754	761	6	18	10	0	408	417	6	13	3	1	228	230	5	4	12	1	120	124	8	17	3	2	179	182	5
18	2	0	79	90	15	1	11	0	274	266	4	15	3	1	86	78	12	6	12	1	697	682	6	19	3	2	788	782	7
20	2	0	112	108	12	3	11	0	252	262	5	17	3	1	289	295	5	8	12	1	110	105	9	21	3	2	633	630	6
22	2	0	270	268	7	5	11	0	814	824	6	19	3	1	192	185	7	10	12	1	107	92	10	0	4	2	1806	1849	7
1	3	0	302	297	3	7	11	0	110	111	9	21	3	1	351	351	6	12	12	1	260	254	6	2	4	2	619	619	4
3	3	0	531	536	4	9	11	0	106	88	10	0	4	1	1130	1133	6	14	12	1	49	62	36	4	4	2	62	51	10
5	3	0	4996	4825	9	11	11	0	432	447	5	2	4	1	135	134	4	16	12	1	740	740	7	6	4	2	368	356	4
7	3	0	529	522	4	13	11	0	204	213	7	4	4	1	175	172	4	1	13	1	419	412	4	8	4	2	98	114	8
9	3	0	884	888	6	15	11	0	793	780	6	6	4	1	746	705	5	3	13	1	327	336	5	10	4	2	2002	2035	10
11	3	0	404	403	4	17	11	0	433	443	6	8	4	1	416	407	4	5	13	1	990	999	8	12	4	2	187	200	6
13	3	0	299	293	4	0	12	0	1494	1530	11	10	4	1	449	431	4	7	13	1	85	96	13	14	4	2	196	196	6
15	3	0	895	889	7	2	12	0	217	206	5	12	4	1	670	682	6	9	13	1	287	303	6	16	4	2	99	29	11
17	3	0	985	987	7	4	12	0	312	304	5	14	4	1	250	250	5	11	13	1	1159	1159	8	18	4	2	496	499	5
19	3	0	271	262	6	6	12	0	596	591	5	16	4	1	557	562	5	13	13	1	183	166	8	20	4	2	271	283	7
21	3	0	332	343	6	8	12	0	180	181	6	18	4	1	243	248	6	15	13	1	205	198	8	1	5	2	995	975	7
0	4	0	2072	2098	6	10	12	0	699	705	6	20	4	1	0	11	1	0	14	1	786	801	6	3	5	2	92	90	7
2	4	0	614	607	4	12	12	0	508	512	5	1	5	1	104	106	5	2	14	1	214	208	6	5	5	2	1876	1822	8
4	4	0	1021	1008	7	14	12	0	102	115	13	3	5	1	422	426	3	4	14	1	192	194	5	7	5	2	231	217	4
6	4	0	1921	1766	9	16	12	0	6	53	6	5	5	1	1351	1309	8	6	14	1	276	281	6	9	5	2	467	468	4
8	4	0	427	424	4	1	13	0	527	525	5	7	5	1	893	875	6	8	14	1	269	259	6	11	5	2	656	653	5
10	4	0	446	443	4	3	13	0	168	181	7	9	5	1	483	469	4	10	14	1	294	310	6	13	5	2	46	44	29
12	4	0	255	254	5	5	13	0	370	369	5	11	5	1	299	316	4	12	14	1	168	164	8	15	5	2	299	300	5
14	4	0	755	740	6	7	13	0	470	478	5	13	5	1	549	551	5	14	14	1	122	126	6	17	5	2	704	709	6
16	4	0	2053	2063	13	9	13	0	403	396	5	15	5	1	33	60	32	1	15	1	0	6	1	19	5	2	168	172	6
18	4	0	62	58	21	11	13	0	931	930	7	17	5	1	201	200	7	3	15	1	339	349	5	21	5	2	398	393	6
20	4	0	189	186	8	13	13	0	269	277	6	19	5	1	63	18	22	5	15	1	183	179	7	0	6	2	1089	1107	8
22	4	0	487	490	6	15	13	0	240	245	7	21	5	1	645	643	6	7	15	1	354	363	5	2	6	2	101	109	6
1	5	0	1452	1444	6	0	14	0	1391	1389	10	0	6	1	501	487	4	9	15	1	0	36	1	4	6	2	908	920	7
3	5	0	65	62	9	2	14	0	361	366	5	2	6	1	123	117	5	11	15	1	139	130	10	6	6	2	2488	2417	9
5	5	0	1226	1109	8	4	14	0	208	211	6	4	6	1	262	259	3	13	15	1	198	194	8	8	6	2	300	295	4
7	5	0	885	860	7	6	14	0	691	686	6	6	6	1	940	946	7	0	16	1	152	142	5	10	6	2	68	74	14
9	5	0	55	55	16	8	14	0	130	131	9	8	6	1	537	522	4	2	16	1	225	219	6	12	6	2	352	359	4
11	5	0	368	378	4	10	14	0	1277	1260	8	10	6	1	120	119	8	4	16	1	7	22	7	14	6	2	864	860	7
13	5	0	274	269	5	12	14	0	70	88	22	12	6	1	168	162	4	6	16	1	1283	1279	10	16	6	2	1525	1523	11
15	5	0	246	251	5	14	14	0	52	9	35	14	6	1	0	8	1	8	16	1	328	335	6	18	6	2	0	14	1
17	5	0	509	508	5	1	15	0	281	285	5	16	6	1	1011	1018	8	10	16	1	48	3	42	20	6	2	86	78	16
19	5	0	172	184	8	3	15	0	372	372	5	18	6	1	285	277	6	12	16	1	66	67	21	1	7	2	658	649	5
21	5	0	406	408	6	5	15	0	510	512	5	20	6	1	469	460	6	1	17	1	102	104	13	3	7	2	56	56	14
0	6	0	845	861	6	7	15	0	48	74	34	1	7	1	148	146	5	3	17	1	246	250	7	5	7	2	4578	4463	11
2	6	0	187	188	3	9	15	0	155	167	9	3	7	1	504	507	4	5	17	1	774	778	6	7	7	2	189	189	5
4	6	0	317	324	3	11	15	0	399	398	6	5	7	1	633	634	5	7	17	1	232	227	7	9	7	2	461	468	4
6	6	0	500	484	4	13	15	0	375	385	6	7	7	1	216	206	4	9	17	1	334	336	6	11	7	2	51	65	23
8	6	0	672	654	5	0	16	0	602	595	5	9	7	1	381	391	4	0	18	1	300	302	6	13	7	2	340	332	5
10	6	0	1433	1432	10	2	16	0	221	215	6	11	7	1	47	63	26	2	18	1	106	105	12	15	7	2	970	977	7
12	6	0	182	189	6	4	16	0	180	176	7	13	7	1	70	72	15	4	18	1	301	315	6	17	7	2	1016	1019	8
14	6	0	420	424	5	6	16	0	790	810	6	15	7	1	63	67	20	6	18	1	300	296	7	19	7	2	91	87	15
16	6	0	493	497	5	8	16	0	66	69	21	17	7	1	225	230	7	1	19	1	188	376	6	0	8	2	419	426	4
18	6	0	362	363	5	10	16	0	90	84	15	19	7	1	143	139	10	3	19	1	409	414	6	2	8	2	472	474	4
20	6	0	0	7	1	12	16	0	444	460	6	0	8	1	567	540	4	0	0	2	3249	3369	7	4	8	2	223	231	5
1	7	0	645	622	5	1	17	0	282	286	6	2	8	1	94	75	7	2	0	2	600	620	4	6	8	2	394	388	4
3	7	0	185	186	4	3	17	0	276	275	6	4	8	1	0	10	1	4	0	2	288	292	1	8	8	2	553	556	5
5	7	0	1403	1382	9	5	17	0	1782	1766	12	6	8	1	294	306	4	6	0	2	746	710	5	10	8	2	63	40	16
7	7	0	500	484	4	7	17	0	0	9	1	8	8	1	75	77	12	8	0	2	567	563	4	12	8	2	96	81	11
9	7	0	1175	1162	8	9	17	0	59	52	25	10	8	1	58	61	18	10	0	2	1449	1414	9	14	8	2	520	528	5
11	7	0	637	597	5	0	18	0	341	339	6	12	8	1	505	498	5	12	0	2	998	1004	7	16	8	2	878	881	7
13	7	0	298	298	5	2	18	0	287	283	6	14	8	1	517	517	5	14	0	2	1298	1296	9	18	8	2	15	17	14
15	7	0	252	265	5	4	18	0	88	64	15	16	8	1	581	582	6	16	0	2	794	799	7	1	9	2	493	473	4
17	7	0	353	339	5	6	18	0	289	283	7	18	8	1	301	309	6	18	0	2	629	626	6	3	9	2	81	85	11
19	7	0	660	658	6	8	18	0	299	289	6	20	8	1	317	316	6	20	0	2	145	136	10	5	9	2	503	500	5
21	7	0	610	595	6	1	19	0	185	181	8	1	9	1	929	911	6	22	0	2	362	365	6	7	9	2	445	448	5

Observed and calculated structure factors for K2

h	k	l	10Fo	10Fc	10s
9	9	2	618	630	5
11	9	2	1620	1574	12
13	9	2	178	184	7
15	9	2	203	194	7
17	9	2	695	696	6
19	9	2	278	285	7
0	10	2	4346	4380	12
2	10	2	625	624	5
4	10	2	697	696	6
6	10	2	52	72	21
8	10	2	257	261	5
10	10	2	1826	1836	12
12	10	2	391	376	5
14	10	2	318	323	6
16	10	2	196	197	8
18	10	2	199	200	8
1	11	2	406	412	4
3	11	2	685	687	5
5	11	2	27	31	27
7	11	2	20	3	19
9	11	2	601	596	5
11	11	2	1810	1810	11
13	11	2	75	45	16
15	11	2	114	125	12
17	11	2	62	52	27
0	12	2	1312	1322	9
2	12	2	71	68	13
4	12	2	113	109	9
6	12	2	813	818	6
8	12	2	177	186	7
10	12	2	722	722	6
12	12	2	256	255	6
14	12	2	469	466	5
16	12	2	448	451	6
1	13	2	142	156	8
3	13	2	69	69	15
5	13	2	1754	1773	13
7	13	2	0	8	1
9	13	2	99	97	11
11	13	2	110	117	10
13	13	2	116	116	12
15	13	2	526	525	6
0	14	2	367	373	5
2	14	2	314	308	5
4	14	2	705	705	6
6	14	2	492	486	5
8	14	2	188	186	7
10	14	2	90	86	14
12	14	2	54	25	29
14	14	2	142	152	6
1	15	2	601	594	6
3	15	2	257	254	6
5	15	2	1458	1453	10
7	15	2	464	462	5
9	15	2	39	49	38
11	15	2	402	404	6
13	15	2	139	128	10
0	16	2	963	959	7
2	16	2	146	141	9
4	16	2	60	73	22
6	16	2	516	521	5
8	16	2	14	47	14
10	16	2	752	747	6
1	17	2	267	247	6
3	17	2	370	365	6
5	17	2	94	93	14
7	17	2	96	93	14
9	17	2	161	354	6
0	18	2	710	692	6
2	18	2	63	63	23
4	18	2	258	258	7
6	18	2	189	185	6
1	1	3	221	219	3
3	1	3	563	562	4
5	1	3	118	112	6
7	1	3	346	351	4
9	1	3	284	285	4
11	1	3	1318	1320	9
13	1	3	193	403	5
15	1	3	246	244	6
17	1	3	322	329	5
19	1	3	472	471	5
21	1	3	708	692	6
0	2	3	2124	2135	8
2	2	3	637	633	5
4	2	3	141	134	5
6	2	3	1099	1076	7
8	2	3	637	643	5
10	2	3	124	133	8
12	2	3	687	695	5
14	2	3	322	318	5
16	2	3	1000	1009	7
18	2	3	207	216	7
20	2	3	195	203	8
1	3	3	527	518	4
3	3	3	237	236	3
5	3	3	1027	1004	7
7	3	3	745	715	6
9	3	3	185	189	5
11	3	3	1353	1371	11
13	3	3	5	19	5
15	3	3	157	159	7
17	3	3	259	261	6
19	3	3	129	112	11
21	3	3	406	405	6
0	4	3	2154	2143	8
2	4	3	23	22	22
4	4	3	326	318	4
6	4	3	264	251	4
8	4	3	200	204	5
10	4	3	537	521	5
12	4	3	736	740	6
14	4	3	96	96	11
16	4	3	164	164	8
18	4	3	147	150	9
20	4	3	38	40	38
1	5	3	85	79	8
3	5	3	257	263	4
5	5	3	736	728	6
7	5	3	865	863	7
9	5	3	350	359	5
11	5	3	142	140	7
13	5	3	413	412	5
15	5	3	119	125	9
17	5	3	281	263	6
19	5	3	62	54	24
0	6	3	500	514	4
2	6	3	156	147	5
4	6	3	479	470	4
6	6	3	1232	1249	8
8	6	3	379	375	4
10	6	3	168	171	6
12	6	3	328	322	5
14	6	3	70	80	16
16	6	3	1090	1088	8
18	6	3	404	404	6
20	6	3	426	416	6
1	7	3	186	169	5
3	7	3	220	224	4
5	7	3	1362	1320	10
7	7	3	173	183	6
9	7	3	402	405	4
11	7	3	851	849	7
13	7	3	120	130	10
15	7	3	64	57	20
17	7	3	662	643	6
19	7	3	101	105	14
0	8	3	943	934	7
2	8	3	53	53	17
4	8	3	273	272	4
6	8	3	574	565	5
8	8	3	75	82	13
10	8	3	180	180	6
12	8	3	578	582	5
14	8	3	314	308	5
16	8	3	96	89	13
18	8	3	124	136	12
1	9	3	578	574	5
3	9	3	154	145	6
5	9	3	295	279	5
7	9	3	241	239	5
9	9	3	76	76	14
11	9	3	911	911	7
13	9	3	55	66	25
15	9	3	169	160	8
17	9	3	472	481	6
0	10	3	909	928	7
2	10	3	739	747	6
4	10	3	317	318	4
6	10	3	236	237	5
8	10	3	201	209	6
10	10	3	115	118	9
12	10	3	90	88	13
14	10	3	573	583	6
16	10	3	185	185	8
1	11	3	249	245	5
3	11	3	92	86	10
5	11	3	836	814	7
7	11	3	222	224	6
9	11	3	345	345	5
11	11	3	31	1	31
13	11	3	36	17	36
15	11	3	66	67	22
17	11	3	532	542	6
0	12	3	166	172	6
2	12	3	122	117	5
4	12	3	374	377	5
6	12	3	187	182	6
8	12	3	0	31	1
10	12	3	79	99	15
12	12	3	238	247	7
14	12	3	154	156	9
16	12	3	449	447	6
1	13	3	109	101	5
3	13	3	424	440	5
5	13	3	401	401	5
7	13	3	103	112	11
9	13	3	242	239	6
11	13	3	468	442	5
13	13	3	45	29	45
15	13	3	98	105	14
0	14	3	138	135	8
2	14	3	180	168	7
4	14	3	324	327	5
6	14	3	134	147	9
8	14	3	307	312	6
10	14	3	141	141	9
12	14	3	52	47	34
1	15	3	182	173	7
3	15	3	271	271	6
5	15	3	165	171	6
7	15	3	230	225	7
9	15	3	86	89	15
11	15	3	140	125	6
0	16	3	178	184	8
2	16	3	73	63	17
4	16	3	224	235	7
6	16	3	1121	1118	8
8	16	3	289	286	6
10	16	3	164	153	9
1	17	3	166	172	9
3	17	3	252	269	7
5	17	3	503	491	6
7	17	3	28	27	27
0	18	3	195	198	8
2	18	3	205	208	8
4	18	3	153	138	10
0	0	4	6595	6632	12
2	0	4	375	379	4
4	0	4	609	621	5
6	0	4	344	338	4
8	0	4	101	101	4
10	0	4	2725	2727	12
12	0	4	1006	990	7
14	0	4	372	383	5
16	0	4	90	95	14
18	0	4	477	465	5
20	0	4	243	249	8
1	1	4	322	325	4
3	1	4	68	55	11
5	1	4	220	193	4
7	1	4	0	8	1
9	1	4	1173	1172	9
11	1	4	1709	1707	11
13	1	4	242	230	6
15	1	4	172	174	8
17	1	4	73	42	18
19	1	4	502	502	6
0	2	4	321	347	4
2	2	4	196	203	4
4	2	4	389	390	4
6	2	4	442	464	4
8	2	4	106	106	9
10	2	4	416	422	5
12	2	4	363	371	5
14	2	4	635	633	6
16	2	4	758	757	6
18	2	4	99	94	14
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3	3	4	438	436	4
5	3	4	3400	3387	11
7	3	4	190	190	5
9	3	4	681	688	6
11	3	4	129	125	8
13	3	4	275	271	5
15	3	4	778	772	7
17	3	4	759	760	7
19	3	4	219	230	7
0	4	4	518	551	5
2	4	4	431	421	4
4	4	4	566	581	5
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8	4	4	183	181	6
10	4	4	316	326	5
12	4	4	166	174	7
14	4	4	743	739	6
16	4	4	1473	1493	11
18	4	4	139	128	10
1	5	4	971	965	7
3	5	4	144	137	6
5	5	4	1517	1550	10
7	5	4	387	397	4
9	5	4	87	80	11
11	5	4	909	913	7
13	5	4	120	114	9
15	5	4	269	267	6
17	5	4	122	127	11
19	5	4	116	118	12
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2	6	4	192	206	5
4	6	4	359	351	4
6	6	4	170	173	6
8	6	4	365	357	4
10	6	4	1295	1295	10
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16	6	4	189	184	8
18	6	4	258	254	7
1	7	4	240	223	4
3	7	4	241	236	5
5	7	4	1266	1266	9
7	7	4	380	387	5
9	7	4	904	911	7
11	7	4	750	752	6
13	7	4	255	246	6
15	7	4	240	247	7
17	7	4	430	431	6
0	8	4	1828	1887	11
2	8	4	43	35	31
4	8	4	250	246	5
6	8	4	564	561	5
8	8	4	370	361	5
10	8	4	1074	1082	8
12	8	4	78	78	15
14	8	4	98	96	12
16	8	4	272	271	7
18	8	4	0	25	1
1	9	4	10	28	10
3	9	4	239	246	5
5	9	4	1742	1776	12
7	9	4	486	476	5
9	9	4	0	6	1
11	9	4	223	216	6
13	9	4	98	77	12
15	9	4	494	492	5
17	9	4	609	602	6
0	10	4	843	851	6
2	10	4	0	13	1
4	10	4	445	452	5
6	10	4	211	205	6
8	10	4	270	283	6
10	10	4	440	439	5
12	10	4	238	248	6
14	10	4	816	830	7
16	10	4	406	406	6
1	11	4	163	164	7
3	11	4	318	322	5
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7	11	4	0	15	1
9	11	4	58	49	21
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2	12	4	212	208	6
4	12	4	195	201	6
6	12	4	273	278	6
8	12	4	227	218	6
10	12	4	501	492	5
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14	12	4	36	36	36
1	13	4	305	302	5
3	13	4	131	118	9
5	13	4	239	240	6
7	13	4	277	278	6
9	13	4	396	392	6
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0	14	4	1332	1357	9
2	14	4	213	214	6
4	14	4	321	319	6
6	14	4	447	459	5
8	14	4	126	113	11
10	14	4	982	989	7
12	14	4	58	50	29
1	15	4	244	249	7
3	15	4	177	171	6
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7	15	4	84	65	16
9	15	4	142	163	11
0	16	4	171	174	8
2	16	4	210	204	7
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6	16	4	450	451	6
8	16	4	49	7	49
1	17	4	351	346	6
3	17	4	198	179	8
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9	1	5	290	279	5
11	1	5	210	205	6
13	1	5	160	163	8
15	1	5	117	120	11
17	1	5	703	720	7
19	1	5	374	376	6
0	2	5	761	771	6
2	2	5	149	138	6
4	2	5	193	192	4
6	2	5	455	459	5
8	2	5	267	264	5
10	2	5	64	63	17
12	2	5	727	731	6
14	2	5	59	34	22
16	2	5	207	204	7
18	2	5	96	84	15
1	3	5	120	130	8
3	3	5	237	224	5
5	3	5	548	545	5
7	3	5	105	90	9
9	3	5	105	103	10
11	3	5	240	237	6
13	3	5	239	248	6
15	3	5	30	12	29
17	3	5	509	510	6
0	4	5	125	138	7
2	4	5	87	74	11
4	4	5	90	75	10
6	4	5	657	631	5
8	4	5	307	310	5
10	4	5	274	259	5
12	4	5	459	459	5
14	4	5	264	253	6
16	4	5	598	599	6
18	4	5	248	261	7
1	5	5	140	139	7
3	5	5	232	224	5
5	5	5	602	593	5
7	5	5	596	595	5
9	5	5	339	344	5
11	5	5	281	268	5
13	5	5	368	372	5
15	5	5	51	60	35
17	5	5	156	142	10
0	6	5	369	394	4
2	6	5	55	67	20
4	6	5	24	30	23
6	6	5	462	467	5
8	6	5	338	348	5
10	6	5	40	66	40
12	6	5	249	256	6
14	6	5	0	22	1
16	6	5	675	683	6
1	7	5	94	87	10
3	7	5	419	437	5
5	7	5	166	150	7
7	7	5	312	307	5
9	7	5	276	264	5
11	7	5	340	333	5
13	7	5	175	167	8
15	7	5	123	119	11
17	7	5	65	40	24
0	8	5	709	718	6
2	8	5	188	177	6
4	8	5	87	77	11
6	8	5	545	546	5
8	8	5	95	82	12

Observed and calculated structure factors for K2

h	k	l	10Fo	10Fc	10s
10	8	5	67	61	17
12	8	5	358	352	5
14	8	5	446	455	6
16	8	5	672	652	6
1	9	5	669	674	6
3	9	5	55	23	20
5	9	5	510	503	5
7	9	5	350	338	5
9	9	5	30	40	30
11	9	5	1532	1531	11
13	9	5	159	148	9
15	9	5	153	149	10
0	10	5	1051	1047	8
2	10	5	469	481	5
4	10	5	92	84	12
6	10	5	499	484	5
8	10	5	88	106	13
10	10	5	112	105	6
12	10	5	78	77	16
14	10	5	451	450	6
1	11	5	60	38	19
3	11	5	120	125	9
5	11	5	537	528	5
7	11	5	520	522	5
9	11	5	195	183	7
11	11	5	330	331	6
13	11	5	218	211	8
0	12	5	1019	1037	7
2	12	5	515	515	5
4	12	5	49	41	10
6	12	5	710	717	6
8	12	5	66	62	21
10	12	5	0	22	1
12	12	5	203	209	8
1	13	5	154	152	5
3	13	5	243	237	6
5	13	5	962	967	7
7	13	5	189	189	8
9	13	5	264	268	7
11	13	5	1245	1235	9
0	14	5	959	958	7
2	14	5	185	179	8
4	14	5	310	313	6
6	14	5	430	431	6
8	14	5	171	171	9
10	14	5	140	138	6
1	15	5	90	93	15
3	15	5	299	289	6
5	15	5	20	23	20
7	15	5	337	335	6
0	16	5	292	284	6
2	16	5	251	247	7
4	16	5	115	94	12
0	0	6	2496	2542	11
2	0	6	104	99	10
4	0	6	591	597	5
6	0	6	687	691	5
8	0	6	358	363	5
10	0	6	887	886	7
12	0	6	770	764	7
14	0	6	749	743	6
16	0	6	857	870	8
1	1	6	159	154	7
3	1	6	145	141	7
5	1	6	1667	1687	12
7	1	6	97	107	11
9	1	6	348	347	5
11	1	6	214	228	7
13	1	6	68	70	19
15	1	6	431	429	6
17	1	6	324	314	6
0	2	6	1690	1711	11
2	2	6	192	194	6
4	2	6	165	166	7
6	2	6	494	487	5
8	2	6	220	216	6
10	2	6	817	816	7
12	2	6	312	320	6
14	2	6	0	26	1
16	2	6	380	374	6
1	3	6	236	238	5
3	3	6	72	76	14
5	3	6	822	836	7
7	3	6	81	74	13
9	3	6	978	976	7
11	3	6	1137	1149	8
13	3	6	163	160	8
15	3	6	110	89	12
17	3	6	389	387	6
0	4	6	2302	2379	12
2	4	6	53	40	21
4	4	6	328	331	5
6	4	6	522	527	5
8	4	6	115	112	10
10	4	6	1341	1348	9
12	4	6	187	196	8
14	4	6	46	34	46
16	4	6	199	217	8
1	5	6	277	287	5
3	5	6	297	296	5
5	5	6	504	501	5
7	5	6	60	78	20
9	5	6	263	267	6
11	5	6	331	326	6
13	5	6	81	87	16
15	5	6	275	273	7
0	6	6	121	124	8
2	6	6	63	27	17
4	6	6	408	417	5
6	6	6	909	908	7
8	6	6	306	306	5
10	6	6	85	29	14
12	6	6	184	177	8
14	6	6	771	752	6
1	7	6	526	531	5
3	7	6	117	121	9
5	7	6	2422	2459	13
7	7	6	119	111	10
9	7	6	160	165	5
11	7	6	406	414	5
13	7	6	218	202	7
15	7	6	672	662	6
0	8	6	285	280	5
2	8	6	217	213	6
4	8	6	337	319	5
6	8	6	275	274	6
8	8	6	334	334	6
10	8	6	157	162	9
12	8	6	118	112	12
14	8	6	376	366	6
1	9	6	356	355	5
3	9	6	62	79	20
5	9	6	114	4	10
7	9	6	515	517	5
9	9	6	421	422	5
11	9	6	731	717	6
13	9	6	51	12	41
0	10	6	2098	2158	14
2	10	6	285	287	6
4	10	6	272	277	6
6	10	6	527	535	5
8	10	6	90	76	14
10	10	6	1272	1261	9
12	10	6	213	223	8
1	11	6	141	135	9
3	11	6	327	328	6
5	11	6	444	451	5
7	11	6	128	119	10
9	11	6	439	429	6
11	11	6	775	761	6
0	12	6	512	511	5
2	12	6	112	92	11
4	12	6	119	108	10
6	12	6	863	868	7
8	12	6	50	55	49
10	12	6	374	378	6
1	13	6	46	6	46
3	13	6	0	51	1
5	13	6	1325	1314	9
7	13	6	138	128	10
0	14	6	73	71	20
2	14	6	349	357	6
4	14	6	308	308	7
6	14	6	153	156	10
1	1	7	81	74	13
3	1	7	201	201	6
5	1	7	91	90	12
7	1	7	281	278	6
9	1	7	175	166	8
11	1	7	709	709	6
13	1	7	287	300	7
15	1	7	183	202	9
0	2	7	644	641	5
2	2	7	348	338	5
4	2	7	55	17	23
6	2	7	476	479	5
8	2	7	259	255	6
10	2	7	0	9	1
12	2	7	486	478	6
14	2	7	171	174	9
1	3	7	213	218	6
3	3	7	44	18	44
5	3	7	407	395	5
7	3	7	412	406	5
9	3	7	163	153	8
11	3	7	817	803	7
13	3	7	70	54	21
0	4	7	1038	1028	8
2	4	7	74	61	15
4	4	7	210	203	6
6	4	7	122	123	10
8	4	7	162	161	8
10	4	7	343	346	6
12	4	7	466	464	6
14	4	7	118	105	13
1	5	7	18	5	17
3	5	7	131	124	8
5	5	7	232	223	6
7	5	7	513	518	5
9	5	7	264	254	6
11	5	7	59	41	26
13	5	7	248	247	7
0	6	7	222	223	6
2	6	7	136	132	9
4	6	7	195	203	7
6	6	7	703	706	6
8	6	7	253	255	6
10	6	7	141	142	10
12	6	7	199	206	8
1	7	7	97	96	11
3	7	7	209	218	7
5	7	7	793	789	7
7	7	7	122	114	10
9	7	7	293	290	6
11	7	7	521	526	6
0	8	7	587	577	5
2	8	7	38	42	37
4	8	7	205	205	7
6	8	7	350	343	6
8	8	7	4	7	3
10	8	7	161	148	9
1	9	7	345	354	6
3	9	7	93	84	13
5	9	7	250	238	7
7	9	7	145	145	10
9	9	7	28	9	27
0	10	7	594	598	6
2	10	7	418	417	5
4	10	7	144	146	10
6	10	7	187	193	8
8	10	7	125	111	11
1	11	7	129	134	10
3	11	7	56	59	28
5	11	7	569	557	6
7	11	7	158	158	9
0	12	7	0	12	1
2	12	7	196	204	8
4	12	7	238	252	8
0	0	8	2441	2503	14
2	0	8	153	141	8
4	0	8	194	206	7
6	0	8	669	669	6
8	0	8	41	5	40
10	0	8	1492	1483	10
12	0	8	528	521	6
1	1	8	139	134	9
3	1	8	116	107	11
5	1	8	452	453	5
7	1	8	210	210	7
9	1	8	638	632	6
11	1	8	541	528	6
0	2	8	0	5	1
2	2	8	86	96	15
4	2	8	239	217	7
6	2	8	501	491	5
8	2	8	29	18	28
10	2	8	222	216	8
1	3	8	87	100	14
3	3	8	302	293	6
5	3	8	1781	1784	12
7	3	8	0	5	1
9	3	8	379	372	6
11	3	8	132	109	11
0	4	8	208	226	7
2	4	8	276	281	6
4	4	8	199	202	7
6	4	8	642	648	6
8	4	8	43	13	42
10	4	8	151	149	10
1	5	8	514	521	5
3	5	8	139	150	10
5	5	8	429	433	6
7	5	8	0	18	1
9	5	8	125	109	12
0	6	8	1806	1824	12
2	6	8	192	193	8
4	6	8	305	300	6
6	6	8	459	458	6
8	6	8	143	149	10
1	7	8	9	40	8
3	7	8	144	162	10
5	7	8	890	878	7
7	7	8	222	227	7
0	8	8	921	926	7
2	8	8	46	14	46
4	8	8	53	50	34
6	8	8	400	395	6
1	9	8	48	32	48
3	9	8	121	119	12
5	9	8	1234	1240	10
0	10	8	1024	1012	8
2	10	8	98	93	15
1	1	9	31	26	31
3	1	9	147	140	9
5	1	9	312	318	6
0	2	9	118	135	12
2	2	9	80	93	18
4	2	9	157	159	10
6	2	9	46	20	46
1	3	9	123	121	11
3	3	9	57	3	27
5	3	9	123	98	11
0	4	9	431	415	6
2	4	9	44	53	44
4	4	9	42	60	41
1	5	9	38	18	37
3	5	9	47	60	46

Observed and calculated structure factors for K3

h	k	l	10Fo	10Fc	10s
2	0	0	622	635	4
4	0	0	1360	1369	5
6	0	0	620	619	5
8	0	0	1059	1029	8
10	0	0	3859	3857	9
12	0	0	1356	1369	11
14	0	0	311	302	5
16	0	0	319	317	6
18	0	0	745	735	7
20	0	0	325	322	7
22	0	0	1559	1575	11
1	1	0	712	748	3
3	1	0	336	321	3
5	1	0	681	680	5
7	1	0	425	420	4
9	1	0	1734	1708	9
11	1	0	2945	2886	10
13	1	0	250	251	5
15	1	0	185	177	7
17	1	0	305	295	6
19	1	0	642	638	6
21	1	0	811	801	7
0	2	0	1160	1211	4
2	2	0	337	345	3
4	2	0	634	649	4
6	2	0	61	61	12
8	2	0	232	227	4
10	2	0	602	617	5
12	2	0	311	307	5
14	2	0	854	848	7
16	2	0	754	759	6
18	2	0	113	104	13
20	2	0	201	190	8
22	2	0	352	345	7
1	3	0	413	400	3
3	3	0	514	508	4
7	3	0	498	475	4
9	3	0	1122	1119	7
11	3	0	353	346	4
13	3	0	439	438	5
15	3	0	956	958	7
17	3	0	932	921	7
19	3	0	292	289	7
21	3	0	348	337	7
0	4	0	2393	2478	6
2	4	0	696	704	5
4	4	0	1182	1152	7
6	4	0	3732	3631	8
8	4	0	609	602	5
10	4	0	662	665	5
12	4	0	302	302	5
14	4	0	935	946	7
16	4	0	2024	2024	13
18	4	0	188	182	8
20	4	0	337	329	7
22	4	0	395	407	7
1	5	0	1525	1537	7
3	5	0	53	54	14
5	5	0	3234	3195	8
7	5	0	946	905	6
9	5	0	96	108	10
11	5	0	359	380	5
13	5	0	331	331	5
15	5	0	310	301	6
17	5	0	431	440	6
19	5	0	166	163	10
21	5	0	266	267	8
0	6	0	1038	1037	7
2	6	0	101	110	7
4	6	0	364	381	4
6	6	0	542	531	4
8	6	0	645	627	5
10	6	0	1467	1465	11
12	6	0	316	317	5
14	6	0	460	463	5
16	6	0	508	500	5
18	6	0	403	408	6
20	6	0	78	10	22
1	7	0	764	747	6
3	7	0	219	226	4
5	7	0	1602	1623	9
7	7	0	449	443	4
9	7	0	1304	1309	9
11	7	0	593	555	5
13	7	0	495	505	5
15	7	0	327	327	6
17	7	0	188	179	8
19	7	0	776	781	7
0	8	0	2733	2705	9
2	8	0	154	163	6
4	8	0	536	540	5
6	8	0	607	616	5
8	8	0	503	508	5
10	8	0	1460	1451	9
12	8	0	282	281	6
14	8	0	49	71	42
16	8	0	231	230	7
18	8	0	61	20	31
20	8	0	368	357	7
1	9	0	179	158	6
3	9	0	410	417	4
5	9	0	1828	1853	10
7	9	0	919	911	7
9	9	0	100	107	14
11	9	0	596	583	5
13	9	0	283	290	6
15	9	0	536	545	6
17	9	0	487	493	6
19	9	0	327	327	7
0	10	0	420	431	5
2	10	0	74	75	14
4	10	0	400	403	5
6	10	0	229	230	6
8	10	0	431	440	5
10	10	0	659	670	6
12	10	0	129	136	11
14	10	0	1188	1224	9
16	10	0	317	315	7
18	10	0	635	635	6
1	11	0	406	407	5
3	11	0	285	292	5
5	11	0	1000	1013	7
7	11	0	122	121	10
9	11	0	187	188	7
11	11	0	482	498	6
13	11	0	169	173	9
15	11	0	979	985	8
17	11	0	504	514	6
0	12	0	1157	1180	9
2	12	0	234	234	6
4	12	0	335	325	5
6	12	0	675	691	6
8	12	0	218	227	7
10	12	0	573	569	6
12	12	0	561	558	6
14	12	0	162	174	10
16	12	0	138	139	13
1	13	0	534	543	5
3	13	0	245	249	6
5	13	0	432	435	5
7	13	0	575	566	5
9	13	0	412	409	5
11	13	0	937	939	8
13	13	0	338	339	7
15	13	0	308	318	7
0	14	0	1550	1558	10
2	14	0	412	422	5
4	14	0	211	214	7
6	14	0	769	773	6
8	14	0	138	159	11
10	14	0	1426	1448	10
12	14	0	72	52	25
14	14	0	47	19	47
1	15	0	328	318	6
3	15	0	428	427	5
5	15	0	444	428	5
7	15	0	83	54	18
9	15	0	218	219	8
11	15	0	403	400	6
13	15	0	489	497	6
0	16	0	587	565	6
2	16	0	207	206	8
4	16	0	129	109	11
6	16	0	881	871	7
8	16	0	63	70	31
10	16	0	16	22	16
12	16	0	470	479	7
1	17	0	241	244	8
3	17	0	329	334	7
5	17	0	1892	1885	12
7	17	0	25	39	25
9	17	0	0	11	1
0	18	0	252	259	8
2	18	0	323	328	7
4	18	0	94	97	18
6	18	0	231	236	9
8	18	0	370	353	7
1	19	0	293	301	8
3	19	0	112	102	16
1	1	1	181	166	3
3	1	1	556	547	4
5	1	1	594	600	4
7	1	1	225	208	4
9	1	1	456	443	4
11	1	1	886	891	6
13	1	1	306	310	5
15	1	1	80	87	16
17	1	1	729	728	6
19	1	1	459	478	6
21	1	1	979	968	8
0	2	1	383	332	3
2	2	1	382	397	3
4	2	1	453	455	4
6	2	1	251	235	4
8	2	1	786	801	6
10	2	1	532	555	5
12	2	1	971	969	8
14	2	1	68	60	19
16	2	1	799	803	6
18	2	1	117	82	12
20	2	1	80	90	22
22	2	1	245	236	8
1	3	1	274	280	3
3	3	1	219	209	4
5	3	1	185	164	4
7	3	1	546	535	4
9	3	1	354	358	4
11	3	1	255	264	5
13	3	1	349	358	5
15	3	1	54	19	28
17	3	1	381	374	6
19	3	1	251	241	7
21	3	1	372	380	7
0	4	1	916	921	6
2	4	1	56	24	13
4	4	1	328	317	3
6	4	1	844	811	6
8	4	1	549	548	5
10	4	1	150	125	7
12	4	1	691	709	6
14	4	1	103	290	5
16	4	1	672	679	6
18	4	1	212	220	8
20	4	1	159	152	11
1	5	1	132	150	5
3	5	1	696	705	5
5	5	1	1794	1792	8
7	5	1	852	834	6
9	5	1	515	513	5
11	5	1	154	187	5
13	5	1	754	755	6
15	5	1	283	280	6
17	5	1	258	245	7
19	5	1	120	99	13
21	5	1	905	887	8
0	6	1	258	240	3
2	6	1	246	246	4
4	6	1	307	307	4
6	6	1	869	866	6
8	6	1	487	473	5
10	6	1	72	49	16
12	6	1	143	141	5
14	6	1	7	38	6
16	6	1	1093	1097	9
18	6	1	224	223	8
20	6	1	410	405	6
1	7	1	50	10	17
3	7	1	650	642	5
5	7	1	430	432	4
7	7	1	130	136	8
9	7	1	573	589	5
11	7	1	86	44	13
13	7	1	78	74	16
15	7	1	97	86	14
17	7	1	176	161	9
19	7	1	181	181	10
0	8	1	797	782	6
2	8	1	91	90	9
4	8	1	144	161	7
6	8	1	357	361	4
8	8	1	168	168	7
10	8	1	200	182	6
12	8	1	430	435	5
14	8	1	565	569	6
16	8	1	800	790	7
18	8	1	319	305	7
20	8	1	186	174	10
1	9	1	949	938	7
3	9	1	190	191	6
5	9	1	590	624	5
7	9	1	268	275	5
9	9	1	98	100	12
11	9	1	1717	1719	12
13	9	1	28	27	28
15	9	1	53	33	37
17	9	1	188	168	9
19	9	1	139	166	13
0	10	1	1343	1358	10
2	10	1	827	825	6
4	10	1	392	408	5
6	10	1	369	381	5
8	10	1	112	111	11
10	10	1	298	293	6
12	10	1	80	72	17
14	10	1	732	732	6
16	10	1	288	288	7
18	10	1	350	346	7
1	11	1	332	343	5
3	11	1	285	280	5
5	11	1	601	605	5
7	11	1	440	445	5
9	11	1	434	439	5
11	11	1	415	422	5
13	11	1	90	104	15
15	11	1	0	23	1
17	11	1	359	355	7
0	12	1	1241	1266	10
2	12	1	486	490	5
4	12	1	70	77	18
6	12	1	660	662	6
8	12	1	192	188	7
10	12	1	274	287	6
12	12	1	281	267	6
14	12	1	97	108	16
16	12	1	742	755	7
1	13	1	335	325	5
3	13	1	352	352	5
5	13	1	1051	1061	8
7	13	1	59	76	26
9	13	1	415	413	5
11	13	1	1130	1128	8
13	13	1	110	96	14
15	13	1	228	228	9
0	14	1	659	674	6
2	14	1	326	320	6
4	14	1	553	553	5
6	14	1	182	168	8
8	14	1	314	306	6
10	14	1	155	169	10
12	14	1	96	99	16
14	14	1	468	468	6
1	15	1	53	60	34
3	15	1	284	286	6
5	15	1	323	326	6
7	15	1	270	267	7
9	15	1	76	80	21
11	15	1	225	206	8
13	15	1	128	118	13
0	16	1	330	336	6
2	16	1	275	275	7
4	16	1	87	75	17
6	16	1	1288	1254	9
8	16	1	329	345	7
10	16	1	0	22	1
12	16	1	105	97	16
1	17	1	55	7	42
3	17	1	301	294	7
5	17	1	785	776	7
7	17	1	314	297	7
9	17	1	473	470	6
0	18	1	237	246	8
2	18	1	0	34	1
4	18	1	444	441	6
6	18	1	438	429	6
1	19	1	359	348	7
3	19	1	431	427	7
0	0	2	3651	3702	6
2	0	2	709	729	5
4	0	2	439	439	4
6	0	2	729	708	6
8	0	2	806	787	6
10	0	2	1606	1568	10
12	0	2	893	893	7
14	0	2	1431	1436	10
16	0	2	825	821	7
18	0	2	993	985	7
20	0	2	115	102	14
1	1	2	576	585	5
3	1	2	719	732	6
5	1	2	1232	1231	7
7	1	2	173	168	5
9	1	2	745	745	5
11	1	2	642	643	5
13	1	2	125	112	9
15	1	2	735	744	6
17	1	2	128	128	11
19	1	2	0	20	1
21	1	2	285	273	8
0	2	2	4101	4120	6
2	2	2	341	334	4
4	2	2	506	509	4
6	2	2	406	400	4
8	2	2	281	278	4
10	2	2	1325	1315	10
12	2	2	521	528	5
14	2	2	117	127	10
16	2	2	318	318	6
18	2	2	87	80	17
20	2	2	0	24	1
1	3	2	392	394	4
3	3	2	149	143	5
5	3	2	1281	1254	8
7	3	2	204	203	5
9	3	2	1671	1689	10
11	3	2	1408	1409	11
13	3	2	608	600	5
15	3	2	275	271	6
17	3	2	295	294	6
19	3	2	880	885	7
21	3	2	603	613	7
0	4	2	2158	2139	7
2	4	2	729	722	5
4	4	2	66	80	12
6	4	2	224	203	4
8	4	2	208	212	5
10	4	2	2203	2239	10
12	4	2	262	259	5
14	4	2	316	314	5
16	4	2	78	16	18
18	4	2	546	543	6
20	4	2	411	390	6
1	5	2	1031	1017	8
3	5	2	0	23	1
5	5	2	1703	1687	9
7	5	2	173	170	6
9	5	2	459	457	5
11	5	2	649	649	6
13	5	2	135	117	9
15	5	2	244	236	6
17	5	2	799	803	7
19	5	2	461	449	6
21	5	2	524	521	6
0	6	2	1256	1250	8
2	6	2	37	49	37
4	6	2	968	973	7
6	6	2	2415	2383	9
8	6	2	218	202	5
10	6	2	85	92	14
12	6	2	453	458	5
14	6	2	961	965	7
16	6	2	1452	1472	11
18	6	2	118	100	14
20	6	2	19	29	19
1	7	2	813	799	6
3	7	2	67	55	14
5	7	2	4601	4629	10
7	7	2	172	172	7
9	7	2	558	563	5
11	7	2	117	122	10
13	7	2	427	432	5
15	7	2	1008	1024	8
17	7	2	874	877	7
19	7	2	128	127	13
0	8	2	327	326	4
2	8	2	532	514	5
4	8	2	250	260	5
6	8	2	401	378	5
8	8	2	708	698	6
10	8	2	177	171	7
12	8	2	248	246	6
14	8	2	625	621	6
16	8	2	930	945	8
18	8	2	151	147	11
1	9	2	559	558	5
3	9	2	70	62	16
5	9	2	478	477	5
7	9	2	468	460	5
9	9	2	615	623	5
11	9	2	1629	1621	13
13	9	2	91	74	15

Observed and calculated structure factors for K3

h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ
15	9	2	325	314	6	20	2	3	32	10	31	17	11	3	466	471	6	12	4	4	181	179	8	12	14	4	59	19	37
17	9	2	669	677	6	1	3	3	494	493	4	0	12	3	379	363	5	14	4	4	906	919	7	1	15	4	264	266	7
19	9	2	265	265	8	3	3	3	307	308	4	2	12	3	271	271	6	16	4	4	1438	1461	10	3	15	4	429	426	6
0	10	2	4449	4468	11	5	3	3	1178	1161	9	4	12	3	333	336	5	18	4	4	231	221	8	5	15	4	173	167	10
2	10	2	639	626	5	7	3	3	778	763	6	6	12	3	156	147	8	1	5	4	1081	1064	8	7	15	4	179	170	10
4	10	2	751	747	6	9	3	3	257	250	5	8	12	3	111	118	13	3	5	4	183	173	6	9	15	4	204	196	10
6	10	2	63	43	21	11	3	3	1153	1341	9	10	12	3	277	279	7	5	5	4	1547	1595	11	0	16	4	125	132	13
8	10	2	331	328	5	13	3	3	147	131	8	12	12	3	285	275	7	7	5	4	450	454	5	2	16	4	185	181	9
10	10	2	1940	1956	13	15	3	3	33	52	33	14	12	3	196	194	9	9	5	4	95	89	13	4	16	4	67	65	30
12	10	2	338	321	6	17	3	3	243	217	7	16	12	3	468	462	6	11	5	4	929	928	7	6	16	4	490	486	6
14	10	2	378	391	6	19	3	3	164	165	10	1	13	3	199	214	7	13	5	4	180	173	8	8	16	4	0	8	1
16	10	2	161	162	10	21	3	3	431	432	7	3	13	3	459	465	5	15	5	4	289	290	7	1	17	4	333	325	7
18	10	2	337	335	7	0	4	3	2059	1988	8	5	13	3	454	449	5	17	5	4	65	46	30	3	17	4	220	207	9
1	11	2	290	289	5	2	4	3	73	86	11	7	13	3	119	125	12	19	5	4	90	98	21	1	1	5	94	72	12
3	11	2	749	756	6	4	4	3	418	412	4	9	13	3	360	357	6	0	6	4	2208	2231	10	3	1	5	292	292	5
5	11	2	202	197	7	6	4	3	197	193	5	11	13	3	410	407	6	2	6	4	126	139	9	5	1	5	513	498	5
7	11	2	39	14	39	8	4	3	292	303	5	13	13	3	46	43	46	4	6	4	384	380	5	7	1	5	88	78	13
9	11	2	708	709	6	10	4	3	269	261	5	15	13	3	172	145	11	6	6	4	176	169	7	9	1	5	352	361	5
11	11	2	1734	1748	11	12	4	3	791	789	6	0	14	3	52	17	39	8	6	4	324	322	5	11	1	5	278	278	6
13	11	2	50	36	50	14	4	3	143	115	9	2	14	3	292	287	6	10	6	4	1303	1324	10	13	1	5	137	150	10
15	11	2	324	333	7	16	4	3	284	274	6	4	14	3	482	484	5	12	6	4	406	412	5	15	1	5	90	84	17
17	11	2	130	124	13	18	4	3	141	134	11	6	14	3	256	264	7	14	6	4	257	244	7	17	1	5	742	744	7
0	12	2	1427	1429	10	20	4	3	85	72	21	8	14	3	367	368	6	16	6	4	183	182	9	19	1	5	378	383	7
2	12	2	33	35	33	1	5	3	53	45	18	10	14	3	48	10	47	18	6	4	316	308	7	0	2	5	534	511	5
4	12	2	134	122	9	3	5	3	463	466	4	12	14	3	42	30	41	1	7	4	309	293	5	2	2	5	16	21	15
6	12	2	952	935	7	5	5	3	1122	1125	8	1	15	3	244	240	7	3	7	4	295	294	5	4	2	5	443	443	5
8	12	2	163	178	9	7	5	3	844	835	7	3	15	3	179	190	9	5	7	4	1442	1451	11	6	2	5	459	460	5
10	12	2	828	836	7	9	5	3	384	387	5	5	15	3	511	510	6	7	7	4	388	370	5	8	2	5	440	430	5
12	12	2	279	278	7	11	5	3	225	204	6	7	15	3	127	127	13	9	7	4	983	1008	8	10	2	5	258	260	6
14	12	2	477	475	6	13	5	3	574	579	6	9	15	3	132	151	13	11	7	4	732	729	6	12	2	5	769	781	7
16	12	2	365	374	7	15	5	3	182	173	8	11	15	3	399	394	7	13	7	4	430	427	6	14	2	5	11	2	10
1	13	2	154	148	8	17	5	3	300	307	7	0	16	3	180	172	9	15	7	4	302	307	7	16	2	5	356	343	7
3	13	2	75	62	17	19	5	3	135	138	12	2	16	3	78	88	21	17	7	4	299	309	7	18	2	5	151	167	12
5	13	2	1843	1851	13	0	6	3	722	725	5	4	16	3	161	159	10	0	8	4	1957	1984	11	1	3	5	97	100	12
7	13	2	66	80	23	2	6	3	72	62	13	6	16	3	1108	1095	8	2	8	4	0	12	1	3	3	5	189	184	7
9	13	2	103	102	14	4	6	3	524	516	5	8	16	3	261	269	8	4	8	4	275	275	5	5	3	5	424	430	5
11	13	2	95	83	16	6	6	3	1208	1194	8	10	16	3	142	142	12	6	8	4	570	563	5	7	3	5	123	122	10
13	13	2	104	98	15	8	6	3	346	348	5	1	17	3	75	78	24	8	8	4	412	411	5	9	3	5	189	170	7
15	13	2	574	580	6	10	6	3	42	32	41	3	17	3	304	297	7	10	8	4	1250	1259	9	11	3	5	248	258	6
0	14	2	556	561	6	12	6	3	298	298	6	5	17	3	482	490	6	12	8	4	184	188	8	13	3	5	358	355	6
2	14	2	357	340	6	14	6	3	59	47	25	7	17	3	0	30	1	14	8	4	86	72	18	15	3	5	58	65	33
4	14	2	717	724	6	16	6	3	1156	1156	9	0	18	3	246	262	8	16	8	4	172	183	10	17	3	5	568	570	6
6	14	2	434	432	5	18	6	3	349	356	7	2	18	3	150	149	12	18	8	4	87	80	21	0	4	5	0	22	1
8	14	2	244	237	7	20	6	3	354	365	7	2	0	4	381	382	4	1	9	4	83	82	14	2	4	5	38	7	37
10	14	2	305	264	7	1	7	3	77	74	14	4	0	4	782	803	6	3	9	4	296	292	5	4	4	5	164	165	7
12	14	2	111	68	14	3	7	3	312	325	5	6	0	4	411	408	5	5	9	4	1723	1738	12	6	4	5	700	686	6
14	14	2	444	407	6	5	7	3	1166	1163	9	8	0	4	338	336	5	7	9	4	508	518	5	8	4	5	391	390	5
1	15	2	634	636	6	7	7	3	215	227	6	10	0	4	2774	2784	11	9	9	4	24	29	24	10	4	5	66	54	22
3	15	2	263	264	7	9	7	3	558	560	5	12	0	4	887	902	7	11	9	4	178	178	8	12	4	5	464	482	5
5	15	2	1519	1534	10	11	7	3	768	772	7	14	0	4	460	471	5	13	9	4	131	121	11	14	4	5	292	281	6
7	15	2	587	586	6	13	7	3	141	132	9	16	0	4	108	88	13	15	9	4	370	380	6	16	4	5	691	683	6
9	15	2	47	21	46	15	7	3	203	184	7	18	0	4	695	679	7	17	9	4	583	588	6	18	4	5	264	248	8
11	15	2	397	394	6	17	7	3	608	607	6	20	0	4	162	180	12	0	10	4	968	955	7	1	5	5	176	168	7
13	15	2	145	155	12	19	7	3	145	152	12	1	1	4	245	235	4	2	10	4	0	19	1	3	5	5	392	389	5
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6	16	2	477	472	6	6	8	3	536	539	5	9	1	4	1297	1324	9	10	10	4	572	568	6	11	5	5	303	311	6
8	16	2	65	80	30	8	8	3	52	15	28	11	1	4	1633	1641	12	12	10	4	178	190	9	13	5	5	506	514	6
10	16	2	695	697	7	10	8	3	71	38	18	13	1	4	116	115	11	14	10	4	907	924	8	15	5	5	196	190	9
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3	17	2	438	435	6	14	8	3	337	341	6	17	1	4	35	19	35	1	11	4	263	256	6	0	6	5	231	260	6
5	17	2	222	223	9	16	8	3	300	287	7	19	1	4	581	580	6	3	11	4	379	374	5	2	6	5	121	140	10
7	17	2	71	34	25	18	8	3	144	141	12	0	2	4	255	285	4	5	11	4	1186	1208	9	4	6	5	0	10	1
9	17	2	352	349	7	1	9	3	572	572	5	2	2	4	240	236	5	7	11	4	56	36	27	6	6	5	415	410	5
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4	18	2	313	298	7	7	9	3	194	202	7	8	2	4	52	54	28	13	11	4	134	109	12	12	6	5	272	251	6
6	18	2	416	417	7	9	9	3	148	149	9	10	2	4	415	418	5	15	11	4	839	837	8	14	6	5	86	46	18
1	1	3	267	261	4	11	9	3	918	920	8	12	2	4	326	324	5	0	12	4	850	839	7	16	6	5	741	746	7
3	1	3	741	733	6	13	9	3	80	45	18	14	2	4	620	623	6	2	12	4	266	263	6	1	7	5	0	10	1
5	1	3	396	402	4	15	9	3	63	9	27	16	2	4	752	756	6	4	12	4	183	189	8	3	7	5	490	509	5
7	1	3	198	198	5	17	9	3	525	527	6	18	2	4	70	76	26	6	12	4	343	335	6	5	7	5	58	37	25
9	1	3	411	404	5	0	10	3	932	938	7	20	2	4	129	128	14	8	12	4	290	288	7	7	7	5	271	276	6
11	1	3	1409	1414	9	2	10	3	807	833	7	1	3	4	280	283	4	10	12	4	369	361	6	9	7	5	198	194	5
13	1	3	404	400	5	4	10	3	493	504	5	3	3	4	436	433	4	12	12	4	374	370	6	11	7	5	390	403	6
15	1	3	0	14	1	6	10	3	142	152	9	5	3	4	3440	3477	10	14	12	4	83	59	21	13	7	5	193	193	9
17	1	3	326	337	6	8	10	3	191	200	7	7	3	4	178	160	7	1	13	4	305	306	6	15	7	5	0	9	1
19	1	3	459	463	6	10	10	3	118	93	12	9	3	4	852	869	7	3	13	4	154	150	10	17	7	5	116	93	15
21	1	3	932	922	8	12	10	3	167	174	9	11	3	4	81	77	16	5	13	4	277	287	7	0	8	5	880	886	7
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2	2	3	482	464	4	16	10	3	76	87	24	15	3	4	823	815	7	9	13	4	421	422	6	4	8	5	37	26	37
4	2	3	59	52	14	1	11	3	426	427	5	17	3	4	699	699	7	11	13	4	743	744	7	6	8	5	594	585	6
6	2	3	1143	1119	9	3	11	3	238	234	6	19	3	4	248	249	8	13	13	4	189	192	10	8	8	5	145	141	9
8	2	3	858	860	6	5	11	3	671	675	6	0	4	4	732	755	6	0	14	4	1488	1493	10	10	8	5	116	114	12
10	2	3	529	542	5	7	11	3	142	139	9	2	4	4	456	453	5	2	14	4	263	247	7	12	8	5	314	311	7
12	2	3	698	714	6	9	11	3	485	493	5	4	4	4	716	713	6	4	14	4	330	332	6	14	8	5	490	492	6
14	2	3	285	284	6	11	11	3	146	135	10	6	4	4	1820	1821	11	6	14	4	514	531	6	16	8	5	817	808	7
16	2	3	1158	1163	9	13	11	3	107	82	14	8	4	4	287	298	5	8	14	4	93	123	18	1	9	5	669	674	6
18	2	3	100	109	15	15	11	3	123	119	14	10	4	4	466	478	5	10	14	4	1140	1141	9	3	9	5	95	93	14

Observed and calculated structure factors for K3

h	k	l	10Fo	10Fc	10s
5	9	5	649	640	6
7	9	5	313	301	6
9	9	5	76	85	20
11	9	5	1517	1540	12
13	9	5	55	64	54
15	9	5	47	13	46
0	10	5	1048	1050	8
2	10	5	525	534	5
4	10	5	231	219	7
6	10	5	422	412	5
8	10	5	84	79	16
10	10	5	293	284	7
12	10	5	0	8	1
14	10	5	560	550	6
1	11	5	158	178	9
3	11	5	197	216	8
5	11	5	418	407	6
7	11	5	469	473	5
9	11	5	297	293	7
11	11	5	438	447	6
13	11	5	174	181	11
0	12	5	1223	1208	9
2	12	5	482	488	6
4	12	5	99	82	15
6	12	5	721	710	7
8	12	5	125	117	13
10	12	5	172	166	10
12	12	5	214	216	9
1	13	5	294	281	7
3	13	5	254	261	7
5	13	5	985	1009	8
7	13	5	202	186	8
9	13	5	355	359	7
11	13	5	1220	1212	9
0	14	5	874	860	7
2	14	5	263	261	8
4	14	5	437	434	6
6	14	5	335	347	7
8	14	5	195	206	10
1	15	5	60	45	36
3	15	5	248	244	8
5	15	5	124	143	15
7	15	5	258	263	8
0	16	5	317	298	7
2	16	5	291	297	8
4	16	5	172	175	11
0	0	6	2718	2718	12
2	0	6	143	153	8
4	0	6	664	667	6
6	0	6	695	705	6
8	0	6	499	498	5
10	0	6	958	976	7
12	0	6	719	725	6
14	0	6	843	823	7
16	0	6	886	888	8
1	1	6	204	188	6
3	1	6	138	122	9
5	1	6	1745	1768	12
7	1	6	66	63	21
9	1	6	384	401	5
11	1	6	211	223	8
13	1	6	53	23	43
15	1	6	500	489	6
17	1	6	280	293	8
0	2	6	1673	1695	12
2	2	6	223	210	6
4	2	6	220	212	6
6	2	6	493	482	5
8	2	6	273	267	6
10	2	6	797	802	7
12	2	6	298	284	6
14	2	6	0	11	1
16	2	6	383	370	7
1	3	6	206	194	6
3	3	6	70	46	19
5	3	6	924	917	7
7	3	6	79	81	17
9	3	6	1125	1134	8
11	3	6	1092	1106	8
13	3	6	325	328	7
15	3	6	213	135	8
17	3	6	331	329	7
0	4	6	2540	2525	12
2	4	6	90	85	13
4	4	6	400	408	5
6	4	6	453	461	5
8	4	6	154	161	9
10	4	6	1459	1471	11
12	4	6	256	248	7
14	4	6	105	109	16
16	4	6	238	223	8
1	5	6	285	283	6
3	5	6	363	366	5
5	5	6	405	403	5
7	5	6	86	88	16
9	5	6	228	228	7
11	5	6	346	348	6
13	5	6	65	31	26
15	5	6	206	207	9
0	6	6	74	77	18
2	6	6	14	20	33
4	6	6	491	491	5
6	6	6	861	862	7
8	6	6	274	269	6
10	6	6	60	39	30
12	6	6	198	211	9
14	6	6	838	849	7
1	7	6	637	642	6
3	7	6	159	162	9
5	7	6	2522	2542	13
7	7	6	68	76	22
9	7	6	450	462	6
11	7	6	461	461	6
13	7	6	270	258	7
15	7	6	669	669	7
0	8	6	220	209	7
2	8	6	228	224	7
4	8	6	341	342	6
6	8	6	260	266	7
8	8	6	408	413	6
10	8	6	51	23	50
12	8	6	239	227	8
14	8	6	450	440	6
1	9	6	196	194	6
3	9	6	109	98	13
5	9	6	0	24	1
7	9	6	511	521	6
9	9	6	424	430	6
11	9	6	745	742	7
13	9	6	65	73	30
0	10	6	2180	2198	14
2	10	6	291	304	6
4	10	6	131	332	6
6	10	6	537	542	6
8	10	6	120	117	14
10	10	6	1332	1335	10
12	10	6	161	157	11
1	11	6	52	36	46
3	11	6	356	354	6
5	11	6	149	151	6
7	11	6	69	87	26
9	11	6	539	535	6
11	11	6	707	706	7
0	12	6	597	578	6
2	12	6	102	85	15
4	12	6	140	129	11
6	12	6	959	961	8
8	12	6	66	35	30
10	12	6	468	456	6
1	13	6	31	7	30
3	13	6	34	22	34
5	13	6	1377	1376	10
7	13	6	205	202	9
0	14	6	47	63	46
2	14	6	402	393	7
4	14	6	110	120	7
1	1	7	70	80	20
3	1	7	281	276	6
5	1	7	190	60	8
7	1	7	237	228	7
9	1	7	225	218	8
11	1	7	754	760	7
13	1	7	307	313	7
15	1	7	65	53	33
0	2	7	802	800	7
2	2	7	295	293	6
4	2	7	42	11	41
6	2	7	451	460	6
8	2	7	338	337	6
10	2	7	208	201	8
12	2	7	531	533	6
14	2	7	120	120	15
1	3	7	164	177	9
3	3	7	44	18	43
5	3	7	449	453	5
7	3	7	454	454	6
9	3	7	217	214	8
11	3	7	772	773	7
13	3	7	0	9	1
0	4	7	933	915	7
2	4	7	140	132	10
4	4	7	281	288	7
6	4	7	74	67	21
8	4	7	237	243	7
10	4	7	173	167	10
12	4	7	476	475	6
14	4	7	160	142	11
1	5	7	29	21	28
3	5	7	236	245	7
5	5	7	446	450	6
7	5	7	500	502	6
9	5	7	275	281	7
11	5	7	98	90	17
13	5	7	358	359	7
0	6	7	336	332	6
2	6	7	91	102	16
4	6	7	241	244	7
6	6	7	686	672	7
8	6	7	240	246	8
10	6	7	75	65	23
12	6	7	204	206	9
1	7	7	62	32	26
3	7	7	286	291	6
5	7	7	710	696	7
7	7	7	152	149	10
9	7	7	406	401	6
11	7	7	487	477	6
0	8	7	443	436	6
2	8	7	140	148	11
4	8	7	296	300	7
6	8	7	296	301	7
8	8	7	63	71	32
10	8	7	0	12	1
1	9	7	161	168	6
3	9	7	54	20	38
5	9	7	99	106	16
7	9	7	106	109	16
9	9	7	30	39	29
0	10	7	632	630	6
2	10	7	451	450	6
4	10	7	258	246	8
6	10	7	179	166	10
8	10	7	74	82	25
1	11	7	232	229	8
3	11	7	155	139	11
5	11	7	494	490	6
7	11	7	127	116	14
0	12	7	155	144	11
2	12	7	152	167	11
4	12	7	236	232	9
0	0	8	2555	2563	14
2	0	8	153	155	10
4	0	8	315	315	7
6	0	8	725	718	7
8	0	8	41	28	41
10	0	8	1493	1503	11
1	1	8	88	90	17
3	1	8	109	97	13
5	1	8	400	405	6
7	1	8	208	197	8
9	1	8	737	723	7
11	1	8	502	496	6
0	2	8	42	32	41
2	2	8	94	108	16
4	2	8	260	264	7
6	2	8	526	526	6
8	2	8	0	11	1
10	2	8	234	219	8
1	3	8	168	157	9
3	3	8	301	304	7
5	3	8	1826	1822	12
7	3	8	21	13	20
9	3	8	481	485	6
11	3	8	148	139	12
0	4	8	111	127	14
2	4	8	298	298	7
4	4	8	274	279	7
6	4	8	573	581	6
8	4	8	111	90	14
10	4	8	242	237	8
1	5	8	569	571	6
3	5	8	157	159	10
5	5	8	459	460	6
7	5	8	90	46	18
9	5	8	128	114	14
0	6	8	1864	1880	12
2	6	8	165	170	10
4	6	8	331	331	7
6	6	8	463	461	6
8	6	8	138	138	13
1	7	8	76	84	24
3	7	8	194	195	9
5	7	8	978	977	8
7	7	8	204	210	9
0	8	8	988	975	8
2	8	8	66	56	28
4	8	8	71	63	28
6	8	8	386	397	7
1	9	8	43	5	42
3	9	8	168	161	11
5	9	8	1212	1212	9
0	10	8	1083	1085	9
2	10	8	101	87	17
1	1	9	42	53	42
3	1	9	222	226	9
5	1	9	193	191	9
0	2	9	54	22	53
2	2	9	53	19	52
4	2	9	224	202	9
6	2	9	64	6	34
1	3	9	148	143	12
3	3	9	89	64	19
5	3	9	0	13	1
0	4	9	393	380	7
2	4	9	0	39	1
4	4	9	61	82	40
1	5	9	0	11	1
3	5	9	138	127	13

Observed and calculated structure factors for K5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	650	662	4	4	8	0	455	441	4	3	1	1	468	462	4	7	9	1	290	289	5	7	1	2	160	160	5
4	0	0	1265	1261	6	6	8	0	601	598	5	5	1	1	827	855	6	9	9	1	50	57	30	9	1	2	666	666	5
6	0	0	539	558	4	8	8	0	464	466	5	7	1	1	155	140	5	11	9	1	1635	1655	11	11	1	2	661	659	6
8	0	0	954	926	7	10	8	0	1351	1331	10	9	1	1	446	444	4	13	9	1	35	17	35	13	1	2	80	65	14
10	0	0	3658	3701	11	12	8	0	207	210	7	11	1	1	807	812	6	15	9	1	50	54	43	15	1	2	681	679	6
12	0	0	1372	1382	9	14	8	0	130	132	10	13	1	1	348	345	5	17	9	1	150	156	10	17	1	2	110	95	12
14	0	0	246	241	6	16	8	0	272	276	7	15	1	1	0	34	1	19	9	1	185	194	9	19	1	2	35	14	35
16	0	0	262	249	6	18	8	0	0	24	1	17	1	1	722	723	6	0	10	1	1268	1282	9	21	1	2	129	319	7
18	0	0	639	616	6	20	8	0	343	324	7	19	1	1	474	480	6	2	10	1	796	778	6	0	2	2	4097	4072	8
20	0	0	299	290	7	1	9	0	102	75	9	21	1	1	865	844	8	4	10	1	300	312	5	2	2	2	132	142	3
22	0	0	1614	1618	12	3	9	0	405	411	4	0	2	1	42	48	16	6	10	1	399	412	5	4	2	2	502	501	4
1	1	0	719	745	3	5	9	0	1818	1829	11	2	2	1	445	467	3	8	10	1	146	146	8	6	2	2	445	441	4
3	1	0	240	232	3	7	9	0	894	873	6	4	2	1	474	480	4	10	10	1	275	268	8	8	2	2	282	265	4
5	1	0	499	493	4	9	9	0	64	42	18	6	2	1	297	283	3	12	10	1	38	10	37	10	2	2	1275	1291	9
7	1	0	452	442	4	11	9	0	639	626	6	8	2	1	656	658	5	14	10	1	649	648	6	12	2	2	519	536	5
9	1	0	1676	1663	9	13	9	0	267	262	6	10	2	1	296	309	4	16	10	1	279	287	7	14	2	2	102	107	11
11	1	0	2876	2844	11	15	9	0	535	553	6	12	2	1	941	938	7	18	10	1	288	282	8	16	2	2	343	333	6
13	1	0	306	311	5	17	9	0	483	478	6	14	2	1	125	124	10	1	11	1	227	231	6	18	2	2	75	47	19
15	1	0	253	252	6	19	9	0	259	260	8	16	2	1	680	681	6	3	11	1	231	228	6	20	2	2	0	12	1
17	1	0	303	299	6	0	10	0	287	293	5	18	2	1	38	9	38	5	11	1	680	694	6	1	3	2	386	390	1
19	1	0	596	603	6	2	10	0	0	25	1	20	2	1	172	155	9	7	11	1	491	492	5	3	3	2	227	227	4
21	1	0	757	761	7	4	10	0	400	408	4	22	2	1	203	226	10	9	11	1	165	356	5	5	3	2	1070	1047	7
0	2	0	1286	1313	4	6	10	0	280	285	5	1	3	1	316	319	3	11	11	1	346	343	6	7	3	2	176	176	5
2	2	0	277	295	3	8	10	0	342	346	5	3	3	1	217	234	4	13	11	1	110	131	13	9	3	2	1576	1608	11
4	2	0	668	673	5	10	10	0	543	539	5	5	3	1	313	302	4	15	11	1	86	95	18	11	3	2	1339	1352	9
6	2	0	132	128	5	12	10	0	164	156	8	7	3	1	497	484	4	17	11	1	404	409	6	13	3	2	492	486	5
8	2	0	278	273	4	14	10	0	1174	1182	8	9	3	1	276	275	4	0	12	1	1107	1107	8	15	3	2	193	186	7
10	2	0	657	666	5	16	10	0	215	222	8	11	3	1	230	244	6	2	12	1	491	486	5	17	3	2	300	310	6
12	2	0	332	320	5	18	10	0	549	542	6	13	3	1	281	288	5	4	12	1	109	102	10	19	3	2	865	844	7
14	2	0	862	864	7	1	11	0	326	319	5	15	3	1	17	34	17	6	12	1	631	628	6	21	3	2	517	543	6
16	2	0	721	717	6	3	11	0	258	276	5	17	3	1	326	330	6	8	12	1	162	155	8	0	4	2	1917	1878	8
18	2	0	45	35	45	5	11	0	849	868	6	19	3	1	220	209	8	10	12	1	170	181	9	2	4	2	668	668	5
20	2	0	171	174	10	7	11	0	132	137	9	21	3	1	333	332	7	12	12	1	260	256	7	4	4	2	6	8	5
22	2	0	316	330	7	9	11	0	88	93	14	0	4	1	1068	1073	7	14	12	1	65	66	26	6	4	2	253	236	4
1	3	0	160	161	3	11	11	0	487	489	5	2	4	1	61	72	12	16	12	1	689	700	6	8	4	2	131	140	7
3	3	0	553	558	4	13	11	0	174	169	9	4	4	1	267	262	3	1	13	1	371	356	5	10	4	2	2024	2065	11
5	3	0	4766	4771	9	15	11	0	878	885	8	6	4	1	783	744	5	3	13	1	347	353	5	12	4	2	257	257	6
7	3	0	504	481	4	17	11	0	456	463	6	8	4	1	487	486	4	5	13	1	959	977	8	14	4	2	241	250	6
9	3	0	1027	1019	8	0	12	0	1433	1463	10	10	4	1	264	248	5	7	13	1	53	62	31	16	4	2	0	24	1
11	3	0	315	302	5	2	12	0	245	242	6	12	4	1	700	713	6	9	13	1	339	338	6	18	4	2	499	507	6
13	3	0	167	169	5	4	12	0	261	255	6	14	4	1	277	276	6	11	13	1	1095	1086	9	20	4	2	336	331	7
15	3	0	889	874	7	6	12	0	604	616	5	16	4	1	614	620	6	13	13	1	142	126	12	1	5	2	978	964	7
17	3	0	950	930	7	8	12	0	183	186	7	18	4	1	250	250	7	15	13	1	239	237	8	3	5	2	50	59	17
19	3	0	253	256	7	10	12	0	623	616	6	20	4	1	111	95	14	0	14	1	687	701	6	5	5	2	1817	1772	9
21	3	0	405	389	7	12	12	0	530	514	6	1	5	1	125	123	6	2	14	1	280	274	6	7	5	2	210	198	5
0	4	0	2146	2142	7	14	12	0	85	114	19	3	5	1	566	575	4	4	14	1	441	458	5	9	5	2	422	415	5
2	4	0	635	631	5	16	12	0	129	109	13	5	5	1	1535	1499	9	6	14	1	216	233	7	11	5	2	637	641	6
4	4	0	1100	1090	7	1	13	0	461	469	5	7	5	1	863	844	7	8	14	1	309	290	6	13	5	2	81	59	15
6	4	0	3672	3609	9	3	13	0	199	202	7	9	5	1	558	547	5	10	14	1	206	211	8	15	5	2	250	254	6
8	4	0	518	500	4	5	13	0	362	366	5	11	5	1	281	296	5	12	14	1	144	144	11	17	5	2	750	749	7
10	4	0	497	491	5	7	13	0	487	502	5	13	5	1	633	637	6	14	14	1	406	398	7	19	5	2	414	418	6
12	4	0	274	268	5	9	13	0	457	452	5	15	5	1	153	135	9	1	15	1	52	5	31	21	5	2	473	456	7
14	4	0	873	877	7	11	13	0	876	873	7	17	5	1	220	226	8	3	15	1	107	106	6	0	6	2	1104	1090	7
16	4	0	1989	1971	14	13	13	0	302	306	7	19	5	1	57	43	33	5	15	1	223	229	7	2	6	2	91	95	8
18	4	0	133	120	11	15	13	0	245	252	8	21	5	1	749	755	7	7	15	1	307	310	6	4	6	2	1001	1012	8
20	4	0	262	253	8	0	14	0	1421	1408	9	0	6	1	471	456	4	9	15	1	56	60	30	6	6	2	2350	2313	10
1	5	0	1480	1455	7	2	14	0	395	406	5	2	6	1	194	191	4	11	15	1	142	128	11	8	6	2	260	249	5
3	5	0	66	56	11	4	14	0	209	197	7	4	6	1	239	244	4	13	15	1	152	140	11	10	6	2	0	19	1
5	5	0	3223	3140	9	6	14	0	735	740	6	6	6	1	865	856	6	0	16	1	277	284	7	12	6	2	385	389	5
7	5	0	880	849	6	8	14	0	142	139	10	8	6	1	527	511	5	2	16	1	222	235	8	14	6	2	940	959	7
9	5	0	134	146	7	10	14	0	1306	1318	9	10	6	1	96	85	11	4	16	1	40	24	40	16	6	2	1426	1425	10
11	5	0	339	356	5	12	14	0	55	67	42	12	6	1	344	330	5	6	16	1	1232	1232	9	18	6	2	97	54	16
13	5	0	310	318	5	14	14	0	69	32	25	14	6	1	37	5	37	8	16	1	316	321	7	20	6	2	60	77	37
15	5	0	272	284	6	1	15	0	272	263	6	16	6	1	1010	1019	8	10	16	1	42	40	41	1	7	2	758	746	5
17	5	0	468	464	6	3	15	0	396	405	6	18	6	1	242	253	8	12	16	1	79	66	21	3	7	2	35	30	34
19	5	0	204	206	9	5	15	0	497	498	5	20	6	1	422	420	6	1	17	1	16	51	15	5	7	2	4634	4437	12
21	5	0	292	298	8	7	15	0	13	6	13	1	7	1	91	98	9	3	17	1	278	280	7	7	7	2	179	190	6
0	6	0	887	880	6	9	15	0	140	141	10	3	7	1	591	582	4	5	17	1	728	736	6	9	7	2	492	498	5
2	6	0	150	151	5	11	15	0	395	398	6	5	7	1	475	479	4	7	17	1	247	241	8	11	7	2	137	142	9
4	6	0	390	396	4	13	15	0	426	430	7	7	7	1	188	189	6	9	17	1	412	400	6	13	7	2	368	377	5
6	6	0	575	551	4	0	16	0	583	564	6	9	7	1	490	497	5	0	18	1	286	291	7	15	7	2	992	951	8
8	6	0	675	661	5	2	16	0	193	193	8	11	7	1	0	3	1	2	18	1	65	63	27	17	7	2	914	909	8
10	6	0	1370	1372	9	4	16	0	196	201	8	13	7	1	79	69	15	4	18	1	339	356	7	19	7	2	72	81	25
12	6	0	278	276	5	6	16	0	801	797	7	15	7	1	0	34	1	6	18	1	152	347	7	0	8	2	457	458	4
14	6	0	458	461	5	8	16	0	69	67	21	17	7	1	206	199	8	1	19	1	321	328	8	2	8	2	479	480	4
16	6	0	553	554	6	10	16	0	26	39	25	19	7	1	157	152	10	3	19	1	407	407	7	4	8	2	192	201	6
18	6	0	393	383	6	12	16	0	414	430	7	0	8	1	640	613	5	0	0	2	1210	3369	7	6	8	2	382	376	4
20	6	0	0	22	1	1	17	0	277	271	7	2	8	1	22	28	21	2	0	2	619	647	5	8	8	2	626	619	5
1	7	0	733	705	5	3	17	0	314	310	7	4	8	1	118	120	8	4	0	2	390	380	3	10	8	2	51	48	11
3	7	0	162	167	5	5	17	0	1781	1774	13	6	8	1	284	298	5	6	0	2	782	750	6	12	8	2	186	184	7
5	7	0	1447	1397	10	7	17	0	13	36	13	8	8	1	136	125	8	8	0	2	638	623	5	14	8	2	560	558	6
7	7	0	468	454	5	9	17	0	0	29	1	10	8	1	97	58	11	10	0	2	1428	1380	11	16	8	2	895	880	7
9	7	0	1253	1234	9	0	18	0	333	324	7	12	8	1	472	471	5	12	0	2	908	928	7	18	8	2	74	79	22
11	7	0	544	512	5	2	18	0	324	314	7	14	8	1	559	561	6	14	0	2	1356	1368	10	1	9	2	476	461	5
13	7	0	397	400	5	4	18	0	76	52	22	16	8	1	690	685	6	16	0	2	710	713	7	3	9	2	56	48	20
15	7	0	257	257	7	6	18	0	230	235	8	18	8	1	327	323	7	18	0	2	846	833	7	5	9	2	462	458	5
17	7	0	240	226	7	8	18	0	330	330	7	20	8	1	232	231	8	20	0	2	63	87	30	7	9	2	420	425	5
19	7	0	711	728	7	1	19	0	212	214	9	1	9	1	941	927	6	1	1	2	532	539	4	9	9	2	681	689	6
0	8	0	2609	2563	10	3	19	0	93	88	18	3	9	1	153	141	7	3	1	2	767	765	6	11	9	2	1548	1551	11
2	8	0	159	164	6	1	1	1	160	151	3	5	9	1	427	436	4	5	1	2	1060	1072	8	13	9	2	120	103	11

Observed and calculated structure factors for K5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	309	300	6	20	2	3	91	78	18	17	11	3	508	513	6	10	4	4	331	317	5	10	14	4	1017	1039	9
17	9	2	638	642	6	1	3	3	524	520	4	0	12	3	226	226	7	12	4	4	177	167	8	12	14	4	25	32	24
19	9	2	285	291	8	3	3	3	257	262	4	2	12	3	271	272	6	14	4	4	838	852	7	1	15	4	213	218	8
0	10	2	4413	4326	13	5	3	3	1078	1063	8	4	12	3	346	350	5	16	4	4	1399	1404	11	3	15	4	402	404	6
2	10	2	641	638	5	7	3	3	736	732	6	6	12	3	123	125	10	18	4	4	167	173	10	5	15	4	221	222	8
4	10	2	721	732	6	9	3	3	200	200	6	8	12	3	81	83	16	1	5	4	1008	997	7	7	15	4	127	116	12
6	10	2	110	93	10	11	3	3	1326	1317	10	10	12	3	171	168	9	3	5	4	154	151	7	9	15	4	143	131	11
8	10	2	279	291	6	13	3	3	73	79	17	12	12	3	251	254	7	5	5	4	1515	1545	11	0	16	4	140	137	11
10	10	2	1833	1845	14	15	3	3	100	101	14	14	12	3	149	155	11	7	5	4	408	407	5	2	16	4	195	178	9
12	10	2	329	321	6	17	3	3	241	234	7	16	12	3	413	399	7	9	5	4	137	132	8	4	16	4	153	137	11
14	10	2	363	361	6	19	3	3	142	130	11	1	13	3	242	247	6	11	5	4	897	910	7	6	16	4	429	433	6
16	10	2	222	216	8	21	3	3	404	404	7	3	13	3	457	458	5	13	5	4	158	161	9	8	16	4	32	2	31
18	10	2	300	275	7	0	4	3	2165	2099	9	5	13	3	365	373	6	15	5	4	283	273	7	1	17	4	141	140	7
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3	11	2	716	720	6	4	4	3	370	378	4	9	13	3	281	278	7	19	5	4	135	133	12	1	1	5	75	62	14
5	11	2	115	67	10	6	4	3	228	232	5	11	13	3	385	373	6	0	6	4	2086	2127	11	3	1	5	233	241	6
7	11	2	27	6	27	8	4	3	248	259	5	13	13	3	41	9	41	2	6	4	160	169	7	5	1	5	654	649	5
9	11	2	630	633	6	10	4	3	388	378	5	15	13	3	145	153	12	4	6	4	386	388	5	7	1	5	50	42	31
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13	11	2	54	38	32	14	4	3	107	113	12	2	14	3	235	237	7	8	6	4	353	352	5	11	1	5	229	225	6
15	11	2	239	236	8	16	4	3	209	208	8	4	14	3	392	392	6	10	6	4	1264	1262	9	13	1	5	172	181	8
17	11	2	107	101	15	18	4	3	163	157	10	6	14	3	181	193	8	12	6	4	359	365	6	15	1	5	30	6	30
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4	12	2	59	58	23	3	5	3	363	371	4	12	14	3	28	28	27	18	6	4	271	280	8	0	2	5	698	702	6
6	12	2	839	854	7	5	5	3	890	884	7	1	15	3	185	177	8	1	7	4	274	271	5	2	2	5	85	60	12
8	12	2	171	170	8	7	5	3	845	836	6	3	15	3	229	216	7	3	7	4	247	239	5	4	2	5	450	453	5
10	12	2	778	781	7	9	5	3	420	422	5	5	15	3	418	416	6	5	7	4	1273	1284	10	6	2	5	482	472	5
12	12	2	269	251	7	11	5	3	117	123	10	7	15	3	175	174	9	7	7	4	375	372	5	8	2	5	339	346	5
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3	13	2	81	77	15	19	5	3	94	84	17	2	16	3	74	67	21	15	7	4	250	247	7	16	2	5	248	246	8
5	13	2	1769	1776	11	0	6	3	557	546	5	4	16	3	191	192	9	17	7	4	332	343	7	18	2	5	113	111	16
7	13	2	49	40	40	2	6	3	94	94	9	6	16	3	1070	1071	8	0	8	4	1841	1876	12	1	3	5	124	120	9
9	13	2	112	132	12	4	6	3	467	452	5	8	16	3	258	259	8	2	8	4	0	21	1	3	3	5	198	202	6
11	13	2	121	124	12	6	6	3	1183	1179	9	10	16	3	105	109	15	4	8	4	201	205	6	5	3	5	501	511	5
13	13	2	99	96	15	8	6	3	372	374	5	1	17	3	117	119	14	6	8	4	540	547	5	7	3	5	112	107	10
15	13	2	532	522	6	10	6	3	117	129	10	3	17	3	295	288	7	8	8	4	166	374	5	9	3	5	121	112	10
0	14	2	430	424	5	12	6	3	290	291	6	5	17	3	450	450	6	10	8	4	1139	1154	8	11	3	5	266	275	6
2	14	2	317	328	6	14	6	3	72	85	19	7	17	3	20	14	20	12	8	4	133	134	10	13	3	5	293	294	6
4	14	2	701	702	6	16	6	3	1092	1094	9	0	18	3	212	211	9	14	8	4	127	119	12	15	3	5	54	20	36
6	14	2	416	429	6	18	6	3	373	380	7	2	18	3	179	167	10	16	8	4	232	227	8	17	3	5	522	523	6
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12	14	2	135	61	11	3	7	3	282	287	5	4	0	4	704	724	6	3	9	4	292	285	5	4	4	5	124	133	9
14	14	2	369	376	7	5	7	3	1197	1206	9	6	0	4	426	425	5	5	9	4	1723	1727	13	6	4	5	646	637	5
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3	15	2	260	270	7	9	7	3	486	492	5	10	0	4	2603	2656	13	9	9	4	0	17	1	10	4	5	139	137	9
5	15	2	1430	1446	11	11	7	3	801	805	7	12	0	4	916	929	7	11	9	4	237	212	7	12	4	5	490	490	5
7	15	2	504	513	6	13	7	3	126	129	10	14	0	4	410	404	5	13	9	4	114	106	12	14	4	5	275	269	7
9	15	2	95	90	15	15	7	3	130	133	11	16	0	4	165	154	9	15	9	4	179	391	7	16	4	5	635	638	6
11	15	2	379	383	7	17	7	3	627	619	6	18	0	4	584	587	6	17	9	4	571	569	6	18	4	5	264	266	8
13	15	2	149	136	11	19	7	3	112	118	15	20	0	4	148	165	12	0	10	4	839	844	7	1	5	5	155	150	8
0	16	2	948	928	8	0	8	3	896	879	7	1	1	4	250	248	4	2	10	4	23	20	22	3	5	5	333	320	5
2	16	2	137	126	11	2	8	3	133	137	8	3	1	4	84	70	10	4	10	4	458	473	5	5	5	5	705	708	6
4	16	2	57	65	33	4	8	3	343	350	5	5	1	4	248	238	5	6	10	4	212	200	7	7	5	5	571	572	5
6	16	2	501	498	6	6	8	3	579	578	5	7	1	4	31	24	31	8	10	4	350	351	6	9	5	5	401	403	5
8	16	2	90	79	16	8	8	3	63	42	19	9	1	4	1219	1269	10	10	10	4	469	471	5	11	5	5	255	248	6
10	16	2	700	696	6	10	8	3	76	87	17	11	1	4	1569	1607	13	12	10	4	181	197	9	13	5	5	421	433	6
1	17	2	239	221	8	12	8	3	560	563	5	13	1	4	169	159	8	14	10	4	884	893	7	15	5	5	84	85	18
3	17	2	405	397	6	14	8	3	345	343	6	15	1	4	190	182	8	16	10	4	374	369	7	17	5	5	186	165	10
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7	17	2	0	40	1	18	8	3	161	155	11	19	1	4	552	550	6	3	11	4	356	348	5	2	6	5	108	110	10
9	17	2	353	351	7	1	9	3	572	572	5	0	2	4	305	341	4	5	11	4	1063	1093	8	4	6	5	0	34	1
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2	18	2	68	34	25	5	9	3	257	256	5	4	2	4	416	410	4	9	11	4	57	38	27	8	6	5	315	333	6
4	18	2	226	232	9	7	9	3	205	201	6	6	2	4	464	480	4	11	11	4	0	36	1	10	6	5	54	49	28
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1	1	3	256	248	3	11	9	3	866	866	7	10	2	4	438	450	5	15	11	4	744	749	7	14	6	5	0	8	1
3	1	3	662	648	5	13	9	3	13	12	12	12	2	4	307	325	6	0	12	4	922	912	7	16	6	5	693	680	7
5	1	3	204	203	4	15	9	3	89	80	17	14	2	4	637	638	6	2	12	4	266	256	6	1	7	5	77	58	15
7	1	3	255	250	4	17	9	3	502	497	6	16	2	4	699	725	7	4	12	4	148	148	9	3	7	5	460	471	5
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11	1	3	1330	1342	10	2	10	3	769	780	6	20	2	4	122	118	14	8	12	4	225	241	7	7	7	5	307	306	6
13	1	3	420	425	5	4	10	3	398	406	5	1	3	4	247	256	5	10	12	4	407	403	6	9	7	5	332	334	6
15	1	3	104	96	13	6	10	3	179	183	7	3	3	4	466	452	4	12	12	4	350	344	6	11	7	5	370	367	6
17	1	3	345	346	6	8	10	3	220	222	6	5	3	4	3318	3335	11	14	12	4	53	20	52	13	7	5	172	172	9
19	1	3	455	470	6	10	10	3	78	75	16	7	3	4	170	161	7	1	13	4	271	254	7	15	7	5	56	48	34
21	1	3	837	816	8	12	10	3	111	110	12	9	3	4	779	790	6	3	13	4	127	124	11	17	7	5	40	56	39
0	2	3	2274	2222	8	14	10	3	631	639	6	11	3	4	53	45	27	5	13	4	232	234	7	0	8	5	766	761	6
2	2	3	537	530	4	16	10	3	60	83	35	13	3	4	337	333	5	7	13	4	295	295	6	2	8	5	113	107	11
4	2	3	44	36	22	1	11	3	320	322	5	15	3	4	748	748	6	9	13	4	444	447	6	4	8	5	53	7	27
6	2	3	1069	1060	8	3	11	3	178	184	7	17	3	4	709	709	7	11	13	4	670	691	7	6	8	5	531	531	5
8	2	3	750	741	6	5	11	3	749	755	6	19	3	4	212	220	9	13	13	4	174	170	9	8	8	5	110	114	12
10	2	3	336	352	5	7	11	3	180	189	7	0	4	4	520	537	5	0	14	4	1391	1368	10	10	8	5	54	29	32
12	2	3	693	705	6	9	11	3	409	414	5	2	4	4	423	417	4	2	14	4	251	240	7	12	8	5	332	341	6
14	2	3	321	331	6	11	11	3	64	65	24	4	4	4	634	666	5	4	14	4	292	306	7	14	8	5	485	481	6
16	2	3	1075	1071	8	13	11	3	61	48	26	6	4	4	1824	1813	11	6	14	4	491	503	6	16	8	5	730	727	7
18	2	3	167	176	10	15	11	3	36	46	35	8	4	4	231	231	6	8	14	4	123	112	13	1	9	5	659	665	6

Observed and calculated structure factors for K5

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	9	5	80	65	16	9	1	6	361	360	6	10	8	6	111	101	13	2	4	7	105	97	12	9	1	8	680	676	7
5	9	5	516	512	6	11	1	6	193	206	8	12	8	6	184	182	10	4	4	7	261	264	7	11	1	8	481	477	6
7	9	5	103	105	6	13	1	6	50	47	50	14	8	6	403	390	7	6	4	7	95	92	15	0	2	8	39	4	19
9	9	5	62	51	24	15	1	6	445	441	6	1	9	6	140	135	6	8	4	7	214	206	8	2	2	8	99	84	14
11	9	5	1484	1484	11	17	1	6	297	297	8	3	9	6	91	100	15	10	4	7	245	240	7	4	2	8	254	242	7
13	9	5	104	97	15	0	2	6	1690	1676	13	5	9	6	48	36	48	12	4	7	475	470	6	6	2	8	506	492	6
15	9	5	58	77	19	2	2	6	217	209	6	7	9	6	482	493	6	14	4	7	141	133	12	8	2	8	60	27	31
0	10	5	997	996	8	4	2	6	203	193	6	9	9	6	463	462	6	1	5	7	0	11	1	10	2	8	282	236	7
2	10	5	494	500	5	6	2	6	492	496	5	11	9	6	709	694	6	3	5	7	205	195	7	1	3	8	154	141	10
4	10	5	166	155	8	8	2	6	237	248	7	13	9	6	40	49	39	5	5	7	323	318	6	3	3	8	294	300	7
6	10	5	438	428	5	10	2	6	783	782	7	0	10	6	2136	2104	15	7	5	7	492	496	6	5	3	8	1728	1740	13
8	10	5	92	101	15	12	2	6	291	293	7	2	10	6	107	101	6	9	5	7	300	298	7	7	3	8	59	18	31
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12	10	5	81	51	19	16	2	6	387	386	7	6	10	6	565	560	6	13	5	7	296	294	8	11	3	8	150	154	12
14	10	5	488	484	6	1	3	6	193	197	7	8	10	6	108	98	13	0	6	7	234	234	7	0	4	8	212	227	8
1	11	5	103	107	13	3	3	6	72	78	17	10	10	6	1256	1243	9	2	6	7	86	110	17	2	4	8	285	286	7
3	11	5	187	186	8	5	3	6	784	803	6	12	10	6	179	174	10	4	6	7	206	203	7	4	4	8	245	250	8
5	11	5	465	467	6	7	3	6	75	76	17	1	11	6	78	78	19	6	6	7	661	659	6	6	4	8	573	588	6
7	11	5	485	495	6	9	3	6	1080	1079	9	3	11	6	351	345	6	8	6	7	250	252	7	8	4	8	51	57	50
9	11	5	242	235	7	11	3	6	1058	1068	8	5	11	6	424	438	6	10	6	7	127	126	12	10	4	8	138	149	12
11	11	5	382	386	6	13	3	6	260	255	7	7	11	6	101	102	15	12	6	7	202	197	9	1	5	8	544	536	6
13	11	5	198	193	9	15	3	6	80	85	20	9	11	6	468	462	6	1	7	7	69	61	21	3	5	8	145	145	11
0	12	5	1100	1079	8	0	4	6	2398	2383	13	11	11	6	687	691	6	3	7	7	251	262	7	5	5	8	424	430	6
2	12	5	474	481	6	2	4	6	45	65	44	0	12	6	514	511	6	5	7	7	711	704	6	7	5	8	0	27	1
4	12	5	65	60	21	4	4	6	349	353	5	2	12	6	49	62	48	7	7	7	129	119	12	9	5	8	153	143	11
6	12	5	659	670	6	6	4	6	466	472	5	4	12	6	89	82	17	9	7	7	360	364	7	0	6	8	1836	1805	13
8	12	5	81	95	19	8	4	6	128	121	10	6	12	6	897	895	8	11	7	7	490	487	6	2	6	8	189	182	9
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12	12	5	215	212	9	12	4	6	244	237	7	10	12	6	405	414	7	2	8	7	108	112	11	6	6	8	439	433	6
1	13	5	310	304	6	14	4	6	57	68	35	1	13	6	31	29	31	4	8	7	268	267	7	8	6	8	163	156	11
3	13	5	251	255	7	16	4	6	185	192	10	3	13	6	42	40	42	6	8	7	323	324	7	1	7	8	82	69	20
5	13	5	930	942	8	1	5	6	259	259	6	5	13	6	1291	1312	9	8	8	7	50	33	50	3	7	8	186	168	9
7	13	5	168	168	9	3	5	6	316	321	5	7	13	6	165	166	11	10	8	7	76	68	23	5	7	8	892	879	7
9	13	5	309	298	7	5	5	6	454	450	5	0	14	6	62	39	31	1	9	7	375	368	6	7	7	8	209	215	9
11	13	5	1190	1167	9	7	5	6	75	78	18	2	14	6	382	374	7	3	9	7	55	38	34	0	8	8	925	912	8
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2	14	5	226	226	8	11	5	6	337	344	6	1	1	7	72	72	18	7	9	7	102	109	16	4	8	8	35	26	34
4	14	5	369	369	6	13	5	6	93	69	16	3	1	7	243	242	7	9	9	7	0	4	1	6	8	8	381	389	7
6	14	5	185	184	7	15	5	6	209	221	9	5	1	7	65	50	21	0	10	7	587	582	6	1	9	8	46	27	45
8	14	5	202	195	9	0	6	6	165	158	8	7	1	7	245	241	7	2	10	7	428	427	6	3	9	8	148	156	12
1	15	5	100	83	16	2	6	6	0	13	1	9	1	7	211	214	8	4	10	7	195	191	9	5	9	8	1192	1203	9
3	15	5	253	256	8	4	6	6	494	502	5	11	1	7	706	709	7	6	10	7	191	174	9	0	10	8	1018	998	8
5	15	5	76	69	22	6	6	6	833	832	7	13	1	7	312	320	7	8	10	7	107	105	15	2	10	8	111	100	15
7	15	5	277	289	8	8	6	6	284	286	6	15	1	7	95	120	18	1	11	7	179	174	10	1	1	9	75	46	23
0	16	5	247	249	8	10	6	6	76	91	19	0	2	7	665	657	6	3	11	7	115	114	14	3	1	9	172	187	11
2	16	5	266	259	8	12	6	6	178	183	9	2	2	7	306	299	6	5	11	7	535	529	6	5	1	9	278	267	8
4	16	5	138	128	13	14	6	6	826	826	7	4	2	7	0	9	1	7	11	7	146	140	12	0	2	9	93	79	17
0	0	6	2491	2544	13	1	7	6	595	595	6	6	2	7	440	436	6	0	12	7	54	59	53	2	2	9	77	40	20
2	0	6	110	115	11	3	7	6	152	152	9	8	2	7	295	295	6	2	12	7	165	169	10	4	2	9	226	207	8
4	0	6	624	610	6	5	7	6	2421	2422	14	10	2	7	99	95	15	4	12	7	250	243	8	6	2	9	0	11	1
6	0	6	666	672	6	7	7	6	108	102	13	12	2	7	511	508	6	0	0	8	2417	2459	15	1	3	9	154	144	11
8	0	6	407	407	5	9	7	6	391	397	6	14	2	7	178	164	10	2	0	8	151	142	10	3	3	9	0	26	1
10	0	6	870	879	8	11	7	6	457	469	6	1	3	7	195	189	7	4	0	8	262	266	7	5	3	9	59	54	17
12	0	6	720	731	7	13	7	6	224	228	8	3	3	7	56	28	28	6	0	8	710	706	6	0	4	9	424	415	7
14	0	6	794	783	7	15	7	6	611	625	7	5	3	7	398	393	6	8	0	8	29	12	29	2	4	9	13	49	13
16	0	6	821	826	7	0	8	6	297	292	6	7	3	7	442	434	6	10	0	8	1417	1421	10	4	4	9	78	77	21
1	1	6	158	161	8	2	8	6	201	207	8	9	3	7	176	176	9	1	1	8	110	99	13	1	5	9	0	9	1
3	1	6	145	150	8	4	8	6	288	294	6	11	3	7	755	743	7	3	1	8	110	102	13	3	5	9	129	103	13
5	1	6	1638	1687	13	6	8	6	264	264	7	13	3	7	0	25	1	5	1	8	473	471	6						
7	1	6	80	75	16	8	8	6	361	367	6	0	4	7	990	968	8	7	1	8	200	190	9						

Observed and calculated structure factors for K6

h	k	l	10Fo	10Fc	10s
2	0	0	570	579	4
4	0	0	1283	1287	7
6	0	0	674	686	6
8	0	0	1065	1062	7
10	0	0	1857	1863	13
12	0	0	1353	1351	9
14	0	0	237	225	8
16	0	0	362	368	7
18	0	0	670	648	7
20	0	0	286	287	9
22	0	0	1641	1630	11
1	1	0	629	688	4
1	1	0	262	249	4
5	1	0	617	618	5
7	1	0	497	496	4
9	1	0	1738	1730	11
11	1	0	2926	2908	13
13	1	0	300	295	6
15	1	0	252	248	8
17	1	0	268	279	8
19	1	0	616	598	7
21	1	0	812	827	8
0	2	0	1275	1308	5
2	2	0	255	269	4
4	2	0	684	708	5
6	2	0	130	144	8
8	2	0	284	283	5
10	2	0	648	665	6
12	2	0	303	298	6
14	2	0	849	862	7
16	2	0	746	741	7
18	2	0	59	18	52
20	2	0	188	176	12
22	2	0	340	329	9
1	3	0	325	314	4
3	3	0	415	424	4
5	3	0	4943	5023	11
7	3	0	500	484	5
9	3	0	1023	1027	7
11	3	0	448	431	5
13	3	0	458	459	6
15	3	0	905	928	8
17	3	0	922	919	7
19	3	0	234	230	10
21	3	0	303	305	9
0	4	0	2323	2370	8
2	4	0	621	622	5
4	4	0	1188	1193	9
6	4	0	3671	3644	11
8	4	0	551	552	5
10	4	0	558	563	5
12	4	0	241	222	7
14	4	0	904	911	7
16	4	0	2060	2063	13
18	4	0	129	119	16
20	4	0	240	235	10
22	4	0	406	402	9
1	5	0	1457	1456	9
3	5	0	79	82	12
5	5	0	3188	3215	11
7	5	0	868	844	7
9	5	0	114	122	12
11	5	0	316	335	6
13	5	0	253	277	8
15	5	0	276	285	8
17	5	0	479	472	7
19	5	0	204	204	11
21	5	0	272	290	11
0	6	0	1072	1069	7
2	6	0	103	106	10
4	6	0	369	373	4
6	6	0	495	477	5
8	6	0	588	570	5
10	6	0	1443	1460	11
12	6	0	280	279	7
14	6	0	422	434	6
16	6	0	465	468	7
18	6	0	421	416	7
20	6	0	0	2	1
1	7	0	747	728	6
3	7	0	202	203	6
5	7	0	1530	1556	11
7	7	0	428	429	5
9	7	0	1265	1292	9
11	7	0	647	604	6
13	7	0	433	426	6
15	7	0	271	270	8
17	7	0	212	205	10
19	7	0	693	704	7
0	8	0	2712	2703	12
2	8	0	141	145	9
4	8	0	482	482	5
6	8	0	560	571	5
8	8	0	531	538	6
10	8	0	1397	1391	10
12	8	0	222	220	8
14	8	0	116	101	15
16	8	0	263	238	9
18	8	0	56	33	55
20	8	0	322	310	9
1	9	0	174	152	8
3	9	0	351	358	5
5	9	0	1862	1918	13
7	9	0	899	896	7
9	9	0	105	95	15
11	9	0	566	554	6
13	9	0	277	296	8
15	9	0	572	583	6
17	9	0	508	508	7
19	9	0	281	278	10
0	10	0	445	453	5
2	10	0	19	12	19
4	10	0	450	456	6
6	10	0	214	212	8
8	10	0	356	367	6
10	10	0	601	606	6
12	10	0	144	130	12
14	10	0	1175	1186	9
16	10	0	309	316	8
18	10	0	559	552	7
1	11	0	313	319	6
3	11	0	337	336	6
5	11	0	1010	1030	8
7	11	0	138	145	11
9	11	0	148	139	11
11	11	0	410	421	7
13	11	0	239	241	9
15	11	0	897	906	8
17	11	0	439	453	8
0	12	0	1483	1490	10
2	12	0	220	218	8
4	12	0	323	319	7
6	12	0	675	671	7
8	12	0	144	170	13
10	12	0	632	638	7
12	12	0	547	538	7
14	12	0	151	147	14
16	12	0	106	97	21
1	13	0	501	496	6
3	13	0	204	200	9
5	13	0	469	469	6
7	13	0	486	493	6
9	13	0	464	463	7
11	13	0	962	968	8
13	13	0	314	304	9
15	13	0	254	265	10
0	14	0	1600	1600	11
2	14	0	398	413	7
4	14	0	235	228	9
6	14	0	680	675	6
8	14	0	192	187	11
10	14	0	1384	1396	11
12	14	0	56	75	56
14	14	0	57	11	56
1	15	0	298	294	8
3	15	0	416	407	7
5	15	0	452	456	7
7	15	0	61	26	43
9	15	0	190	194	12
11	15	0	374	367	8
13	15	0	436	443	8
0	16	0	614	602	7
2	16	0	194	184	11
4	16	0	180	175	12
6	16	0	857	859	8
8	16	0	67	57	38
10	16	0	76	44	34
12	16	0	438	444	8
1	17	0	249	240	10
3	17	0	314	329	9
5	17	0	1869	1897	15
7	17	0	50	41	49
9	17	0	58	50	58
0	18	0	232	230	11
2	18	0	289	292	9
4	18	0	140	120	16
6	18	0	239	243	11
8	18	0	336	335	9
1	19	0	262	252	10
3	19	0	62	73	61
1	1	1	157	149	5
3	1	1	536	529	4
5	1	1	654	665	5
7	1	1	126	114	8
9	1	1	401	385	5
11	1	1	900	915	7
13	1	1	308	290	6
15	1	1	43	22	43
17	1	1	717	725	6
19	1	1	465	481	7
21	1	1	919	902	8
0	2	1	298	261	4
2	2	1	425	447	4
4	2	1	414	412	4
6	2	1	204	187	5
8	2	1	742	748	6
10	2	1	394	416	5
12	2	1	969	977	8
14	2	1	103	95	16
16	2	1	771	780	7
18	2	1	53	39	53
20	2	1	170	174	13
22	2	1	216	222	12
1	3	1	292	298	4
3	3	1	222	201	5
5	3	1	221	215	5
7	3	1	514	510	5
9	3	1	301	305	5
11	3	1	282	284	6
13	3	1	313	322	7
15	3	1	33	25	32
17	3	1	330	336	7
19	3	1	217	210	10
21	3	1	386	373	8
0	4	1	931	938	7
2	4	1	56	67	21
4	4	1	264	249	4
6	4	1	840	800	6
8	4	1	541	534	5
10	4	1	231	207	7
12	4	1	702	713	6
14	4	1	257	261	8
16	4	1	676	674	7
18	4	1	223	223	10
20	4	1	70	91	40
1	5	1	111	114	9
3	5	1	626	643	5
5	5	1	1736	1718	10
7	5	1	882	874	7
9	5	1	497	494	5
11	5	1	381	403	6
13	5	1	674	684	6
15	5	1	171	159	11
17	5	1	243	240	9
19	5	1	13	34	12
21	5	1	829	809	8
0	6	1	298	273	4
2	6	1	208	201	6
4	6	1	310	303	4
6	6	1	892	889	7
8	6	1	442	440	5
10	6	1	44	21	44
12	6	1	377	368	6
14	6	1	0	19	1
16	6	1	1102	1096	9
18	6	1	243	236	10
20	6	1	433	431	8
1	7	1	75	90	16
3	7	1	596	589	5
5	7	1	441	454	5
7	7	1	170	166	8
9	7	1	479	498	6
11	7	1	66	2	27
13	7	1	69	67	27
15	7	1	19	31	38
17	7	1	176	176	11
19	7	1	160	149	14
0	8	1	819	789	6
2	8	1	0	46	1
4	8	1	89	91	16
6	8	1	340	353	5
8	8	1	183	184	9
10	8	1	149	138	11
12	8	1	483	491	6
14	8	1	548	557	6
16	8	1	771	761	7
18	8	1	287	300	9
20	8	1	227	231	12
1	9	1	939	917	7
3	9	1	211	197	7
5	9	1	534	555	6
7	9	1	338	337	6
9	9	1	97	101	17
11	9	1	1711	1739	12
13	9	1	0	13	1
15	9	1	62	43	45
17	9	1	191	190	12
19	9	1	181	179	13
0	10	1	1336	1338	9
2	10	1	801	788	7
4	10	1	340	341	6
6	10	1	404	418	6
8	10	1	140	123	12
10	10	1	295	290	7
12	10	1	34	47	34
14	10	1	651	653	7
16	10	1	308	326	9
18	10	1	290	286	9
1	11	1	248	254	7
3	11	1	270	261	7
5	11	1	631	642	6
7	11	1	491	500	6
9	11	1	356	363	7
11	11	1	390	389	7
13	11	1	121	106	16
15	11	1	51	81	51
17	11	1	403	406	8
0	12	1	1221	1228	9
2	12	1	476	471	6
4	12	1	82	74	21
6	12	1	663	660	6
8	12	1	205	205	9
10	12	1	228	246	9
12	12	1	309	291	8
14	12	1	51	66	50
16	12	1	765	777	8
1	13	1	334	326	7
3	13	1	332	332	7
5	13	1	1025	1048	8
7	13	1	106	100	17
9	13	1	377	376	7
11	13	1	1118	1118	9
13	13	1	92	105	25
15	13	1	249	233	10
0	14	1	675	687	7
2	14	1	290	296	8
4	14	1	462	479	7
6	14	1	231	231	9
8	14	1	301	297	8
10	14	1	186	195	12
12	14	1	162	125	13
14	14	1	425	413	8
1	15	1	24	7	24
3	15	1	257	268	9
5	15	1	298	304	8
7	15	1	315	321	8
9	15	1	74	64	32
11	15	1	189	175	12
13	15	1	142	122	16
0	16	1	172	360	7
2	16	1	254	242	9
4	16	1	73	48	30
6	16	1	1254	1258	10
8	16	1	274	280	10
10	16	1	62	12	62
12	16	1	119	109	20
1	17	1	57	40	56
3	17	1	290	294	9
5	17	1	742	748	8
7	17	1	259	269	10
9	17	1	435	429	8
0	18	1	262	258	10
2	18	1	74	55	36
4	18	1	385	383	8
6	18	1	392	373	8
1	19	1	312	332	10
3	19	1	396	387	9
0	0	2	3647	3635	9
2	0	2	632	646	5
4	0	2	474	472	4
6	0	2	725	695	6
8	0	2	687	673	6
10	0	2	1501	1478	10
12	0	2	876	871	7
14	0	2	1353	1368	10
16	0	2	808	812	7
18	0	2	836	824	7
20	0	2	56	77	56
22	0	2	194	207	13
1	1	2	508	518	4
3	1	2	672	670	5
5	1	2	1244	1232	9
7	1	2	160	160	7
9	1	2	683	679	6
11	1	2	585	576	6
13	1	2	137	141	12
15	1	2	707	709	6
17	1	2	89	87	21
19	1	2	48	20	47
21	1	2	264	256	10
0	2	2	4304	4184	10
2	2	2	302	305	4
4	2	2	464	469	5
6	2	2	391	390	4
8	2	2	211	204	6
10	2	2	1341	1342	10
12	2	2	553	546	6
14	2	2	117	125	14
16	2	2	298	294	8
18	2	2	105	70	19
20	2	2	58	2	57
1	3	2	362	365	4
3	3	2	192	190	5
5	3	2	1246	1226	8
7	3	2	125	121	9
9	3	2	1643	1661	12
11	3	2	1471	1456	11
13	3	2	515	505	6
15	3	2	217	212	9
17	3	2	280	283	8
19	3	2	817	820	7
21	3	2	632	625	7
0	4	2	2206	2172	9
2	4	2	722	714	5
4	4	2	55	36	22
6	4	2	345	330	5
8	4	2	238	254	6
10	4	2	2133	2176	13
12	4	2	245	247	7
14	4	2	260	261	8
16	4	2	93	79	20
18	4	2	558	546	7
20	4	2	344	334	9
1	5	2	1056	1030	8
3	5	2	102	100	10
5	5	2	1803	1771	11
7	5	2	188	162	8
9	5	2	479	473	5
11	5	2	651	646	6
13	5	2	43	42	43
15	5	2	273	276	8
17	5	2	772	758	7
19	5	2	416	418	8
21	5	2	474	464	8
0	6	2	1248	1222	8
2	6	2	119	118	9
4	6	2	1043	1053	8
6	6	2	2410	2354	12
8	6	2	239	235	7
10	6	2	123	65	13
12	6	2	158	161	6
14	6	2	948	957	8
16	6	2	1496	1508	11
18	6	2	9	40	9
20	6	2	79	73	34
1	7	2	710	707	6
3	7	2	105	114	12
5	7	2	4608	4673	14
7	7	2	188	189	8
9	7	2	514	524	5
11	7	2	95	18	18
13	7	2	434	443	6
15	7	2	982	986	8
17	7	2	915	917	8
19	7	2	46	66	45
0	8	2	342	343	5
2	8	2	444	439	5
4	8	2	279	294	6
6	8	2	410	393	5
8	8	2	624	624	6
10	8	2	68	74	28
12	8	2	215	217	9
14	8	2	597	605	6
16	8	2	928	929	8
18	8	2	111	87	19
1	9	2	497	481	6
3	9	2	54	46	43
5	9	2	467	465	6
7	9	2	437	421	6
9	9	2	667	673	6

Observed and calculated structure factors for K6

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1576	1583	11	16	2	3	1159	1156	9	13	11	3	67	65	41	4	4	4	709	729	6	4	14	4	342	337	8
13	9	2	89	111	22	18	2	3	137	153	15	15	11	3	79	61	32	6	4	4	1830	1854	13	6	14	4	452	460	7
15	9	2	296	296	8	20	2	3	110	102	22	17	11	3	495	503	8	8	4	4	250	261	7	8	14	4	176	153	13
17	9	2	642	638	7	1	3	3	501	499	5	0	12	3	349	351	7	10	4	4	385	398	6	10	14	4	1122	1098	10
19	9	2	284	275	10	3	3	3	290	294	5	2	12	3	255	259	8	12	4	4	118	119	15	12	14	4	48	33	48
0	10	2	4556	4526	15	5	3	3	1172	1136	9	4	12	3	330	330	7	14	4	4	870	882	7	1	15	4	255	258	10
2	10	2	607	616	6	7	3	3	774	757	6	6	12	3	180	164	11	16	4	4	1498	1490	11	3	15	4	407	400	8
4	10	2	726	739	7	9	3	3	228	226	7	8	12	3	135	126	14	18	4	4	173	173	13	5	15	4	206	202	11
6	10	2	31	8	30	11	3	3	1341	1352	10	10	12	3	236	238	9	1	5	4	1021	993	8	7	15	4	169	152	14
8	10	2	357	355	6	13	3	3	111	107	16	12	12	3	263	279	10	3	5	4	137	139	11	9	15	4	152	185	16
10	10	2	1929	1943	16	15	3	3	69	97	31	14	12	3	144	154	16	5	5	4	1573	1609	11	0	16	4	146	170	16
12	10	2	313	314	8	17	3	3	224	225	10	16	12	3	484	480	8	7	5	4	409	402	6	2	16	4	159	172	15
14	10	2	359	356	8	19	3	3	134	131	16	1	13	3	229	229	9	9	5	4	113	115	15	4	16	4	112	113	21
16	10	2	107	130	21	21	3	3	449	440	8	3	13	3	439	437	7	11	5	4	878	891	8	6	16	4	483	489	8
18	10	2	303	315	10	0	4	3	2105	2010	11	5	13	3	439	438	7	13	5	4	125	128	15	8	16	4	0	9	1
1	11	2	102	305	7	2	4	3	38	64	37	7	13	3	107	109	17	15	5	4	268	280	9	1	17	4	301	314	10
3	11	2	728	726	7	4	4	3	371	368	5	9	13	3	304	307	8	17	5	4	82	92	29	3	17	4	239	218	11
5	11	2	188	183	9	6	4	3	189	194	8	11	13	3	424	410	8	19	5	4	118	130	20	1	1	5	50	60	50
7	11	2	41	35	41	8	4	3	286	296	6	13	13	3	28	31	27	0	6	4	2269	2260	13	3	1	5	257	270	7
9	11	2	708	714	6	10	4	3	360	346	6	15	13	3	154	145	16	2	6	4	120	140	13	5	1	5	563	562	6
11	11	2	1784	1791	14	12	4	3	777	772	7	0	14	3	0	27	1	4	6	4	377	377	6	7	1	5	36	20	35
13	11	2	23	23	23	14	4	3	88	100	21	2	14	3	240	249	9	6	6	4	190	197	9	9	1	5	303	323	7
15	11	2	223	230	11	16	4	3	263	254	8	4	14	3	397	406	7	8	6	4	277	286	7	11	1	5	286	293	8
17	11	2	106	109	23	18	4	3	109	131	20	6	14	3	189	200	11	10	6	4	1326	1329	10	13	1	5	151	149	13
0	12	2	1409	1401	10	20	4	3	0	27	1	8	14	3	344	351	8	12	6	4	359	365	7	15	1	5	58	4	57
2	12	2	0	22	1	1	5	3	81	82	16	10	14	3	33	34	32	14	6	4	231	230	9	17	1	5	745	739	7
4	12	2	102	94	17	3	5	3	418	423	5	12	14	3	0	16	1	16	6	4	142	150	15	19	1	5	349	378	9
6	12	2	855	864	7	5	5	3	1031	1042	7	1	15	3	195	180	11	18	6	4	312	304	9	0	2	5	582	562	6
8	12	2	182	187	10	7	5	3	867	866	7	3	15	3	198	190	11	1	7	4	294	288	7	2	2	5	72	61	24
10	12	2	814	802	8	9	5	3	364	376	6	5	15	3	511	499	7	3	7	4	268	258	7	4	2	5	408	407	6
12	12	2	247	258	9	11	5	3	200	202	9	7	15	3	193	192	12	5	7	4	1408	1406	10	6	2	5	435	437	6
14	12	2	517	494	7	13	5	3	524	522	6	9	15	3	110	117	20	7	7	4	362	349	6	8	2	5	394	389	6
16	12	2	356	374	9	15	5	3	106	64	18	11	15	3	375	375	8	9	7	4	980	1008	8	10	2	5	164	150	11
1	13	2	137	140	13	17	5	3	320	306	8	0	16	3	215	213	11	11	7	4	767	768	7	12	2	5	783	778	7
3	13	2	43	41	42	19	5	3	78	76	33	2	16	3	72	77	36	13	7	4	370	359	7	14	2	5	0	25	1
5	13	2	1886	1888	13	0	6	3	673	671	6	4	16	3	152	175	15	15	7	4	259	258	9	16	2	5	313	312	9
7	13	2	65	66	35	2	6	3	95	83	14	6	16	3	1115	1116	9	17	7	4	306	326	9	18	2	5	127	129	18
9	13	2	103	113	19	4	6	3	517	503	6	8	16	3	218	225	11	0	8	4	1955	2001	14	1	3	5	104	108	15
11	13	2	48	62	48	6	6	3	1174	1197	9	10	16	3	141	151	17	2	8	4	0	6	1	3	3	5	179	184	9
13	13	2	133	143	17	8	6	3	322	311	6	1	17	3	111	116	21	4	8	4	235	230	8	5	3	5	468	473	6
15	13	2	537	556	8	10	6	3	68	82	28	3	17	3	310	301	9	6	8	4	520	518	6	7	3	5	107	121	16
0	14	2	517	521	6	12	6	3	341	332	7	5	17	3	481	479	8	8	8	4	424	428	6	9	3	5	126	127	14
2	14	2	320	316	7	14	6	3	43	64	42	7	17	3	0	10	1	10	8	4	1206	1212	9	11	3	5	243	253	9
4	14	2	755	757	7	16	6	3	1153	1156	9	0	18	3	230	234	12	12	8	4	124	137	16	13	3	5	336	318	8
6	14	2	463	454	7	18	6	3	363	366	8	2	18	3	174	168	14	14	8	4	97	93	23	15	3	5	50	26	49
8	14	2	222	226	10	20	6	3	402	393	8	4	18	3	205	193	12	16	8	4	203	189	11	17	3	5	526	531	8
10	14	2	207	199	11	1	7	3	148	126	10	0	0	4	6936	6828	15	18	8	4	111	89	21	0	4	5	31	25	30
12	14	2	83	73	29	3	7	3	278	292	6	2	0	4	346	347	5	1	9	4	67	77	29	2	4	5	64	37	30
14	14	2	410	412	8	5	7	3	1180	1173	9	4	0	4	713	739	6	3	9	4	239	243	8	4	4	5	119	125	14
1	15	2	596	584	7	7	7	3	198	209	8	6	0	4	361	342	5	5	9	4	1773	1787	12	6	4	5	688	682	7
3	15	2	297	295	8	9	7	3	501	496	6	8	0	4	374	376	6	7	9	4	495	504	6	8	4	5	363	381	7
5	15	2	1508	1517	11	11	7	3	793	794	7	10	0	4	2733	2785	15	9	9	4	0	23	1	10	4	5	128	111	14
7	15	2	528	528	7	13	7	3	122	129	15	12	0	4	912	911	8	11	9	4	160	164	12	12	4	5	497	490	6
9	15	2	48	56	47	15	7	3	143	137	13	14	0	4	388	399	7	13	9	4	129	135	16	14	4	5	248	258	9
11	15	2	359	364	9	17	7	3	582	590	7	16	0	4	49	61	48	15	9	4	403	411	8	16	4	5	685	687	7
13	15	2	178	177	14	19	7	3	113	115	21	18	0	4	629	617	7	17	9	4	584	588	8	18	4	5	246	250	11
0	16	2	1004	998	8	0	8	3	763	745	6	20	0	4	162	166	16	0	10	4	963	957	8	1	5	5	148	134	11
2	16	2	150	148	13	2	8	3	159	147	9	1	1	4	232	226	6	2	10	4	0	38	1	3	5	5	353	347	6
4	16	2	100	121	22	4	8	3	329	329	6	3	1	4	83	67	16	4	10	4	510	522	6	5	5	5	832	838	7
6	16	2	438	435	8	6	8	3	542	532	6	5	1	4	172	157	8	6	10	4	231	243	9	7	5	5	610	606	6
8	16	2	49	51	48	8	8	3	34	13	33	7	1	4	43	55	42	8	10	4	160	364	7	9	5	5	352	361	7
10	16	2	744	730	8	10	8	3	0	22	1	9	1	4	1298	1317	10	10	10	4	537	517	7	11	5	5	337	317	7
1	17	2	231	209	11	12	8	3	580	581	6	11	1	4	1628	1665	12	12	10	4	173	170	12	13	5	5	459	458	7
3	17	2	399	402	8	14	8	3	345	340	7	13	1	4	149	150	12	14	10	4	902	902	8	15	5	5	117	97	18
5	17	2	217	203	11	16	8	3	253	245	10	15	1	4	170	175	11	16	10	4	453	440	8	17	5	5	174	177	14
7	17	2	37	37	36	18	8	3	146	131	15	17	1	4	27	36	27	1	11	4	205	192	9	0	6	5	260	287	7
9	17	2	188	179	9	1	9	3	575	563	6	19	1	4	553	548	8	3	11	4	392	393	7	2	6	5	114	112	15
0	18	2	824	807	8	3	9	3	70	52	25	0	2	4	316	332	5	5	11	4	1199	1221	9	4	6	5	22	7	21
2	18	2	36	24	36	5	9	3	170	165	10	2	2	4	174	184	8	7	11	4	64	49	35	6	6	5	438	441	6
4	18	2	260	269	11	7	9	3	225	237	9	4	2	4	430	432	5	9	11	4	89	80	23	8	6	5	282	291	8
6	18	2	399	403	9	9	9	3	131	127	14	6	2	4	455	477	5	11	11	4	47	18	47	10	6	5	28	13	27
1	1	3	248	241	5	11	9	3	942	933	8	8	2	4	91	95	18	13	11	4	149	162	15	12	6	5	269	269	9
3	1	3	706	702	6	13	9	3	0	32	1	10	2	4	481	450	6	15	11	4	770	764	7	14	6	5	0	28	1
5	1	3	343	344	4	15	9	3	73	67	34	12	2	4	303	308	7	0	12	4	929	933	8	16	6	5	740	747	8
7	1	3	286	276	5	17	9	3	527	530	8	14	2	4	645	638	7	2	12	4	235	232	9	1	7	5	44	46	43
9	1	3	338	342	6	0	10	3	887	897	7	16	2	4	746	749	7	4	12	4	214	201	9	3	7	5	465	479	6
11	1	3	1417	1429	11	2	10	3	783	788	7	18	2	4	22	3	22	6	12	4	324	326	8	5	7	5	138	44	12
13	1	3	382	378	6	4	10	3	427	432	6	20	2	4	125	119	20	8	12	4	210	224	10	7	7	5	280	290	8
15	1	3	88	89	21	6	10	3	185	173	9	1	3	4	211	229	7	10	12	4	420	420	7	9	7	5	322	335	7
17	1	3	357	354	7	8	10	3	208	199	9	3	3	4	387	378	5	12	12	4	376	367	8	11	7	5	363	374	8
19	1	3	458	470	8	10	10	3	88	85	21	5	3	4	3486	3519	14	14	12	4	39	53	39	13	7	5	180	170	12
21	1	3	904	868	8	12	10	3	128	146	15	7	3	4	165	164	10	1	13	4	262	265	9	15	7	5	16	52	36
0	2	3	2543	2455	10	14	10	3	650	642	7	9	3	4	786	799	7	3	13	4	129	119	15	17	7	5	92	72	27
2	2	3	544	519	5	16	10	3	116	110	20	11	3	4	138	140	12	5	13	4	292	305	8	0	8	5	862	869	8
4	2	3	115	99	10	1	11	3	343	351	7	13	3	4	402	399	7	7	13	4	276	284	9	2	8	5	117	109	14
6	2	3	1157	1128	8	3	11	3	198	206	9	15	3	4	808	796	8	9	13	4	477	461	7	4	8	5	60	32	37
8	2	3	823	817	7	5	11	3	704	696	7	17	3	4	697	705	7	11	13	4	764	760	8	6	8	5	571	566	6
10	2	3	421	433	5	7	11	3	195	200	10	19	3	4	192	201	13	13	13	4	155	168	16	8	8	5	166	146	11
12	2	3	745	748	7	9	11	3	422	420	7	0	4	4	672	698	6	0	14	4	1529	1516	11	10	8	5	58	82	57
14	2	3	324	303	7	11	11	3	137	124	15	2	4	4	408	412	5	2	14	4	257	246	10	12	8	5	355	363	8

Observed and calculated structure factors for K6

h	k	l	10Fo	10Fc	10s
14	8	5	479	474	7
16	8	5	794	787	8
1	9	5	669	666	7
3	9	5	107	99	16
5	9	5	602	596	7
7	9	5	356	344	7
9	9	5	90	83	22
11	9	5	1581	1563	11
13	9	5	96	74	23
15	9	5	77	73	37
0	10	5	1057	1051	9
2	10	5	513	515	6
4	10	5	191	180	10
6	10	5	451	436	7
8	10	5	72	90	31
10	10	5	284	284	9
12	10	5	47	25	47
14	10	5	507	491	8
1	11	5	106	112	18
3	11	5	203	202	10
5	11	5	448	445	7
7	11	5	503	503	7
9	11	5	252	237	9
11	11	5	400	407	8
13	11	5	172	178	14
0	12	5	1166	1162	9
2	12	5	484	471	7
4	12	5	76	79	31
6	12	5	689	693	7
8	12	5	120	131	18
10	12	5	143	134	16
12	12	5	228	242	12
1	13	5	286	283	9
3	13	5	234	244	10
5	13	5	996	998	9
7	13	5	200	201	12
9	13	5	324	332	9
11	13	5	1190	1200	10
0	14	5	900	875	8
2	14	5	253	243	10
4	14	5	371	383	8
6	14	5	400	398	8
8	14	5	191	199	13
1	15	5	66	84	54
3	15	5	219	230	11
5	15	5	117	111	20
7	15	5	301	300	10
0	16	5	295	294	10
2	16	5	256	263	11
4	16	5	164	145	15
0	0	6	2705	2678	15
2	0	6	109	103	16
4	0	6	681	690	6
6	0	6	675	691	7
8	0	6	425	436	7
10	0	6	933	935	8
12	0	6	689	691	7
14	0	6	796	793	8
16	0	6	873	890	8
1	1	6	144	146	12
3	1	6	101	94	17
5	1	6	1775	1784	12
7	1	6	74	71	25
9	1	6	363	365	7
11	1	6	248	259	9
13	1	6	0	9	1
15	1	6	471	464	8
17	1	6	298	304	10
0	2	6	1722	1737	12
2	2	6	200	187	9
4	2	6	178	170	10
6	2	6	476	467	6
8	2	6	217	210	9
10	2	6	808	818	7
12	2	6	302	302	8
14	2	6	32	18	31
16	2	6	351	360	9
1	3	6	172	169	11
3	3	6	63	69	34
5	3	6	904	889	8
7	3	6	40	42	39
9	3	6	1112	1120	9
11	3	6	1107	1126	9
13	3	6	251	263	10
15	3	6	108	100	21
17	3	6	312	315	9
0	4	6	2571	2542	15
2	4	6	97	94	18
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6	4	6	518	520	6
8	4	6	187	189	11
10	4	6	1425	1445	11
12	4	6	237	230	10
14	4	6	95	74	23
16	4	6	249	258	11
1	5	6	302	301	7
3	5	6	304	302	7
5	5	6	460	458	6
7	5	6	112	105	16
9	5	6	263	259	9
11	5	6	355	341	8
13	5	6	84	79	29
15	5	6	229	241	11
0	6	6	119	102	15
2	6	6	27	3	26
4	6	6	526	526	6
6	6	6	857	857	8
8	6	6	283	285	8
10	6	6	71	64	33
12	6	6	163	168	13
14	6	6	829	831	8
1	7	6	590	582	6
3	7	6	93	110	21
5	7	6	2567	2564	17
7	7	6	65	99	19
9	7	6	424	420	7
11	7	6	183	400	8
13	7	6	289	274	9
15	7	6	677	654	7
0	8	6	265	245	8
2	8	6	186	185	11
4	8	6	351	356	7
6	8	6	265	265	9
8	8	6	361	371	8
10	8	6	97	94	23
12	8	6	219	209	11
14	8	6	437	426	8
1	9	6	364	359	7
3	9	6	60	106	60
5	9	6	0	25	1
7	9	6	495	494	7
9	9	6	459	453	7
11	9	6	735	732	7
13	9	6	43	43	42
0	10	6	2278	2255	18
2	10	6	288	289	9
4	10	6	330	320	8
6	10	6	515	505	7
8	10	6	138	136	16
10	10	6	1337	1328	10
12	10	6	188	178	13
1	11	6	79	56	29
3	11	6	358	345	8
5	11	6	371	371	8
7	11	6	84	87	28
9	11	6	525	522	8
11	11	6	745	743	8
0	12	6	550	551	7
2	12	6	86	63	26
4	12	6	103	104	22
6	12	6	908	913	8
8	12	6	0	50	1
10	12	6	438	429	8
1	13	6	14	10	14
3	13	6	0	20	1
5	13	6	1423	1414	11
7	13	6	183	186	14
0	14	6	0	47	1
2	14	6	367	366	9
4	14	6	344	346	9
6	14	6	146	145	17
1	1	7	79	76	27
3	1	7	260	257	8
5	1	7	38	16	38
7	1	7	252	262	9
9	1	7	181	184	12
11	1	7	757	769	8
13	1	7	288	299	10
15	1	7	103	117	24
0	2	7	782	764	7
2	2	7	316	309	7
4	2	7	30	24	30
6	2	7	470	470	7
8	2	7	328	320	8
10	2	7	148	139	14
12	2	7	535	539	7
14	2	7	158	139	14
1	3	7	190	187	10
3	3	7	0	18	1
5	3	7	432	438	7
7	3	7	441	446	7
9	3	7	182	190	12
11	3	7	784	776	8
13	3	7	0	12	1
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2	4	7	120	100	16
4	4	7	255	255	9
6	4	7	72	80	34
8	4	7	230	222	10
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14	4	7	118	125	21
1	5	7	0	3	1
3	5	7	232	212	9
5	5	7	397	395	7
7	5	7	515	521	7
9	5	7	273	270	9
11	5	7	97	76	24
13	5	7	311	317	10
0	6	7	301	285	8
2	6	7	115	121	17
4	6	7	234	225	10
6	6	7	679	679	7
8	6	7	223	227	10
10	6	7	62	100	61
12	6	7	233	225	11
1	7	7	36	66	35
3	7	7	250	263	9
5	7	7	716	706	7
7	7	7	132	125	16
9	7	7	338	360	9
11	7	7	487	496	8
0	8	7	459	468	7
2	8	7	122	110	17
4	8	7	262	253	9
6	8	7	295	308	9
8	8	7	0	58	1
10	8	7	0	40	1
1	9	7	359	357	8
3	9	7	0	20	1
5	9	7	147	165	15
7	9	7	138	136	16
9	9	7	31	30	32
0	10	7	610	599	7
2	10	7	423	429	8
4	10	7	203	198	12
6	10	7	192	169	12
8	10	7	99	90	25
1	11	7	182	181	13
3	11	7	115	123	21
5	11	7	504	507	8
7	11	7	152	159	16
0	12	7	122	126	20
2	12	7	166	173	14
4	12	7	233	218	11
0	0	8	2566	2602	18
2	0	8	137	130	15
4	0	8	268	274	9
6	0	8	667	681	7
8	0	8	42	56	41
10	0	8	1479	1507	11
12	0	8	472	479	8
1	1	8	98	81	22
3	1	8	112	111	19
5	1	8	456	450	7
7	1	8	162	175	14
9	1	8	721	711	8
11	1	8	502	508	8
0	2	8	35	5	35
2	2	8	77	74	32
4	2	8	250	257	10
6	2	8	513	500	7
8	2	8	71	31	40
10	2	8	244	240	11
1	3	8	131	129	16
3	3	8	280	267	9
5	3	8	1833	1856	13
7	3	8	62	20	55
9	3	8	465	441	8
11	3	8	70	104	48
0	4	8	134	165	16
2	4	8	280	278	9
4	4	8	288	291	9
6	4	8	592	606	7
8	4	8	78	60	34
10	4	8	186	181	11
1	5	8	543	533	7
3	5	8	147	139	15
5	5	8	472	465	8
7	5	8	65	21	50
9	5	8	140	136	17
0	6	8	1910	1906	13
2	6	8	162	161	14
4	6	8	314	322	9
6	6	8	474	476	8
8	6	8	122	118	21
1	7	8	81	80	30
3	7	8	163	171	14
5	7	8	969	958	9
7	7	8	195	196	12
0	8	8	1013	1001	8
2	8	8	33	48	32
4	8	8	29	38	29
6	8	8	352	366	9
1	9	8	0	3	1
3	9	8	106	130	24
5	9	8	1233	1242	10
0	10	8	1073	1081	9
2	10	8	104	111	25
1	1	9	0	43	1
3	1	9	213	199	12
5	1	9	341	244	9
0	2	9	50	29	50
2	2	9	86	50	28
4	2	9	169	177	15
6	2	9	10	8	10
1	3	9	121	135	20
3	3	9	92	40	27
5	3	9	54	42	53
0	4	9	385	389	9
2	4	9	97	56	26
4	4	9	73	69	42
1	5	9	49	11	49
3	5	9	123	107	20

Observed and calculated structure factors for K7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	644	656	4	4	8	0	391	378	4	3	1	1	456	455	4	7	9	1	332	334	5	7	1	2	173	169	5
4	0	0	1218	1229	6	6	8	0	572	571	5	5	1	1	896	898	6	9	9	1	58	51	26	9	1	2	646	640	5
6	0	0	589	597	5	8	8	0	463	463	5	7	1	1	103	87	8	11	9	1	1687	1692	13	11	1	2	653	649	6
8	0	0	875	852	6	10	8	0	1311	1323	10	9	1	1	437	438	4	13	9	1	81	63	16	13	1	2	55	51	30
10	0	0	1626	1688	10	12	8	0	165	170	8	11	1	1	850	849	7	15	9	1	104	95	15	15	1	2	641	652	6
12	0	0	1383	1393	9	14	8	0	170	171	9	13	1	1	372	360	5	17	9	1	188	180	10	17	1	2	58	59	32
14	0	0	184	177	7	16	8	0	306	302	7	15	1	1	72	60	19	19	9	1	183	183	10	19	1	2	44	17	43
16	0	0	225	218	7	18	8	0	75	35	21	17	1	1	721	732	6	0	10	1	1187	1235	9	21	1	2	362	342	7
18	0	0	573	550	6	20	8	0	315	319	8	19	1	1	456	469	6	2	10	1	757	759	6	0	2	2	4067	4100	8
20	0	0	240	243	8	1	9	0	94	78	11	21	1	1	876	860	8	4	10	1	245	251	6	2	2	2	334	333	4
22	0	0	1672	1691	12	3	9	0	401	402	4	0	2	1	81	109	7	6	10	1	445	458	5	4	2	2	495	488	4
1	1	0	691	731	3	5	9	0	1885	1881	11	2	2	1	474	496	4	8	10	1	162	170	8	6	2	2	447	439	4
3	1	0	183	175	3	7	9	0	886	866	7	4	2	1	503	510	4	10	10	1	238	245	7	8	2	2	267	262	5
5	1	0	435	441	4	9	9	0	55	25	29	6	2	1	250	235	4	12	10	1	57	18	32	10	2	2	1297	1301	9
7	1	0	478	476	4	11	9	0	615	608	6	8	2	1	595	606	5	14	10	1	597	594	6	12	2	2	543	545	6
9	1	0	1696	1687	9	13	9	0	257	261	7	10	2	1	246	265	5	16	10	1	285	286	7	14	2	2	114	117	12
11	1	0	2884	2865	11	15	9	0	542	558	6	12	2	1	948	960	7	18	10	1	261	267	8	16	2	2	365	352	6
13	1	0	323	328	5	17	9	0	495	492	6	14	2	1	162	160	8	1	11	1	209	212	7	18	2	2	0	31	1
15	1	0	321	308	6	19	9	0	261	251	9	16	2	1	666	686	6	3	11	1	257	253	6	20	2	2	51	22	50
17	1	0	312	314	6	0	10	0	287	305	5	18	2	1	67	40	25	5	11	1	688	686	6	1	3	2	389	383	4
19	1	0	594	606	6	2	10	0	64	53	20	20	2	1	157	173	12	7	11	1	528	529	5	3	3	2	303	300	4
21	1	0	768	770	7	4	10	0	457	456	5	22	2	1	209	218	10	9	11	1	333	326	6	5	3	2	1021	1003	7
0	2	0	1341	1358	4	6	10	0	283	272	5	1	3	1	330	342	4	11	11	1	379	374	6	7	3	2	135	133	7
2	2	0	246	254	3	8	10	0	280	282	6	3	3	1	242	237	4	13	11	1	119	121	13	9	3	2	1585	1614	10
4	2	0	693	704	5	10	10	0	492	499	5	5	3	1	351	340	4	15	11	1	76	91	24	11	3	2	1383	1378	9
6	2	0	151	159	5	12	10	0	155	154	10	7	3	1	482	478	4	17	11	1	452	458	7	13	3	2	453	439	5
8	2	0	303	299	4	14	10	0	1184	1194	9	9	3	1	225	220	5	0	12	1	1100	1098	8	15	3	2	162	138	9
10	2	0	675	694	6	16	10	0	218	213	8	11	3	1	223	241	6	2	12	1	483	488	5	17	3	2	327	324	6
12	2	0	318	322	5	18	10	0	514	521	7	13	3	1	254	264	6	4	12	1	99	106	13	19	3	2	827	831	7
14	2	0	865	872	7	1	11	0	286	278	5	15	3	1	0	45	1	6	12	1	626	630	6	21	3	2	520	535	7
16	2	0	695	711	6	3	11	0	294	294	5	17	3	1	301	304	6	8	12	1	142	146	10	0	4	2	1890	1890	8
18	2	0	35	24	35	5	11	0	927	906	7	19	3	1	192	196	9	10	12	1	181	175	9	2	4	2	657	654	5
20	2	0	187	176	10	7	11	0	169	169	8	21	3	1	339	328	7	12	12	1	279	279	7	4	4	2	72	33	11
22	2	0	126	319	8	9	11	0	70	62	22	0	4	1	1051	1055	7	14	12	1	32	39	32	6	4	2	314	298	4
1	3	0	321	316	3	11	11	0	459	472	5	2	4	1	70	83	11	16	12	1	726	714	7	8	4	2	114	120	9
3	3	0	583	577	4	13	11	0	167	171	9	4	4	1	267	254	3	1	13	1	384	375	5	10	4	2	1990	2026	11
5	3	0	4635	4771	8	15	11	0	869	882	7	6	4	1	802	773	6	3	13	1	377	372	5	12	4	2	297	294	5
7	3	0	498	487	4	17	11	0	401	413	7	8	4	1	488	486	4	5	13	1	936	950	7	14	4	2	241	233	7
9	3	0	993	992	8	0	12	0	1547	1564	10	10	4	1	278	253	5	7	13	1	71	71	21	16	4	2	13	27	12
11	3	0	330	326	5	2	12	0	266	258	6	12	4	1	713	727	6	9	13	1	314	314	6	18	4	2	496	487	6
13	3	0	343	341	5	4	12	0	242	241	6	14	4	1	250	260	6	11	13	1	1099	1086	9	20	4	2	329	317	7
15	3	0	829	831	7	6	12	0	614	618	6	16	4	1	643	649	6	13	13	1	164	140	11	1	5	2	975	965	7
17	3	0	954	951	8	8	12	0	161	168	9	18	4	1	251	258	7	15	13	1	282	272	8	3	5	2	103	110	8
19	3	0	212	215	8	10	12	0	650	652	6	20	4	1	107	87	16	0	14	1	667	676	6	5	5	2	1864	1833	9
21	3	0	445	429	7	12	12	0	504	505	6	1	5	1	113	110	7	2	14	1	275	270	6	7	5	2	206	203	6
0	4	0	2065	2081	6	14	12	0	91	84	19	3	5	1	495	508	4	4	14	1	397	406	6	9	5	2	414	410	5
2	4	0	579	585	4	16	12	0	112	103	17	5	5	1	1527	1482	9	6	14	1	287	284	7	11	5	2	657	645	6
4	4	0	1106	1102	7	1	13	0	457	450	5	7	5	1	902	887	7	8	14	1	296	301	7	13	5	2	37	20	37
6	4	0	3642	3627	9	3	13	0	158	161	9	9	5	1	575	568	5	10	14	1	187	189	9	15	5	2	245	262	7
8	4	0	471	473	4	5	13	0	407	407	5	11	5	1	289	299	5	12	14	1	182	181	10	17	5	2	722	728	7
10	4	0	428	421	5	7	13	0	471	474	5	13	5	1	556	570	5	14	14	1	378	375	7	19	5	2	423	416	6
12	4	0	277	269	5	9	13	0	518	514	6	15	5	1	117	106	12	1	15	1	29	20	29	21	5	2	452	447	7
14	4	0	887	881	7	11	13	0	928	925	8	17	5	1	226	226	8	3	15	1	294	290	7	0	6	2	1078	1066	7
16	4	0	1966	2008	14	13	13	0	279	289	8	19	5	1	45	21	44	5	15	1	264	258	7	2	6	2	139	153	6
18	4	0	90	86	18	15	13	0	206	231	10	21	5	1	743	731	7	7	15	1	347	345	7	4	6	2	1069	1080	8
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1	5	0	1414	1407	7	2	14	0	388	391	6	2	6	1	186	174	5	11	15	1	133	122	14	8	6	2	273	276	5
3	5	0	47	48	19	4	14	0	218	218	7	4	6	1	195	196	5	13	15	1	134	138	14	10	6	2	24	25	24
5	5	0	3200	3149	9	6	14	0	701	709	6	6	6	1	874	878	7	0	16	1	256	253	7	12	6	2	346	356	5
7	5	0	833	812	7	8	14	0	105	108	15	8	6	1	516	499	5	2	16	1	240	244	8	14	6	2	983	991	8
9	5	0	161	169	7	10	14	0	1290	1325	10	10	6	1	134	127	9	4	16	1	0	9	1	16	6	2	1433	1465	10
11	5	0	126	351	5	12	14	0	69	87	14	12	6	1	340	328	5	6	16	1	1272	1268	9	18	6	2	62	28	33
13	5	0	139	336	5	14	14	0	54	22	53	14	6	1	9	23	8	8	16	1	313	309	7	20	6	2	103	104	18
15	5	0	261	277	7	1	15	0	233	232	7	16	6	1	1032	1035	8	10	16	1	77	72	25	1	7	2	714	694	5
17	5	0	491	489	6	3	15	0	418	417	6	18	6	1	286	278	7	12	16	1	83	85	25	3	7	2	0	8	1
19	5	0	228	240	8	5	15	0	519	530	6	20	6	1	419	425	7	1	17	1	85	94	20	5	7	2	4542	4474	11
21	5	0	129	336	7	7	15	0	33	21	33	1	7	1	142	145	6	3	17	1	324	307	7	7	7	2	207	207	6
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2	6	0	167	168	5	11	15	0	390	379	7	5	7	1	418	415	4	7	17	1	225	222	9	11	7	2	113	109	11
4	6	0	413	420	4	13	15	0	410	415	7	7	7	1	195	200	6	9	17	1	399	382	7	13	7	2	336	332	6
6	6	0	557	530	5	0	16	0	610	601	6	9	7	1	444	452	5	0	18	1	282	290	8	15	7	2	903	929	8
8	6	0	679	665	5	2	16	0	182	179	9	11	7	1	25	20	25	2	18	1	71	77	29	17	7	2	960	958	8
10	6	0	1347	1350	9	4	16	0	236	245	8	13	7	1	80	61	17	4	18	1	327	329	7	19	7	2	13	43	12
12	6	0	276	276	6	6	16	0	859	850	7	15	7	1	0	33	1	6	18	1	329	317	8	0	8	2	478	490	5
14	6	0	461	465	5	8	16	0	61	58	17	17	7	1	195	199	9	1	19	1	338	334	8	2	8	2	444	436	5
16	6	0	558	560	6	10	16	0	24	48	23	19	7	1	128	128	13	3	19	1	398	403	7	4	8	2	186	189	6
18	6	0	387	376	6	12	16	0	406	421	7	0	8	1	668	651	5	0	0	2	3336	3307	7	6	8	2	411	399	5
20	6	0	42	37	42	1	17	0	268	263	8	2	8	1	31	4	31	2	0	2	566	585	4	8	8	2	570	575	5
1	7	0	710	695	5	3	17	0	277	284	8	4	8	1	86	109	12	4	0	2	384	389	4	10	8	2	0	6	1
3	7	0	109	116	8	5	17	0	1867	1858	13	6	8	1	296	308	5	6	0	2	777	725	5	12	8	2	158	157	9
5	7	0	1377	1357	9	7	17	0	65	47	32	8	8	1	124	135	10	8	0	2	519	514	5	14	8	2	561	553	6
7	7	0	466	455	4	9	17	0	35	44	34	10	8	1	77	66	17	10	0	2	1390	1327	11	16	8	2	870	881	8
9	7	0	1253	1235	9	0	18	0	319	316	7	12	8	1	506	511	6	12	0	2	957	952	7	18	8	2	42	58	42
11	7	0	571	539	6	2	18	0	296	301	8	14	8	1	558	559	6	14	0	2	1308	1328	9	1	9	2	438	432	5
13	7	0	350	351	5	4	18	0	79	62	25	16	8	1	723	715	7	16	0	2	685	684	6	3	9	2	66	34	19
15	7	0	211	219	8	6	18	0	240	234	9	18	8	1	332	341	7	18	0	2	789	787	7	5	9	2	484	455	5
17	7	0	261	264	7	8	18	0	329	319	8	20	8	1	250	245	9	20	0	2	60	63	40	7	9	2	406	404	5
19	7	0	687	697	7	1	19	0	198	195	10	1	9	1	947	943	7	1	1	2	491	494	4	9	9	2	729	741	6
0	8	0	2621	2571	10	3	19	0	79	52	25	3	9	1	119	125	8	3	1	2	771	770	6	11	9	2	1592	1578	11
2	8	0	152	152	6	1	1	1	171	162	3	5	9	1	351	362	5	5	1	2	1061	1052	6	13	9	2	97	96	15

Observed and calculated structure factors for K7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	317	321	7	20	2	3	94	116	20	17	11	3	556	554	7	8	4	4	207	207	7	8	14	4	92	93	20
17	9	2	619	634	6	1	3	3	545	540	5	0	12	3	218	219	7	10	4	4	265	286	6	10	14	4	1050	1047	8
19	9	2	302	302	8	3	3	3	244	237	6	2	12	3	291	279	6	12	4	4	175	175	8	12	14	4	59	49	58
0	10	2	4445	4405	12	5	3	3	1076	1046	8	4	12	3	349	355	6	14	4	4	840	848	7	1	15	4	198	195	9
2	10	2	662	672	6	7	3	3	742	727	6	6	12	3	138	131	10	16	4	4	1431	1436	11	3	15	4	402	405	7
4	10	2	716	738	6	9	3	3	180	182	7	8	12	3	75	69	20	18	4	4	125	142	14	5	15	4	261	253	8
6	10	2	71	74	19	11	3	3	1323	1327	10	10	12	3	157	161	10	1	5	4	974	969	8	7	15	4	109	102	16
8	10	2	252	259	6	13	3	3	66	63	23	12	12	3	283	271	7	3	5	4	152	142	8	9	15	4	96	105	20
10	10	2	1825	1856	14	15	3	3	114	130	12	14	12	3	126	126	14	5	5	4	1511	1549	11	0	16	4	149	161	13
12	10	2	311	321	6	17	3	3	248	256	7	16	12	3	415	405	7	7	5	4	392	390	5	2	16	4	173	169	11
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16	10	2	244	233	8	21	3	3	400	398	7	3	13	3	465	467	5	11	5	4	912	915	7	6	16	4	469	475	7
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7	11	2	25	2	24	8	4	3	261	264	5	13	13	3	0	12	1	0	6	4	2107	2155	11	3	1	5	222	228	6
9	11	2	639	642	6	10	4	3	408	389	5	15	13	3	204	174	10	2	6	4	182	187	7	5	1	5	688	684	6
11	11	2	1767	1770	12	12	4	3	783	785	6	0	14	3	41	8	40	4	6	4	407	409	5	7	1	5	0	11	1
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15	11	2	213	212	9	16	4	3	218	223	8	4	14	3	347	346	6	8	6	4	375	367	5	11	1	5	241	244	7
17	11	2	82	66	24	18	4	3	172	163	10	6	14	3	150	157	11	10	6	4	1233	1251	9	13	1	5	200	197	8
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4	12	2	0	16	1	3	5	3	322	335	4	12	14	3	0	58	1	16	6	4	229	216	8	19	1	5	369	365	7
6	12	2	825	839	7	5	5	3	871	861	6	1	15	3	165	164	10	18	6	4	275	274	8	0	2	5	744	742	6
8	12	2	145	155	10	7	5	3	864	869	7	3	15	3	225	216	8	1	7	4	259	254	6	2	2	5	84	80	15
10	12	2	789	795	7	9	5	3	449	448	5	5	15	3	472	454	6	3	7	4	190	188	7	4	2	5	474	476	5
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7	13	2	0	40	1	2	6	3	99	98	11	6	16	3	1122	1119	9	17	7	4	381	381	7	18	2	5	65	80	35
9	13	2	160	161	10	4	6	3	428	412	5	8	16	3	260	261	9	0	8	4	1836	1899	12	1	3	5	120	131	10
11	13	2	110	107	15	6	6	3	1193	1195	9	10	16	3	104	85	19	2	8	4	0	19	1	3	3	5	204	209	7
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15	13	2	505	515	7	10	6	3	166	169	8	3	17	3	314	315	8	6	8	4	521	520	5	7	3	5	98	101	13
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2	14	2	317	311	6	14	6	3	96	100	15	7	17	3	0	23	1	10	8	4	1149	1155	9	11	3	5	292	289	6
4	14	2	729	742	6	16	6	3	1126	1115	9	0	18	3	201	215	10	12	8	4	87	98	18	13	3	5	275	274	7
6	14	2	449	448	6	18	6	3	397	402	7	2	18	3	176	181	11	14	8	4	154	146	11	15	3	5	65	15	29
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12	14	2	70	58	29	3	7	3	266	292	5	2	0	4	381	383	4	1	9	4	41	31	41	2	4	5	73	48	18
14	14	2	396	406	7	5	7	3	1159	1160	9	4	0	4	685	691	5	3	9	4	277	281	6	4	4	5	130	121	10
1	15	2	514	520	6	7	7	3	171	170	8	6	0	4	401	392	5	5	9	4	1762	1771	13	6	4	5	678	657	6
3	15	2	303	296	7	9	7	3	467	471	5	8	0	4	237	245	6	7	9	4	491	492	5	8	4	5	345	354	6
5	15	2	1469	1480	11	11	7	3	817	826	7	10	0	4	2644	2652	12	9	9	4	60	40	27	10	4	5	141	138	10
7	15	2	480	481	6	13	7	3	120	126	12	12	0	4	936	947	8	11	9	4	221	199	8	12	4	5	507	504	6
9	15	2	146	155	12	15	7	3	145	150	11	14	0	4	334	340	6	13	9	4	123	116	13	14	4	5	259	258	7
11	15	2	376	380	7	17	7	3	615	617	7	16	0	4	177	188	10	15	9	4	390	387	7	16	4	5	663	669	7
13	15	2	152	139	13	19	7	3	81	88	25	18	0	4	544	533	6	17	9	4	579	580	7	18	4	5	279	282	8
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2	16	2	130	127	13	2	8	3	127	115	9	1	1	4	248	241	5	2	10	4	81	80	17	3	5	5	283	284	6
4	16	2	0	42	1	4	8	3	341	343	5	1	1	4	106	93	9	4	10	4	495	512	6	5	5	5	691	700	6
6	16	2	456	461	6	6	8	3	578	577	5	5	1	4	299	283	5	6	10	4	193	211	8	7	5	5	591	606	6
8	16	2	48	74	47	8	8	3	31	33	30	7	1	4	64	50	20	8	10	4	301	296	6	9	5	5	410	420	5
10	16	2	736	730	7	10	8	3	82	88	17	9	1	4	1262	1269	10	10	10	4	451	439	6	11	5	5	245	252	7
1	17	2	230	232	9	12	8	3	605	598	6	11	1	4	1607	1624	10	12	10	4	202	198	9	13	5	5	378	380	6
3	17	2	375	370	7	14	8	3	358	354	6	13	1	4	179	181	9	14	10	4	907	915	8	15	5	5	59	66	19
5	17	2	148	150	13	16	8	3	214	185	9	15	1	4	201	213	8	16	10	4	420	368	7	17	5	5	169	164	11
7	17	2	0	26	1	18	8	3	168	171	11	17	1	4	0	11	1	1	11	4	151	150	10	0	6	5	378	410	5
9	17	2	391	387	7	1	9	3	583	583	6	19	1	4	544	556	6	3	11	4	349	349	6	2	6	5	78	101	17
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4	18	2	217	218	9	7	9	3	231	217	6	4	2	4	441	435	5	9	11	4	23	25	23	8	6	5	322	332	6
6	18	2	423	419	7	9	9	3	81	70	17	6	2	4	441	468	5	11	11	4	0	16	1	10	6	5	72	78	21
1	1	3	270	260	4	11	9	3	877	889	7	8	2	4	110	111	11	13	11	4	116	108	15	12	6	5	230	232	8
3	1	3	634	628	5	13	9	3	19	32	19	10	2	4	465	473	5	15	11	4	746	741	7	14	6	5	40	2	40
5	1	3	193	177	5	15	9	3	107	108	16	12	2	4	317	326	6	0	12	4	984	989	8	16	6	5	707	692	7
7	1	3	285	291	5	17	9	3	518	522	6	14	2	4	651	654	6	2	12	4	261	258	7	1	7	5	99	81	13
9	1	3	369	375	5	0	10	3	802	815	6	16	2	4	728	727	6	4	12	4	125	139	12	3	7	5	478	480	5
11	1	3	1402	1381	10	2	10	3	750	756	6	18	2	4	17	8	17	6	12	4	283	280	7	5	7	5	0	7	1
13	1	3	427	433	5	4	10	3	355	354	5	20	2	4	139	127	13	8	12	4	199	212	9	7	7	5	317	310	6
15	1	3	119	131	12	6	10	3	212	207	7	1	3	4	227	227	5	10	12	4	423	432	6	9	7	5	300	305	6
17	1	3	360	356	6	8	10	3	234	232	7	3	3	4	474	469	5	12	12	4	348	337	7	11	7	5	364	367	6
19	1	3	456	462	6	10	10	3	59	48	30	5	3	4	3291	3347	11	14	12	4	54	10	54	13	7	5	180	161	9
21	1	3	868	829	8	12	10	3	85	88	19	7	3	4	157	166	8	1	13	4	227	234	8	15	7	5	0	48	1
0	2	3	2220	2194	8	14	10	3	579	581	6	9	3	4	758	767	6	3	13	4	69	94	26	17	7	5	65	59	38
2	2	3	571	555	5	16	10	3	73	74	26	11	3	4	61	63	25	5	13	4	261	256	7	0	8	5	774	784	6
4	2	3	23	19	22	1	11	3	292	306	6	13	3	4	292	304	6	7	13	4	279	274	7	2	8	5	137	131	10
6	2	3	1117	1100	8	3	11	3	183	197	8	15	3	4	716	722	6	9	13	4	506	498	6	4	8	5	26	17	25
8	2	3	707	703	6	5	11	3	745	743	7	17	3	4	728	733	7	11	13	4	722	727	7	6	8	5	544	538	6
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12	2	3	719	731	6	9	11	3	191	191	6	0	4	4	482	505	5	0	14	4	1406	1414	11	10	8	5	29	34	29
14	2	3	361	353	6	11	11	3	99	97	15	2	4	4	394	385	4	2	14	4	244	236	8	12	8	5	375	380	6
16	2	3	1089	1091	8	13	11	3	0	40	1	4	4	4	647	666	5	4	14	4	311	320	7	14	8	5	477	480	6
18	2	3	234	223	8	15	11	3	28	58	27	6	4	4	1846	1841	11	6	14	4	477	482	6	16	8	5	783	760	7

Observed and calculated structure factors for K7

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	9	5	679	687	6	7	1	6	92	58	14	8	8	6	345	347	6	13	3	7	40	45	40	5	1	8	506	517	6
3	9	5	64	60	24	9	1	6	161	161	6	10	8	6	143	135	12	0	4	7	996	980	8	7	1	8	174	181	10
5	9	5	487	477	6	11	1	6	236	223	7	12	8	6	168	168	11	2	4	7	98	92	15	9	1	8	685	678	7
7	9	5	337	334	6	13	1	6	64	52	31	14	8	6	391	386	7	4	4	7	256	258	7	11	1	8	493	478	7
9	9	5	54	42	42	15	1	6	419	414	7	1	9	6	325	323	6	6	4	7	81	89	19	0	2	8	104	11	16
11	9	5	1520	1529	11	17	1	6	334	332	8	3	9	6	100	110	15	8	4	7	193	199	9	2	2	8	74	66	23
13	9	5	103	121	17	0	2	6	1689	1697	13	5	9	6	52	42	52	10	4	7	260	250	8	4	2	8	253	260	8
15	9	5	106	106	18	2	2	6	194	196	7	7	9	6	473	477	6	12	4	7	468	474	7	6	2	8	515	498	6
0	10	5	969	969	7	4	2	6	199	182	7	9	9	6	488	490	6	14	4	7	141	120	14	8	2	8	22	41	22
2	10	5	496	498	6	6	2	6	492	493	6	11	9	6	734	720	7	1	5	7	14	9	13	10	2	8	247	252	9
4	10	5	113	118	13	8	2	6	246	240	7	13	9	6	55	44	55	3	5	7	174	174	9	1	3	8	123	121	13
6	10	5	475	462	6	10	2	6	774	791	7	0	10	6	2142	2167	15	5	5	7	306	310	7	3	3	8	324	314	7
8	10	5	130	128	12	12	2	6	318	303	7	2	10	6	315	324	7	7	5	7	514	516	6	5	3	8	1785	1767	13
10	10	5	247	247	8	14	2	6	46	20	46	4	10	6	320	318	7	9	5	7	320	316	7	7	3	8	54	23	53
12	10	5	68	72	32	16	2	6	397	406	7	6	10	6	559	552	6	11	5	7	29	33	28	9	3	8	420	416	7
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3	11	5	190	205	9	5	3	6	776	777	7	12	10	6	187	180	11	2	6	7	111	114	14	2	4	8	269	268	8
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7	11	5	513	522	6	9	3	6	1089	1090	9	3	11	6	353	347	7	6	6	7	687	680	7	6	4	8	592	604	6
9	11	5	219	213	9	11	3	6	1101	1090	9	5	11	6	444	455	6	8	6	7	241	245	8	8	4	8	0	30	1
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13	11	5	179	184	11	15	3	6	53	46	52	9	11	6	466	456	7	12	6	7	206	201	10	1	5	8	526	527	6
0	12	5	1084	1080	8	0	4	6	2363	2413	13	11	11	6	723	719	7	1	7	7	106	81	14	3	5	8	141	140	12
2	12	5	481	481	6	2	4	6	60	67	24	0	12	6	486	494	6	3	7	7	257	261	7	5	5	8	424	424	7
4	12	5	51	54	50	4	4	6	329	333	6	2	12	6	20	40	19	5	7	7	707	688	7	7	5	8	39	16	39
6	12	5	665	675	7	6	4	6	496	513	5	4	12	6	43	56	42	7	7	7	137	121	13	9	5	8	169	172	12
8	12	5	90	91	20	8	4	6	102	110	14	6	12	6	908	906	8	9	7	7	342	343	7	0	6	8	1840	1859	13
10	12	5	95	88	19	10	4	6	1369	1363	10	8	12	6	10	34	9	11	7	7	500	506	7	2	6	8	196	190	10
12	12	5	234	231	9	12	4	6	263	270	8	10	12	6	429	419	7	0	8	7	528	526	6	4	6	8	347	339	7
1	13	5	329	325	7	14	4	6	43	61	42	1	13	6	69	22	28	2	8	7	82	93	21	6	6	8	479	462	6
3	13	5	254	271	8	16	4	6	207	200	10	3	13	6	58	60	49	4	8	7	267	265	8	8	6	8	174	167	11
5	13	5	941	931	8	1	5	6	267	256	6	5	13	6	1387	1388	11	6	8	7	333	331	7	1	7	8	49	51	49
7	13	5	187	176	10	3	5	6	278	282	6	7	13	6	160	165	12	8	8	7	69	27	29	3	7	8	148	130	12
9	13	5	279	283	8	5	5	6	548	482	6	0	14	6	54	48	53	10	8	7	91	74	21	5	7	8	889	884	8
11	13	5	1197	1183	10	7	5	6	77	77	20	2	14	6	372	358	7	1	9	7	379	383	7	7	7	8	205	215	10
0	14	5	876	865	8	9	5	6	241	239	7	4	14	6	335	334	8	3	9	7	53	47	52	0	8	8	942	940	8
2	14	5	224	228	9	11	5	6	357	355	6	6	14	6	137	138	14	5	9	7	244	249	8	2	8	8	27	41	27
4	14	5	335	331	7	13	5	6	92	88	19	1	1	7	84	81	17	7	9	7	131	123	13	4	8	8	0	3	1
6	14	5	434	432	7	15	5	6	253	246	9	3	1	7	227	238	7	9	9	7	74	4	26	6	8	8	377	372	7
8	14	5	228	206	9	0	6	6	185	188	8	5	1	7	36	67	36	0	10	7	539	556	6	1	9	8	31	19	31
1	15	5	89	102	21	2	6	6	68	18	22	7	1	7	287	271	7	2	10	7	418	419	7	3	9	8	132	150	14
3	15	5	234	244	9	4	6	6	528	535	6	9	1	7	210	215	8	4	10	7	168	161	11	5	9	8	1220	1245	10
5	15	5	46	81	46	6	6	6	815	830	7	11	1	7	733	738	7	6	10	7	205	192	10	0	10	8	1021	1026	9
7	15	5	320	316	8	8	6	6	299	302	7	13	1	7	329	334	7	8	10	7	119	121	16	2	10	8	135	137	14
0	16	5	223	217	9	10	6	6	112	126	14	15	1	7	139	135	14	1	11	7	162	163	12	1	1	9	46	56	45
2	16	5	262	264	9	12	6	6	173	164	10	0	2	7	645	653	6	3	11	7	131	123	14	3	1	9	178	172	11
4	16	5	111	115	18	14	6	6	842	839	7	2	2	7	304	311	6	5	11	7	546	530	6	5	1	9	280	291	8
0	0	6	2529	2529	13	1	7	6	565	568	6	4	2	7	44	25	43	7	11	7	150	163	13	0	2	9	94	93	19
2	0	6	92	75	14	3	7	6	157	155	10	6	2	7	464	461	6	0	12	7	68	42	31	2	2	9	0	51	1
4	0	6	632	641	6	5	7	6	2401	2450	14	8	2	7	294	281	7	2	12	7	159	180	12	4	2	9	234	222	9
6	0	6	689	696	6	7	7	6	102	116	15	10	2	7	79	83	21	4	12	7	239	244	9	6	2	9	52	5	52
8	0	6	342	346	6	9	7	6	172	173	6	12	2	7	528	529	6	0	0	8	2467	2476	15	1	3	9	155	152	12
10	0	6	859	851	7	11	7	6	463	460	6	14	2	7	187	193	11	2	0	8	138	141	12	3	3	9	48	7	47
12	0	6	740	750	7	13	7	6	207	202	10	1	3	7	194	195	8	4	0	8	229	238	8	5	3	9	62	70	43
14	0	6	770	776	7	15	7	6	621	623	7	3	3	7	59	27	30	6	0	8	709	698	7	0	4	9	423	420	7
16	0	6	818	824	7	0	8	6	327	327	6	5	3	7	394	385	6	8	0	8	32	15	31	2	4	9	0	52	1
1	1	6	119	129	11	2	8	6	193	190	8	7	3	7	457	442	6	10	0	8	1422	1434	11	4	4	9	86	70	21
3	1	6	168	160	8	4	8	6	293	290	7	9	3	7	167	157	10	1	1	8	109	94	15	1	5	9	26	5	26
5	1	6	1677	1703	13	6	8	6	266	272	7	11	3	7	760	756	7	3	1	8	118	122	14	3	5	9	97	88	20

Observed and calculated structure factors for K8

h	k	l	10Fo	10Fc	10s
2	0	0	559	571	4
4	0	0	1211	1199	6
6	0	0	734	742	5
8	0	0	1109	1103	7
10	0	0	4149	3913	11
12	0	0	1369	1407	9
14	0	0	217	216	7
16	0	0	427	426	6
18	0	0	545	549	6
20	0	0	363	366	7
22	0	0	1754	1785	12
1	1	0	629	656	3
3	1	0	187	184	4
5	1	0	569	576	5
7	1	0	544	550	4
9	1	0	1721	1699	10
11	1	0	3100	2964	11
13	1	0	393	396	5
15	1	0	271	282	6
17	1	0	296	296	7
19	1	0	575	574	6
21	1	0	851	857	8
0	2	0	1343	1373	4
2	2	0	212	226	3
4	2	0	708	730	5
6	2	0	209	214	4
8	2	0	324	324	4
10	2	0	671	667	6
12	2	0	320	314	5
14	2	0	872	871	7
16	2	0	750	754	7
18	2	0	84	93	20
20	2	0	150	141	12
22	2	0	303	300	8
1	3	0	261	256	3
3	3	0	334	349	4
7	3	0	513	502	4
9	3	0	914	917	7
11	3	0	529	525	5
13	3	0	436	433	5
15	3	0	955	964	8
17	3	0	969	971	8
19	3	0	239	245	8
21	3	0	263	262	9
0	4	0	2294	2277	7
2	4	0	527	542	4
4	4	0	1205	1194	7
6	4	0	4030	3714	9
8	4	0	456	457	5
10	4	0	494	491	5
12	4	0	167	162	8
14	4	0	820	832	7
16	4	0	2152	2129	14
18	4	0	60	55	33
20	4	0	178	178	11
22	4	0	441	445	7
1	5	0	1410	1394	7
3	5	0	138	131	6
5	5	0	3450	3244	9
7	5	0	823	817	6
9	5	0	79	87	15
11	5	0	299	315	5
13	5	0	196	205	8
15	5	0	270	276	7
17	5	0	509	529	6
19	5	0	174	184	11
21	5	0	344	353	8
0	6	0	1061	1084	8
2	6	0	91	100	9
4	6	0	287	295	4
6	6	0	429	413	4
8	6	0	522	510	5
10	6	0	1534	1521	12
12	6	0	221	225	7
14	6	0	392	404	6
16	6	0	399	415	6
18	6	0	423	420	6
20	6	0	28	25	27
1	7	0	735	726	6
3	7	0	184	179	5
5	7	0	1503	1488	10
7	7	0	403	398	5
9	7	0	1270	1266	9
11	7	0	672	641	6
13	7	0	314	317	6
15	7	0	241	256	7
17	7	0	266	270	8
19	7	0	641	665	7
21	7	0	675	673	7
0	8	0	2840	2754	10
2	8	0	120	113	8
4	8	0	479	491	5
6	8	0	531	540	5
8	8	0	573	579	5
10	8	0	1340	1346	10
12	8	0	156	157	9
14	8	0	122	104	12
16	8	0	245	249	8
18	8	0	53	46	52
20	8	0	314	302	8
1	9	0	183	175	6
3	9	0	296	295	5
5	9	0	1986	1976	11
7	9	0	908	903	7
9	9	0	93	119	16
11	9	0	573	551	6
13	9	0	311	302	6
15	9	0	676	686	7
17	9	0	554	553	6
19	9	0	239	218	10
0	10	0	412	423	5
2	10	0	0	3	1
4	10	0	456	466	5
6	10	0	232	231	6
8	10	0	260	270	6
10	10	0	560	566	6
12	10	0	155	153	10
14	10	0	1139	1136	9
16	10	0	323	336	7
18	10	0	435	440	7
1	11	0	263	255	6
3	11	0	345	356	5
5	11	0	986	1004	8
7	11	0	119	131	12
9	11	0	115	120	13
11	11	0	156	157	6
13	11	0	288	298	7
15	11	0	836	833	7
17	11	0	417	437	7
0	12	0	1522	1543	10
2	12	0	154	160	9
4	12	0	361	365	5
6	12	0	659	662	6
8	12	0	123	146	12
10	12	0	730	726	7
12	12	0	548	548	6
14	12	0	131	147	14
16	12	0	62	51	42
1	13	0	501	507	5
3	13	0	148	149	9
5	13	0	448	441	5
7	13	0	442	450	6
9	13	0	444	445	6
11	13	0	975	986	8
13	13	0	255	258	8
15	13	0	246	250	9
0	14	0	1595	1588	11
2	14	0	396	392	6
4	14	0	211	206	8
6	14	0	585	606	6
8	14	0	217	207	8
10	14	0	1335	1346	10
12	14	0	96	107	20
14	14	0	0	9	1
1	15	0	335	326	6
3	15	0	345	350	6
5	15	0	508	489	6
7	15	0	0	5	1
9	15	0	214	225	9
11	15	0	367	374	7
13	15	0	384	385	7
0	16	0	594	598	6
2	16	0	170	172	10
4	16	0	176	173	10
6	16	0	822	834	7
8	16	0	0	37	1
10	16	0	99	60	20
12	16	0	459	456	7
1	17	0	227	224	9
3	17	0	319	312	7
5	17	0	1880	1890	14
7	17	0	0	19	1
9	17	0	66	56	35
0	18	0	288	271	8
2	18	0	237	249	9
4	18	0	140	136	13
6	18	0	292	286	8
8	18	0	271	273	9
1	19	0	218	205	10
3	19	0	75	80	30
1	1	1	125	115	4
3	1	1	446	440	4
5	1	1	718	742	5
7	1	1	63	21	14
9	1	1	292	285	4
11	1	1	885	894	7
13	1	1	289	281	6
15	1	1	152	148	9
17	1	1	715	715	6
19	1	1	472	492	6
21	1	1	817	809	7
0	2	1	217	182	4
2	2	1	524	547	4
4	2	1	315	320	4
6	2	1	220	200	4
8	2	1	637	640	5
10	2	1	211	229	6
12	2	1	952	962	7
14	2	1	55	80	33
16	2	1	715	729	6
18	2	1	16	6	15
20	2	1	264	275	8
22	2	1	217	217	10
1	3	1	304	310	4
3	3	1	214	215	4
5	3	1	246	244	4
7	3	1	477	481	4
9	3	1	287	287	5
11	3	1	320	328	5
13	3	1	282	285	6
15	3	1	59	57	29
17	3	1	314	313	7
19	3	1	204	207	10
21	3	1	378	388	7
0	4	1	988	1000	7
2	4	1	125	129	6
4	4	1	181	172	5
6	4	1	803	761	5
8	4	1	477	477	4
10	4	1	390	367	5
12	4	1	687	687	6
14	4	1	240	238	7
16	4	1	617	626	6
18	4	1	218	224	9
20	4	1	57	16	50
1	5	1	48	72	20
3	5	1	498	518	4
5	5	1	1585	1555	9
7	5	1	925	899	7
9	5	1	428	424	5
11	5	1	381	397	5
13	5	1	609	608	6
15	5	1	0	2	1
17	5	1	210	209	9
19	5	1	0	9	1
21	5	1	719	717	7
0	6	1	339	315	4
2	6	1	144	137	6
4	6	1	341	347	4
6	6	1	926	935	7
8	6	1	459	456	5
10	6	1	62	48	23
12	6	1	407	409	5
14	6	1	42	35	41
16	6	1	1098	1091	8
18	6	1	252	257	8
20	6	1	464	468	7
1	7	1	131	124	7
3	7	1	536	524	4
5	7	1	592	603	5
7	7	1	186	184	6
9	7	1	405	418	5
11	7	1	41	41	41
13	7	1	54	67	37
15	7	1	80	65	20
17	7	1	194	195	10
19	7	1	156	141	12
0	8	1	731	705	6
2	8	1	55	34	20
4	8	1	4	8	4
6	8	1	328	347	5
8	8	1	111	134	11
10	8	1	16	27	16
12	8	1	507	511	6
14	8	1	526	534	6
16	8	1	660	665	6
18	8	1	102	102	8
20	8	1	297	308	8
1	9	1	911	882	7
3	9	1	138	142	9
5	9	1	492	515	5
7	9	1	362	379	5
9	9	1	83	104	17
11	9	1	1758	1755	14
13	9	1	80	53	20
15	9	1	134	124	12
17	9	1	182	171	10
19	9	1	186	188	11
0	10	1	1176	1405	9
2	10	1	767	770	7
4	10	1	274	281	6
6	10	1	434	442	5
8	10	1	129	120	11
10	10	1	348	342	6
12	10	1	16	32	15
14	10	1	625	630	6
16	10	1	404	405	7
18	10	1	224	225	10
1	11	1	160	166	8
3	11	1	176	178	8
5	11	1	719	731	6
7	11	1	542	532	5
9	11	1	298	307	6
11	11	1	320	314	6
13	11	1	131	136	12
15	11	1	216	205	9
17	11	1	411	427	7
0	12	1	1163	1153	9
2	12	1	499	504	5
4	12	1	77	83	18
6	12	1	688	678	6
8	12	1	165	168	9
10	12	1	144	159	11
12	12	1	287	279	7
14	12	1	14	58	13
16	12	1	795	791	7
1	13	1	351	354	6
3	13	1	302	309	6
5	13	1	1052	1071	8
7	13	1	125	127	12
9	13	1	361	353	6
11	13	1	1185	1165	9
13	13	1	123	133	15
15	13	1	194	186	11
0	14	1	776	797	7
2	14	1	238	241	7
4	14	1	431	431	6
6	14	1	264	265	7
8	14	1	279	271	7
10	14	1	287	301	8
12	14	1	126	138	15
14	14	1	382	366	7
1	15	1	23	24	23
3	15	1	302	304	7
5	15	1	220	227	8
7	15	1	365	364	7
9	15	1	0	40	1
11	15	1	162	147	12
13	15	1	179	175	12
0	16	1	398	398	6
2	16	1	234	220	8
4	16	1	44	15	43
6	16	1	1274	1274	9
8	16	1	284	281	8
10	16	1	33	29	32
12	16	1	95	107	23
1	17	1	83	71	22
3	17	1	272	263	8
5	17	1	790	807	7
7	17	1	258	252	8
9	17	1	388	379	7
0	18	1	277	288	8
2	18	1	59	88	55
4	18	1	341	344	8
6	18	1	305	308	8
8	18	1	0	51	1
1	19	1	339	349	8
3	19	1	379	388	8
0	0	2	3241	3576	7
2	0	2	548	574	5
4	0	2	460	472	4
6	0	2	753	722	5
8	0	2	598	581	5
10	0	2	1526	1470	11
12	0	2	886	885	7
14	0	2	1346	1337	9
16	0	2	869	862	7
18	0	2	646	644	6
20	0	2	129	108	14
22	0	2	309	313	8
1	1	2	455	471	4
3	1	2	607	611	5
5	1	2	1254	1265	8
7	1	2	147	139	6
9	1	2	643	634	5
11	1	2	521	510	5
13	1	2	174	164	8
15	1	2	749	722	6
17	1	2	48	60	48
19	1	2	19	12	18
21	1	2	235	231	9
0	2	2	4219	4232	8
2	2	2	280	278	4
4	2	2	422	417	4
6	2	2	383	377	4
8	2	2	145	126	7
10	2	2	1398	1402	11
12	2	2	594	589	6
14	2	2	82	87	17
16	2	2	280	274	7
18	2	2	48	47	48
20	2	2	89	69	21
1	3	2	348	347	4
3	3	2	260	252	4
5	3	2	1227	1219	9
7	3	2	72	71	14
9	3	2	1590	1585	11
11	3	2	1504	1519	12
13	3	2	369	365	5
15	3	2	208	206	8
17	3	2	310	304	7
19	3	2	784	788	7
21	3	2	674	680	7
0	4	2	2196	2178	8
2	4	2	693	694	5
6	4	2	454	441	4
8	4	2	272	278	5
10	4	2	2159	2172	12
12	4	2	200	208	7
14	4	2	234	224	7
16	4	2	131	147	12
18	4	2	576	563	6
20	4	2	305	309	8
1	5	2	1081	1063	8
3	5	2	160	157	6
5	5	2	1846	1822	9
7	5	2	151	147	7
9	5	2	519	529	5
11	5	2	665	664	6
13	5	2	50	3	50
15	5	2	339	326	6
17	5	2	746	744	7
19	5	2	392	389	7
21	5	2	425	415	7
0	6	2	1172	1183	9
2	6	2	161	171	6
4	6	2	1022	1024	7
6	6	2	2478	2379	10
8	6	2	308	303	5
10	6	2	83	79	17
12	6	2	304	301	6
14	6	2	899	908	8
16	6	2	1556	1565	12
18	6	2	43	30	42
20	6	2	108	86	19
1	7	2	620	615	5
3	7	2	149	150	7
5	7	2	5019	4699	12
7	7	2	197	201	6
9	7	2	476	491	5
11	7	2	70	61	21
13	7	2	429	434	6
15	7	2	1008	1015	8
17	7	2	1015	1014	9
19	7	2	79	84	27
0	8	2	331	350	4
2	8	2	409	398	4
4	8	2	341	347	5
6	8	2	400	391	5
8	8	2	525	536	5
10	8	2	41	7	41
12	8	2	175	173	9
14	8	2	591	599	6
16	8	2	925	929	7
18	8	2	0	32	1
1	9	2	459	444	5
3	9	2	19	47	38
5	9	2	451	450	5
7	9	2	410	404	5
9	9	2	653	650	6

Observed and calculated structure factors for K8

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1581	1564	11	16	2	3	1089	1101	9	13	11	3	59	33	39	4	4	4	695	711	5	4	14	4	316	320	7
13	9	2	187	191	9	18	2	3	193	193	10	15	11	3	18	50	18	6	4	4	1905	1904	12	6	14	4	406	403	7
15	9	2	232	235	8	20	2	3	176	196	12	17	11	3	522	522	7	8	4	4	181	189	8	8	14	4	180	176	11
17	9	2	660	662	7	1	3	3	497	487	4	0	12	3	281	287	6	10	4	4	354	361	6	10	14	4	1058	1053	9
19	9	2	278	280	9	3	3	3	285	285	4	2	12	3	305	297	6	12	4	4	86	97	17	12	14	4	42	63	41
0	10	2	4699	4565	13	5	3	3	1101	1098	8	4	12	3	331	338	6	14	4	4	826	821	7	1	15	4	294	285	8
2	10	2	587	575	5	7	3	3	772	750	6	6	12	3	185	182	9	16	4	4	1560	1550	11	3	15	4	359	353	7
4	10	2	700	695	6	9	3	3	223	222	6	8	12	3	89	82	17	18	4	4	129	124	15	5	15	4	224	231	9
6	10	2	65	27	22	11	3	3	1377	1384	10	10	12	3	168	165	10	1	5	4	937	933	7	7	15	4	141	131	13
8	10	2	359	356	5	13	3	3	59	72	28	12	12	3	268	272	8	3	5	4	110	107	11	9	15	4	214	212	10
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12	10	2	356	366	6	17	3	3	260	247	8	16	12	3	527	498	7	7	5	4	374	368	5	2	16	4	167	165	12
14	10	2	319	325	7	19	3	3	136	127	14	1	13	3	255	252	7	9	5	4	93	93	15	4	16	4	117	106	16
16	10	2	114	109	16	21	3	3	450	439	7	3	13	3	400	411	6	11	5	4	849	873	7	6	16	4	460	467	7
18	10	2	277	273	9	0	4	3	2160	2056	9	5	13	3	464	463	6	13	5	4	63	69	28	8	16	4	40	24	39
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3	11	2	665	655	6	4	4	3	310	313	4	9	13	3	287	284	7	17	5	4	149	139	13	3	17	4	212	210	10
5	11	2	124	122	11	6	4	3	216	220	6	11	13	3	459	451	7	19	5	4	118	111	16	5	17	4	1408	1415	10
7	11	2	49	61	49	8	4	3	243	252	6	13	13	3	0	5	1	0	6	4	2252	2269	11	1	1	5	58	29	24
9	11	2	697	710	6	10	4	3	487	474	5	15	13	3	108	93	20	2	6	4	133	137	9	3	1	5	196	207	7
11	11	2	1856	1852	12	12	4	3	740	748	6	0	14	3	113	120	14	4	6	4	329	332	5	5	1	5	608	610	6
13	11	2	39	47	39	14	4	3	107	81	14	2	14	3	190	198	9	6	6	4	229	230	6	7	1	5	36	10	16
15	11	2	145	132	13	16	4	3	209	212	9	4	14	3	355	361	7	8	6	4	248	240	6	9	1	5	240	248	7
17	11	2	109	101	18	18	4	3	140	128	13	6	14	3	172	174	10	10	6	4	1351	1364	10	11	1	5	286	275	6
0	12	2	1414	1431	11	20	4	3	38	37	37	8	14	3	327	321	7	12	6	4	319	312	6	13	1	5	136	144	11
2	12	2	22	47	21	1	5	3	121	117	8	10	14	3	116	127	16	14	6	4	226	210	8	15	1	5	105	97	16
4	12	2	97	91	14	3	5	3	330	338	4	12	14	3	0	20	1	16	6	4	118	115	15	17	1	5	736	728	7
6	12	2	802	804	6	5	5	3	915	905	6	1	15	3	165	159	10	18	6	4	297	300	8	19	1	5	377	381	8
8	12	2	210	217	8	7	5	3	883	884	7	3	15	3	237	242	8	1	7	4	109	293	5	0	2	5	614	610	5
10	12	2	760	779	7	9	5	3	329	320	5	5	15	3	423	434	7	3	7	4	230	229	6	2	2	5	152	134	8
12	12	2	246	233	8	11	5	3	206	199	7	7	15	3	240	234	9	5	7	4	1328	1350	10	4	2	5	336	337	5
14	12	2	461	456	7	13	5	3	463	460	5	9	15	3	80	86	26	7	7	4	321	319	6	6	2	5	440	436	5
16	12	2	392	401	8	15	5	3	81	74	20	11	15	3	369	353	8	9	7	4	978	991	8	8	2	5	324	319	6
1	13	2	114	110	13	17	5	3	272	276	8	0	16	3	254	255	8	11	7	4	808	796	7	10	2	5	48	24	48
3	13	2	23	1	22	19	5	3	69	48	32	2	16	3	67	64	28	13	7	4	265	263	7	12	2	5	763	765	6
5	13	2	1878	1889	14	0	6	3	628	637	5	4	16	3	189	202	10	15	7	4	225	238	9	14	2	5	0	9	1
7	13	2	81	43	19	2	6	3	147	127	7	6	16	3	1139	1132	9	17	7	4	371	376	7	16	2	5	276	278	8
9	13	2	87	73	19	4	6	3	557	544	5	8	16	3	235	239	9	0	8	4	1968	2032	12	18	2	5	97	97	20
11	13	2	0	51	1	6	6	3	1214	1227	9	10	16	3	173	187	12	2	8	4	31	6	30	1	3	5	104	105	12
13	13	2	176	176	11	8	6	3	316	314	5	1	17	3	151	143	13	4	8	4	269	243	6	3	3	5	190	195	7
15	13	2	550	567	7	10	6	3	113	116	12	3	17	3	287	283	8	6	8	4	483	495	5	5	3	5	475	486	5
0	14	2	446	447	6	12	6	3	358	367	6	5	17	3	533	533	7	8	8	4	440	449	5	7	3	5	107	117	12
2	14	2	275	272	7	14	6	3	19	60	19	7	17	3	22	4	22	10	8	4	1170	1175	9	9	3	5	116	130	10
4	14	2	768	762	7	16	6	3	1153	1143	9	0	18	3	203	206	10	12	8	4	93	89	17	11	3	5	221	228	8
6	14	2	483	486	6	18	6	3	388	385	7	2	18	3	183	199	12	14	8	4	100	82	18	13	3	5	291	287	7
8	14	2	194	191	9	20	6	3	455	423	7	4	18	3	166	162	12	16	8	4	203	201	10	15	3	5	0	1	1
10	14	2	110	105	16	1	7	3	163	146	7	0	0	4	6284	6873	12	18	8	4	93	97	23	17	3	5	527	519	7
12	14	2	81	61	24	3	7	3	210	224	6	2	0	4	317	326	4	1	9	4	89	87	15	0	4	5	63	63	23
14	14	2	395	399	7	5	7	3	1305	1286	9	4	0	4	621	650	5	3	9	4	179	179	8	2	4	5	103	71	12
1	15	2	585	575	6	7	7	3	196	197	7	6	0	4	321	280	5	5	9	4	1831	1810	13	4	4	5	84	75	16
3	15	2	277	290	7	9	7	3	424	424	5	8	0	4	410	410	5	7	9	4	511	508	5	6	4	5	668	664	6
5	15	2	1529	1532	11	11	7	3	840	829	7	10	0	4	2843	2848	13	9	9	4	26	46	26	8	4	5	331	345	6
7	15	2	469	473	6	13	7	3	129	129	12	12	0	4	970	957	8	11	9	4	166	165	10	10	4	5	236	215	7
9	15	2	57	37	56	15	7	3	53	59	52	14	0	4	386	387	6	13	9	4	134	140	13	12	4	5	470	464	6
11	15	2	368	361	7	17	7	3	604	610	6	16	0	4	47	17	46	15	9	4	489	495	7	14	4	5	230	236	9
13	15	2	197	184	11	19	7	3	87	103	24	18	0	4	551	536	6	17	9	4	630	628	7	16	4	5	666	649	7
0	16	2	1028	1029	8	0	8	3	824	810	6	20	0	4	253	239	9	0	10	4	908	923	7	18	4	5	240	245	10
2	16	2	170	170	10	2	8	3	74	84	17	1	1	4	233	233	5	2	10	4	40	51	40	1	5	5	118	114	11
4	16	2	121	133	15	4	8	3	258	252	6	3	1	4	113	101	9	4	10	4	538	533	6	3	5	5	264	264	6
6	16	2	455	455	7	6	8	3	530	535	5	5	1	4	200	164	6	6	10	4	230	230	7	5	5	5	740	739	6
8	16	2	41	2	40	8	8	3	31	40	31	7	1	4	78	78	17	8	10	4	299	289	7	7	5	5	617	620	6
10	16	2	767	764	7	10	8	3	96	109	15	9	1	4	1255	1280	10	10	10	4	483	472	6	9	5	5	319	307	6
1	17	2	245	241	9	12	8	3	594	594	6	11	1	4	1699	1708	13	12	10	4	164	182	11	11	5	5	326	322	6
3	17	2	369	370	7	14	8	3	313	318	7	13	1	4	225	226	8	14	10	4	870	857	7	13	5	5	413	405	6
5	17	2	137	133	14	16	8	3	199	164	10	15	1	4	184	186	9	16	10	4	459	453	7	15	5	5	47	20	46
7	17	2	65	63	37	18	8	3	139	131	14	17	1	4	52	23	52	1	11	4	154	152	10	17	5	5	154	151	13
9	17	2	385	381	8	1	9	3	536	536	5	19	1	4	535	530	7	3	11	4	405	402	6	0	6	5	263	291	6
0	18	2	802	785	7	3	9	3	92	85	14	0	2	4	356	370	4	5	11	4	1193	1196	9	2	6	5	77	77	18
2	18	2	52	28	52	5	9	3	215	196	7	2	2	4	159	155	7	7	11	4	60	31	33	4	6	5	0	28	1
4	18	2	267	274	9	7	9	3	273	272	6	4	2	4	458	455	4	9	11	4	63	76	32	6	6	5	471	465	5
6	18	2	161	368	8	9	9	3	125	120	11	6	2	4	407	428	5	11	11	4	90	66	18	8	6	5	293	306	6
1	1	3	199	195	5	11	9	3	960	945	8	8	2	4	128	134	10	13	11	4	208	207	10	10	6	5	0	21	1
3	1	3	623	635	5	13	9	3	0	19	1	10	2	4	448	456	5	15	11	4	690	692	7	12	6	5	290	291	7
5	1	3	260	265	4	15	9	3	139	133	13	12	2	4	316	313	6	0	12	4	962	980	8	14	6	5	88	46	20
7	1	3	345	353	4	17	9	3	522	515	7	14	2	4	642	644	6	2	12	4	183	173	9	16	6	5	732	744	7
9	1	3	258	251	5	0	10	3	935	951	7	16	2	4	760	754	7	4	12	4	260	247	7	1	7	5	70	66	21
11	1	3	1431	1406	10	2	10	3	755	756	6	18	2	4	101	95	19	6	12	4	331	321	7	3	7	5	442	444	5
13	1	3	367	371	6	4	10	3	375	376	5	20	2	4	75	93	31	8	12	4	193	191	9	5	7	5	148	134	10
15	1	3	207	212	8	6	10	3	198	192	8	1	3	4	168	175	6	10	12	4	508	502	6	7	7	5	295	287	6
17	1	3	339	340	7	8	10	3	176	180	8	3	3	4	335	326	4	12	12	4	375	379	7	9	7	5	284	282	7
19	1	3	464	482	7	10	10	3	138	131	11	5	3	4	3583	3564	11	14	12	4	77	61	28	11	7	5	347	345	6
21	1	3	780	772	8	12	10	3	137	133	12	7	3	4	170	179	8	1	13	4	278	277	7	13	7	5	159	161	11
0	2	3	2379	2371	9	14	10	3	619	608	7	9	3	4	715	715	6	3	13	4	94	90	17	15	7	5	117	120	16
2	2	3	607	606	5	16	10	3	190	179	11	11	3	4	219	212	7	5	13	4	283	281	7	17	7	5	48	64	48
4	2	3	207	199	5	1	11	3	271	279	6	13	3	4	375	378	6	7	13	4	241	250	8	0	8	5	813	812	7
6	2	3	1125	1114	8	3	11	3	118	116	12	15	3	4	821	829	7	9	13	4	432	435	7	2	8	5	151	162	10
8	2	3	738	735	6	5	11	3	763	768	6	17	3	4	736	743	7	11	13	4	780	776	7	4	8	5	108	95	13
10	2	3	253	251	6	7	11	3	228	226	7	19	3	4	224	218	10	13	13	4	130	134	15	6	8	5	569	561	6
12	2	3	733	734	6	9	11	3	357	359	6	0	4	4	640	652	5	0	14	4	1514	1508	11	8	8	5	116	108	13
14	2	3	301	294	6	11	11	3	70	61	25	2	4	4	188	163	4	2	14	4	234	234	8	10	8	5	30	5	30

Observed and calculated structure factors for K8

h	k	l	10Fo	10Fc	10s
12	8	5	374	369	7
14	8	5	457	458	7
16	8	5	717	713	7
1	9	5	652	653	6
3	9	5	82	67	18
5	9	5	592	579	6
7	9	5	369	361	6
9	9	5	104	83	15
11	9	5	1578	1576	11
13	9	5	110	110	17
15	9	5	146	126	13
0	10	5	1099	1094	8
2	10	5	498	505	5
4	10	5	135	133	11
6	10	5	483	456	6
8	10	5	83	94	19
10	10	5	346	328	7
12	10	5	0	14	1
14	10	5	479	478	7
1	11	5	58	50	33
3	11	5	150	148	11
5	11	5	509	513	6
7	11	5	530	526	6
9	11	5	207	198	9
11	11	5	160	147	7
13	11	5	185	195	11
0	12	5	1078	1101	9
2	12	5	491	489	6
4	12	5	66	70	31
6	12	5	713	705	7
8	12	5	104	108	18
10	12	5	83	69	25
12	12	5	238	229	9
1	13	5	314	305	7
3	13	5	224	226	9
5	13	5	1018	1018	9
7	13	5	215	216	10
9	13	5	327	310	8
11	13	5	1258	1230	9
0	14	5	967	954	8
2	14	5	200	202	10
4	14	5	335	340	8
6	14	5	428	425	7
8	14	5	180	183	11
10	14	5	319	335	8
1	15	5	91	111	23
3	15	5	240	247	9
5	15	5	64	48	42
7	15	5	325	333	8
0	16	5	318	316	8
2	16	5	239	246	10
4	16	5	107	122	20
0	0	6	2492	2628	13
2	0	6	77	70	19
4	0	6	674	692	6
6	0	6	678	676	6
8	0	6	389	384	6
10	0	6	922	910	7
12	0	6	685	684	7
14	0	6	761	760	7
16	0	6	896	915	8
1	1	6	143	134	10
3	1	6	63	52	24
5	1	6	1750	1795	13
7	1	6	98	91	15
9	1	6	354	346	6
11	1	6	289	287	7
13	1	6	41	15	41
15	1	6	459	461	7
17	1	6	316	320	8
0	2	6	1740	1772	13
2	2	6	162	157	9
4	2	6	148	136	9
6	2	6	502	459	5
8	2	6	179	161	9
10	2	6	858	868	7
12	2	6	339	331	7
14	2	6	32	7	31
16	2	6	339	346	8
1	3	6	167	165	8
3	3	6	87	86	15
5	3	6	863	872	7
7	3	6	57	5	33
9	3	6	1055	1060	8
11	3	6	1161	1164	9
13	3	6	158	169	12
15	3	6	86	94	23
17	3	6	317	322	8
0	4	6	2516	2543	13
2	4	6	79	91	18
4	4	6	344	347	6
6	4	6	558	572	6
8	4	6	222	218	8
10	4	6	1437	1430	11
12	4	6	215	200	9
14	4	6	0	48	1
16	4	6	295	294	8
1	5	6	340	333	6
3	5	6	281	264	6
5	5	6	530	503	5
7	5	6	125	121	12
9	5	6	302	300	7
11	5	6	129	124	7
13	5	6	102	110	18
15	5	6	284	294	9
0	6	6	102	116	15
2	6	6	0	21	1
4	6	6	488	489	5
6	6	6	867	871	7
8	6	6	123	125	7
10	6	6	35	39	34
12	6	6	128	126	13
14	6	6	807	793	7
16	6	6	779	778	7
1	7	6	519	525	6
3	7	6	90	73	16
5	7	6	2572	2581	15
7	7	6	108	112	15
9	7	6	371	387	7
11	7	6	338	350	7
13	7	6	276	266	8
15	7	6	692	681	7
0	8	6	251	252	7
2	8	6	158	163	10
4	8	6	380	390	6
6	8	6	256	266	8
8	8	6	330	321	7
10	8	6	155	148	11
12	8	6	196	178	10
14	8	6	421	415	7
1	9	6	354	339	6
3	9	6	99	110	16
5	9	6	57	23	37
7	9	6	466	484	6
9	9	6	434	437	7
11	9	6	727	716	7
13	9	6	54	18	54
0	10	6	2290	2271	15
2	10	6	256	266	8
4	10	6	288	284	7
6	10	6	463	479	6
8	10	6	129	129	16
10	10	6	1353	1339	10
12	10	6	209	210	10
1	11	6	86	85	20
3	11	6	312	300	7
5	11	6	393	403	7
7	11	6	84	71	23
9	11	6	524	513	7
11	11	6	794	786	7
0	12	6	569	571	6
2	12	6	76	77	25
4	12	6	103	101	18
6	12	6	873	869	7
8	12	6	71	74	32
10	12	6	419	412	7
1	13	6	60	28	45
3	13	6	0	8	1
5	13	6	1411	1408	11
7	13	6	173	161	12
0	14	6	53	18	53
2	14	6	336	325	8
4	14	6	357	351	8
6	14	6	187	167	11
1	1	7	45	58	44
3	1	7	206	218	8
5	1	7	21	23	20
7	1	7	292	283	7
9	1	7	115	135	15
11	1	7	754	752	7
13	1	7	274	288	8
15	1	7	180	186	12
0	2	7	747	731	6
2	2	7	331	339	6
4	2	7	93	56	16
6	2	7	482	482	6
8	2	7	284	283	7
10	2	7	21	54	21
12	2	7	513	511	6
14	2	7	142	138	14
1	3	7	197	197	8
3	3	7	53	18	38
5	3	7	431	431	6
7	3	7	427	429	6
9	3	7	173	182	11
11	3	7	812	794	7
13	3	7	0	25	1
0	4	7	980	969	8
2	4	7	89	61	17
4	4	7	205	200	8
6	4	7	119	100	13
8	4	7	187	192	10
10	4	7	309	319	8
12	4	7	456	466	7
14	4	7	101	101	20
1	5	7	65	23	27
3	5	7	146	162	11
5	5	7	313	315	7
7	5	7	511	531	6
9	5	7	228	230	9
11	5	7	77	79	26
13	5	7	260	277	9
0	6	7	273	278	7
2	6	7	129	127	12
4	6	7	237	245	8
6	6	7	677	683	6
8	6	7	224	227	9
10	6	7	108	109	18
12	6	7	236	240	10
1	7	7	99	86	16
3	7	7	222	223	9
5	7	7	762	762	7
7	7	7	118	114	15
9	7	7	318	306	8
11	7	7	518	509	7
0	8	7	512	502	6
2	8	7	81	63	21
4	8	7	202	187	9
6	8	7	334	315	7
8	8	7	82	25	23
10	8	7	101	110	19
12	8	7	385	378	8
1	9	7	317	327	7
3	9	7	26	40	26
5	9	7	190	185	10
7	9	7	167	168	11
9	9	7	0	34	1
11	9	7	607	595	7
0	10	7	616	613	6
2	10	7	412	414	7
4	10	7	178	175	11
6	10	7	171	169	12
8	10	7	97	81	20
1	11	7	151	147	12
3	11	7	47	74	46
5	11	7	541	535	7
7	11	7	162	167	12
0	12	7	96	88	19
2	12	7	192	200	10
4	12	7	238	218	9
6	12	7	79	85	28
1	13	7	179	172	12
0	0	8	2502	2616	16
2	0	8	136	120	12
4	0	8	233	227	8
6	0	8	625	646	7
8	0	8	63	62	16
10	0	8	1542	1541	11
12	0	8	505	497	7
1	1	8	78	82	22
3	1	8	126	134	14
5	1	8	443	448	6
7	1	8	129	154	15
9	1	8	708	694	7
11	1	8	523	528	7
0	2	8	41	14	41
2	2	8	88	66	19
4	2	8	277	267	8
6	2	8	477	468	6
8	2	8	50	53	49
10	2	8	241	239	9
1	3	8	78	99	25
3	3	8	236	241	9
5	3	8	1835	1869	13
7	3	8	14	5	13
9	3	8	394	394	7
11	3	8	96	64	21
0	4	8	190	180	9
2	4	8	242	245	8
4	4	8	281	276	8
6	4	8	621	633	6
8	4	8	13	15	13
10	4	8	179	165	11
1	5	8	502	508	6
3	5	8	113	136	16
5	5	8	475	487	7
7	5	8	33	8	32
9	5	8	134	112	14
0	6	8	1886	1897	13
2	6	8	159	156	12
4	6	8	279	296	8
6	6	8	473	479	7
8	6	8	77	87	28
1	7	8	73	78	29
3	7	8	142	151	13
5	7	8	924	921	8
7	7	8	166	181	12
0	8	8	1028	1022	8
2	8	8	43	49	43
4	8	8	39	53	38
6	8	8	336	352	8
1	9	8	0	5	1
3	9	8	102	80	20
5	9	8	1248	1261	9
0	10	8	1067	1037	9
2	10	8	132	118	15
1	1	9	21	16	21
3	1	9	175	165	11
5	1	9	261	263	9
0	2	9	64	50	40
2	2	9	52	89	51
4	2	9	129	129	15
6	2	9	0	5	1
1	3	9	111	110	18
3	3	9	0	14	1
5	3	9	77	62	27
0	4	9	401	388	7
2	4	9	33	65	32
4	4	9	86	53	24
1	5	9	0	4	1
3	5	9	46	68	45
0	6	9	0	73	1

Observed and calculated structure factors for K9

h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ	h	k	l	10Fo	10Fc	10σ
2	0	0	637	655	4	4	8	0	369	358	4	3	1	1	484	480	3	7	9	1	324	319	4	7	1	2	203	194	4
4	0	0	1271	1257	5	6	8	0	551	553	4	5	1	1	809	848	5	9	9	1	38	52	37	9	1	2	654	646	5
6	0	0	588	588	4	8	8	0	460	458	4	7	1	1	157	131	4	11	9	1	1689	1694	12	11	1	2	648	640	5
8	0	0	864	842	6	10	8	0	1377	1355	9	9	1	1	481	477	4	13	9	1	52	43	20	13	1	2	66	65	13
10	0	0	1853	1679	10	12	8	0	186	193	6	11	1	1	874	881	6	15	9	1	69	48	16	15	1	2	656	657	6
12	0	0	1372	1369	10	14	8	0	176	174	7	13	1	1	387	383	4	17	9	1	188	184	8	17	1	2	60	66	18
14	0	0	190	183	5	16	8	0	262	271	6	15	1	1	40	10	39	19	9	1	170	176	8	19	1	2	22	30	21
16	0	0	210	220	6	18	8	0	0	31	1	17	1	1	725	736	6	0	10	1	1198	1210	8	21	1	2	344	320	6
18	0	0	621	612	6	20	8	0	345	330	6	19	1	1	447	467	5	2	10	1	786	785	6	0	2	2	3969	4116	8
20	0	0	187	204	8	1	9	0	89	78	8	21	1	1	941	924	7	4	10	1	281	287	4	2	2	2	321	316	3
22	0	0	1609	1625	11	3	9	0	410	410	4	0	2	1	58	51	8	6	10	1	423	435	4	4	2	2	504	487	4
1	1	0	672	710	3	5	9	0	1871	1877	10	2	2	1	452	478	3	8	10	1	177	181	6	6	2	2	429	420	4
3	1	0	171	170	3	7	9	0	874	875	6	4	2	1	522	525	4	10	10	1	243	235	5	8	2	2	280	270	3
5	1	0	447	446	3	9	9	0	42	21	30	6	2	1	243	234	3	12	10	1	35	1	35	10	2	2	1286	1284	10
7	1	0	500	492	4	11	9	0	605	589	5	8	2	1	636	643	4	14	10	1	616	621	6	12	2	2	525	538	5
9	1	0	1794	1733	8	13	9	0	292	291	5	10	2	1	351	358	4	16	10	1	227	241	7	14	2	2	142	144	7
11	1	0	2948	2831	10	15	9	0	490	499	5	12	2	1	966	971	7	18	10	1	285	287	7	16	2	2	317	335	5
13	1	0	311	314	4	17	9	0	477	473	5	14	2	1	162	154	6	1	11	1	238	243	5	18	2	2	85	60	12
15	1	0	280	286	5	19	9	0	287	283	6	16	2	1	728	725	6	3	11	1	292	290	4	20	2	2	89	64	13
17	1	0	280	281	5	0	10	0	291	308	4	18	2	1	47	31	27	5	11	1	647	656	5	1	3	2	358	351	3
19	1	0	640	636	6	2	10	0	74	68	11	20	2	1	133	131	12	7	11	1	523	527	5	3	3	2	307	312	3
21	1	0	743	751	6	4	10	0	481	493	4	22	2	1	185	192	9	9	11	1	351	349	5	5	3	2	1017	999	6
0	2	0	1332	1361	4	6	10	0	281	275	4	1	3	1	327	332	3	11	11	1	397	407	5	7	3	2	107	109	6
2	2	0	227	248	3	8	10	0	302	311	4	3	3	1	236	237	3	13	11	1	107	108	10	9	3	2	1701	1694	9
4	2	0	717	732	5	10	10	0	507	525	5	5	3	1	319	313	3	15	11	1	40	45	40	11	3	2	1345	1341	10
6	2	0	147	152	4	12	10	0	114	112	9	7	3	1	512	503	4	17	11	1	439	446	6	13	3	2	478	481	5
8	2	0	301	300	3	14	10	0	1221	1238	8	9	3	1	244	242	4	0	12	1	1137	1147	8	15	3	2	154	148	7
10	2	0	685	708	5	16	10	0	204	202	7	11	3	1	223	225	4	2	12	1	479	471	5	17	3	2	282	295	5
12	2	0	293	282	4	18	10	0	576	567	6	13	3	1	279	284	4	4	12	1	98	95	10	19	3	2	847	858	7
14	2	0	873	873	6	1	11	0	305	294	4	15	3	1	19	27	19	6	12	1	612	620	5	21	3	2	497	502	6
16	2	0	695	695	6	3	11	0	300	297	4	17	3	1	308	313	5	8	12	1	169	168	6	0	4	2	1909	1935	7
18	2	0	72	67	15	5	11	0	919	935	7	19	3	1	197	209	7	10	12	1	209	223	6	2	4	2	665	672	4
20	2	0	219	200	7	7	11	0	176	177	6	21	3	1	316	322	6	12	12	1	287	284	6	4	4	2	18	24	18
22	2	0	352	344	6	9	11	0	63	68	15	0	4	1	974	1009	6	14	12	1	42	44	41	6	4	2	288	273	1
1	3	0	339	341	3	11	11	0	455	469	5	2	4	1	46	62	13	16	12	1	706	709	6	8	4	2	136	133	5
3	3	0	568	575	4	13	11	0	146	150	8	4	4	1	295	287	3	1	13	1	369	357	4	10	4	2	2043	2054	10
5	3	0	5071	4767	8	15	11	0	921	925	7	6	4	1	826	798	5	3	13	1	384	389	4	12	4	2	306	318	4
7	3	0	496	482	4	17	11	0	391	408	6	8	4	1	525	521	4	5	13	1	942	949	7	14	4	2	254	257	5
9	3	0	1045	1036	7	0	12	0	1520	1553	11	10	4	1	193	178	5	7	13	1	64	63	16	16	4	2	16	12	15
11	3	0	316	308	4	2	12	0	260	259	5	12	4	1	729	741	6	9	13	1	325	326	5	18	4	2	480	479	5
13	3	0	370	369	4	4	12	0	232	224	5	14	4	1	264	263	5	11	13	1	1067	1072	8	20	4	2	347	339	6
15	3	0	838	833	6	6	12	0	622	635	5	16	4	1	689	680	6	13	13	1	149	139	9	1	5	2	960	962	6
17	3	0	936	934	7	8	12	0	142	151	7	18	4	1	262	262	6	15	13	1	297	284	6	3	5	2	117	118	5
19	3	0	204	223	7	10	12	0	633	627	6	20	4	1	105	115	13	0	14	1	617	633	5	5	5	2	1887	1815	8
21	3	0	415	423	6	12	12	0	513	509	5	1	5	1	119	123	4	2	14	1	299	301	5	7	5	2	198	187	4
0	4	0	2095	2111	6	14	12	0	62	79	22	3	5	1	562	562	4	4	14	1	423	428	5	9	5	2	400	394	4
2	4	0	564	572	4	16	12	0	129	113	10	5	5	1	1614	1577	8	6	14	1	270	263	5	11	5	2	648	641	5
4	4	0	1134	1145	7	1	13	0	422	425	4	7	5	1	899	884	6	8	14	1	341	326	5	13	5	2	0	16	1
6	4	0	1786	1576	9	3	13	0	146	160	7	9	5	1	587	587	5	10	14	1	153	152	8	15	5	2	243	247	6
8	4	0	494	480	4	5	13	0	430	426	5	11	5	1	288	310	4	12	14	1	180	173	8	17	5	2	740	743	6
10	4	0	449	449	4	7	13	0	478	474	5	13	5	1	594	601	5	14	14	1	411	410	6	19	5	2	427	427	5
12	4	0	268	265	4	9	13	0	560	558	5	15	5	1	178	181	7	1	15	1	0	25	1	21	5	2	484	468	6
14	4	0	939	947	7	11	13	0	908	913	7	17	5	1	238	226	6	3	15	1	270	273	6	0	6	2	1093	1076	8
16	4	0	1980	1972	13	13	13	0	299	300	6	19	5	1	32	42	32	5	15	1	285	281	6	2	6	2	160	169	4
18	4	0	104	89	11	15	13	0	234	237	7	21	5	1	792	784	7	7	15	1	324	330	6	4	6	2	1130	1129	7
20	4	0	275	262	6	0	14	0	1502	1511	10	0	6	1	466	455	4	9	15	1	66	72	19	6	6	2	2332	2275	9
1	5	0	1410	1398	6	2	14	0	403	406	5	2	6	1	201	195	3	11	15	1	154	133	8	8	6	2	271	269	4
3	5	0	41	40	14	4	14	0	207	208	6	4	6	1	196	193	4	13	15	1	117	126	12	10	6	2	28	37	27
5	5	0	3309	3161	8	6	14	0	697	718	6	6	6	1	869	857	6	0	16	1	239	246	6	12	6	2	348	356	4
7	5	0	820	805	6	8	14	0	79	110	15	8	6	1	520	511	4	2	16	1	265	260	6	14	6	2	1026	1039	8
9	5	0	214	220	4	10	14	0	1351	1361	10	10	6	1	111	110	7	4	16	1	34	24	33	16	6	2	1429	1427	11
11	5	0	316	317	4	12	14	0	94	86	14	12	6	1	321	318	4	6	16	1	1258	1261	9	18	6	2	42	42	42
13	5	0	353	361	4	14	14	0	49	25	48	14	6	1	0	25	1	8	16	1	308	307	6	20	6	2	112	101	12
15	5	0	276	282	5	1	15	0	221	224	6	16	6	1	1066	1059	8	10	16	1	88	81	15	1	7	2	744	721	5
17	5	0	477	476	5	3	15	0	392	409	5	18	6	1	281	284	6	12	16	1	106	90	13	3	7	2	42	10	19
19	5	0	228	234	7	5	15	0	531	524	5	20	6	1	417	414	6	1	17	1	68	74	18	5	7	2	4579	4495	11
21	5	0	278	277	7	7	15	0	25	17	24	1	7	1	134	128	5	3	17	1	334	331	6	7	7	2	205	206	5
0	6	0	914	922	6	9	15	0	97	97	13	3	7	1	625	616	5	5	17	1	694	688	6	9	7	2	480	489	5
2	6	0	148	153	4	11	15	0	381	374	6	5	7	1	368	355	3	7	17	1	246	237	7	11	7	2	99	111	9
4	6	0	436	446	4	13	15	0	421	425	6	7	7	1	189	192	5	9	17	1	418	411	6	13	7	2	338	347	5
6	6	0	555	548	4	0	16	0	603	601	6	9	7	1	481	490	4	0	18	1	275	280	6	15	7	2	903	914	7
8	6	0	668	651	5	2	16	0	156	161	8	11	7	1	21	6	21	2	18	1	59	60	25	17	7	2	914	924	7
10	6	0	1326	1315	10	4	16	0	258	264	6	13	7	1	49	56	22	4	18	1	328	344	6	19	7	2	48	52	47
12	6	0	295	307	4	6	16	0	842	841	7	15	7	1	85	71	12	6	18	1	373	363	6	0	8	2	483	494	4
14	6	0	478	471	5	8	16	0	67	55	19	17	7	1	188	188	7	1	19	1	318	313	6	2	8	2	439	421	4
16	6	0	543	553	5	10	16	0	34	31	34	19	7	1	138	135	9	3	19	1	392	407	6	4	8	2	178	186	5
18	6	0	374	379	5	12	16	0	407	401	6	0	8	1	704	696	5	0	0	2	3133	3315	7	6	8	2	420	404	4
20	6	0	95	19	14	1	17	0	264	252	6	2	8	1	6	43	6	2	0	2	549	572	4	8	8	2	568	576	5
1	7	0	753	741	5	3	17	0	305	300	6	4	8	1	140	145	5	4	0	2	442	439	4	10	8	2	36	49	36
3	7	0	99	100	6	5	17	0	1898	1890	15	6	8	1	309	315	4	6	0	2	769	746	5	12	8	2	204	204	6
5	7	0	1401	1373	9	7	17	0	58	61	28	8	8	1	143	149	6	8	0	2	539	522	4	14	8	2	573	581	5
7	7	0	437	422	4	9	17	0	67	53	22	10	8	1	134	114	7	10	0	2	1371	1327	10	16	8	2	874	888	7
9	7	0	1284	1269	8	0	18	0	305	294	6	12	8	1	501	504	5	12	0	2	904	899	7	18	8	2	102	74	12
11	7	0	546	514	5	2	18	0	305	301	6	14	8	1	576	574	5	14	0	2	1347	1355	9	1	9	2	418	410	4
13	7	0	367	376	4	4	18	0	66	63	22	16	8	1	787	774	6	16	0	2	664	666	6	3	9	2	27	22	26
15	7	0	220	221	6	6	18	0	217	226	8	18	8	1	348	354	6	18	0	2	863	857	7	5	9	2	445	436	4
17	7	0	214	221	6	8	18	0	327	321	6	20	8	1	227	222	7	20	0	2	53	44	28	7	9	2	388	379	4
19	7	0	723	724	6	1	19	0	200	199	8	1	9	1	978	959	6	1	1	2	477	486	4	9	9	2	752	764	6
0	8	0	2594	2566	9	3	19	0	70	55	22	3	9	1	159	149	5	3	1	2	758	758	5	11	9	2	1574	1563	10
2	8	0	148	152	5	1	1	1	182	170	3	5	9	1	386	400	4	5	1	2	1077	1078	7	13	9	2	85	69	12

Observed and calculated structure factors for K9

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	365	361	5	20	2	3	77	68	17	17	11	3	546	562	6	12	4	4	164	164	7	12	14	4	71	47	19
17	9	2	590	600	6	1	3	3	555	553	4	0	12	3	273	258	5	14	4	4	896	904	7	1	15	4	183	179	8
19	9	2	299	301	6	3	3	3	260	256	3	2	12	3	266	263	5	16	4	4	1383	1401	10	3	15	4	420	405	5
0	10	2	4369	4409	12	5	3	3	1100	1076	7	4	12	3	336	340	5	18	4	4	141	146	9	5	15	4	242	239	7
2	10	2	683	674	5	7	3	3	765	737	6	6	12	3	122	121	8	1	5	4	969	974	7	7	15	4	123	130	11
4	10	2	753	760	6	9	3	3	188	182	5	8	12	3	80	91	13	3	5	4	156	152	5	9	15	4	110	96	12
6	10	2	79	67	11	11	3	3	1320	1312	9	10	12	3	205	201	6	5	5	4	1515	1550	10	0	16	4	154	158	9
8	10	2	266	277	5	13	3	3	70	79	14	12	12	3	283	276	6	7	5	4	402	387	4	2	16	4	164	149	9
10	10	2	1881	1869	12	15	3	3	86	97	12	14	12	3	129	133	10	9	5	4	186	192	6	4	16	4	200	196	8
12	10	2	309	301	5	17	3	3	218	242	6	16	12	3	421	403	6	11	5	4	894	902	6	6	16	4	462	464	6
14	10	2	371	375	5	19	3	3	124	134	11	1	13	3	245	238	6	13	5	4	202	205	6	8	16	4	0	11	1
16	10	2	222	225	7	21	3	3	400	401	6	3	13	3	475	486	5	15	5	4	270	270	6	1	17	4	324	336	6
18	10	2	295	284	6	0	4	3	2072	2071	8	5	13	3	330	336	5	17	5	4	93	91	13	3	17	4	195	190	8
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5	11	2	103	92	9	6	4	3	212	200	4	11	13	3	353	352	6	2	6	4	161	165	6	5	1	5	633	634	5
7	11	2	48	18	21	8	4	3	280	292	4	13	13	3	0	9	1	4	6	4	402	410	4	7	1	5	38	41	38
9	11	2	661	676	5	10	4	3	338	331	4	0	14	3	57	40	20	6	6	4	161	160	6	9	1	5	376	393	4
11	11	2	1767	1747	11	12	4	3	810	798	6	2	14	3	262	263	6	8	6	4	351	349	4	11	1	5	278	269	5
13	11	2	51	62	26	14	4	3	122	111	8	4	14	3	379	375	5	10	6	4	1232	1248	8	13	1	5	213	209	6
15	11	2	269	262	6	16	4	3	253	251	6	6	14	3	181	180	7	12	6	4	387	397	5	15	1	5	49	19	27
17	11	2	76	81	18	18	4	3	162	166	8	8	14	3	383	379	5	14	6	4	268	268	6	17	1	5	737	738	6
0	12	2	1357	1346	9	20	4	3	44	59	43	10	14	3	41	26	40	16	6	4	192	206	7	19	1	5	356	369	6
2	12	2	18	28	18	1	5	3	59	65	11	12	14	3	62	51	23	18	6	4	284	279	7	0	2	5	695	700	5
4	12	2	45	16	26	3	5	3	372	376	4	1	15	3	175	166	7	1	7	4	329	285	4	2	2	5	74	57	11
6	12	2	840	841	6	5	5	3	959	935	6	3	15	3	192	194	7	3	7	4	192	181	5	4	2	5	490	498	4
8	12	2	125	136	8	7	5	3	881	869	6	5	15	3	477	482	5	5	7	4	1286	1284	9	6	2	5	448	442	4
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12	12	2	233	220	6	11	5	3	138	129	7	9	15	3	142	125	9	9	7	4	996	989	7	10	2	5	147	134	7
14	12	2	577	575	6	13	5	3	446	451	5	11	15	3	345	342	6	11	7	4	701	705	6	12	2	5	759	757	6
16	12	2	357	357	6	15	5	3	87	91	12	0	16	3	133	110	10	13	7	4	323	322	5	14	2	5	85	76	13
1	13	2	208	208	6	17	5	3	282	288	6	2	16	3	100	93	12	15	7	4	210	219	7	16	2	5	275	277	6
3	13	2	70	72	14	19	5	3	96	77	13	4	16	3	191	197	7	17	7	4	340	342	6	18	2	5	79	89	16
5	13	2	1885	1866	13	0	6	3	529	533	4	6	16	3	1124	1113	8	0	8	4	1825	1897	11	1	3	5	140	136	6
7	13	2	50	55	25	2	6	3	90	83	8	8	16	3	250	252	7	2	8	4	0	9	1	3	3	5	205	205	5
9	13	2	176	175	7	4	6	3	429	407	4	10	16	3	77	81	18	4	8	4	138	141	7	5	3	5	529	529	5
11	13	2	109	103	10	6	6	3	1189	1175	8	1	17	3	142	142	9	6	8	4	508	504	5	7	3	5	97	108	9
13	13	2	102	104	12	8	6	3	376	368	4	3	17	3	332	335	6	8	8	4	365	366	4	9	3	5	92	87	10
15	13	2	515	517	6	10	6	3	151	151	6	5	17	3	409	407	6	10	8	4	1163	1181	8	11	3	5	296	291	5
0	14	2	446	439	5	12	6	3	284	285	5	7	17	3	0	15	1	12	8	4	102	116	10	13	3	5	309	293	5
2	14	2	305	304	5	14	6	3	102	103	10	0	18	3	223	227	7	14	8	4	149	152	8	15	3	5	25	32	25
4	14	2	736	751	6	16	6	3	1131	1132	8	2	18	3	171	164	9	16	8	4	218	217	7	17	3	5	513	509	5
6	14	2	425	423	5	18	6	3	405	409	6	0	0	4	6274	6558	11	18	8	4	44	34	44	0	4	5	77	59	11
8	14	2	178	184	7	20	6	3	370	378	6	2	0	4	390	394	4	1	9	4	28	33	28	2	4	5	56	34	16
10	14	2	169	169	8	1	7	3	174	177	5	4	0	4	708	738	5	3	9	4	289	287	5	4	4	5	131	144	7
12	14	2	127	79	10	3	7	3	313	318	4	6	0	4	416	410	4	5	9	4	1760	1767	12	6	4	5	680	670	5
14	14	2	407	418	6	5	7	3	1121	1115	8	8	0	4	223	233	5	7	9	4	503	501	5	8	4	5	382	376	4
1	15	2	509	507	5	7	7	3	171	174	6	10	0	4	2599	2622	12	9	9	4	60	37	17	10	4	5	96	86	10
3	15	2	286	296	6	9	7	3	482	490	5	12	0	4	926	924	7	11	9	4	183	184	7	12	4	5	512	516	5
5	15	2	1463	1479	11	11	7	3	808	800	6	14	0	4	353	350	5	13	9	4	147	134	8	14	4	5	269	258	6
7	15	2	497	504	5	13	7	3	136	134	8	16	0	4	194	187	7	15	9	4	332	345	6	16	4	5	693	689	6
9	15	2	166	169	8	15	7	3	170	170	7	18	0	4	593	583	6	17	9	4	557	563	6	18	4	5	277	284	7
11	15	2	359	362	6	17	7	3	606	602	6	20	0	4	136	101	11	0	10	4	839	863	7	1	5	5	177	163	6
13	15	2	146	136	10	19	7	3	100	101	13	1	1	4	209	204	4	2	10	4	89	87	10	3	5	5	324	323	4
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2	16	2	136	128	9	2	8	3	136	146	6	5	1	4	294	293	4	6	10	4	221	214	6	7	5	5	603	597	5
4	16	2	26	40	25	4	8	3	353	366	4	7	1	4	83	75	10	8	10	4	322	321	5	9	5	5	425	435	5
6	16	2	453	456	5	6	8	3	570	572	5	9	1	4	1312	1322	9	10	10	4	482	470	5	11	5	5	277	266	5
8	16	2	65	71	22	8	8	3	15	20	14	11	1	4	1578	1592	12	12	10	4	165	165	8	13	5	5	403	406	5
10	16	2	712	707	6	10	8	3	51	51	20	13	1	4	174	169	6	14	10	4	938	947	7	15	5	5	125	123	10
1	17	2	239	233	6	12	8	3	589	592	5	15	1	4	204	212	6	16	10	4	352	361	6	17	5	5	170	164	9
3	17	2	386	386	6	14	8	3	373	367	5	17	1	4	42	37	41	1	11	4	173	153	6	0	6	5	351	387	4
5	17	2	180	177	8	16	8	3	238	240	6	19	1	4	580	578	6	3	11	4	348	361	5	2	6	5	108	112	8
7	17	2	14	7	13	18	8	3	189	182	8	0	2	4	339	364	3	5	11	4	1137	1164	8	4	6	5	57	69	17
9	17	2	403	397	6	1	9	3	578	583	5	2	2	4	159	166	5	7	11	4	86	87	13	6	6	5	421	412	4
0	18	2	777	772	7	3	9	3	86	84	10	4	2	4	450	452	4	9	11	4	30	20	30	8	6	5	135	339	5
2	18	2	50	14	36	5	9	3	315	311	4	6	2	4	452	467	4	11	11	4	24	10	24	10	6	5	69	62	15
4	18	2	206	213	8	7	9	3	232	231	5	8	2	4	119	111	7	13	11	4	100	94	12	12	6	5	230	225	6
6	18	2	415	417	6	9	9	3	79	81	12	10	2	4	466	477	4	15	11	4	794	789	7	14	6	5	0	4	1
1	1	3	276	276	3	11	9	3	880	888	7	12	2	4	295	299	5	0	12	4	954	966	7	16	6	5	718	713	6
3	1	3	672	663	5	13	9	3	0	17	1	14	2	4	658	652	6	2	12	4	272	272	5	1	7	5	92	79	10
5	1	3	240	230	3	15	9	3	71	73	17	16	2	4	704	713	6	4	12	4	109	112	10	3	7	5	492	503	5
7	1	3	255	252	4	17	9	3	522	522	5	18	2	4	53	43	28	6	12	4	279	288	5	5	7	5	0	23	1
9	1	3	414	421	4	0	10	3	774	791	6	20	2	4	145	145	10	8	12	4	211	211	6	7	7	5	305	313	5
11	1	3	1393	1406	11	2	10	3	771	785	6	1	3	4	213	244	4	10	12	4	401	398	5	9	7	5	333	330	5
13	1	3	444	455	4	4	10	3	394	389	4	3	3	4	484	469	4	12	12	4	335	335	6	11	7	5	376	377	5
15	1	3	88	74	11	6	10	3	186	187	6	5	3	4	3347	3339	10	14	12	4	19	5	39	13	7	5	169	164	7
17	1	3	360	362	5	8	10	3	253	247	5	7	3	4	164	162	5	1	13	4	213	212	6	15	7	5	0	21	1
19	1	3	452	456	5	10	10	3	28	33	27	9	3	4	802	805	6	3	13	4	82	89	13	17	7	5	69	63	20
21	1	3	924	894	7	12	10	3	107	104	10	11	3	4	31	52	31	5	13	4	285	271	6	0	8	5	810	823	6
0	2	3	2234	2249	8	14	10	3	599	605	5	13	3	4	327	331	5	7	13	4	266	270	6	2	8	5	105	98	9
2	2	3	545	526	4	16	10	3	14	29	14	15	3	4	706	714	6	9	13	4	538	535	5	4	8	5	32	9	31
4	2	3	0	16	1	1	11	3	338	340	4	17	3	4	714	717	6	11	13	4	717	715	6	6	8	5	553	544	5
6	2	3	1136	1106	7	3	11	3	240	234	5	19	3	4	192	194	8	13	13	4	171	166	8	8	8	5	137	133	8
8	2	3	741	734	5	5	11	3	716	708	6	0	4	4	496	508	4	0	14	4	1454	1447	10	10	8	5	60	71	20
10	2	3	407	411	4	7	11	3	210	222	5	2	4	4	370	360	4	2	14	4	247	243	6	12	8	5	372	373	5
12	2	3	732	738	5	9	11	3	405	410	5	4	4	4	702	716	5	4	14	4	307	314	6	14	8	5	494	492	5
14	2	3	348	350	5	11	11	3	131	131	8	6	4	4	1812	1794	10	6	14	4	485	491	5	16	8	5	806	802	7
16	2	3	1129	1123	8	13	11	3	57	63	23	8	4	4	195	211	5	8	14	4	96	87	13	1	9	5	688	689	6
18	2	3	219	214	7	15	11	3	87	96	15	10	4	4	287	295	5	10	14	4	1080	1076	8	3	9	5	62	71	17

Observed and calculated structure factors for K9

h	k	l	10Fo	10Fc	10σ
5	9	5	517	501	5
7	9	5	135	129	5
9	9	5	52	49	25
11	9	5	1507	1524	11
13	9	5	105	104	12
15	9	5	75	73	19
0	10	5	941	951	7
2	10	5	514	513	5
4	10	5	157	142	7
6	10	5	452	450	5
8	10	5	138	134	8
10	10	5	239	239	6
12	10	5	56	57	25
14	10	5	469	473	6
1	11	5	105	112	10
3	11	5	239	239	6
5	11	5	446	445	5
7	11	5	518	521	5
9	11	5	246	235	6
11	11	5	427	433	6
13	11	5	176	173	8
0	12	5	1102	1111	8
2	12	5	466	470	5
4	12	5	67	66	18
6	12	5	670	665	6
8	12	5	105	108	12
10	12	5	118	120	11
12	12	5	232	238	7
1	13	5	102	105	6
3	13	5	278	282	6
5	13	5	930	928	7
7	13	5	171	171	8
9	13	5	293	295	6
11	13	5	1170	1167	9
0	14	5	849	831	7
2	14	5	263	256	6
4	14	5	356	351	6
6	14	5	419	412	6
8	14	5	234	227	7
1	15	5	97	107	13
3	15	5	224	227	7
5	15	5	106	101	13
7	15	5	305	304	7
0	16	5	217	212	8
2	16	5	261	277	7
4	16	5	119	129	12
0	0	6	2458	2541	12
2	0	6	75	80	12
4	0	6	640	655	5
6	0	6	681	686	5
8	0	6	356	356	5
10	0	6	858	863	7
12	0	6	721	722	6
14	0	6	795	782	7
16	0	6	808	812	7
1	1	6	122	126	8
3	1	6	155	152	6
5	1	6	1684	1709	12
7	1	6	51	46	21
9	1	6	362	357	5
11	1	6	225	227	6
13	1	6	9	45	9
15	1	6	454	427	5
17	1	6	320	320	7
0	2	6	1670	1688	11
2	2	6	205	196	5
4	2	6	202	197	5
6	2	6	498	492	5
8	2	6	262	254	5
10	2	6	769	768	6
12	2	6	287	297	6
14	2	6	46	33	46
16	2	6	387	394	6
1	3	6	176	175	6
3	3	6	129	128	7
5	3	6	769	775	6
7	3	6	18	38	18
9	3	6	1135	1135	9
11	3	6	1047	1063	8
13	3	6	255	256	6
15	3	6	60	57	23
0	4	6	2380	2426	12
2	4	6	58	73	17
4	4	6	328	334	5
6	4	6	488	501	5
8	4	6	117	118	8
10	4	6	1391	1379	9
12	4	6	301	282	6
14	4	6	62	77	23
16	4	6	207	212	7
1	5	6	250	246	5
3	5	6	295	291	5
5	5	6	462	455	5
7	5	6	85	78	11
9	5	6	211	210	6
11	5	6	343	356	5
13	5	6	95	92	13
15	5	6	203	216	8
0	6	6	183	187	6
2	6	6	44	41	31
4	6	6	571	581	5
6	6	6	810	800	6
8	6	6	101	102	5
10	6	6	163	146	7
12	6	6	146	160	9
14	6	6	880	877	7
1	7	6	591	594	5
3	7	6	168	175	7
5	7	6	2399	2446	13
7	7	6	107	109	10
9	7	6	388	392	5
11	7	6	457	461	5
13	7	6	211	204	7
15	7	6	607	597	6
0	8	6	331	324	5
2	8	6	176	178	7
4	8	6	282	288	5
6	8	6	274	275	6
8	8	6	344	344	5
10	8	6	112	103	10
12	8	6	215	200	7
14	8	6	414	404	6
1	9	6	305	302	5
3	9	6	118	122	9
5	9	6	64	53	19
7	9	6	468	462	5
9	9	6	517	514	5
11	9	6	708	706	6
13	9	6	82	66	16
0	10	6	2104	2152	14
2	10	6	322	331	5
4	10	6	351	344	5
6	10	6	548	548	5
8	10	6	93	83	13
10	10	6	1259	1250	8
12	10	6	169	159	8
1	11	6	66	60	18
3	11	6	338	333	5
5	11	6	447	440	5
7	11	6	83	86	16
9	11	6	494	489	5
11	11	6	714	697	6
0	12	6	501	502	5
2	12	6	36	33	36
4	12	6	36	41	36
6	12	6	907	908	7
8	12	6	44	14	43
10	12	6	422	426	6
1	13	6	0	30	1
3	13	6	49	44	39
5	13	6	1427	1392	9
7	13	6	184	181	8
0	14	6	29	19	29
2	14	6	355	358	6
4	14	6	353	341	6
1	1	7	70	78	14
3	1	7	263	258	5
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7	1	7	258	253	6
9	1	7	245	235	6
11	1	7	734	746	6
13	1	7	346	346	6
15	1	7	113	108	12
0	2	7	686	672	6
2	2	7	300	302	5
4	2	7	0	28	1
6	2	7	452	456	5
8	2	7	300	298	6
10	2	7	134	122	10
12	2	7	544	540	5
14	2	7	191	184	8
1	3	7	182	186	6
3	3	7	0	26	1
5	3	7	385	384	5
7	3	7	455	456	5
9	3	7	182	173	7
11	3	7	755	741	6
13	3	7	0	36	1
0	4	7	958	951	7
2	4	7	114	112	9
4	4	7	283	284	5
6	4	7	72	69	15
8	4	7	206	225	7
10	4	7	194	200	7
12	4	7	468	477	6
14	4	7	148	128	10
1	5	7	23	23	23
3	5	7	196	210	7
5	5	7	355	355	5
7	5	7	506	509	5
9	5	7	337	335	6
11	5	7	58	47	24
13	5	7	274	279	7
0	6	7	212	225	6
2	6	7	89	105	13
4	6	7	191	186	7
6	6	7	671	658	6
8	6	7	239	249	7
10	6	7	142	143	9
12	6	7	194	195	8
1	7	7	53	64	23
3	7	7	272	280	6
5	7	7	660	651	6
7	7	7	125	131	10
9	7	7	171	166	6
11	7	7	489	483	6
0	8	7	486	482	5
2	8	7	125	127	9
4	8	7	299	298	6
6	8	7	320	318	6
8	8	7	64	46	21
10	8	7	39	30	38
1	9	7	393	392	5
3	9	7	41	26	40
5	9	7	228	222	7
7	9	7	115	112	11
9	9	7	75	10	17
0	10	7	534	540	5
2	10	7	426	429	5
4	10	7	182	177	8
6	10	7	193	185	8
8	10	7	132	121	10
1	11	7	183	187	8
3	11	7	139	141	10
5	11	7	508	504	6
7	11	7	159	160	9
0	12	7	74	74	19
2	12	7	152	161	9
4	12	7	245	245	7
0	0	8	2381	2458	14
2	0	8	139	147	9
4	0	8	270	268	6
6	0	8	699	703	6
8	0	8	43	25	43
10	0	8	1436	1405	11
1	1	8	78	77	14
3	1	8	121	134	10
5	1	8	509	513	5
7	1	8	172	167	8
9	1	8	701	709	6
11	1	8	459	460	6
0	2	8	116	3	10
2	2	8	65	67	18
4	2	8	272	269	6
6	2	8	505	491	5
8	2	8	49	41	40
10	2	8	261	251	7
1	3	8	136	131	9
3	3	8	314	319	6
5	3	8	1750	1747	12
7	3	8	41	20	40
9	3	8	452	445	6
11	3	8	157	150	9
0	4	8	252	248	6
2	4	8	257	254	6
4	4	8	277	271	6
6	4	8	582	580	6
8	4	8	54	39	30
10	4	8	130	127	11
1	5	8	518	528	5
3	5	8	141	149	9
5	5	8	420	422	6
7	5	8	9	11	8
9	5	8	180	179	8
0	6	8	1815	1856	12
2	6	8	168	184	9
4	6	8	348	346	6
6	6	8	461	454	6
8	6	8	166	157	8
1	7	8	54	69	28
3	7	8	136	130	10
5	7	8	891	896	7
7	7	8	208	206	7
0	8	8	930	933	7
2	8	8	48	48	44
4	8	8	0	12	1
6	8	8	367	358	6
1	9	8	0	26	1
3	9	8	164	155	9
5	9	8	1220	1230	9
0	10	8	1025	1026	8
2	10	8	145	142	10
1	1	9	74	67	19
3	1	9	205	197	8
5	1	9	242	247	7
0	2	9	74	62	18
2	2	9	34	26	33
4	2	9	262	251	7
6	2	9	15	19	15
1	3	9	174	172	9
3	3	9	22	27	22
5	3	9	71	46	18
0	4	9	420	410	6
2	4	9	63	53	20
4	4	9	84	71	16
1	5	9	48	13	47
3	5	9	112	107	12

Observed and calculated structure factors for K10

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	592	606	4	2	8	0	150	144	7	1	1	1	143	126	4	5	9	1	492	514	5	3	1	2	677	686	5
4	0	0	1261	1285	6	4	8	0	503	495	5	3	1	1	506	493	4	7	9	1	345	339	5	5	1	2	1219	1218	8
6	0	0	638	661	5	6	8	0	582	588	5	5	1	1	699	716	5	9	9	1	90	99	16	7	1	2	157	158	6
8	0	0	1015	1027	7	8	8	0	525	537	5	7	1	1	96	86	9	11	9	1	1723	1719	13	9	1	2	683	679	6
10	0	0	3752	3804	11	10	8	0	1372	1362	10	9	1	1	361	358	4	13	9	1	29	25	29	11	1	2	571	579	5
12	0	0	1365	1399	9	12	8	0	199	199	8	11	1	1	866	885	7	15	9	1	61	69	39	13	1	2	131	134	11
14	0	0	257	237	6	14	8	0	101	101	16	13	1	1	301	304	6	17	9	1	165	182	12	15	1	2	714	700	7
16	0	0	332	320	6	16	8	0	254	260	8	15	1	1	48	52	48	19	9	1	160	179	13	17	1	2	61	78	33
18	0	0	630	622	7	18	8	0	0	24	1	17	1	1	721	726	7	0	10	1	1333	1340	9	19	1	2	0	17	1
20	0	0	297	299	8	20	8	0	332	310	8	19	1	1	454	471	6	2	10	1	779	768	6	21	1	2	248	266	10
22	0	0	1629	1651	12	1	9	0	168	147	7	21	1	1	875	860	8	4	10	1	326	334	5	0	2	2	4190	4158	8
1	1	0	644	683	4	3	9	0	378	387	5	0	2	1	216	176	4	6	10	1	410	415	5	2	2	2	315	314	4
3	1	0	235	224	4	5	9	0	1842	1890	11	2	2	1	465	477	4	8	10	1	109	117	13	4	2	2	467	468	4
5	1	0	575	577	5	7	9	0	896	890	7	4	2	1	387	389	4	10	10	1	292	291	7	6	2	2	405	401	4
7	1	0	487	491	4	9	9	0	83	80	18	6	2	1	244	229	4	12	10	1	22	28	21	8	2	2	227	215	5
9	1	0	1718	1716	9	11	9	0	590	571	6	8	2	1	691	699	5	14	10	1	648	648	6	10	2	2	1331	1337	9
11	1	0	2871	2893	11	13	9	0	272	272	7	10	2	1	327	350	5	16	10	1	323	333	8	12	2	2	548	569	5
13	1	0	312	317	6	15	9	0	582	587	6	12	2	1	980	975	7	18	10	1	284	283	9	14	2	2	120	115	12
15	1	0	243	242	7	17	9	0	508	512	6	14	2	1	86	84	17	1	11	1	218	227	7	16	2	2	318	309	6
17	1	0	286	290	7	19	9	0	264	262	9	16	2	1	731	747	7	3	11	1	217	219	7	18	2	2	80	54	22
19	1	0	601	598	6	0	10	0	401	416	5	18	2	1	58	19	38	5	11	1	679	684	6	20	2	2	49	13	49
21	1	0	791	791	7	2	10	0	0	4	1	20	2	1	194	201	11	7	11	1	514	513	6	1	3	2	363	364	4
0	2	0	1309	1328	5	4	10	0	426	448	5	22	2	1	213	220	11	9	11	1	334	345	6	3	3	2	225	220	4
2	2	0	242	254	3	6	10	0	228	238	7	1	3	1	295	291	4	11	11	1	377	369	6	5	3	2	1207	1192	9
4	2	0	697	716	6	8	10	0	325	333	6	3	3	1	218	209	4	13	11	1	134	140	13	7	3	2	108	121	9
6	2	0	152	161	6	10	10	0	576	583	6	5	3	1	243	232	4	15	11	1	102	113	19	9	3	2	1631	1648	11
8	2	0	296	297	4	12	10	0	138	138	11	7	3	1	490	494	4	17	11	1	401	411	7	11	3	2	1427	1442	9
10	2	0	639	656	6	14	10	0	1198	1178	9	9	3	1	296	301	5	0	12	1	1168	1187	9	13	3	2	477	479	5
12	2	0	304	301	5	16	10	0	298	297	8	11	3	1	270	280	6	2	12	1	489	482	5	15	3	2	205	200	8
14	2	0	851	867	7	18	10	0	516	519	7	13	3	1	302	309	6	4	12	1	93	85	16	17	3	2	292	291	7
16	2	0	717	725	6	1	11	0	323	315	5	15	3	1	12	13	12	6	12	1	668	660	6	19	3	2	825	821	8
18	2	0	18	10	17	3	11	0	331	330	6	17	3	1	337	331	7	8	12	1	169	172	10	21	3	2	593	604	7
20	2	0	173	159	11	5	11	0	972	1005	7	19	3	1	214	211	9	10	12	1	211	208	8	0	4	2	2161	2113	8
22	2	0	322	316	8	7	11	0	142	144	10	21	3	1	341	358	8	12	12	1	282	271	7	2	4	2	704	689	5
1	3	0	331	323	4	9	11	0	132	131	11	0	4	1	979	989	7	14	12	1	67	62	14	4	4	2	4	43	4
3	3	0	431	443	4	11	11	0	420	425	6	2	4	1	80	88	11	16	12	1	761	755	7	6	4	2	330	313	4
5	3	0	4998	4976	9	13	11	0	232	240	8	4	4	1	233	229	4	1	13	1	354	336	6	8	4	2	220	227	6
7	3	0	497	483	4	15	11	0	878	881	8	6	4	1	823	782	6	3	13	1	322	333	6	10	4	2	2102	2143	12
9	3	0	1004	1006	7	17	11	0	440	447	7	8	4	1	489	491	5	5	13	1	1022	1025	8	12	4	2	225	234	7
11	3	0	412	416	5	0	12	0	1503	1490	10	10	4	1	274	248	5	7	13	1	115	103	14	14	4	2	252	262	7
13	3	0	429	436	5	2	12	0	217	220	7	12	4	1	697	705	6	9	13	1	364	370	7	16	4	2	82	67	20
15	3	0	907	907	7	4	12	0	338	336	6	14	4	1	248	252	7	11	13	1	1127	1112	9	18	4	2	546	536	6
17	3	0	951	942	8	6	12	0	649	663	6	16	4	1	636	647	6	13	13	1	117	107	15	20	4	2	310	315	8
19	3	0	239	241	9	8	12	0	194	189	8	18	4	1	244	235	8	15	13	1	245	230	9	1	5	2	1050	1025	7
21	3	0	327	317	8	10	12	0	638	640	6	20	4	1	83	79	25	0	14	1	708	723	6	3	5	2	91	83	10
0	4	0	2303	2309	7	12	12	0	551	549	6	1	5	1	86	94	10	2	14	1	273	267	7	5	5	2	1793	1757	9
2	4	0	595	596	5	14	12	0	136	154	14	3	5	1	578	591	4	4	14	1	468	466	6	7	5	2	172	172	7
4	4	0	1209	1204	8	16	12	0	108	92	19	5	5	1	1636	1637	9	6	14	1	235	238	8	9	5	2	481	488	5
6	4	0	1711	1648	9	1	13	0	486	489	5	7	5	1	698	877	7	8	14	1	276	268	7	11	5	2	658	642	6
8	4	0	519	512	5	3	13	0	148	158	11	9	5	1	494	482	5	10	14	1	217	221	9	13	5	2	38	52	37
10	4	0	514	520	5	5	13	0	427	423	6	11	5	1	344	371	5	12	14	1	115	136	18	15	5	2	248	268	8
12	4	0	223	219	7	7	13	0	476	476	6	13	5	1	647	647	6	14	14	1	399	392	7	17	5	2	765	754	7
14	4	0	893	900	8	9	13	0	471	471	6	15	5	1	101	109	16	1	15	1	28	8	27	19	5	2	407	409	7
16	4	0	2029	2021	14	11	13	0	948	939	8	17	5	1	238	226	8	3	15	1	291	297	7	21	5	2	447	450	7
18	4	0	129	117	13	13	13	0	271	279	8	19	5	1	69	46	31	5	15	1	275	265	8	0	6	2	1182	1176	7
20	4	0	268	231	8	15	13	0	245	248	9	21	5	1	784	771	7	7	15	1	146	339	7	2	6	2	129	132	7
22	4	0	388	396	8	0	14	0	1570	1553	12	0	6	1	346	320	4	9	15	1	60	61	43	4	6	2	1051	1046	7
1	5	0	1451	1451	8	2	14	0	413	412	6	2	6	1	181	175	5	11	15	1	177	160	11	6	6	2	2390	2159	11
3	5	0	113	107	8	4	14	0	218	209	8	4	6	1	318	314	4	13	15	1	143	146	15	8	6	2	270	264	6
5	5	0	3195	3202	9	6	14	0	658	668	6	6	6	1	871	881	6	0	16	1	352	348	7	10	6	2	31	47	31
7	5	0	852	823	6	8	14	0	162	177	11	8	6	1	459	455	5	2	16	1	249	237	8	12	6	2	358	361	6
9	5	0	115	122	10	10	14	0	1369	1377	10	10	6	1	58	36	29	4	16	1	0	31	1	14	6	2	941	952	8
11	5	0	314	340	5	12	14	0	37	89	16	12	6	1	389	375	5	6	16	1	1253	1262	9	16	6	2	1500	1480	11
13	5	0	254	264	7	14	14	0	0	10	1	14	6	1	0	25	1	8	16	1	280	291	8	18	6	2	0	36	1
15	5	0	293	290	7	1	15	0	316	306	7	16	6	1	1077	1068	8	10	16	1	11	17	11	20	6	2	80	67	29
17	5	0	549	500	6	3	15	0	402	399	6	18	6	1	229	240	9	12	16	1	106	98	20	1	7	2	720	703	6
19	5	0	181	196	11	5	15	0	464	466	6	20	6	1	429	436	7	1	17	1	27	36	27	3	7	2	86	94	13
21	5	0	294	302	8	7	15	0	49	14	49	1	7	1	101	99	10	3	17	1	283	276	8	5	7	2	4563	4618	12
0	6	0	1015	1022	7	9	15	0	219	205	9	3	7	1	555	551	5	5	17	1	737	751	7	7	7	2	214	202	6
2	6	0	116	123	7	11	15	0	373	378	7	5	7	1	497	496	5	7	17	1	249	249	9	9	7	2	507	520	5
4	6	0	364	374	4	13	15	0	437	433	7	7	7	1	183	184	7	9	17	1	429	419	7	11	7	2	25	40	25
6	6	0	498	484	4	0	16	0	567	563	6	9	7	1	471	486	5	0	18	1	270	279	9	13	7	2	419	422	6
8	6	0	608	585	5	2	16	0	171	167	11	11	7	1	49	13	48	2	18	1	81	76	28	15	7	2	969	977	8
10	6	0	1438	1444	12	4	16	0	185	184	10	13	7	1	90	90	17	4	18	1	372	365	7	17	7	2	937	950	8
12	6	0	260	264	6	6	16	0	834	849	7	15	7	1	0	15	1	6	18	1	350	349	8	19	7	2	68	75	36
14	6	0	436	434	5	8	16	0	19	36	19	17	7	1	180	177	11	1	19	1	151	144	8	0	8	2	370	365	5
16	6	0	465	467	6	10	16	0	0	10	1	19	7	1	161	143	12	3	19	1	185	198	8	2	8	2	438	440	5
18	6	0	403	398	6	12	16	0	443	442	7	0	8	1	756	731	6	0	0	2	3550	3575	8	4	8	2	291	299	5
20	6	0	0	7	1	1	17	0	255	244	9	2	8	1	15	9	14	2	0	2	605	621	5	6	8	2	378	375	5
1	7	0	752	729	6	3	17	0	321	304	8	4	8	1	103	77	11	4	0	2	488	481	4	8	8	2	587	608	6
3	7	0	189	192	6	5	17	0	1852	1861	14	6	8	1	327	344	5	6	0	2	764	733	5	10	8	2	0	61	1
5	7	0	1515	1514	10	7	17	0	25	18	24	8	8	1	145	152	9	8	0	2	654	640	5	12	8	2	205	206	8
7	7	0	431	426	5	9	17	0	9	42	9	10	8	1	117	92	12	10	0	2	1505	1453	11	14	8	2	617	609	6
9	7	0	1294	1292	9	0	18	0	236	258	10	12	8	1	491	490	6	12	0	2	874	877	7	16	8	2	909	902	7
11	7	0	625	585	6	2	18	0	295	288	9	14	8	1	549	540	6	14	0	2	1374	1380	11	18	8	2	77	78	28
13	7	0	404	397	5	4	18	0	104	108	21	16	8	1	724	721	7	16	0	2	775	784	7	1	9	2	483	473	6
15	7	0	259	266	7	6	18	0	242	240	10	18	8	1	311	308	8	18	0	2	794	778	7	3	9	2	53	27	32
17	7	0	227	226	9	8	18	0	124	119	8	20	8	1	240	254	10	20	0	2	105	77	18	5	9	2	443	436	5
19	7	0	700	700	7	1	19	0	227	234	11	1	9	1	930	906	7	22	0	2	212	234	11	7	9	2	415	408	5
0	8	0	2753	2694	10	3	19	0	63	66	54	3	9	1	168	165	8	1	1	2	525	525	4	9	9	2	675	678	6

Observed and calculated structure factors for K10

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1568	1564	11	16	2	3	1105	1114	9	13	11	3	40	38	39	4	4	4	717	736	6	4	14	4	317	326	7
13	9	2	139	146	12	18	2	3	160	161	12	15	11	3	51	33	50	6	4	4	1832	1840	12	6	14	4	434	450	7
15	9	2	284	283	8	20	2	3	122	120	17	17	11	3	519	510	7	8	4	4	240	235	7	8	14	4	155	145	13
17	9	2	626	640	7	1	3	3	515	497	4	0	12	3	299	304	7	10	4	4	361	371	6	10	14	4	1076	1079	8
19	9	2	273	286	9	3	3	3	291	289	4	2	12	3	287	271	6	12	4	4	123	125	13	12	14	4	48	48	48
0	10	2	4610	4491	13	5	3	3	1121	1113	8	4	12	3	323	338	6	14	4	4	865	875	7	1	15	4	262	264	8
2	10	2	625	619	6	7	3	3	754	741	6	6	12	3	156	157	10	16	4	4	1465	1459	11	3	15	4	401	398	7
4	10	2	727	728	6	9	3	3	228	222	7	8	12	3	106	95	15	18	4	4	177	168	12	5	15	4	216	206	9
6	10	2	25	22	24	11	3	3	1348	1347	10	10	12	3	197	207	9	1	5	4	980	985	8	7	15	4	159	138	13
8	10	2	317	329	6	13	3	3	91	91	16	12	12	3	271	272	8	3	5	4	131	112	10	9	15	4	188	191	11
10	10	2	1886	1904	14	15	3	3	94	103	17	14	12	3	138	155	14	5	5	4	1566	1606	12	0	16	4	132	141	16
12	10	2	349	348	6	17	3	3	239	237	8	16	12	3	471	469	7	7	5	4	384	380	5	2	16	4	164	161	13
14	10	2	350	347	7	19	3	3	121	139	17	1	13	3	228	237	8	9	5	4	116	116	13	4	16	4	119	117	17
16	10	2	164	158	12	21	3	3	419	418	7	3	13	3	427	434	6	11	5	4	878	893	7	6	16	4	492	482	7
18	10	2	307	298	8	0	4	3	2134	2042	9	5	13	3	428	428	6	13	5	4	122	114	13	8	16	4	58	23	57
1	11	2	316	310	6	2	4	3	56	56	20	7	13	3	112	106	15	15	5	4	280	286	8	1	17	4	327	321	8
3	11	2	705	708	6	4	4	3	359	356	4	9	13	3	307	304	7	17	5	4	78	107	28	3	17	4	197	197	11
5	11	2	146	147	10	6	4	3	206	208	6	11	13	3	412	407	7	19	5	4	126	128	16	5	17	4	1387	1391	10
7	11	2	64	35	25	8	4	3	271	270	6	13	13	3	0	31	1	0	6	4	2227	2239	12	1	1	5	47	43	47
9	11	2	699	701	6	10	4	3	381	372	5	15	13	3	165	148	13	2	6	4	136	152	10	3	1	5	239	249	7
11	11	2	1755	1773	12	12	4	3	773	776	7	0	14	3	63	61	31	4	6	4	379	374	5	5	1	5	590	578	6
13	11	2	52	29	52	14	4	3	104	94	15	2	14	3	208	225	9	6	6	4	203	200	8	7	1	5	46	6	46
15	11	2	224	217	9	16	4	3	210	240	8	4	14	3	187	396	6	8	6	4	296	299	6	9	1	5	293	303	6
17	11	2	113	106	18	18	4	3	152	148	12	6	14	3	178	193	10	10	6	4	1307	1312	9	11	1	5	279	270	7
0	12	2	1391	1393	9	20	4	3	0	14	1	8	14	3	325	321	7	12	6	4	369	362	6	13	1	5	161	155	10
2	12	2	49	12	49	1	5	3	97	102	11	10	14	3	104	59	18	14	6	4	221	234	9	15	1	5	52	24	52
4	12	2	113	96	13	3	5	3	383	388	4	12	14	3	27	16	26	16	6	4	165	153	12	17	1	5	722	739	7
6	12	2	848	858	7	5	5	3	1002	980	7	1	15	3	192	183	10	18	6	4	298	294	8	19	1	5	351	370	8
8	12	2	213	205	8	7	5	3	879	872	6	3	15	3	216	225	9	1	7	4	294	294	6	0	2	5	610	594	6
10	12	2	776	796	7	9	5	3	364	365	5	5	15	3	453	456	7	3	7	4	244	239	7	2	2	5	81	76	18
12	12	2	240	246	9	11	5	3	191	179	8	7	15	3	214	205	10	5	7	4	1343	1369	9	4	2	5	395	393	5
14	12	2	483	480	7	13	5	3	488	489	5	9	15	3	133	112	15	7	7	4	359	343	6	6	2	5	468	453	5
16	12	2	372	381	8	15	5	3	62	21	33	11	15	3	365	355	8	9	7	4	1007	1011	8	8	2	5	373	370	5
1	13	2	141	149	11	17	5	3	288	293	8	0	16	3	202	198	10	11	7	4	766	751	7	10	2	5	127	120	12
3	13	2	15	56	14	19	5	3	101	85	20	2	16	3	115	74	16	13	7	4	338	332	7	12	2	5	781	779	7
5	13	2	1778	1852	15	0	6	3	642	647	6	4	16	3	196	190	10	15	7	4	229	252	9	14	2	5	0	18	1
7	13	2	58	50	41	2	6	3	121	103	9	6	16	3	1128	1110	9	17	7	4	353	342	7	16	2	5	320	303	7
9	13	2	127	111	13	4	6	3	538	516	5	8	16	3	237	241	9	0	8	4	1960	1986	12	18	2	5	130	114	16
11	13	2	47	77	46	6	6	3	1196	1197	8	10	16	3	142	144	15	2	8	4	28	1	28	1	3	5	99	101	14
13	13	2	121	124	16	8	6	3	331	321	5	1	17	3	118	114	17	4	8	4	242	240	7	3	3	5	187	187	8
15	13	2	540	533	7	10	6	3	110	100	13	3	17	3	297	290	8	6	8	4	540	530	6	5	3	5	470	476	5
0	14	2	466	479	6	12	6	3	329	330	6	5	17	3	478	480	7	8	8	4	415	426	6	7	3	5	111	116	13
2	14	2	311	306	7	14	6	3	59	61	15	7	17	3	43	9	42	10	8	4	1177	1190	9	9	3	5	137	138	11
4	14	2	746	751	7	16	6	3	1120	1126	9	0	18	3	206	214	11	12	8	4	114	122	15	11	3	5	235	250	8
6	14	2	462	462	6	18	6	3	362	365	7	2	18	3	174	186	12	14	8	4	80	88	24	13	3	5	314	307	7
8	14	2	192	212	10	20	6	3	398	394	8	4	18	3	177	180	12	16	8	4	208	206	10	15	3	5	0	20	1
10	14	2	173	172	11	1	7	3	142	132	9	0	0	4	6923	6770	13	18	8	4	106	80	20	17	3	5	530	534	7
12	14	2	69	66	35	3	7	3	252	259	6	2	0	4	357	355	4	1	9	4	81	76	19	0	4	5	115	58	13
14	14	2	403	404	7	5	7	3	1229	1205	9	4	0	4	708	718	6	3	9	4	262	259	6	2	4	5	77	49	19
1	15	2	584	590	6	7	7	3	193	195	7	6	0	4	367	362	5	5	9	4	1741	1768	11	4	4	5	91	108	16
3	15	2	302	304	7	9	7	3	480	481	5	8	0	4	358	357	5	7	9	4	500	503	6	6	4	5	673	667	6
5	15	2	1499	1505	11	11	7	3	793	804	7	10	0	4	2731	2749	13	9	9	4	39	12	39	8	4	5	342	351	6
7	15	2	506	502	6	13	7	3	102	116	16	12	0	4	945	936	8	11	9	4	175	171	10	10	4	5	147	140	11
9	15	2	109	57	17	15	7	3	120	123	15	14	0	4	404	406	6	13	9	4	125	111	14	12	4	5	491	483	6
11	15	2	371	374	7	17	7	3	593	599	6	16	0	4	71	85	28	15	9	4	408	415	7	14	4	5	247	248	8
13	15	2	179	173	12	19	7	3	110	114	20	18	0	4	606	588	7	17	9	4	591	597	7	16	4	5	655	658	7
0	16	2	978	978	8	0	8	3	805	784	7	20	0	4	190	172	12	0	10	4	932	930	7	18	4	5	243	256	10
2	16	2	149	142	13	2	8	3	131	123	10	1	1	4	222	224	5	2	10	4	0	50	1	1	5	5	122	126	12
4	16	2	105	115	18	4	8	3	115	321	5	3	1	4	72	75	17	4	10	4	513	519	5	3	5	5	329	320	6
6	16	2	440	438	7	6	8	3	551	546	5	5	1	4	187	173	7	6	10	4	222	231	8	5	5	5	812	790	6
8	16	2	60	57	49	8	8	3	51	17	50	7	1	4	69	55	21	8	10	4	336	333	6	7	5	5	601	603	6
10	16	2	734	724	7	10	8	3	64	49	27	9	1	4	1283	1309	10	10	10	4	493	492	6	9	5	5	348	351	6
1	17	2	217	224	9	12	8	3	576	590	6	11	1	4	1629	1651	13	12	10	4	178	179	11	11	5	5	310	301	7
3	17	2	387	376	7	14	8	3	321	326	7	13	1	4	170	164	9	14	10	4	902	896	7	13	5	5	445	434	6
5	17	2	171	173	12	16	8	3	240	221	9	15	1	4	163	169	10	16	10	4	419	421	7	15	5	5	79	63	26
7	17	2	59	36	59	18	8	3	139	147	14	17	1	4	7	35	7	1	11	4	194	190	8	17	5	5	171	168	12
9	17	2	382	376	8	1	9	3	544	550	6	19	1	4	555	545	7	3	11	4	385	386	6	0	6	5	281	300	6
0	18	2	820	800	7	3	9	3	83	74	17	0	2	4	330	345	4	5	11	4	1157	1200	9	2	6	5	86	100	18
2	18	2	33	17	32	5	9	3	202	193	8	2	2	4	174	175	7	7	11	4	48	48	48	4	6	5	21	10	21
4	18	2	246	259	10	7	9	3	247	245	7	4	2	4	450	443	5	9	11	4	92	74	19	6	6	5	438	428	5
6	18	2	395	395	8	9	9	3	131	128	11	6	2	4	450	470	5	11	11	4	50	15	50	8	6	5	291	299	7
1	1	3	226	223	4	11	9	3	894	921	8	8	2	4	111	113	13	13	11	4	179	161	11	10	6	5	57	13	38
3	1	3	682	675	5	13	9	3	54	11	53	10	2	4	440	445	5	15	11	4	739	742	7	12	6	5	271	273	8
5	1	3	298	302	4	15	9	3	104	91	18	12	2	4	321	311	6	0	12	4	914	934	7	14	6	5	73	36	27
7	1	3	292	297	5	17	9	3	511	527	7	14	2	4	643	643	6	2	12	4	234	230	8	16	6	5	736	729	7
9	1	3	316	323	5	0	10	3	897	914	7	16	2	4	728	731	7	4	12	4	199	214	9	1	7	5	53	56	46
11	1	3	1386	1400	10	2	10	3	764	764	6	18	2	4	0	21	1	6	12	4	314	323	7	3	7	5	450	460	5
13	1	3	401	392	5	4	10	3	428	426	5	20	2	4	114	106	19	8	12	4	218	235	9	5	7	5	83	74	20
15	1	3	115	116	14	6	10	3	180	178	8	1	3	4	221	227	6	10	12	4	420	425	7	7	7	5	300	296	6
17	1	3	356	347	7	8	10	3	167	185	9	3	3	4	404	387	5	12	12	4	401	375	7	9	7	5	333	329	6
19	1	3	460	457	7	10	10	3	100	91	16	5	3	4	3378	3487	12	14	12	4	56	61	55	11	7	5	351	160	7
21	1	3	867	825	8	12	10	3	121	130	14	7	3	4	166	162	8	1	13	4	259	263	8	13	7	5	196	188	10
0	2	3	2436	2392	9	14	10	3	628	632	6	9	3	4	768	784	6	3	13	4	109	91	15	15	7	5	19	58	19
2	2	3	569	554	4	16	10	3	106	121	19	11	3	4	126	133	12	5	13	4	284	274	7	17	7	5	69	75	39
4	2	3	128	129	8	1	11	3	329	332	6	13	3	4	392	385	6	7	13	4	269	267	8	0	8	5	831	835	7
6	2	3	1125	1105	8	3	11	3	154	166	10	15	3	4	789	777	7	9	13	4	468	462	7	2	8	5	131	131	11
8	2	3	775	770	6	5	11	3	737	729	6	17	3	4	726	721	7	11	13	4	757	740	7	4	8	5	54	39	43
10	2	3	364	366	5	7	11	3	207	205	8	19	3	4	207	211	11	13	13	4	144	149	14	6	8	5	574	559	6
12	2	3	734	730	6	9	11	3	400	403	6	0	4	4	628	653	6	0	14	4	1469	1483	11	8	8	5	117	126	14
14	2	3	296	294	6	11	11	3	104	102	16	2	4	4	407	389	5	2	14	4	254	244	8	10	8	5	26	46	26

Observed and calculated structure factors for K10

h	k	l	10Fo	10Fc	10s
12	8	5	155	156	7
14	8	5	476	462	7
16	8	5	752	749	7
1	9	5	651	653	6
3	9	5	67	76	27
5	9	5	582	570	6
7	9	5	143	144	7
9	9	5	87	84	20
11	9	5	1512	1540	11
13	9	5	70	92	34
15	9	5	94	89	23
0	10	5	1055	1047	8
2	10	5	485	498	6
4	10	5	173	172	10
6	10	5	448	439	6
8	10	5	85	87	21
10	10	5	295	286	8
12	10	5	56	40	55
14	10	5	506	490	7
1	11	5	106	98	16
3	11	5	183	184	9
5	11	5	473	469	6
7	11	5	511	511	6
9	11	5	223	230	9
11	11	5	388	397	7
13	11	5	184	198	12
0	12	5	1147	1131	9
2	12	5	473	482	6
4	12	5	91	79	19
6	12	5	679	691	7
8	12	5	105	105	18
10	12	5	102	103	20
12	12	5	234	226	10
1	13	5	280	291	8
3	13	5	234	241	9
5	13	5	986	981	8
7	13	5	205	200	10
9	13	5	332	326	8
11	13	5	1207	1192	9
0	14	5	908	895	8
2	14	5	240	228	9
4	14	5	379	374	7
6	14	5	396	395	7
8	14	5	171	183	12
10	14	5	251	264	10
1	15	5	88	85	23
3	15	5	243	246	9
5	15	5	89	90	24
7	15	5	314	315	9
0	16	5	299	292	9
2	16	5	272	261	9
4	16	5	132	135	17
0	0	6	2629	2650	13
2	0	6	93	86	17
4	0	6	701	700	6
6	0	6	688	687	6
8	0	6	407	407	6
10	0	6	905	911	7
12	0	6	696	700	6
14	0	6	795	799	7
16	0	6	883	864	8
1	1	6	147	155	11
3	1	6	102	105	15
5	1	6	1748	1766	14
7	1	6	76	74	22
9	1	6	373	373	6
11	1	6	259	255	8
13	1	6	54	11	54
15	1	6	455	453	7
17	1	6	315	313	9
0	2	6	1687	1720	13
2	2	6	184	183	8
4	2	6	182	176	9
6	2	6	473	472	6
8	2	6	219	217	8
10	2	6	805	817	7
12	2	6	310	312	7
14	2	6	0	10	1
16	2	6	375	365	7
1	3	6	190	174	8
3	3	6	88	83	18
5	3	6	855	874	7
7	3	6	0	34	1
9	3	6	1083	1108	8
11	3	6	1101	1121	9
13	3	6	226	247	9
15	3	6	62	89	48
17	3	6	316	320	8
0	4	6	2470	2518	14
2	4	6	85	74	18
4	4	6	387	383	6
6	4	6	518	515	6
8	4	6	154	173	11
10	4	6	1405	1414	11
12	4	6	235	228	9
14	4	6	95	80	22
16	4	6	216	245	10
1	5	6	298	303	6
3	5	6	305	306	6
5	5	6	466	455	6
7	5	6	95	102	17
9	5	6	269	269	8
11	5	6	336	340	7
13	5	6	47	80	47
15	5	6	229	238	10
0	6	6	121	117	13
2	6	6	52	13	51
4	6	6	516	518	6
6	6	6	847	852	7
8	6	6	300	298	7
10	6	6	93	68	20
12	6	6	169	154	11
14	6	6	826	826	8
1	7	6	578	577	6
3	7	6	100	110	16
5	7	6	2500	2537	15
7	7	6	104	109	16
9	7	6	407	416	6
11	7	6	384	403	7
13	7	6	265	261	9
15	7	6	672	648	7
0	8	6	271	252	7
2	8	6	190	183	10
4	8	6	365	368	6
6	8	6	255	257	8
8	8	6	359	360	7
10	8	6	104	103	18
12	8	6	211	205	10
14	8	6	445	428	7
1	9	6	360	350	6
3	9	6	121	124	14
5	9	6	50	42	50
7	9	6	492	485	6
9	9	6	473	462	7
11	9	6	727	715	7
13	9	6	16	17	15
0	10	6	2257	2224	16
2	10	6	277	288	8
4	10	6	318	311	7
6	10	6	506	513	6
8	10	6	132	122	15
10	10	6	1294	1303	10
12	10	6	176	189	12
1	11	6	67	58	31
3	11	6	351	337	7
5	11	6	375	383	7
7	11	6	96	81	21
9	11	6	522	511	7
11	11	6	728	732	7
0	12	6	549	551	6
2	12	6	0	54	1
4	12	6	106	105	19
6	12	6	908	907	8
8	12	6	84	69	26
10	12	6	439	426	7
1	13	6	45	3	44
3	13	6	40	39	40
5	13	6	1371	1380	10
7	13	6	165	172	13
0	14	6	25	19	24
2	14	6	354	355	8
4	14	6	360	341	8
6	14	6	133	141	16
1	1	7	73	58	23
3	1	7	247	246	8
5	1	7	32	11	32
7	1	7	266	272	8
9	1	7	174	173	11
11	1	7	750	742	7
13	1	7	291	302	9
15	1	7	119	133	19
0	2	7	734	742	7
2	2	7	320	312	7
4	2	7	28	32	27
6	2	7	465	461	6
8	2	7	305	311	7
10	2	7	125	113	15
12	2	7	534	525	7
14	2	7	157	139	13
1	3	7	167	178	10
3	3	7	37	19	36
5	3	7	414	419	6
7	3	7	440	439	6
9	3	7	205	196	10
11	3	7	782	767	7
13	3	7	45	24	44
0	4	7	975	956	8
2	4	7	90	91	20
4	4	7	246	238	8
6	4	7	86	88	21
8	4	7	216	206	9
10	4	7	249	246	9
12	4	7	478	479	7
14	4	7	116	114	19
1	5	7	0	13	1
3	5	7	189	201	10
5	5	7	374	369	7
7	5	7	505	521	6
9	5	7	256	260	9
11	5	7	79	70	28
13	5	7	294	299	9
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2	6	7	133	116	13
4	6	7	227	235	9
6	6	7	677	671	7
8	6	7	214	226	10
10	6	7	99	104	20
12	6	7	213	222	11
1	7	7	61	65	38
3	7	7	219	250	9
5	7	7	715	715	7
7	7	7	121	124	16
9	7	7	144	350	8
11	7	7	494	488	7
0	8	7	472	473	6
2	8	7	85	91	23
4	8	7	250	241	9
6	8	7	320	319	7
8	8	7	0	46	1
10	8	7	45	55	45
1	9	7	351	350	7
3	9	7	63	28	39
5	9	7	169	166	12
7	9	7	158	142	13
9	9	7	40	33	40
0	10	7	612	605	7
2	10	7	423	418	7
4	10	7	218	205	10
6	10	7	195	171	11
8	10	7	97	86	22
1	11	7	173	172	13
3	11	7	88	102	26
5	11	7	510	516	7
7	11	7	148	159	15
0	12	7	99	106	22
2	12	7	182	177	12
4	12	7	214	221	11
0	0	8	2553	2574	16
2	0	8	114	128	16
4	0	8	282	274	8
6	0	8	684	680	7
8	0	8	0	47	1
10	0	8	1503	1491	11
12	0	8	463	484	7
1	1	8	77	81	26
3	1	8	120	117	15
5	1	8	443	446	7
7	1	8	167	169	12
9	1	8	720	711	7
11	1	8	498	503	7
0	2	8	52	5	51
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4	2	8	256	268	9
6	2	8	502	494	7
8	2	8	0	49	1
10	2	8	244	237	10
1	3	8	138	126	13
3	3	8	260	276	9
5	3	8	1848	1835	13
7	3	8	0	16	1
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11	3	8	101	102	22
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2	4	8	250	261	9
4	4	8	281	289	8
6	4	8	574	598	7
8	4	8	47	51	46
10	4	8	179	173	12
1	5	8	528	532	7
3	5	8	117	125	18
5	5	8	466	466	7
7	5	8	54	10	53
9	5	8	136	130	16
0	6	8	1893	1884	14
2	6	8	182	180	11
4	6	8	349	327	7
6	6	8	478	470	7
8	6	8	125	132	18
1	7	8	89	81	24
3	7	8	155	156	13
5	7	8	925	935	8
7	7	8	192	193	12
0	8	8	975	981	8
2	8	8	67	52	16
4	8	8	23	52	22
6	8	8	377	376	8
1	9	8	0	5	1
3	9	8	139	137	15
5	9	8	1223	1224	9
0	10	8	1060	1056	9
2	10	8	130	126	16
1	1	9	0	27	1
3	1	9	199	188	11
5	1	9	242	240	10
0	2	9	0	28	1
2	2	9	56	55	56
4	2	9	185	166	12
6	2	9	25	5	24
1	3	9	102	123	22
3	3	9	69	33	37
5	3	9	36	46	35
0	4	9	408	400	8
2	4	9	54	52	54
4	4	9	37	61	36
1	5	9	32	11	32
3	5	9	91	102	25

Observed and calculated structure factors for K11

h	k	l	10Fo	10Fc	10s
2	0	0	470	498	3
4	0	0	1385	1370	5
6	0	0	604	614	4
8	0	0	1262	1246	8
10	0	0	3960	3917	10
12	0	0	1309	1336	11
14	0	0	106	297	5
16	0	0	161	361	5
18	0	0	900	870	7
20	0	0	337	338	6
22	0	0	1495	1503	11
1	1	0	706	739	3
3	1	0	448	435	4
5	1	0	751	757	5
7	1	0	380	374	3
9	1	0	1682	1696	9
11	1	0	2856	2886	10
13	1	0	169	173	7
15	1	0	123	124	10
17	1	0	267	268	6
19	1	0	612	599	6
21	1	0	825	824	7
0	2	0	1133	1182	4
2	2	0	377	386	3
4	2	0	626	631	5
6	2	0	33	23	32
8	2	0	208	199	4
10	2	0	580	596	5
12	2	0	309	307	4
14	2	0	834	824	7
16	2	0	757	771	6
18	2	0	152	150	9
20	2	0	181	185	9
22	2	0	160	164	7
1	3	0	399	387	3
3	3	0	341	350	3
5	3	0	4990	5036	8
7	3	0	429	410	4
9	3	0	1120	1116	7
11	3	0	350	340	4
13	3	0	572	574	5
15	3	0	995	997	8
17	3	0	894	901	8
19	3	0	265	266	7
21	3	0	310	301	7
0	4	0	2605	2572	6
2	4	0	830	822	6
4	4	0	1164	1158	7
6	4	0	3628	3592	8
8	4	0	737	727	5
10	4	0	751	753	6
12	4	0	308	307	5
14	4	0	927	933	7
16	4	0	2048	2036	13
18	4	0	248	249	7
20	4	0	392	372	6
1	5	0	1603	1582	7
3	5	0	87	82	7
5	5	0	3273	3214	8
7	5	0	962	934	7
9	5	0	87	91	10
11	5	0	365	386	4
13	5	0	304	306	5
15	5	0	298	308	6
17	5	0	380	393	5
19	5	0	161	153	9
21	5	0	229	232	8
0	6	0	1088	1085	7
2	6	0	92	12	6
4	6	0	330	345	3
6	6	0	535	522	4
8	6	0	561	554	5
10	6	0	1489	1497	11
12	6	0	366	375	5
14	6	0	429	428	5
16	6	0	527	512	5
18	6	0	457	465	5
20	6	0	0	35	1
1	7	0	755	743	6
3	7	0	344	355	4
5	7	0	1727	1698	9
7	7	0	490	487	4
9	7	0	1298	1294	8
11	7	0	610	565	5
13	7	0	631	634	5
15	7	0	374	377	5
17	7	0	136	130	10
19	7	0	754	764	7
0	8	0	2777	2709	9
2	8	0	157	151	5
4	8	0	579	570	5
6	8	0	644	649	5
8	8	0	556	563	5
10	8	0	1464	1481	12
12	8	0	325	334	5
14	8	0	64	49	21
16	8	0	218	215	7
18	8	0	80	63	19
20	8	0	166	357	7
1	9	0	194	186	5
3	9	0	169	382	4
5	9	0	1840	1839	10
7	9	0	965	944	8
9	9	0	146	151	7
11	9	0	587	578	5
13	9	0	314	317	6
15	9	0	519	536	6
17	9	0	503	505	6
19	9	0	354	371	7
0	10	0	461	481	4
2	10	0	151	171	7
4	10	0	342	353	4
6	10	0	247	202	5
8	10	0	576	586	5
10	10	0	703	721	6
12	10	0	149	151	9
14	10	0	1191	1192	9
16	10	0	351	353	6
18	10	0	731	732	7
1	11	0	450	444	5
3	11	0	340	352	4
5	11	0	1027	1034	8
7	11	0	136	139	8
9	11	0	193	194	7
11	11	0	520	530	5
13	11	0	213	214	7
15	11	0	1017	1021	8
17	11	0	528	542	6
0	12	0	1325	1351	9
2	12	0	233	226	5
4	12	0	359	361	5
6	12	0	709	716	6
8	12	0	219	227	6
10	12	0	541	543	5
12	12	0	597	590	5
14	12	0	213	212	7
16	12	0	154	156	11
1	13	0	538	554	5
3	13	0	331	334	5
5	13	0	446	447	5
7	13	0	615	616	5
9	13	0	162	161	5
11	13	0	928	940	7
13	13	0	376	386	6
15	13	0	341	352	7
0	14	0	1578	1578	10
2	14	0	494	494	5
4	14	0	198	199	7
6	14	0	786	785	7
8	14	0	255	246	6
10	14	0	1469	1485	10
12	14	0	45	43	44
14	14	0	66	70	28
1	15	0	351	351	5
3	15	0	460	454	5
5	15	0	425	418	5
7	15	0	107	94	13
9	15	0	253	248	7
11	15	0	398	408	6
13	15	0	535	544	6
0	16	0	555	559	5
2	16	0	240	244	7
4	16	0	76	73	18
6	16	0	888	886	7
8	16	0	107	92	13
10	16	0	36	34	35
12	16	0	493	496	6
1	17	0	240	242	7
3	17	0	398	403	6
5	17	0	1880	1876	12
7	17	0	31	46	30
9	17	0	0	23	1
0	18	0	228	234	8
2	18	0	355	361	6
4	18	0	128	108	12
6	18	0	205	215	9
8	18	0	420	415	6
1	19	0	363	361	6
3	19	0	126	117	13
1	1	1	192	180	3
3	1	1	716	703	6
5	1	1	498	511	4
7	1	1	121	303	3
9	1	1	509	508	4
11	1	1	896	899	6
13	1	1	240	232	5
15	1	1	169	161	7
17	1	1	717	726	6
19	1	1	511	524	6
21	1	1	1026	1013	8
0	2	1	503	444	3
2	2	1	225	248	3
4	2	1	473	479	4
6	2	1	252	238	3
8	2	1	984	989	7
10	2	1	628	655	5
12	2	1	964	963	8
14	2	1	91	94	13
16	2	1	841	843	7
18	2	1	168	169	8
20	2	1	20	38	19
22	2	1	258	258	8
1	3	1	244	247	3
3	3	1	155	150	4
5	3	1	128	122	5
7	3	1	540	533	4
9	3	1	363	378	4
11	3	1	251	252	5
13	3	1	400	409	5
15	3	1	52	41	27
17	3	1	399	399	5
19	3	1	221	222	7
21	3	1	383	388	6
0	4	1	872	888	6
2	4	1	81	54	7
4	4	1	171	161	4
6	4	1	881	831	6
8	4	1	625	612	5
10	4	1	87	58	11
12	4	1	683	701	6
14	4	1	152	144	5
16	4	1	693	696	6
18	4	1	197	196	8
20	4	1	186	190	9
1	5	1	171	182	4
3	5	1	919	914	6
5	5	1	1926	1907	8
7	5	1	782	768	6
9	5	1	561	562	5
11	5	1	192	417	4
13	5	1	878	899	7
15	5	1	157	158	5
17	5	1	260	260	6
19	5	1	71	66	21
21	5	1	972	970	8
0	6	1	208	180	3
2	6	1	122	321	3
4	6	1	135	331	3
6	6	1	826	823	6
8	6	1	416	401	4
10	6	1	85	92	12
12	6	1	353	337	5
14	6	1	109	17	11
16	6	1	1087	1097	8
18	6	1	184	182	8
20	6	1	191	384	6
1	7	1	35	45	35
3	7	1	682	667	5
5	7	1	412	409	4
7	7	1	135	106	7
9	7	1	637	657	5
11	7	1	120	69	9
13	7	1	85	76	14
15	7	1	141	117	9
17	7	1	138	138	10
19	7	1	213	212	8
0	8	1	845	829	6
2	8	1	176	187	5
4	8	1	205	220	5
6	8	1	365	378	4
8	8	1	261	268	5
10	8	1	238	233	5
12	8	1	404	402	5
14	8	1	619	614	6
16	8	1	838	838	7
18	8	1	255	258	7
20	8	1	113	121	15
1	9	1	973	939	7
3	9	1	302	298	4
5	9	1	669	698	5
7	9	1	232	224	5
9	9	1	96	81	11
11	9	1	1713	1715	12
13	9	1	97	108	13
15	9	1	96	91	13
17	9	1	178	175	9
19	9	1	196	211	9
0	10	1	1367	1371	10
2	10	1	843	836	6
4	10	1	475	490	5
6	10	1	322	330	5
8	10	1	74	83	15
10	10	1	292	293	5
12	10	1	116	117	11
14	10	1	764	771	6
16	10	1	256	267	7
18	10	1	392	377	6
1	11	1	398	405	4
3	11	1	337	334	4
5	11	1	579	582	5
7	11	1	391	391	5
9	11	1	501	499	5
11	11	1	442	451	5
13	11	1	76	74	18
15	11	1	66	30	24
17	11	1	320	321	7
0	12	1	1292	1323	9
2	12	1	444	432	5
4	12	1	83	89	12
6	12	1	665	660	6
8	12	1	266	269	6
10	12	1	340	335	5
12	12	1	256	256	7
14	12	1	58	81	30
16	12	1	763	767	7
1	13	1	296	281	5
3	13	1	317	320	5
5	13	1	1071	1084	8
7	13	1	81	72	14
9	13	1	436	441	5
11	13	1	1103	1109	8
13	13	1	54	56	35
15	13	1	243	228	8
0	14	1	637	653	6
2	14	1	371	363	5
4	14	1	617	626	6
6	14	1	127	115	10
8	14	1	319	320	6
10	14	1	137	140	10
12	14	1	52	51	39
14	14	1	526	528	6
1	15	1	93	95	13
3	15	1	223	238	7
5	15	1	349	345	6
7	15	1	222	221	7
9	15	1	115	116	12
11	15	1	230	227	8
13	15	1	66	59	25
0	16	1	346	343	6
2	16	1	246	250	7
4	16	1	63	94	25
6	16	1	1237	1236	9
8	16	1	311	316	6
10	16	1	0	14	1
12	16	1	96	93	17
1	17	1	73	60	20
3	17	1	307	295	6
5	17	1	770	779	7
7	17	1	329	327	7
9	17	1	541	525	6
0	18	1	237	246	8
2	18	1	0	14	1
4	18	1	485	493	6
6	18	1	482	475	6
1	19	1	337	344	7
3	19	1	397	397	6
0	0	2	3727	3811	7
2	0	2	842	855	6
4	0	2	445	442	4
6	0	2	699	682	5
8	0	2	997	985	7
10	0	2	1666	1621	10
12	0	2	872	877	7
14	0	2	1431	1426	10
16	0	2	848	866	7
18	0	2	1147	1121	9
20	0	2	119	135	13
1	1	2	586	593	4
3	1	2	654	638	5
5	1	2	1298	1285	7
7	1	2	219	208	4
9	1	2	733	734	6
11	1	2	651	656	6
13	1	2	192	180	6
15	1	2	763	772	6
17	1	2	146	140	9
19	1	2	68	53	22
21	1	2	276	271	7
0	2	2	4155	4134	7
2	2	2	303	300	3
4	2	2	503	498	4
6	2	2	396	388	4
8	2	2	258	247	4
10	2	2	1325	1319	10
12	2	2	561	529	5
14	2	2	152	154	8
16	2	2	322	318	5
18	2	2	133	118	11
20	2	2	78	34	20
1	3	2	403	400	3
3	3	2	6	35	6
5	3	2	1344	1320	8
7	3	2	261	263	4
9	3	2	1683	1679	10
11	3	2	1398	1421	11
13	3	2	737	734	6
15	3	2	331	320	5
17	3	2	280	274	6
19	3	2	848	856	7
21	3	2	676	648	6
0	4	2	2248	2219	7
2	4	2	831	827	6
4	4	2	80	96	9
6	4	2	174	166	5
8	4	2	325	334	4
10	4	2	2247	2292	11
12	4	2	273	268	5
14	4	2	290	292	5
16	4	2	56	28	26
18	4	2	613	604	6
20	4	2	432	420	6
1	5	2	1057	1040	8
3	5	2	36	20	32
5	5	2	1709	1658	9
7	5	2	166	155	6
9	5	2	461	465	5
11	5	2	635	635	6
13	5	2	154	146	8
15	5	2	221	217	7
17	5	2	833	838	7
19	5	2	464	457	6
21	5	2	551	551	6
0	6	2	1326	1296	8
2	6	2	63	53	11
4	6	2	928	945	6
6	6	2	2442	2387	10
8	6	2	125	118	8
10	6	2	132	140	8
12	6	2	489	497	5
14	6	2	917	924	7
16	6	2	1484	1478	11
18	6	2	161	151	9
20	6	2	73	12	24
1	7	2	837	825	6
3	7	2	188	193	5
5	7	2	4705	4673	11
7	7	2	187	192	6
9	7	2	549	548	5
11	7	2	127	127	9
13	7	2	546	554	5
15	7	2	1043	1050	8
17	7	2	820	823	7
19	7	2	98	102	15
0	8	2	299	299	4
2	8	2	557	546	5
4	8	2	281	292	4
6	8	2	369	355	4
8	8	2	778	783	6
10	8	2	205	206	6
12	8	2	296	302	5
14	8	2	605	618	6
16	8	2	1013	965	8
18	8	2	187	189	9
1	9	2	603	598	5
3	9	2	89	74	11
5	9	2	485	484	5
7	9	2	500	498	5
9	9	2	578	588	5
11	9	2	1627	1632	13
13	9	2	40	49	40

Observed and calculated structure factors for K11

h	k	l	10Fo	10Fc	10s
15	9	2	312	303	6
17	9	2	686	682	6
19	9	2	224	230	9
0	10	2	4540	4483	12
2	10	2	547	554	5
4	10	2	701	713	6
6	10	2	63	37	18
8	10	2	445	450	5
10	10	2	1974	1987	13
12	10	2	323	319	6
14	10	2	396	374	6
16	10	2	128	129	12
18	10	2	429	418	6
1	11	2	245	244	5
3	11	2	820	829	7
5	11	2	230	233	6
7	11	2	26	6	26
9	11	2	703	710	6
11	11	2	1712	1720	11
13	11	2	80	26	17
15	11	2	390	379	6
17	11	2	171	162	10
0	12	2	1402	1429	10
2	12	2	42	46	41
4	12	2	180	179	7
6	12	2	976	977	8
8	12	2	189	195	7
10	12	2	817	829	7
12	12	2	352	333	6
14	12	2	454	450	6
16	12	2	358	364	7
1	13	2	118	126	9
3	13	2	46	23	14
5	13	2	1818	1846	13
7	13	2	123	134	10
9	13	2	70	72	19
11	13	2	122	87	12
13	13	2	128	132	12
15	13	2	607	605	6
0	14	2	617	603	5
2	14	2	399	404	5
4	14	2	690	698	6
6	14	2	440	426	5
8	14	2	308	304	6
10	14	2	324	328	6
12	14	2	64	70	27
14	14	2	360	370	6
1	15	2	691	678	6
3	15	2	264	272	6
5	15	2	1564	1517	11
7	15	2	654	639	6
9	15	2	41	27	41
11	15	2	415	407	6
13	15	2	201	188	9
0	16	2	917	906	7
2	16	2	173	169	9
4	16	2	176	186	8
6	16	2	451	449	6
8	16	2	70	70	23
10	16	2	697	698	7
1	17	2	166	164	9
3	17	2	496	489	6
5	17	2	246	249	7
7	17	2	78	55	20
9	17	2	304	309	7
0	18	2	819	804	7
2	18	2	14	22	34
4	18	2	299	300	7
6	18	2	438	427	6
1	1	3	282	275	3
3	1	3	868	853	6
5	1	3	474	483	4
7	1	3	136	126	6
9	1	3	452	459	5
11	1	3	1427	1423	11
13	1	3	328	334	5
15	1	3	75	85	17
17	1	3	327	338	6
19	1	3	501	503	6
21	1	3	990	970	8
0	2	3	2668	2614	8
2	2	3	365	353	4
4	2	3	25	28	24
6	2	3	1129	1113	9
8	2	3	1005	1006	8
10	2	3	622	640	5
12	2	3	692	716	6
14	2	3	316	312	5
16	2	3	1209	1208	10
18	2	3	67	43	23
20	2	3	52	42	51
1	3	3	479	473	4
3	3	3	357	357	4
5	3	3	1235	1211	9
7	3	3	777	764	6
9	3	3	261	259	5
11	3	3	1353	1335	9
13	3	3	165	174	8
15	3	3	0	23	1
17	3	3	179	192	8
19	3	3	152	147	10
21	3	3	465	452	6
0	4	3	2018	1961	8
2	4	3	140	150	5
4	4	3	451	451	4
6	4	3	187	175	5
8	4	3	347	355	4
10	4	3	222	208	5
12	4	3	760	772	6
14	4	3	164	160	8
16	4	3	284	282	6
18	4	3	111	107	13
20	4	3	106	101	15
1	5	3	33	20	32
3	5	3	605	613	5
5	5	3	1245	1215	10
7	5	3	776	778	6
9	5	3	417	422	5
11	5	3	242	227	5
13	5	3	695	701	6
15	5	3	244	241	7
17	5	3	326	321	6
19	5	3	105	113	15
0	6	3	774	781	6
2	6	3	0	12	1
4	6	3	545	531	5
6	6	3	1149	1161	8
8	6	3	306	298	4
10	6	3	36	24	35
12	6	3	294	295	5
14	6	3	55	56	28
16	6	3	1160	1160	9
18	6	3	311	320	7
20	6	3	349	347	7
1	7	3	39	29	38
3	7	3	343	359	4
5	7	3	1171	1151	8
7	7	3	255	260	5
9	7	3	616	623	5
11	7	3	745	752	6
13	7	3	130	138	10
15	7	3	205	205	7
17	7	3	578	581	6
19	7	3	192	187	9
0	8	3	712	706	5
2	8	3	266	270	4
4	8	3	435	436	4
6	8	3	527	523	5
8	8	3	75	86	14
10	8	3	71	77	16
12	8	3	513	513	5
14	8	3	384	381	5
16	8	3	137	122	6
18	8	3	95	89	17
1	9	3	583	577	5
3	9	3	22	20	22
5	9	3	52	42	23
7	9	3	164	148	7
9	9	3	135	138	9
11	9	3	908	913	7
13	9	3	117	121	11
15	9	3	57	43	31
17	9	3	527	527	6
0	10	3	940	950	7
2	10	3	858	851	6
4	10	3	565	572	5
6	10	3	120	110	9
8	10	3	183	190	7
10	10	3	88	95	14
12	10	3	198	207	7
14	10	3	773	770	7
16	10	3	71	66	23
1	11	3	469	474	5
3	11	3	295	299	5
5	11	3	666	658	6
7	11	3	101	90	11
9	11	3	555	554	5
11	11	3	182	158	8
13	11	3	125	120	11
15	11	3	164	164	10
17	11	3	428	441	6
0	12	3	412	410	5
2	12	3	221	207	6
4	12	3	351	349	5
6	12	3	159	146	8
8	12	3	204	206	7
10	12	3	308	317	6
12	12	3	249	258	7
14	12	3	150	160	10
16	12	3	462	468	6
1	13	3	183	181	7
3	13	3	423	433	5
5	13	3	469	468	5
7	13	3	125	138	10
9	13	3	387	380	6
11	13	3	375	387	6
13	13	3	93	91	17
0	14	3	40	5	40
2	14	3	326	323	6
4	14	3	540	544	5
6	14	3	294	305	6
8	14	3	387	386	6
10	14	3	12	13	12
12	14	3	60	62	30
1	15	3	274	261	6
3	15	3	129	131	10
5	15	3	520	521	6
7	15	3	82	91	18
9	15	3	197	188	8
11	15	3	423	411	6
0	16	3	186	176	8
2	16	3	73	57	20
4	16	3	130	140	11
6	16	3	1081	1072	9
8	16	3	224	226	8
10	16	3	156	151	10
1	17	3	78	26	19
3	17	3	278	284	7
5	17	3	492	489	6
7	17	3	62	52	31
0	18	3	260	261	7
2	18	3	111	116	14
0	0	4	6665	6796	11
2	0	4	301	301	4
4	0	4	795	815	6
6	0	4	438	428	4
8	0	4	471	477	5
10	0	4	2821	2804	12
12	0	4	885	876	7
14	0	4	463	473	5
16	0	4	57	67	29
18	0	4	799	796	7
20	0	4	181	183	9
1	1	4	228	228	4
3	1	4	23	34	22
5	1	4	93	72	10
7	1	4	31	17	31
9	1	4	1300	1318	9
11	1	4	1598	1632	12
13	1	4	68	50	19
15	1	4	91	88	14
17	1	4	48	61	48
19	1	4	550	546	6
0	2	4	238	257	4
2	2	4	267	265	4
4	2	4	371	374	4
6	2	4	549	558	5
8	2	4	41	26	40
10	2	4	385	398	5
12	2	4	325	324	5
14	2	4	593	598	6
16	2	4	770	769	7
18	2	4	135	115	11
20	2	4	134	120	12
1	3	4	279	287	4
3	3	4	341	330	4
5	3	4	3491	3506	11
7	3	4	100	115	10
9	3	4	863	870	6
11	3	4	70	67	17
13	3	4	489	496	5
15	3	4	829	841	7
17	3	4	676	680	6
19	3	4	215	227	9
0	4	4	790	802	6
2	4	4	541	536	5
4	4	4	686	718	6
6	4	4	1795	1788	11
8	4	4	391	396	5
10	4	4	516	536	5
12	4	4	180	183	7
14	4	4	886	907	7
16	4	4	1473	1460	10
18	4	4	278	283	7
1	5	4	1100	1096	8
3	5	4	160	156	6
5	5	4	1571	1591	11
7	5	4	472	470	5
9	5	4	85	73	13
11	5	4	926	940	7
13	5	4	154	147	8
15	5	4	293	287	6
17	5	4	0	9	1
19	5	4	105	90	16
0	6	4	2227	2263	10
2	6	4	71	71	13
4	6	4	150	156	4
6	6	4	171	176	7
8	6	4	270	264	5
10	6	4	1361	1353	10
12	6	4	460	452	5
14	6	4	205	211	7
16	6	4	208	185	8
18	6	4	350	351	7
1	7	4	304	291	4
3	7	4	397	394	4
5	7	4	1502	1501	11
7	7	4	401	399	5
9	7	4	970	990	8
11	7	4	741	737	6
13	7	4	542	534	5
15	7	4	344	349	6
17	7	4	259	265	8
0	8	4	1927	1984	11
2	8	4	63	9	17
4	8	4	286	290	5
6	8	4	598	590	6
8	8	4	462	465	5
10	8	4	1270	1281	9
12	8	4	225	230	7
14	8	4	81	63	18
16	8	4	160	171	10
18	8	4	121	121	13
1	9	4	113	104	9
3	9	4	276	275	5
5	9	4	1725	1728	12
7	9	4	530	535	5
9	9	4	55	61	26
11	9	4	151	171	9
13	9	4	127	136	11
15	9	4	379	372	6
17	9	4	598	598	6
0	10	4	991	992	7
2	10	4	87	85	12
4	10	4	429	435	5
6	10	4	283	270	5
8	10	4	544	538	5
10	10	4	625	610	6
12	10	4	179	196	9
14	10	4	888	897	7
16	10	4	465	477	6
1	11	4	284	287	5
3	11	4	425	425	5
5	11	4	1216	1227	9
7	11	4	62	45	21
9	11	4	113	108	11
11	11	4	53	65	24
13	11	4	150	143	10
15	11	4	872	870	7
0	12	4	811	816	6
2	12	4	272	262	6
4	12	4	219	215	7
6	12	4	356	355	5
8	12	4	277	297	6
10	12	4	334	336	6
12	12	4	407	400	6
14	12	4	95	84	17
1	13	4	314	313	6
3	13	4	214	209	7
5	13	4	294	297	6
7	13	4	373	374	6
9	13	4	377	389	6
11	13	4	745	745	7
13	13	4	209	225	9
0	14	4	1523	1511	11
2	14	4	306	298	6
4	14	4	313	321	6
6	14	4	540	539	6
8	14	4	199	188	8
10	14	4	1182	1171	9
12	14	4	23	9	23
1	15	4	304	295	6
3	15	4	443	444	6
5	15	4	149	157	10
7	15	4	217	210	8
9	15	4	237	222	8
0	16	4	159	123	9
2	16	4	222	213	8
4	16	4	22	34	21
6	16	4	501	499	6
8	16	4	20	12	19
1	17	4	312	317	7
3	17	4	275	263	7
1	1	5	77	81	13
3	1	5	373	391	4
5	1	5	455	442	5
7	1	5	135	132	8
9	1	5	389	406	5
11	1	5	289	286	6
13	1	5	84	92	15
15	1	5	132	140	11
17	1	5	739	738	7
19	1	5	418	422	6
0	2	5	448	447	5
2	2	5	63	68	17
4	2	5	457	454	5
6	2	5	463	460	5
8	2	5	544	548	5
10	2	5	315	320	5
12	2	5	765	773	7
14	2	5	0	29	1
16	2	5	168	168	6
18	2	5	240	235	8
1	3	5	106	90	9
3	3	5	143	139	7
5	3	5	386	395	4
7	3	5	112	114	10
9	3	5	173	169	7
11	3	5	270	262	6
13	3	5	404	395	5
15	3	5	100	80	14
17	3	5	580	577	6
0	4	5	43	10	35
2	4	5	35	42	35
4	4	5	188	199	6
6	4	5	704	692	6
8	4	5	422	433	5
10	4	5	13	11	13
12	4	5	475	478	5
14	4	5	321	323	6
16	4	5	679	695	6
18	4	5	214	210	8
1	5	5	180	175	6
3	5	5	523	510	5
5	5	5	954	947	7
7	5	5	526	532	5
9	5	5	410	415	5
11	5	5	343	328	5
13	5	5	619	614	6
15	5	5	252	244	7
17	5	5	187	198	9
0	6	5	183	216	6
2	6	5	189	187	6
4	6	5	49	24	28
6	6	5	394	386	5
8	6	5	240	251	6
10	6	5	76	73	15
12	6	5	257	249	6
14	6	5	15	22	15
16	6	5	744	740	7
1	7	5	0	28	1
3	7	5	496	514	5
5	7	5	40	23	39
7	7	5	269	258	6
9	7	5	437	439	5
11	7	5	406	415	5
13	7	5	193	197	8
15	7	5	52	15	52
17	7	5	115	106	14
0	8	5	895	907	7
2	8	5	0	19	1
4	8	5	69	60	17
6	8	5	596	590	5
8	8	5	212	208	7
10	8	5	158	153	8
12	8	5	286	292	6
14	8	5	522	520	6
16	8	5	839	845	7
1	9	5	661	663	6
3	9	5	175	163	7

Observed and calculated structure factors for K11

h	k	l	10Fo	10Fc	10s
5	9	5	689	685	6
7	9	5	283	271	6
9	9	5	63	74	22
11	9	5	1478	1528	12
13	9	5	0	23	1
15	9	5	21	29	20
0	10	5	1066	1056	8
2	10	5	535	541	5
4	10	5	281	282	6
6	10	5	381	371	5
8	10	5	49	52	44
10	10	5	280	276	6
12	10	5	77	12	20
14	10	5	578	572	6
1	11	5	216	224	7
3	11	5	246	245	6
5	11	5	398	388	5
7	11	5	419	428	5
9	11	5	338	332	6
11	11	5	463	466	6
13	11	5	150	159	11
0	12	5	1228	1244	10
2	12	5	442	447	5
4	12	5	68	70	21
6	12	5	703	706	6
8	12	5	181	173	8
10	12	5	196	205	9
12	12	5	200	207	9
1	13	5	245	244	7
3	13	5	235	242	7
5	13	5	1027	1020	8
7	13	5	184	187	9
9	13	5	407	385	6
11	13	5	1182	1190	9
0	14	5	842	840	7
2	14	5	300	293	6
4	14	5	499	495	6
6	14	5	298	303	7
8	14	5	214	214	8
1	15	5	44	12	43
3	15	5	197	211	9
5	15	5	174	162	9
7	15	5	222	218	8
0	16	5	305	304	7
2	16	5	279	276	7
0	0	6	2715	2755	12
2	0	6	210	206	6
4	0	6	648	666	6
6	0	6	716	714	6
8	0	6	595	598	6
10	0	6	992	1008	8
12	0	6	701	703	7
14	0	6	834	818	7
16	0	6	925	925	8
1	1	6	214	193	6
3	1	6	68	78	16
5	1	6	1780	1797	12
7	1	6	50	48	31
9	1	6	396	390	5
11	1	6	219	215	7
13	1	6	53	27	39
15	1	6	507	513	6
17	1	6	284	282	8
0	2	6	1684	1694	12
2	2	6	199	199	6
4	2	6	193	204	7
6	2	6	474	477	5
8	2	6	244	248	6
10	2	6	781	795	7
12	2	6	275	281	6
14	2	6	65	27	24
16	2	6	375	374	6
1	3	6	205	194	6
3	3	6	27	35	26
5	3	6	939	947	7
7	3	6	102	112	12
9	3	6	1133	1132	8
11	3	6	1086	1110	9
13	3	6	409	410	6
15	3	6	167	167	10
0	4	6	2521	2557	12
2	4	6	124	130	9
4	4	6	413	418	5
6	4	6	421	436	5
8	4	6	232	224	6
10	4	6	1506	1505	11
12	4	6	232	247	7
14	4	6	97	98	16
16	4	6	229	219	8
1	5	6	278	290	5
3	5	6	383	383	5
5	5	6	393	379	5
7	5	6	111	103	11
9	5	6	224	227	7
11	5	6	359	363	6
13	5	6	0	17	1
15	5	6	177	184	10
0	6	6	67	60	17
2	6	6	78	76	15
4	6	6	481	478	5
6	6	6	866	863	7
8	6	6	209	215	7
10	6	6	36	20	35
12	6	6	240	242	7
14	6	6	813	821	7
1	7	6	653	655	6
3	7	6	107	95	11
5	7	6	2523	2550	14
7	7	6	93	87	14
9	7	6	461	459	5
11	7	6	459	467	6
13	7	6	352	341	6
15	7	6	709	677	7
0	8	6	200	188	7
2	8	6	227	237	7
4	8	6	348	353	5
6	8	6	263	255	6
8	8	6	456	458	5
10	8	6	37	11	37
12	8	6	277	262	7
14	8	6	447	440	6
1	9	6	421	418	5
3	9	6	83	81	15
5	9	6	0	25	1
7	9	6	534	546	6
9	9	6	412	399	6
11	9	6	751	743	7
13	9	6	83	102	21
0	10	6	2203	2191	14
2	10	6	245	250	7
4	10	6	314	312	6
6	10	6	540	539	6
8	10	6	214	206	8
10	10	6	1334	1342	10
12	10	6	170	162	10
1	11	6	32	11	32
3	11	6	407	403	6
5	11	6	315	328	7
7	11	6	110	99	13
9	11	6	546	533	6
11	11	6	672	681	7
0	12	6	576	577	6
2	12	6	86	88	17
4	12	6	170	163	9
6	12	6	991	978	8
8	12	6	70	44	23
10	12	6	460	452	6
1	13	6	20	15	19
3	13	6	38	25	37
5	13	6	1372	1363	10
7	13	6	240	240	8
0	14	6	78	85	21
2	14	6	463	445	6
4	14	6	298	299	7
1	1	7	104	85	11
3	1	7	332	335	5
5	1	7	83	95	15
7	1	7	179	186	8
9	1	7	236	243	7
11	1	7	754	756	7
13	1	7	257	265	7
15	1	7	39	11	39
0	2	7	831	823	7
2	2	7	240	238	6
4	2	7	0	4	1
6	2	7	440	441	5
8	2	7	408	409	5
10	2	7	249	249	7
12	2	7	536	535	6
14	2	7	124	128	13
1	3	7	167	166	8
3	3	7	27	8	26
5	3	7	465	470	5
7	3	7	452	448	5
9	3	7	227	220	7
11	3	7	767	755	7
13	3	7	27	28	27
0	4	7	905	885	7
2	4	7	172	169	8
4	4	7	320	318	6
6	4	7	36	53	35
8	4	7	287	279	6
10	4	7	129	129	12
12	4	7	458	459	6
14	4	7	191	181	9
1	5	7	40	36	40
3	5	7	331	323	6
5	5	7	499	495	6
7	5	7	452	462	5
9	5	7	303	304	6
11	5	7	134	103	12
13	5	7	431	438	6
0	6	7	340	353	6
2	6	7	66	74	21
4	6	7	250	249	7
6	6	7	640	646	6
8	6	7	210	214	8
10	6	7	0	38	1
12	6	7	198	203	9
1	7	7	49	10	39
3	7	7	312	311	6
5	7	7	693	682	6
7	7	7	158	157	10
9	7	7	442	445	6
11	7	7	461	459	6
0	8	7	415	405	5
2	8	7	201	204	8
4	8	7	336	330	6
6	8	7	274	280	7
8	8	7	132	135	12
10	8	7	46	41	46
1	9	7	353	369	6
3	9	7	0	35	1
5	9	7	17	68	17
7	9	7	81	75	18
9	9	7	22	29	21
0	10	7	629	637	6
2	10	7	447	452	6
4	10	7	290	276	7
6	10	7	155	143	10
8	10	7	64	72	29
1	11	7	244	251	7
3	11	7	184	182	9
5	11	7	488	476	6
7	11	7	86	92	19
0	12	7	179	180	9
2	12	7	126	128	12
4	12	7	242	236	8
0	0	8	2522	2559	14
2	0	8	119	111	12
4	0	8	322	323	6
6	0	8	721	719	7
8	0	8	135	112	11
10	0	8	1515	1494	11
1	1	8	75	87	19
3	1	8	69	54	20
5	1	8	389	384	6
7	1	8	211	214	8
9	1	8	711	710	7
11	1	8	484	490	6
0	2	8	76	42	17
2	2	8	124	112	11
4	2	8	234	229	7
6	2	8	538	533	6
8	2	8	37	5	37
10	2	8	224	211	8
1	3	8	175	166	8
3	3	8	258	246	7
5	3	8	1822	1821	12
7	3	8	33	37	32
9	3	8	489	487	6
11	3	8	149	145	11
0	4	8	110	105	12
2	4	8	339	341	6
4	4	8	298	287	6
6	4	8	564	563	6
8	4	8	143	153	11
10	4	8	265	259	7
1	5	8	580	580	6
3	5	8	128	133	11
5	5	8	459	457	6
7	5	8	43	50	42
9	5	8	120	113	13
0	6	8	1881	1881	15
2	6	8	140	140	11
4	6	8	325	323	6
6	6	8	470	454	6
8	6	8	127	112	12
1	7	8	118	90	12
3	7	8	248	247	7
5	7	8	999	988	8
7	7	8	216	215	8
0	8	8	972	972	8
2	8	8	77	70	21
4	8	8	76	72	22
6	8	8	396	414	7
1	9	8	10	13	9
3	9	8	182	167	9
5	9	8	1186	1203	9
0	10	8	1092	1093	8
2	10	8	84	55	19
1	1	9	53	58	42
3	1	9	279	277	7
5	1	9	165	158	10
0	2	9	61	53	29
2	2	9	67	24	23
4	2	9	204	205	9
6	2	9	0	5	1
1	3	9	155	141	10
3	3	9	87	86	18
5	3	9	58	21	38
0	4	9	378	367	6
2	4	9	0	17	1
4	4	9	80	100	21
1	5	9	44	12	44
3	5	9	180	189	10

Observed and calculated structure factors for K12

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	662	684	5	0	8	0	2594	2580	13	3	19	0	183	170	18	1	9	1	915	891	7	20	0	2	218	207	16
4	0	0	1050	1060	8	2	8	0	176	157	10	1	1	1	141	138	7	3	9	1	69	17	37	22	0	2	482	477	10
6	0	0	614	625	6	4	8	0	549	539	6	3	1	1	307	305	5	5	9	1	388	406	7	1	1	2	503	516	6
8	0	0	1070	1066	8	6	8	0	641	659	7	5	1	1	993	1012	7	7	9	1	148	349	8	3	1	2	724	719	6
10	0	0	3835	3812	14	8	8	0	501	500	7	7	1	1	46	24	46	9	9	1	39	29	38	5	1	2	1024	1031	7
12	0	0	1447	1456	11	10	8	0	1176	1139	9	9	1	1	247	240	8	11	9	1	1680	1713	13	7	1	2	76	72	24
14	0	0	257	256	11	12	8	0	105	105	24	11	1	1	710	721	7	13	9	1	142	152	19	9	1	2	579	574	6
16	0	0	408	396	8	14	8	0	111	98	24	13	1	1	271	272	10	15	9	1	226	232	14	11	1	2	578	572	7
18	0	0	368	368	10	16	8	0	336	339	10	15	1	1	316	308	9	17	9	1	74	106	74	13	1	2	87	34	32
20	0	0	470	451	9	18	8	0	0	31	1	17	1	1	665	679	8	19	9	1	199	225	18	15	1	2	676	676	7
22	0	0	1903	1921	15	20	8	0	291	272	13	19	1	1	536	526	9	0	10	1	1424	1433	11	17	1	2	0	44	1
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3	1	0	235	231	5	3	9	0	306	294	7	0	2	1	154	175	7	4	10	1	154	158	14	21	1	2	296	281	13
5	1	0	518	516	5	5	9	0	1904	1941	12	2	2	1	594	594	5	6	10	1	514	510	7	0	2	2	4123	4117	9
7	1	0	409	422	5	7	9	0	870	864	8	4	2	1	333	337	6	8	10	1	131	137	18	2	2	2	363	361	5
9	1	0	1462	1458	11	9	9	0	115	104	22	6	2	1	246	244	7	10	10	1	165	174	9	4	2	2	451	445	5
11	1	0	3084	3032	14	11	9	0	666	650	7	8	2	1	484	497	6	12	10	1	0	19	1	6	2	2	486	481	5
13	1	0	490	492	7	13	9	0	230	223	12	10	2	1	131	118	16	14	10	1	595	595	8	8	2	2	129	136	15
15	1	0	264	271	10	15	9	0	783	797	8	12	2	1	851	855	7	16	10	1	516	510	9	10	2	2	1383	1386	11
17	1	0	366	389	10	17	9	0	581	583	9	14	2	1	136	118	18	18	10	1	165	151	20	12	2	2	597	594	7
19	1	0	477	477	9	19	9	0	99	124	37	16	2	1	538	545	8	1	11	1	70	61	39	14	2	2	54	21	54
21	1	0	865	871	9	0	10	0	289	309	8	18	2	1	49	17	48	3	11	1	65	51	55	16	2	2	265	293	12
0	2	0	1245	1308	6	2	10	0	123	138	17	20	2	1	389	369	10	5	11	1	856	855	8	18	2	2	50	53	50
2	2	0	315	329	5	4	10	0	302	308	8	22	2	1	269	244	14	7	11	1	531	529	7	20	2	2	121	143	29
4	2	0	551	574	6	6	10	0	271	276	9	1	3	1	385	389	5	9	11	1	263	252	10	1	3	2	505	500	5
6	2	0	181	183	8	8	10	0	235	250	11	3	3	1	279	263	6	11	11	1	158	171	17	3	3	2	190	189	8
8	2	0	261	263	7	10	10	0	501	504	8	5	3	1	407	400	5	13	11	1	165	164	17	5	3	2	1169	1145	8
10	2	0	587	579	6	12	10	0	321	308	10	7	3	1	379	388	6	15	11	1	370	356	10	7	3	2	204	207	9
12	2	0	475	465	7	14	10	0	986	1011	9	9	3	1	222	224	9	17	11	1	452	457	10	9	3	2	1278	1272	9
14	2	0	854	842	8	16	10	0	312	324	11	11	3	1	357	382	8	0	12	1	950	974	8	11	3	2	1537	1585	11
16	2	0	810	812	8	18	10	0	338	337	12	13	3	1	208	197	12	2	12	1	566	568	7	13	3	2	234	233	11
18	2	0	205	205	14	1	11	0	246	228	10	15	3	1	129	129	20	4	12	1	142	156	17	15	3	2	241	234	12
20	2	0	52	50	51	3	11	0	277	272	9	17	3	1	261	267	12	6	12	1	724	736	7	17	3	2	424	431	9
22	2	0	197	219	19	5	11	0	729	727	7	19	3	1	192	184	16	8	12	1	83	101	36	19	3	2	717	724	9
1	3	0	272	269	5	7	11	0	44	81	44	21	3	1	372	376	11	10	12	1	33	4	33	21	3	2	707	720	9
3	3	0	450	451	5	9	11	0	43	78	43	0	4	1	1218	1222	8	12	12	1	240	234	13	0	4	2	1796	1772	11
5	3	0	4881	4859	10	11	11	0	398	425	9	2	4	1	155	165	9	14	12	1	40	61	40	2	4	2	614	611	6
7	3	0	555	547	5	13	11	0	266	275	11	4	4	1	115	102	12	16	12	1	782	765	9	4	4	2	120	106	13
9	3	0	771	758	7	15	11	0	672	689	8	6	4	1	655	629	6	1	13	1	475	458	8	6	4	2	449	439	6
11	3	0	471	482	6	17	11	0	465	457	10	8	4	1	362	364	6	3	13	1	282	291	10	8	4	2	130	128	16
13	3	0	276	268	10	0	12	0	1511	1560	12	10	4	1	645	634	7	5	13	1	1036	1044	9	10	4	2	1980	2008	13
15	3	0	954	937	8	2	12	0	150	146	16	12	4	1	639	643	7	7	13	1	125	118	21	12	4	2	140	135	18
17	3	0	1040	1015	9	4	12	0	360	352	8	14	4	1	259	256	11	9	13	1	296	276	11	14	4	2	105	133	25
19	3	0	282	290	12	6	12	0	559	559	7	16	4	1	472	477	8	11	13	1	1240	1245	10	16	4	2	73	68	51
21	3	0	262	267	14	8	12	0	180	159	14	18	4	1	218	232	14	13	13	1	196	200	16	18	4	2	523	528	9
0	4	0	2000	2030	9	10	12	0	781	782	8	20	4	1	87	66	45	15	13	1	118	138	29	20	4	2	239	251	15
2	4	0	655	650	6	12	12	0	517	516	9	22	4	1	292	294	14	0	14	1	908	935	8	1	5	2	1007	977	7
4	4	0	902	901	7	14	12	0	95	119	36	1	5	1	102	107	14	2	14	1	171	154	15	3	5	2	87	94	19
6	4	0	1943	1874	11	16	12	0	0	12	1	3	5	1	366	373	5	4	14	1	183	180	9	5	5	2	1925	1873	13
8	4	0	387	385	6	1	13	0	568	568	7	5	5	1	1143	1105	8	6	14	1	294	287	10	7	5	2	216	223	10
10	4	0	446	448	6	3	13	0	234	232	11	7	5	1	874	854	7	8	14	1	261	247	12	9	5	2	512	501	6
12	4	0	205	206	12	5	13	0	350	346	9	9	5	1	405	400	7	10	14	1	418	439	10	11	5	2	671	671	7
14	4	0	594	586	7	7	13	0	470	481	8	11	5	1	282	311	9	12	14	1	174	154	18	13	5	2	56	32	55
16	4	0	2166	2155	16	9	13	0	319	311	10	13	5	1	545	546	7	14	14	1	294	282	13	15	5	2	352	344	10
18	4	0	0	8	1	11	13	0	948	948	9	15	5	1	246	228	12	1	15	1	47	4	47	17	5	2	672	673	8
20	4	0	137	129	25	13	13	0	276	273	13	17	5	1	180	177	16	3	15	1	177	178	9	19	5	2	319	332	12
22	4	0	546	540	10	15	13	0	279	276	13	19	5	1	0	12	1	5	15	1	78	108	45	21	5	2	339	332	12
1	5	0	1419	1454	10	0	14	0	1342	1342	10	21	5	1	554	536	10	7	15	1	384	374	10	0	6	2	1128	1119	9
3	5	0	80	74	19	2	14	0	363	363	9	0	6	1	542	526	5	9	15	1	26	16	25	2	6	2	59	63	39
5	5	0	1137	1081	11	4	14	0	216	213	13	2	6	1	116	80	13	11	15	1	161	129	20	4	6	2	792	791	7
7	5	0	924	911	7	6	14	0	660	670	8	4	6	1	291	294	6	13	15	1	233	227	15	6	6	2	2556	2499	14
9	5	0	46	49	45	8	14	0	170	180	17	6	6	1	1031	1017	8	0	16	1	434	412	9	8	6	2	300	304	8
11	5	0	379	413	8	10	14	0	1204	1194	10	8	6	1	533	531	7	2	16	1	180	175	15	10	6	2	163	175	15
13	5	0	174	180	14	12	14	0	113	104	31	10	6	1	134	134	18	4	16	1	70	69	70	12	6	2	314	323	10
15	5	0	193	207	14	14	14	0	57	11	56	12	6	1	378	373	8	6	16	1	1303	1315	10	14	6	2	751	742	8
17	5	0	495	517	9	1	15	0	352	329	9	14	6	1	0	12	1	8	16	1	360	344	11	16	6	2	1612	1615	13
19	5	0	142	156	23	3	15	0	313	320	10	16	6	1	985	1001	9	10	16	1	49	60	48	18	6	2	70	66	69
21	5	0	488	478	10	5	15	0	538	540	8	18	6	1	302	293	12	12	16	1	51	51	51	20	6	2	91	74	44
0	6	0	803	812	7	7	15	0	104	125	29	20	6	1	500	490	10	1	17	1	114	125	28	1	7	2	614	603	6
2	6	0	173	189	9	9	15	0	217	213	15	1	7	1	163	156	10	3	17	1	209	198	15	3	7	2	137	144	14
4	6	0	215	219	8	11	15	0	425	419	10	3	7	1	465	469	5	5	17	1	863	867	9	5	7	2	4530	4459	14
6	6	0	438	434	6	13	15	0	331	347	13	5	7	1	828	841	7	7	17	1	244	238	14	7	7	2	183	172	12
8	6	0	629	617	6	0	16	0	608	613	8	7	7	1	212	205	10	9	17	1	266	283	14	9	7	2	436	438	7
10	6	0	1473	1505	11	2	16	0	270	266	12	9	7	1	309	318	9	0	18	1	313	317	12	11	7	2	0	28	1
12	6	0	111	121	23	4	16	0	164	147	18	11	7	1	77	115	39	2	18	1	124	123	27	13	7	2	370	358	9
14	6	0	382	379	9	6	16	0	738	762	8	13	7	1	45	45	44	4	18	1	288	306	13	15	7	2	982	1009	9
16	6	0	456	457	9	8	16	0	70	101	70	15	7	1	161	175	17	6	18	1	265	262	14	17	7	2	1096	1092	10
18	6	0	371	383	11	10	16	0	137	135	24	17	7	1	257	266	13	8	18	1	149	141	23	19	7	2	143	114	23
20	6	0	84	23	50	12	16	0	461	481	11	19	7	1	154	153	21	1	19	1	440	434	10	0	8	2	412	404	6
1	7	0	567	560	6	1	17	0	341	320	11	0	8	1	439	423	6	3	19	1	391	404	12	2	8	2	498	507	6
3	7	0	273	274	7	3	17	0	327	316	11	2	8	1	147	126	12	0	0	2	3301	3350	9	4	8	2	244	259	9
5	7	0	1359	1359	9	5	17	0	1741	1744	13	4	8	1	110	92	18	2	0	2	649	651	5	6	8	2	408	393	7
7	7	0	546	521	6	7	17	0	61	70	61	6	8	1	299	295	8	4	0	2	183	187	9	8	8	2	523	531	7
9	7	0	1099	1070	8	9	17	0	59	55	59	8	8	1	0	53	1	6	0	2	707	679	6	10	8	2	116	133	22
11	7	0	681	646	7	0	18	0	386	392	11	10	8	1	184	190	13	8	0	2	615	597	6	12	8	2	0	2	1
13	7	0	216	243	12	2	18	0	243	256	14	12	8	1	495	498	8	10	0	2	1474	1458	10	14	8	2	485	485	8
15	7	0	307	301	10	4	18	0	107	95	32	14	8	1	507	505	8	12	0	2	1067	1077	9	16	8	2	879	891	9
17	7	0	416	422	10	6	18	0	344	334	12	16	8	1	443	440	9	14	0	2	1244	1238	9	18	8	2	28	34	28
19	7	0	589	605	9	8	18	0	273	263	14	18	8	1	292	284	12	16	0	2	914	890	8	20	8	2	159	148	23
21	7	0	611	609	10	1	19	0	130	154	26	20	8	1	376	377	12	18	0	2	466	469	9	1	9	2	498	494	6

Observed and calculated structure factors for K12

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	9	2	166	156	13	8	2	3	632	614	6	3	11	3	0	2	1	15	3	4	833	819	8	9	13	4	312	308	12
5	9	2	564	562	7	10	2	3	85	60	31	5	11	3	903	889	8	17	3	4	794	788	9	11	13	4	758	767	9
7	9	2	488	491	7	12	2	3	654	666	7	7	11	3	221	219	12	19	3	4	252	253	15	13	13	4	132	158	27
9	9	2	550	541	7	14	2	3	326	328	10	9	11	3	323	320	10	0	4	4	539	544	6	0	14	4	1317	1316	10
11	9	2	1594	1584	12	16	2	3	908	927	9	11	11	3	121	83	23	2	4	4	486	466	6	2	14	4	209	215	14
13	9	2	251	246	12	18	2	3	199	216	16	13	11	3	59	12	59	4	4	4	478	491	7	4	14	4	342	320	10
15	9	2	89	82	39	20	2	3	290	283	13	15	11	3	214	193	16	6	4	4	2054	2061	16	6	14	4	448	447	10
17	9	2	754	750	9	1	3	3	514	505	5	17	11	3	529	549	10	8	4	4	146	151	17	8	14	4	172	163	19
19	9	2	263	267	15	3	3	3	240	238	8	0	12	3	135	113	18	10	4	4	335	351	9	10	14	4	919	932	9
0	10	2	4374	4391	16	5	3	3	969	951	8	2	12	3	343	350	9	12	4	4	129	156	22	12	14	4	104	60	34
2	10	2	576	556	7	7	3	3	715	705	7	4	12	3	413	407	8	14	4	4	602	619	8	1	15	4	308	293	11
4	10	2	661	660	7	9	3	3	174	182	13	6	12	3	227	231	12	16	4	4	1583	1583	12	3	15	4	349	338	11
6	10	2	104	97	23	11	3	3	1386	1411	11	8	12	3	0	12	1	18	4	4	82	97	58	5	15	4	290	273	12
8	10	2	304	310	9	13	3	3	31	12	30	10	12	3	0	21	1	1	5	4	935	935	8	7	15	4	0	31	1
10	10	2	1821	1844	13	15	3	3	212	214	13	12	12	3	233	214	14	3	5	4	133	133	16	9	15	4	191	195	19
12	10	2	419	406	9	17	3	3	265	269	12	14	12	3	114	169	31	5	5	4	1551	1559	11	0	16	4	201	199	16
14	10	2	280	292	12	19	3	3	144	103	22	16	12	3	501	470	10	7	5	4	406	405	8	2	16	4	279	257	12
16	10	2	133	153	24	21	3	3	410	422	11	1	13	3	372	365	9	9	5	4	103	8	24	4	16	4	62	67	61
18	10	2	192	173	17	0	4	3	2297	2203	12	3	13	3	401	405	9	11	5	4	906	919	8	6	16	4	424	423	11
1	11	2	457	465	7	2	4	3	0	8	1	5	13	3	435	451	9	13	5	4	0	27	1	8	16	4	0	35	1
3	11	2	686	689	7	4	4	3	283	280	7	7	13	3	128	109	22	15	5	4	238	243	13	1	17	4	358	362	12
5	11	2	49	33	49	6	4	3	297	288	8	9	13	3	228	209	13	17	5	4	146	152	22	3	17	4	225	215	15
7	11	2	0	7	1	8	4	3	152	168	15	11	13	3	521	523	9	19	5	4	96	94	42	5	17	4	1332	1311	11
9	11	2	560	560	8	10	4	3	686	688	8	13	13	3	0	53	1	0	6	4	2016	2064	15	1	1	5	54	30	53
11	11	2	1888	1880	14	12	4	3	677	685	7	15	13	3	96	39	40	2	6	4	187	201	12	3	1	5	111	124	22
13	11	2	66	42	66	14	4	3	102	100	26	0	14	3	246	249	12	4	6	4	293	291	9	5	1	5	810	798	8
15	11	2	49	27	48	16	4	3	114	94	25	2	14	3	108	112	25	6	6	4	165	188	14	7	1	5	0	44	1
17	11	2	50	60	49	18	4	3	112	123	29	4	14	3	324	302	10	8	6	4	326	322	9	9	1	5	222	213	12
0	12	2	1347	1333	10	20	4	3	92	107	45	6	14	3	130	141	22	10	6	4	1330	1343	10	11	1	5	134	157	20
2	12	2	169	150	14	1	5	3	79	77	23	8	14	3	303	307	11	12	6	4	228	213	12	13	1	5	128	137	23
4	12	2	199	177	13	3	5	3	215	220	9	10	14	3	288	270	12	14	6	4	200	191	14	15	1	5	200	212	16
6	12	2	801	785	7	5	5	3	588	566	6	12	14	3	32	51	31	16	6	4	168	165	19	17	1	5	700	699	9
8	12	2	221	210	13	7	5	3	841	839	7	1	15	3	181	170	16	18	6	4	259	257	14	19	1	5	396	404	12
10	12	2	656	658	8	9	5	3	308	305	9	3	15	3	299	304	11	1	7	4	211	197	11	0	2	5	828	826	8
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14	12	2	402	407	10	13	5	3	408	414	9	7	15	3	222	243	15	5	7	4	1225	1236	10	4	2	5	320	329	9
16	12	2	544	521	9	15	5	3	253	270	12	9	15	3	61	59	60	7	7	4	401	396	8	6	2	5	469	460	7
1	13	2	121	131	21	17	5	3	223	240	15	11	15	3	352	326	12	9	7	4	835	844	8	8	2	5	228	226	12
3	13	2	39	0	38	19	5	3	14	25	13	0	16	3	245	247	14	11	7	4	787	782	8	10	2	5	205	217	14
5	13	2	1729	1750	12	0	6	3	462	476	6	2	16	3	57	28	57	13	7	4	183	193	16	12	2	5	694	680	8
7	13	2	0	35	1	2	6	3	183	170	11	4	16	3	277	275	13	15	7	4	263	267	13	14	2	5	0	32	1
9	13	2	65	38	64	4	6	3	520	497	6	6	16	3	1143	1153	10	17	7	4	481	491	10	16	2	5	115	129	30
11	13	2	121	137	25	6	6	3	1286	1300	10	8	16	3	304	306	12	0	8	4	1847	1882	13	18	2	5	114	93	32
13	13	2	174	171	19	8	6	3	381	374	8	10	16	3	207	205	17	2	8	4	0	39	1	1	3	5	137	133	16
15	13	2	551	569	10	10	6	3	171	184	15	1	17	3	197	196	17	4	8	4	289	288	9	3	3	5	239	239	10
0	14	2	312	317	10	12	6	3	331	340	9	3	17	3	229	236	15	6	8	4	594	589	7	5	3	5	569	578	7
2	14	2	318	325	10	14	6	3	94	84	31	5	17	3	566	570	10	8	8	4	387	385	8	7	3	5	79	78	36
4	14	2	689	695	8	16	6	3	1075	1073	10	7	17	3	29	26	28	10	8	4	1003	998	9	9	3	5	81	95	38
6	14	2	531	509	8	18	6	3	433	424	10	0	18	3	174	193	20	12	8	4	50	50	49	11	3	5	202	205	14
8	14	2	226	206	14	20	6	3	436	438	11	2	18	3	208	223	17	14	8	4	88	72	40	13	3	5	201	215	15
10	14	2	23	23	23	1	7	3	184	164	11	4	18	3	110	118	14	16	8	4	315	287	12	15	3	5	56	55	56
12	14	2	48	7	47	3	7	3	144	174	15	0	0	4	6628	6686	13	18	8	4	0	30	1	17	3	5	491	485	10
14	14	2	296	296	13	5	7	3	1472	1486	11	2	0	4	353	349	6	1	9	4	29	26	29	0	4	5	173	188	14
1	15	2	639	646	8	7	7	3	197	199	12	4	0	4	504	510	6	3	9	4	154	169	15	2	4	5	81	90	34
3	15	2	236	223	12	9	7	3	333	337	9	6	0	4	293	287	8	5	9	4	1814	1810	13	4	4	5	46	35	45
5	15	2	1439	1456	11	11	7	3	880	888	8	8	0	4	390	397	8	7	9	4	476	469	8	6	4	5	608	598	7
7	15	2	449	449	9	13	7	3	156	155	17	10	0	4	2797	2815	17	9	9	4	76	43	43	8	4	5	272	292	10
9	15	2	16	21	15	15	7	3	10	18	9	12	0	4	1036	1023	9	11	9	4	238	239	13	10	4	5	391	392	9
11	15	2	448	429	10	17	7	3	679	661	9	14	0	4	406	406	9	13	9	4	95	75	34	12	4	5	445	426	9
13	15	2	127	144	28	19	7	3	131	108	26	16	0	4	45	7	44	15	9	4	578	592	9	14	4	5	262	262	13
0	16	2	957	960	9	0	8	3	1034	1018	8	18	0	4	381	409	11	17	9	4	662	650	9	16	4	5	549	545	9
2	16	2	200	181	15	2	8	3	0	19	1	20	0	4	306	324	14	0	10	4	821	834	8	18	4	5	238	243	16
4	16	2	112	101	27	4	8	3	205	205	12	1	1	4	399	398	6	2	10	4	36	59	35	1	5	5	143	135	16
6	16	2	600	596	9	6	8	3	555	551	7	3	1	4	43	29	43	4	10	4	424	414	8	3	5	5	179	186	14
8	16	2	88	10	42	8	8	3	110	108	23	5	1	4	171	162	13	6	10	4	181	185	14	5	5	5	494	480	7
10	16	2	798	797	9	10	8	3	276	280	10	7	1	4	74	52	38	8	10	4	273	279	11	7	5	5	573	576	7
1	17	2	290	277	12	12	8	3	548	557	8	9	1	4	1063	1075	9	10	10	4	427	419	9	9	5	5	306	294	10
3	17	2	409	396	10	14	8	3	260	292	12	11	1	4	1787	1799	12	12	10	4	303	299	11	11	5	5	267	267	11
5	17	2	10	36	9	16	8	3	0	14	1	13	1	4	284	283	11	14	10	4	737	748	9	13	5	5	385	375	10
7	17	2	172	176	19	18	8	3	118	95	10	15	1	4	153	159	19	16	10	4	464	435	10	15	5	5	162	183	20
9	17	2	319	329	13	1	9	3	559	574	7	17	1	4	96	79	35	1	11	4	174	160	15	17	5	5	158	117	21
0	18	2	642	639	9	3	9	3	165	176	14	19	1	4	448	438	10	3	11	4	338	331	9	0	6	5	371	408	8
2	18	2	109	94	32	5	9	3	285	269	9	0	2	4	330	351	7	5	11	4	946	950	8	2	6	5	43	41	43
4	18	2	293	291	13	7	9	3	234	225	11	2	2	4	213	214	10	7	11	4	41	28	41	4	6	5	58	10	57
6	18	2	335	366	13	9	9	3	14	49	13	4	2	4	354	350	7	9	11	4	39	49	38	6	6	5	522	522	7
1	1	3	182	188	8	11	9	3	923	930	8	6	2	4	430	448	7	11	11	4	63	12	63	8	6	5	339	359	9
3	1	3	521	523	5	13	9	3	97	103	34	8	2	4	75	101	19	13	11	4	164	175	21	10	6	5	88	81	32
5	1	3	0	17	1	15	9	3	251	217	13	10	2	4	407	397	8	15	11	4	559	559	10	12	6	5	245	258	13
7	1	3	392	393	6	17	9	3	446	440	10	12	2	4	404	415	8	0	12	4	1027	1021	9	14	6	5	50	27	50
9	1	3	197	207	12	0	10	3	998	1020	9	14	2	4	618	621	8	2	12	4	145	149	19	16	6	5	680	667	9
11	1	3	1250	1251	9	2	10	3	714	734	7	16	2	4	799	794	8	4	12	4	231	258	12	1	7	5	106	93	24
13	1	3	369	364	8	4	10	3	242	244	11	18	2	4	186	196	19	6	12	4	268	262	11	3	7	5	407	409	8
15	1	3	352	359	10	6	10	3	275	274	10	20	2	4	0	17	1	8	12	4	167	194	18	5	7	5	271	275	10
17	1	3	306	319	11	8	10	3	198	189	13	1	3	4	167	158	11	10	12	4	573	573	9	7	7	5	301	303	10
19	1	3	516	516	10	10	10	3	193	189	14	3	3	4	377	370	7	12	12	4	163	169	11	9	7	5	212	215	14
21	1	3	553	549	10	12	10	3	60	78	59	5	3	4	1435	1429	15	14	12	4	63	45	63	11	7	5	296	298	11
0	2	3	2073	2042	11	14	10	3	586	569	9	7	3	4	207	203	12	1	13	4	359	349	9	13	7	5	132	133	23
2	2	3	686	670	6	16	10	3	293	292	13	9	3	4	587	588	7	3	13	4	200	178	14	15	7	5	202	203	17
4	2	3	213	216	8	18	10	3	108	84	35	11	3	4	185	194	14	5	13	4	255	235	12	17	7	5	0	9	1
6	2	3	1068	1043	9	1	11	3	171	188	14	13	3	4	256	254	11	7	13	4	296	295	12	0	8	5	649	654	7

Observed and calculated structure factors for K12

h	k	l	10Fo	10Fc	10s
2	8	5	187	199	14
4	8	5	126	139	20
6	8	5	563	553	8
8	8	5	87	76	35
10	8	5	144	141	20
12	8	5	349	347	11
14	8	5	446	450	10
16	8	5	559	556	10
1	9	5	675	672	8
3	9	5	65	6	65
5	9	5	533	520	8
7	9	5	332	334	10
9	9	5	69	20	68
11	9	5	1562	1555	12
13	9	5	187	174	18
15	9	5	226	202	16
0	10	5	1158	1131	10
2	10	5	473	475	8
4	10	5	0	34	1
6	10	5	540	518	8
8	10	5	0	92	1
10	10	5	366	360	10
12	10	5	128	88	26
14	10	5	457	442	10
1	11	5	61	13	61
3	11	5	49	67	48
5	11	5	594	592	8
7	11	5	511	516	9
9	11	5	171	159	18
11	11	5	248	255	14
13	11	5	201	212	18
0	12	5	980	999	9
2	12	5	535	535	9
4	12	5	0	12	1
6	12	5	757	756	8
8	12	5	84	66	45
10	12	5	85	38	47
12	12	5	201	197	17
1	13	5	408	192	10
3	13	5	188	195	16
5	13	5	987	1012	10
7	13	5	196	203	17
9	13	5	241	244	15
11	13	5	1308	1310	11
0	14	5	1069	1070	9
2	14	5	127	131	25
4	14	5	302	300	12
6	14	5	451	444	10
8	14	5	168	156	20
10	14	5	436	448	11
1	15	5	98	88	17
3	15	5	324	310	12
5	15	5	0	36	1
7	15	5	355	344	11
0	16	5	323	329	12
2	16	5	221	211	16
4	16	5	59	61	59
0	0	6	2548	2534	17
2	0	6	133	128	19
4	0	6	535	527	7
6	0	6	689	702	7
8	0	6	381	393	9
10	0	6	905	909	9
12	0	6	778	785	8
14	0	6	704	692	9
16	0	6	921	921	9
1	1	6	174	169	14
3	1	6	108	105	23
5	1	6	1665	1658	13
7	1	6	165	169	15
9	1	6	305	312	11
11	1	6	226	236	13
13	1	6	84	77	45
15	1	6	447	426	10
17	1	6	303	315	13
0	2	6	1724	1729	12
2	2	6	188	200	13
4	2	6	137	133	18
6	2	6	482	492	8
8	2	6	171	166	16
10	2	6	862	872	8
12	2	6	344	340	11
14	2	6	81	75	51
16	2	6	349	344	12
1	3	6	272	278	10
3	3	6	58	19	57
5	3	6	869	874	8
7	3	6	106	100	25
9	3	6	859	852	8
11	3	6	1215	1222	10
13	3	6	62	86	61
15	3	6	132	130	26
17	3	6	429	418	11
0	4	6	2320	2315	18
2	4	6	82	47	14
4	4	6	306	308	10
6	4	6	545	556	8
8	4	6	146	133	19
10	4	6	1335	1311	11
12	4	6	126	140	25
14	4	6	51	19	51
16	4	6	204	233	18
1	5	6	104	105	10
3	5	6	284	298	10
5	5	6	549	551	8
7	5	6	48	89	48
9	5	6	280	285	11
11	5	6	308	301	11
13	5	6	80	96	51
15	5	6	304	313	13
0	6	6	137	91	18
2	6	6	73	79	46
4	6	6	302	314	10
6	6	6	979	980	9
8	6	6	308	312	11
10	6	6	69	67	68
12	6	6	158	176	20
14	6	6	687	670	9
16	6	6	850	839	9
1	7	6	469	483	8
3	7	6	68	62	67
5	7	6	2438	2474	16
7	7	6	115	114	25
9	7	6	311	332	11
11	7	6	366	381	11
13	7	6	251	231	14
15	7	6	710	702	9
0	8	6	264	271	11
2	8	6	247	234	12
4	8	6	294	324	11
6	8	6	288	281	11
8	8	6	306	324	11
10	8	6	228	223	14
12	8	6	63	55	63
14	8	6	329	327	12
1	9	6	394	384	9
3	9	6	72	42	55
5	9	6	66	52	65
7	9	6	553	548	9
9	9	6	360	361	11
11	9	6	731	733	9
13	9	6	35	53	35
0	10	6	2184	2186	17
2	10	6	239	236	12
4	10	6	239	235	13
6	10	6	524	538	9
8	10	6	124	106	26
10	10	6	1294	1289	11
12	10	6	260	268	14
1	11	6	200	190	15
3	11	6	343	322	11
5	11	6	493	485	9
7	11	6	141	143	22
9	11	6	395	400	11
11	11	6	833	820	9
0	12	6	516	521	9
2	12	6	128	138	24
4	12	6	114	143	29
6	12	6	829	837	9
8	12	6	96	71	41
10	12	6	348	347	12
1	13	6	0	5	1
3	13	6	85	8	45
5	13	6	1301	1299	11
7	13	6	112	107	33
0	14	6	132	113	26
2	14	6	361	364	12
4	14	6	305	298	13
6	14	6	165	179	21
1	1	7	72	79	51
3	1	7	178	177	16
5	1	7	194	129	14
7	1	7	274	275	12
9	1	7	76	118	61
11	1	7	698	688	9
13	1	7	253	261	15
15	1	7	268	262	15
0	2	7	633	632	8
2	2	7	367	339	9
4	2	7	0	17	1
6	2	7	483	494	9
8	2	7	250	249	13
10	2	7	55	87	55
12	2	7	434	433	10
14	2	7	205	181	18
1	3	7	247	247	11
3	3	7	0	18	-1
5	3	7	404	410	9
7	3	7	382	375	10
9	3	7	136	138	23
11	3	7	860	848	9
13	3	7	67	50	66
0	4	7	1107	1088	9
2	4	7	39	31	19
4	4	7	134	155	21
6	4	7	178	163	16
8	4	7	127	131	24
10	4	7	455	472	10
12	4	7	439	442	10
14	4	7	81	106	64
1	5	7	0	14	1
3	5	7	92	91	33
5	5	7	137	135	21
7	5	7	498	508	9
9	5	7	210	215	15
11	5	7	22	27	22
13	5	7	270	248	14
0	6	7	221	211	13
2	6	7	122	142	24
4	6	7	194	209	16
6	6	7	734	743	8
8	6	7	240	256	14
10	6	7	154	138	21
12	6	7	206	215	17
1	7	7	104	118	28
3	7	7	162	187	18
5	7	7	910	905	9
7	7	7	97	103	15
9	7	7	269	249	13
11	7	7	572	566	10
0	8	7	664	649	8
2	8	7	0	10	1
4	8	7	154	143	19
6	8	7	345	348	11
8	8	7	0	29	1
10	8	7	243	235	15
12	8	7	158	169	12
1	9	7	321	332	12
3	9	7	115	108	28
5	9	7	264	257	13
7	9	7	162	152	21
9	9	7	0	1	1
11	9	7	577	561	10
0	10	7	644	641	9
2	10	7	428	420	10
4	10	7	92	109	40
6	10	7	234	195	15
8	10	7	78	105	78
1	11	7	124	104	27
3	11	7	18	17	17
5	11	7	605	597	9
7	11	7	133	148	27
0	12	7	70	26	69
2	12	7	219	226	16
4	12	7	270	270	14
6	12	7	126	119	28
1	13	7	252	231	14
0	0	8	2513	2532	17
2	0	8	135	137	22
4	0	8	157	147	20
6	0	8	642	642	9
8	0	8	29	46	28
10	0	8	1556	1532	12
12	0	8	539	546	10
1	1	8	160	176	19
3	1	8	75	96	61
5	1	8	430	428	10
7	1	8	241	233	15
9	1	8	583	574	9
11	1	8	582	583	10
0	2	8	0	11	1
2	2	8	105	107	29
4	2	8	192	198	17
6	2	8	496	491	9
8	2	8	0	24	1
10	2	8	206	199	17
1	3	8	111	80	28
3	3	8	249	253	13
5	3	8	1815	1815	14
7	3	8	0	1	1
9	3	8	308	315	13
11	3	8	115	70	33
0	4	8	193	224	17
2	4	8	289	309	12
4	4	8	138	153	23
6	4	8	712	710	9
8	4	8	0	13	1
10	4	8	164	167	22
1	5	8	501	511	9
3	5	8	180	166	18
5	5	8	426	428	10
7	5	8	48	29	47
9	5	8	118	61	29
0	6	8	1822	1810	14
2	6	8	171	172	18
4	6	8	269	263	13
6	6	8	456	466	10
8	6	8	123	115	28
1	7	8	0	13	1
3	7	8	218	206	15
5	7	8	884	871	9
7	7	8	224	237	17
0	8	8	930	928	9
2	8	8	104	24	32
4	8	8	74	73	73
6	8	8	399	410	11
1	9	8	0	33	-1
3	9	8	67	67	67
5	9	8	1252	1261	11
0	10	8	1007	1012	10
2	10	8	57	17	56
1	1	9	0	8	1
3	1	9	120	123	30
5	1	9	381	375	11
7	1	9	84	104	64
0	2	9	160	180	22
2	2	9	107	117	35
4	2	9	94	109	43
6	2	9	29	41	29
1	3	9	88	96	49
3	3	9	0	1	1
5	3	9	132	139	28
0	4	9	421	412	11
2	4	9	32	52	31
4	4	9	43	62	43
1	5	9	66	25	66
3	5	9	47	42	47
0	6	9	106	132	37

Observed and calculated structure factors for K13

h	k	l	10Fo	10Fc	10s
2	0	0	714	711	1
4	0	0	1290	1262	5
6	0	0	515	525	4
8	0	0	778	752	5
10	0	0	1803	1582	8
12	0	0	1345	1352	9
14	0	0	167	162	5
16	0	0	166	167	6
18	0	0	566	552	5
20	0	0	137	156	8
22	0	0	1642	1657	11
1	1	0	735	771	3
3	1	0	188	183	2
5	1	0	410	419	3
7	1	0	467	458	4
9	1	0	1724	1690	7
11	1	0	3000	2864	9
13	1	0	293	296	4
15	1	0	295	299	4
17	1	0	305	307	4
19	1	0	605	600	5
21	1	0	746	749	6
0	2	0	1315	1351	3
2	2	0	262	276	2
4	2	0	695	697	5
6	2	0	118	130	4
8	2	0	288	285	3
10	2	0	685	692	5
12	2	0	311	315	4
14	2	0	860	849	6
16	2	0	699	700	5
18	2	0	63	69	15
20	2	0	180	183	7
22	2	0	343	340	5
1	3	0	371	359	3
3	3	0	642	648	5
7	3	0	529	515	4
9	3	0	1047	1039	8
11	3	0	260	255	4
13	3	0	318	318	4
15	3	0	768	762	6
17	3	0	924	930	7
19	3	0	203	212	6
21	3	0	492	478	5
0	4	0	1993	2026	5
2	4	0	583	589	4
4	4	0	1077	1072	6
6	4	0	3725	3618	7
8	4	0	507	487	4
10	4	0	406	414	4
12	4	0	292	294	4
14	4	0	895	896	6
16	4	0	2007	1990	11
18	4	0	96	83	10
20	4	0	259	254	6
1	5	0	1410	1411	6
3	5	0	24	12	24
5	5	0	3140	3105	7
7	5	0	832	818	6
9	5	0	188	200	4
11	5	0	139	362	4
13	5	0	386	392	4
15	5	0	240	240	5
17	5	0	479	476	5
19	5	0	236	249	6
21	5	0	294	299	6
0	6	0	803	819	5
2	6	0	217	220	3
4	6	0	502	503	3
6	6	0	624	607	5
8	6	0	726	708	5
10	6	0	1257	1251	9
12	6	0	272	275	4
14	6	0	500	503	4
16	6	0	623	617	5
18	6	0	356	356	5
20	6	0	65	68	18
1	7	0	684	664	5
3	7	0	112	112	5
5	7	0	1329	1318	8
7	7	0	484	479	4
9	7	0	1203	1199	9
11	7	0	568	536	5
13	7	0	359	360	4
15	7	0	207	215	5
17	7	0	258	260	5
19	7	0	661	676	6
0	8	0	2499	2461	8
2	8	0	199	199	3
4	8	0	356	350	3
6	8	0	580	584	4
8	8	0	395	399	4
10	8	0	1285	1278	10
12	8	0	187	196	5
14	8	0	191	182	5
16	8	0	302	314	5
18	8	0	77	66	13
20	8	0	311	300	6
1	9	0	30	10	29
3	9	0	440	448	4
5	9	0	1834	1837	9
7	9	0	823	825	6
9	9	0	40	45	26
11	9	0	665	648	5
13	9	0	260	260	5
15	9	0	465	470	5
17	9	0	459	455	5
19	9	0	242	245	6
0	10	0	283	298	3
2	10	0	62	63	11
4	10	0	452	471	4
6	10	0	256	250	4
8	10	0	293	300	4
10	10	0	492	502	4
12	10	0	132	143	7
14	10	0	1193	1204	8
16	10	0	178	172	6
18	10	0	559	560	5
1	11	0	288	281	4
3	11	0	256	262	4
5	11	0	847	850	6
7	11	0	158	162	5
9	11	0	58	44	15
11	11	0	491	499	5
13	11	0	116	122	8
15	11	0	882	870	7
17	11	0	390	396	5
0	12	0	1571	1584	10
2	12	0	296	293	4
4	12	0	153	157	6
6	12	0	583	585	5
8	12	0	136	151	6
10	12	0	625	625	5
12	12	0	476	475	5
14	12	0	33	28	33
16	12	0	134	122	9
1	13	0	405	411	4
3	13	0	146	160	6
5	13	0	426	428	4
7	13	0	456	465	4
9	13	0	578	575	5
11	13	0	923	922	7
13	13	0	299	306	5
15	13	0	213	226	6
0	14	0	1464	1456	11
2	14	0	373	378	4
4	14	0	223	226	5
6	14	0	727	734	5
8	14	0	75	82	12
10	14	0	1288	1293	8
12	14	0	83	87	13
14	14	0	36	27	35
1	15	0	186	180	5
3	15	0	424	433	4
5	15	0	535	548	5
7	15	0	49	19	22
9	15	0	30	38	29
11	15	0	357	358	5
13	15	0	420	410	5
0	16	0	642	639	5
2	16	0	174	174	6
4	16	0	297	298	5
6	16	0	843	851	7
8	16	0	67	72	16
10	16	0	72	57	14
12	16	0	397	399	5
1	17	0	300	296	5
3	17	0	279	272	5
5	17	0	1870	1862	13
7	17	0	94	86	11
9	17	0	78	83	15
0	18	0	326	317	5
2	18	0	321	319	5
4	18	0	81	30	13
6	18	0	242	252	6
8	18	0	341	338	5
1	19	0	197	192	7
3	19	0	67	59	17
1	1	1	192	176	2
3	1	1	467	462	3
5	1	1	917	946	5
7	1	1	125	108	4
9	1	1	503	497	4
11	1	1	848	862	6
13	1	1	408	405	4
15	1	1	64	49	12
17	1	1	729	736	6
19	1	1	457	471	5
21	1	1	936	897	7
0	2	1	155	187	3
2	2	1	471	499	3
4	2	1	555	560	4
6	2	1	261	235	2
8	2	1	576	590	4
10	2	1	256	272	3
12	2	1	967	969	7
14	2	1	208	193	4
16	2	1	672	677	5
18	2	1	92	76	10
20	2	1	144	147	7
22	2	1	198	198	7
1	3	1	346	351	3
3	3	1	249	242	3
5	3	1	385	374	3
7	3	1	496	494	4
9	3	1	194	199	3
11	3	1	212	215	4
13	3	1	254	258	4
15	3	1	34	43	34
17	3	1	290	294	5
19	3	1	197	196	6
21	3	1	288	300	6
0	4	1	1071	1061	5
2	4	1	72	78	6
4	4	1	278	270	3
6	4	1	821	778	5
8	4	1	510	510	4
10	4	1	234	211	4
12	4	1	740	754	5
14	4	1	254	255	4
16	4	1	675	671	5
18	4	1	269	272	5
20	4	1	131	104	8
1	5	1	124	124	4
3	5	1	518	524	3
5	5	1	1492	1487	7
7	5	1	898	893	6
9	5	1	627	623	5
11	5	1	256	281	4
13	5	1	550	552	5
15	5	1	153	146	6
17	5	1	222	227	5
19	5	1	0	14	1
21	5	1	745	736	6
0	6	1	580	556	4
2	6	1	171	173	3
4	6	1	158	156	3
6	6	1	848	854	6
8	6	1	536	526	4
10	6	1	184	180	4
12	6	1	316	314	4
14	6	1	51	52	17
16	6	1	1025	1030	7
18	6	1	315	309	5
20	6	1	432	429	5
1	7	1	181	168	3
3	7	1	601	599	4
5	7	1	349	349	3
7	7	1	222	216	4
9	7	1	436	448	4
11	7	1	27	13	26
13	7	1	56	49	14
15	7	1	50	59	20
17	7	1	216	212	6
19	7	1	104	114	11
0	8	1	672	647	5
2	8	1	31	30	31
4	8	1	128	142	5
6	8	1	290	294	3
8	8	1	143	143	5
10	8	1	94	85	8
12	8	1	517	528	4
14	8	1	583	584	5
16	8	1	757	757	6
18	8	1	365	369	5
20	8	1	228	236	6
1	9	1	984	965	7
3	9	1	133	137	5
5	9	1	293	313	4
7	9	1	325	331	4
9	9	1	37	24	36
11	9	1	1636	1679	10
13	9	1	73	65	12
15	9	1	98	89	9
17	9	1	182	185	7
19	9	1	182	185	7
0	10	1	1174	1166	9
2	10	1	771	772	5
4	10	1	251	255	4
6	10	1	449	449	4
8	10	1	209	203	4
10	10	1	213	212	5
12	10	1	19	26	19
14	10	1	594	586	5
16	10	1	217	225	6
18	10	1	276	266	6
1	11	1	200	200	4
3	11	1	293	285	4
5	11	1	671	681	5
7	11	1	555	556	5
9	11	1	320	315	4
11	11	1	385	384	4
13	11	1	95	113	10
15	11	1	53	57	22
17	11	1	487	489	5
0	12	1	1091	1100	8
2	12	1	467	460	4
4	12	1	112	111	7
6	12	1	600	606	5
8	12	1	168	169	6
10	12	1	186	198	6
12	12	1	294	286	5
14	12	1	0	18	1
16	12	1	696	694	6
1	13	1	367	366	4
3	13	1	401	401	4
5	13	1	895	901	7
7	13	1	54	62	17
9	13	1	295	302	5
11	13	1	1068	1057	7
13	13	1	150	158	7
15	13	1	303	310	5
0	14	1	615	633	5
2	14	1	292	293	4
4	14	1	385	383	4
6	14	1	292	301	5
8	14	1	332	330	5
10	14	1	135	147	8
12	14	1	198	208	6
14	14	1	387	380	5
1	15	1	52	51	18
3	15	1	270	270	5
5	15	1	261	260	5
7	15	1	354	352	5
9	15	1	82	71	12
11	15	1	114	101	9
13	15	1	130	132	9
0	16	1	201	211	6
2	16	1	246	249	5
4	16	1	0	4	1
6	16	1	1259	1273	9
8	16	1	292	296	5
10	16	1	114	107	10
12	16	1	86	84	13
1	17	1	87	92	11
3	17	1	346	346	5
5	17	1	663	664	5
7	17	1	216	221	6
9	17	1	405	399	5
0	18	1	295	303	5
2	18	1	86	78	12
4	18	1	314	309	5
6	18	1	320	327	5
1	19	1	316	310	5
3	19	1	397	396	5
0	0	2	2978	3229	6
2	0	2	576	590	4
4	0	2	368	364	3
6	0	2	732	701	4
8	0	2	495	480	4
10	0	2	1294	1288	8
12	0	2	948	957	6
14	0	2	1283	1283	8
16	0	2	629	630	5
18	0	2	832	827	6
20	0	2	39	57	38
1	1	2	514	512	4
3	1	2	802	822	6
5	1	2	921	954	6
7	1	2	156	151	3
9	1	2	654	648	4
11	1	2	697	698	5
13	1	2	27	15	27
15	1	2	596	593	5
17	1	2	80	64	11
19	1	2	20	11	19
21	1	2	179	166	5
2	2	2	168	170	3
4	2	2	549	537	4
6	2	2	492	486	3
8	2	2	317	308	3
10	2	2	1245	1230	8
12	2	2	508	510	4
14	2	2	104	116	8
16	2	2	381	371	4
18	2	2	12	36	11
20	2	2	95	93	11
1	3	2	404	404	3
3	3	2	297	299	3
5	3	2	966	958	7
7	3	2	147	142	4
9	3	2	1600	1630	8
11	3	2	1334	1361	9
13	3	2	470	468	4
15	3	2	240	140	4
17	3	2	323	322	5
19	3	2	813	818	7
21	3	2	464	472	5
0	4	2	1825	1786	6
2	4	2	609	600	4
4	4	2	51	18	9
6	4	2	266	241	3
8	4	2	58	65	10
10	4	2	1890	1933	9
12	4	2	314	309	4
14	4	2	261	253	4
16	4	2	83	75	10
18	4	2	449	447	5
20	4	2	297	305	6
1	5	2	903	896	6
3	5	2	93	96	5
5	5	2	1864	1821	7
7	5	2	251	237	3
9	5	2	349	334	3
11	5	2	609	609	5
13	5	2	32	6	31
15	5	2	222	221	5
17	5	2	703	712	6
19	5	2	412	401	5
21	5	2	469	455	5
0	6	2	1075	1058	7
2	6	2	147	153	4
4	6	2	1111	1129	7
6	6	2	2297	2290	8
8	6	2	256	249	4
10	6	2	65	41	11
12	6	2	360	360	4
14	6	2	1007	1025	7
16	6	2	1426	1443	10
18	6	2	52	46	22
20	6	2	109	104	10
1	7	2	745	735	5
3	7	2	60	55	10
5	7	2	4425	4407	9
7	7	2	204	189	4
9	7	2	482	486	4
11	7	2	135	150	6
13	7	2	308	299	4
15	7	2	836	852	6
17	7	2	937	940	7
19	7	2	11	29	11
0	8	2	528	533	4
2	8	2	438	434	4
4	8	2	125	135	5
6	8	2	458	448	4
8	8	2	555	570	5
10	8	2	0	19	1
12	8	2	152	163	6
14	8	2	527	529	5
16	8	2	873	883	6
18	8	2	81	63	13
1	9	2	436	400	4
3	9	2	48	40	16
5	9	2	483	468	4
7	9	2	402	396	4
9	9	2	783	789	6
11	9	2	1581	1579	11
13	9	2	48	48	21
15	9	2	344	345	5
17	9	2	587	598	5

Observed and calculated structure factors for K13

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
19	9	2	301	298	6	3	3	3	232	234	1	2	12	3	257	260	4	14	4	4	845	860	6	1	15	4	146	143	7
0	10	2	4553	4362	10	5	3	3	1060	1035	7	4	12	3	346	351	4	16	4	4	1380	1407	9	3	15	4	431	422	5
2	10	2	725	718	5	7	3	3	748	729	5	6	12	3	122	111	7	18	4	4	143	140	8	5	15	4	269	259	5
4	10	2	783	793	6	9	3	3	168	164	4	8	12	3	85	87	10	1	5	4	999	983	7	7	15	4	100	97	11
6	10	2	118	113	6	11	3	3	1284	1309	10	10	12	3	170	168	6	3	5	4	176	178	4	9	15	4	65	51	17
8	10	2	236	235	4	13	3	3	64	69	12	12	12	3	276	271	5	5	5	4	1467	1506	9	0	16	4	201	191	6
10	10	2	1791	1814	11	15	3	3	113	118	8	14	12	3	91	104	12	7	5	4	407	402	4	2	16	4	165	163	7
12	10	2	283	282	5	17	3	3	252	253	5	16	12	3	177	172	5	9	5	4	203	191	4	4	16	4	210	223	6
14	10	2	385	381	5	19	3	3	116	112	10	1	13	3	252	249	4	11	5	4	905	924	7	6	16	4	488	477	5
16	10	2	265	269	6	21	3	3	400	393	5	3	13	3	486	491	4	13	5	4	241	235	5	8	16	4	40	7	39
18	10	2	262	255	6	0	4	3	2240	2108	7	5	13	3	283	285	5	15	5	4	249	241	5	1	17	4	378	372	5
1	11	2	388	391	4	2	4	3	51	54	10	7	13	3	125	134	8	17	5	4	84	96	13	3	17	4	186	172	7
3	11	2	712	716	5	4	4	3	384	382	3	9	13	3	225	231	5	19	5	4	175	167	7	1	1	5	87	87	7
5	11	2	75	66	10	6	4	3	222	208	3	11	13	3	143	135	5	0	6	4	2116	2111	9	3	1	5	228	219	4
7	11	2	0	12	1	8	4	3	272	282	3	13	13	3	29	34	29	2	6	4	212	216	4	5	1	5	697	701	5
9	11	2	624	623	5	10	4	3	373	365	4	15	13	3	232	216	6	4	6	4	448	455	4	7	1	5	39	25	25
11	11	2	1779	1787	12	12	4	3	799	804	6	0	14	3	40	38	31	6	6	4	128	109	6	9	1	5	402	411	4
13	11	2	50	46	20	14	4	3	109	111	8	2	14	3	259	253	5	8	6	4	403	395	4	11	1	5	256	252	4
15	11	2	245	241	6	16	4	3	231	230	5	4	14	3	324	328	5	10	6	4	1172	1192	8	13	1	5	218	230	5
17	11	2	52	52	26	18	4	3	183	176	6	6	14	3	145	145	7	12	6	4	171	369	4	15	1	5	0	9	1
0	12	2	1301	1285	8	20	4	3	48	57	29	8	14	3	378	382	5	14	6	4	303	300	5	17	1	5	745	741	6
2	12	2	23	8	22	1	5	3	61	59	9	10	14	3	43	30	43	16	6	4	250	251	5	19	1	5	358	367	5
4	12	2	28	19	28	3	5	3	342	350	3	12	14	3	92	87	12	18	6	4	257	262	6	0	2	5	781	773	5
6	12	2	845	853	6	5	5	3	870	859	6	1	15	3	135	135	7	1	7	4	243	234	4	2	2	5	73	67	9
8	12	2	98	104	9	7	5	3	869	874	6	3	15	3	193	197	6	3	7	4	176	184	5	4	2	5	523	526	4
10	12	2	782	773	6	9	5	3	498	499	4	5	15	3	461	463	5	5	7	4	1240	1260	10	6	2	5	447	440	4
12	12	2	239	227	5	11	5	3	105	101	7	7	15	3	218	217	6	7	7	4	400	395	4	8	2	5	314	308	4
14	12	2	602	596	5	13	5	3	415	410	4	9	15	3	123	122	9	9	7	4	923	945	6	10	2	5	82	75	9
16	12	2	176	182	5	15	5	3	76	60	11	11	15	3	332	312	5	11	7	4	724	724	5	12	2	5	757	750	5
1	13	2	260	257	4	17	5	3	291	290	5	0	16	3	80	73	12	13	7	4	307	310	5	14	2	5	106	110	9
3	13	2	117	121	7	19	5	3	65	51	17	2	16	3	98	90	10	15	7	4	216	215	6	16	2	5	247	231	6
5	13	2	1831	1841	11	0	6	3	447	450	4	4	16	3	209	213	6	17	7	4	381	377	5	18	2	5	77	57	15
7	13	2	55	19	16	2	6	3	104	91	6	6	16	3	1134	1126	8	0	8	4	1800	1825	9	1	3	5	150	146	5
9	13	2	230	226	5	4	6	3	387	366	3	8	16	3	243	248	6	2	8	4	49	49	16	3	3	5	221	213	4
11	13	2	133	147	8	6	6	3	1167	1172	7	10	16	3	63	44	18	4	8	4	140	140	6	5	3	5	566	578	4
13	13	2	88	88	11	8	6	3	376	375	4	1	17	3	144	153	7	6	8	4	533	526	4	7	3	5	108	105	7
15	13	2	471	478	5	10	6	3	196	200	5	3	17	3	342	350	5	8	8	4	305	315	4	9	3	5	69	57	11
0	14	2	424	419	4	12	6	3	284	286	4	5	17	3	386	381	5	10	8	4	1099	1117	8	11	3	5	303	305	4
2	14	2	333	327	4	14	6	3	124	126	7	7	17	3	29	24	29	12	8	4	99	117	9	13	3	5	270	266	5
4	14	2	713	719	6	16	6	3	1114	1119	8	0	18	3	201	210	7	14	8	4	170	157	6	15	3	5	47	21	27
6	14	2	461	458	5	18	6	3	434	431	5	2	18	3	178	180	7	16	8	4	258	259	6	17	3	5	506	497	5
8	14	2	190	196	6	20	6	3	392	398	5	4	18	3	152	142	8	18	8	4	16	3	15	0	4	5	83	90	8
10	14	2	148	155	7	1	7	3	217	208	4	2	0	4	427	435	4	1	9	4	0	29	1	2	4	5	56	43	13
12	14	2	65	54	16	3	7	3	307	315	3	4	0	4	733	746	5	3	9	4	325	319	4	4	4	5	132	131	6
14	14	2	387	392	5	5	7	3	1133	1115	7	6	0	4	461	447	4	5	9	4	1728	1742	10	6	4	5	675	660	5
1	15	2	502	505	5	7	7	3	149	151	5	8	0	4	175	172	4	7	9	4	469	467	4	8	4	5	363	372	4
3	15	2	285	283	5	9	7	3	464	470	4	10	0	4	2491	2542	10	9	9	4	105	94	8	10	4	5	110	111	7
5	15	2	1442	1441	10	11	7	3	822	819	6	12	0	4	901	920	7	11	9	4	238	230	5	12	4	5	520	531	5
7	15	2	510	500	5	13	7	3	130	129	7	14	0	4	316	328	4	13	9	4	119	116	8	14	4	5	253	253	5
9	15	2	190	188	6	15	7	3	150	165	7	16	0	4	256	250	5	15	9	4	316	320	5	16	4	5	685	692	6
11	15	2	175	183	5	17	7	3	621	618	5	18	0	4	532	534	5	17	9	4	534	544	5	18	4	5	298	294	6
13	15	2	121	110	9	19	7	3	76	74	16	20	0	4	79	72	15	0	10	4	846	855	6	1	5	5	185	159	4
0	16	2	1015	1017	8	0	8	3	897	870	6	1	1	4	259	249	3	2	10	4	77	82	10	3	5	5	305	304	4
2	16	2	101	104	9	2	8	3	123	135	6	3	1	4	97	87	6	4	10	4	508	515	4	5	5	5	714	706	5
4	16	2	44	20	32	4	8	3	361	365	4	5	1	4	324	313	3	6	10	4	225	227	5	7	5	5	606	608	5
6	16	2	487	491	5	6	8	3	588	584	5	7	1	4	59	46	11	8	10	4	312	312	4	9	5	5	448	461	4
8	16	2	81	95	13	8	8	3	38	26	27	9	1	4	1268	1277	9	10	10	4	456	459	4	11	5	5	253	242	5
10	16	2	698	702	6	10	8	3	91	89	9	11	1	4	1581	1622	10	12	10	4	192	188	6	13	5	5	368	371	5
1	17	2	223	228	6	12	8	3	601	605	5	13	1	4	167	162	5	14	10	4	938	926	7	15	5	5	100	95	10
3	17	2	380	385	5	14	8	3	381	382	4	15	1	4	233	219	5	16	10	4	355	344	5	17	5	5	171	164	7
5	17	2	170	171	7	16	8	3	218	206	6	17	1	4	69	10	14	1	11	4	143	145	6	0	6	5	422	454	4
7	17	2	14	7	14	18	8	3	206	197	7	19	1	4	548	553	5	3	11	4	326	326	4	2	6	5	104	105	7
9	17	2	404	395	5	1	9	3	588	596	5	0	2	4	336	361	3	5	11	4	1083	1101	8	4	6	5	87	96	9
0	18	2	738	733	6	3	9	3	98	85	7	2	2	4	189	188	4	7	11	4	67	77	13	6	6	5	422	419	4
2	18	2	17	19	16	5	9	3	397	388	4	4	2	4	433	428	3	9	11	4	0	7	1	8	6	5	344	348	4
4	18	2	180	195	7	7	9	3	245	238	4	6	2	4	466	488	4	11	11	4	46	34	26	10	6	5	123	116	7
6	18	2	443	431	5	9	9	3	54	42	15	8	2	4	93	98	7	13	11	4	93	74	11	12	6	5	232	219	5
1	1	3	291	282	3	11	9	3	855	870	6	10	2	4	460	462	4	15	11	4	752	741	6	14	6	5	56	26	17
3	1	3	643	636	4	13	9	3	33	40	33	12	2	4	315	323	4	0	12	4	1015	996	7	16	6	5	685	689	6
5	1	3	155	157	4	15	9	3	114	105	9	14	2	4	636	638	5	2	12	4	286	292	4	1	7	5	105	96	7
7	1	3	270	269	3	17	9	3	520	521	5	16	2	4	726	724	6	4	12	4	62	66	15	3	7	5	486	499	4
9	1	3	427	428	4	0	10	3	743	749	5	18	2	4	66	46	15	6	12	4	252	252	5	5	7	5	30	33	30
11	1	3	1392	1393	9	2	10	3	753	765	5	20	2	4	132	133	9	8	12	4	212	205	5	7	7	5	317	324	4
13	1	3	462	466	4	4	10	3	344	353	4	1	3	4	260	267	3	10	12	4	198	398	5	9	7	5	303	301	4
15	1	3	122	113	7	6	10	3	201	201	5	3	3	4	536	518	4	12	12	4	107	311	5	11	7	5	372	377	4
17	1	3	163	167	4	8	10	3	259	262	4	5	3	4	3129	3260	9	14	12	4	9	40	9	13	7	5	143	152	7
19	1	3	448	466	5	10	10	3	13	16	13	7	3	4	189	190	4	1	13	4	204	204	5	15	7	5	36	31	16
21	1	3	889	877	7	12	10	3	68	79	13	9	3	4	796	806	6	3	13	4	110	91	8	17	7	5	21	44	21
0	2	3	2222	2139	7	14	10	3	567	573	5	11	3	4	17	6	16	5	13	4	281	274	5	0	8	5	788	791	6
2	2	3	553	540	4	16	10	3	0	14	1	13	3	4	282	288	4	7	13	4	264	268	5	2	8	5	116	109	7
4	2	3	35	45	16	1	11	3	297	297	4	15	3	4	657	660	5	9	13	4	547	548	5	4	8	5	0	5	1
6	2	3	1107	1094	8	3	11	3	226	232	4	17	3	4	712	720	5	11	13	4	707	720	6	6	8	5	528	526	5
8	2	3	711	698	5	5	11	3	733	739	5	19	3	4	192	187	7	13	13	4	168	176	7	8	8	5	125	133	7
10	2	3	371	352	4	7	11	3	253	251	5	0	4	4	438	463	4	0	14	4	1376	1402	10	10	8	5	53	52	18
12	2	3	743	748	5	9	11	3	379	382	4	2	4	4	387	377	3	2	14	4	233	227	5	12	8	5	403	398	5
14	2	3	385	379	4	11	11	3	120	111	8	4	4	4	639	667	5	4	14	4	322	322	5	14	8	5	498	501	5
16	2	3	1085	1103	8	13	11	3	71	49	14	6	4	4	1808	1837	9	6	14	4	497	507	5	16	8	5	804	796	6
18	2	3	269	254	5	15	11	3	77	83	15	8	4	4	209	215	4	8	14	4	63	68	18	1	9	5	696	694	6
20	2	3	103	96	11	17	11	3	589	577	5	10	4	4	250	261	4	10	14	4	1028	1027	8	3	9	5	71	69	12
1	3	3	582	564	4	0	12	3	226	218	4	12	4	4	185	195	5	12	14	4	11	48	10	5	9	5	442	440	5

Observed and calculated structure factors for K13

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	9	5	147	138	4	13	1	6	71	69	13	14	8	6	178	171	5	6	4	7	69	78	13	0	2	8	0	8	1
9	9	5	37	30	37	15	1	6	393	382	5	1	9	6	296	296	5	8	4	7	211	211	6	2	2	8	98	80	9
11	9	5	1522	1521	10	17	1	6	322	319	6	3	9	6	105	109	8	10	4	7	214	223	6	4	2	8	269	262	5
13	9	5	112	119	10	0	2	6	1656	1659	10	5	9	6	0	43	1	12	4	7	488	484	5	6	2	8	517	508	5
15	9	5	101	108	11	2	2	6	218	224	4	7	9	6	477	470	5	14	4	7	136	124	9	8	2	8	31	34	10
0	10	5	936	927	7	4	2	6	218	221	4	9	9	6	528	529	5	1	5	7	31	26	30	10	2	8	254	247	6
2	10	5	503	507	5	6	2	6	522	525	4	11	9	6	723	720	6	3	5	7	204	195	5	1	3	8	165	147	6
4	10	5	134	124	7	8	2	6	267	274	5	13	9	6	70	70	16	5	5	7	103	113	5	3	3	8	344	344	5
6	10	5	461	459	4	10	2	6	741	736	6	0	10	6	2143	2138	12	7	5	7	501	513	5	5	3	8	1699	1720	10
8	10	5	137	148	7	12	2	6	289	282	5	2	10	6	161	159	5	9	5	7	355	357	5	7	3	8	11	8	11
10	10	5	226	222	6	14	2	6	0	19	1	4	10	6	161	165	5	11	5	7	54	25	21	9	3	8	442	443	5
12	10	5	53	76	23	16	2	6	431	426	5	6	10	6	586	577	5	13	5	7	256	252	6	11	3	8	180	184	7
14	10	5	448	445	5	1	3	6	211	204	4	8	10	6	69	55	15	0	6	7	171	180	6	0	4	8	278	277	5
1	11	5	84	89	10	3	3	6	129	119	6	10	10	6	1204	1211	8	2	6	7	103	108	9	2	4	8	266	266	5
3	11	5	232	237	5	5	3	6	747	760	6	12	10	6	166	158	7	4	6	7	160	159	6	4	4	8	269	249	5
5	11	5	461	458	5	7	3	6	70	66	11	1	11	6	114	101	9	6	6	7	666	667	5	6	4	8	596	605	5
7	11	5	533	538	5	9	3	6	1078	1103	8	3	11	6	357	356	5	8	6	7	248	252	5	8	4	8	13	37	12
9	11	5	211	215	6	11	3	6	1057	1077	7	5	11	6	460	466	5	10	6	7	188	175	6	10	4	8	102	99	11
11	11	5	423	419	5	13	3	6	243	253	6	7	11	6	110	111	9	12	6	7	196	195	7	1	5	8	525	533	5
13	11	5	171	173	7	15	3	6	49	53	26	9	11	6	445	444	5	1	7	7	79	76	11	3	5	8	162	160	7
0	12	5	1065	1075	8	0	4	6	2329	2353	10	11	11	6	717	725	6	3	7	7	279	277	5	5	5	8	398	399	5
2	12	5	459	462	5	2	4	6	40	36	23	0	12	6	484	464	5	5	7	7	665	655	6	7	5	8	26	20	26
4	12	5	50	54	22	4	4	6	344	339	4	2	12	6	47	43	27	7	7	7	127	122	8	9	5	8	180	190	7
6	12	5	655	655	5	6	4	6	472	473	4	4	12	6	32	31	32	9	7	7	360	356	5	0	6	8	1853	1835	13
8	12	5	109	109	9	8	4	6	72	77	12	6	12	6	928	921	7	11	7	7	495	496	5	2	6	8	216	213	6
10	12	5	111	102	9	10	4	6	1283	1317	8	8	12	6	0	1	1	0	8	7	543	524	5	4	6	8	169	171	5
12	12	5	247	242	6	12	4	6	274	272	5	10	12	6	401	398	5	2	8	7	111	116	9	6	6	8	427	425	5
1	13	5	125	115	5	14	4	6	89	81	12	1	13	6	87	71	11	4	8	7	308	301	5	8	6	8	180	183	7
3	13	5	295	290	5	16	4	6	175	177	7	3	13	6	91	84	11	6	8	7	340	333	5	1	7	8	61	46	19
5	13	5	890	899	7	1	5	6	219	207	4	5	13	6	1385	1378	9	8	8	7	34	33	34	3	7	8	135	132	8
7	13	5	179	171	6	3	5	6	295	297	4	7	13	6	142	149	8	10	8	7	44	56	43	5	7	8	887	887	6
9	13	5	279	278	5	5	5	6	460	456	4	0	14	6	24	36	23	1	9	7	403	404	5	7	7	8	227	230	6
11	13	5	1181	1163	8	7	5	6	42	46	28	2	14	6	382	372	5	1	9	7	0	36	1	0	8	8	894	896	7
0	14	5	851	835	7	9	5	6	178	187	6	4	14	6	331	324	5	5	9	7	255	273	6	2	8	8	16	21	35
2	14	5	253	251	6	11	5	6	372	381	5	1	1	7	85	82	10	7	9	7	115	113	9	4	8	8	12	7	12
4	14	5	325	325	5	13	5	6	83	89	12	3	1	7	262	250	4	9	9	7	36	34	35	6	8	8	374	375	5
6	14	5	445	440	5	15	5	6	216	204	6	5	1	7	89	79	9	0	10	7	521	515	5	1	9	8	66	57	17
8	14	5	225	228	6	0	6	6	196	193	5	7	1	7	272	267	5	2	10	7	421	422	5	3	9	8	183	178	7
1	15	5	123	121	8	2	6	6	25	24	25	9	1	7	236	244	5	4	10	7	152	157	7	5	9	8	1222	1224	8
3	15	5	214	227	6	4	6	6	558	577	5	11	1	7	745	743	6	6	10	7	200	192	6	0	10	8	1060	1030	8
5	15	5	83	81	13	6	6	6	811	820	6	13	1	7	340	356	5	8	10	7	150	138	8	2	10	8	137	137	9
7	15	5	119	116	6	8	6	6	290	288	5	15	1	7	141	134	8	1	11	7	155	165	8	1	1	9	69	72	16
0	16	5	190	183	7	10	6	6	155	155	7	0	2	7	635	631	5	3	11	7	146	147	8	3	1	9	195	184	6
2	16	5	274	268	6	12	6	6	181	173	6	2	2	7	307	301	4	5	11	7	527	528	5	5	1	9	290	291	6
4	16	5	108	101	11	14	6	6	858	863	6	4	2	7	29	48	28	7	11	7	171	175	8	0	2	9	103	104	10
0	0	6	2456	2503	10	1	7	6	601	601	5	6	2	7	464	460	4	0	12	7	97	40	11	2	2	9	0	30	1
2	0	6	97	90	8	3	7	6	194	195	5	8	2	7	284	290	5	2	12	7	169	162	7	4	2	9	275	272	6
4	0	6	601	622	5	5	7	6	2375	2402	12	10	2	7	80	89	13	4	12	7	270	256	6	6	2	9	3	13	3
6	0	6	690	702	5	7	7	6	98	103	9	12	2	7	542	542	5	0	0	8	2359	2426	12	1	3	9	178	175	7
8	0	6	342	337	4	9	7	6	384	382	5	14	2	7	212	214	7	2	0	8	168	169	6	3	3	9	0	8	1
10	0	6	833	853	6	11	7	6	481	496	5	1	3	7	189	189	5	4	0	8	271	271	5	5	3	9	96	79	11
12	0	6	750	753	5	13	7	6	181	175	7	3	3	7	54	29	17	6	0	8	720	729	6	0	4	9	435	432	5
14	0	6	758	750	5	15	7	6	563	563	5	5	3	7	353	360	4	8	0	8	56	58	20	2	4	9	59	52	19
16	0	6	814	800	6	0	8	6	158	155	4	7	3	7	459	458	4	10	0	8	1370	1366	9	4	4	9	71	67	15
1	1	6	144	141	6	2	8	6	195	194	5	9	3	7	171	160	6	1	1	8	111	102	9	1	5	9	0	12	1
3	1	6	200	197	4	4	8	6	249	254	5	11	3	7	747	744	6	3	1	8	122	118	8	3	5	9	111	103	10
5	1	6	1650	1652	10	6	8	6	101	102	5	13	3	7	36	46	16	5	1	8	531	535	5						
7	1	6	67	67	12	8	8	6	344	344	5	0	4	7	1005	984	7	7	1	8	193	188	6						
9	1	6	166	370	4	10	8	6	114	122	9	2	4	7	107	103	8	9	1	8	684	682	5						
11	1	6	188	193	6	12	8	6	193	175	6	4	4	7	281	282	5	11	1	8	485	477	5						

Observed and calculated structure factors for K14

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	663	682	3	2	8	0	205	201	4	1	1	1	146	130	3	5	9	1	567	588	5	3	1	2	745	752	5
4	0	0	1403	1410	5	4	8	0	579	571	5	3	1	1	529	518	4	7	9	1	312	313	4	5	1	2	1206	1208	7
6	0	0	573	592	4	6	8	0	637	642	5	5	1	1	621	640	4	9	9	1	116	119	9	7	1	2	125	119	5
8	0	0	994	988	8	8	8	0	498	502	5	7	1	1	156	139	4	11	9	1	1725	1722	12	9	1	2	770	762	6
10	0	0	3820	3818	10	10	8	0	1394	1396	11	9	1	1	395	382	4	13	9	1	29	16	28	11	1	2	638	641	5
12	0	0	1327	1351	10	12	8	0	284	283	5	11	1	1	885	891	7	15	9	1	0	13	1	13	1	2	112	121	9
14	0	0	314	311	5	14	8	0	49	54	29	13	1	1	304	302	4	17	9	1	169	185	9	15	1	2	706	719	6
16	0	0	306	298	5	16	8	0	251	258	6	15	1	1	0	22	1	19	9	1	157	167	9	17	1	2	144	140	8
18	0	0	678	672	6	18	8	0	31	21	30	17	1	1	742	741	6	0	10	1	1324	1361	10	19	1	2	0	6	1
20	0	0	312	309	6	20	8	0	331	324	7	19	1	1	449	464	5	2	10	1	816	800	6	21	1	2	279	271	7
22	0	0	1575	1605	11	1	9	0	136	116	6	21	1	1	947	934	7	4	10	1	390	396	4	0	2	2	4156	4100	7
1	1	0	722	751	3	3	9	0	454	458	4	0	2	1	317	268	3	6	10	1	386	385	5	2	2	2	370	374	3
3	1	0	330	321	3	5	9	0	1811	1835	10	2	2	1	428	451	3	8	10	1	100	108	10	4	2	2	542	539	4
5	1	0	677	685	3	7	9	0	875	869	6	4	2	1	388	393	3	10	10	1	301	295	5	6	2	2	445	436	4
7	1	0	436	432	4	9	9	0	68	58	15	6	2	1	269	256	3	12	10	1	61	62	21	8	2	2	292	283	4
9	1	0	1715	1700	8	11	9	0	615	612	6	8	2	1	738	744	5	14	10	1	710	701	6	10	2	2	1114	1306	10
11	1	0	2917	2925	10	13	9	0	252	259	5	10	2	1	441	470	4	16	10	1	294	310	6	12	2	2	513	522	5
13	1	0	253	250	5	15	9	0	559	555	5	12	2	1	985	989	7	18	10	1	332	318	6	14	2	2	88	101	11
15	1	0	196	195	6	17	9	0	468	480	5	14	2	1	37	48	16	1	11	1	271	278	5	16	2	2	333	336	5
17	1	0	299	302	5	19	9	0	290	283	7	16	2	1	766	783	6	3	11	1	234	230	5	18	2	2	85	61	13
19	1	0	630	625	6	0	10	0	447	474	5	18	2	1	83	56	14	5	11	1	660	665	5	20	2	2	0	10	1
21	1	0	800	818	7	2	10	0	62	67	15	20	2	1	151	153	9	7	11	1	489	491	5	1	3	2	421	411	4
0	2	0	1199	1225	4	4	10	0	385	400	4	22	2	1	240	241	7	9	11	1	378	381	5	3	3	2	139	138	4
2	2	0	321	337	3	6	10	0	233	214	5	1	3	1	274	273	3	11	11	1	389	392	5	5	3	2	1280	1286	7
4	2	0	624	650	5	8	10	0	412	415	4	3	3	1	212	205	3	13	11	1	136	139	9	7	3	2	198	194	4
6	2	0	79	84	7	10	10	0	668	666	5	5	3	1	185	179	3	15	11	1	59	73	27	9	3	2	1669	1664	9
8	2	0	233	234	4	12	10	0	148	150	8	7	3	1	522	519	4	17	11	1	382	388	6	11	3	2	1434	1449	10
10	2	0	593	608	5	14	10	0	1202	1206	9	9	3	1	334	341	4	0	12	1	1234	1256	9	13	3	2	574	578	5
12	2	0	322	319	4	16	10	0	327	321	6	11	3	1	262	268	4	2	12	1	474	480	5	15	3	2	264	257	5
14	2	0	848	847	6	18	10	0	587	599	6	13	3	1	339	346	4	4	12	1	82	80	12	17	3	2	292	290	6
16	2	0	755	752	6	1	11	0	407	399	5	15	3	1	7	2	7	6	12	1	668	661	6	19	3	2	870	857	7
18	2	0	71	66	16	3	11	0	292	289	5	17	3	1	360	367	5	8	12	1	180	186	7	21	3	2	622	633	6
20	2	0	175	170	8	5	11	0	1002	1002	8	19	3	1	225	230	7	10	12	1	277	267	6	0	4	2	2120	2109	7
22	2	0	335	336	6	7	11	0	97	101	10	21	3	1	373	375	6	12	12	1	279	265	6	2	4	2	659	654	5
1	3	0	420	413	3	9	11	0	189	194	7	0	4	1	960	964	6	14	12	1	85	86	15	4	4	2	118	131	5
3	3	0	508	515	4	11	11	0	469	479	5	2	4	1	62	73	10	16	12	1	767	764	7	6	4	2	225	207	4
5	3	0	4979	4962	8	13	11	0	206	209	7	4	4	1	266	260	3	1	13	1	324	312	5	8	4	2	186	196	5
7	3	0	538	513	4	15	11	0	921	934	7	6	4	1	827	793	6	3	13	1	339	340	5	10	4	2	2151	2183	10
9	3	0	1122	1114	9	17	11	0	491	518	6	8	4	1	514	509	4	5	13	1	1053	1063	8	12	4	2	198	201	6
11	3	0	360	354	4	0	12	0	1372	1412	11	10	4	1	208	182	5	7	13	1	100	97	11	14	4	2	329	328	5
13	3	0	434	430	5	2	12	0	255	259	5	12	4	1	707	717	6	9	13	1	403	412	5	16	4	2	40	41	40
15	3	0	923	934	7	4	12	0	318	314	5	14	4	1	260	259	5	11	13	1	1116	1118	8	18	4	2	554	540	5
17	3	0	916	909	7	6	12	0	664	665	6	16	4	1	672	669	6	13	13	1	102	90	13	20	4	2	353	341	6
19	3	0	280	285	6	8	12	0	234	238	6	18	4	1	225	226	6	15	13	1	231	229	8	1	5	2	1021	989	7
21	3	0	339	332	6	10	12	0	587	588	5	20	4	1	113	109	12	0	14	1	695	710	6	3	5	2	40	8	20
0	4	0	2449	2450	6	12	12	0	559	551	6	1	5	1	104	112	6	2	14	1	292	292	5	5	5	2	1722	1677	8
2	4	0	667	672	5	14	12	0	147	157	9	3	5	1	649	649	4	4	14	1	518	526	5	7	5	2	204	199	5
4	4	0	1179	1177	7	16	12	0	139	136	11	5	5	1	1754	1747	8	6	14	1	194	200	7	9	5	2	456	450	4
6	4	0	3707	3659	8	1	13	0	529	531	5	7	5	1	859	856	6	8	14	1	280	277	6	11	5	2	615	620	5
8	4	0	592	589	5	3	13	0	208	210	6	9	5	1	492	483	5	10	14	1	188	197	8	13	5	2	128	116	8
10	4	0	617	617	5	5	13	0	450	449	5	11	5	1	358	378	4	12	14	1	113	113	12	15	5	2	237	236	6
12	4	0	267	266	5	7	13	0	535	539	5	13	5	1	709	705	6	14	14	1	446	435	6	17	5	2	774	782	6
14	4	0	937	934	7	9	13	0	448	441	5	15	5	1	211	206	6	1	15	1	39	22	39	19	5	2	431	421	6
16	4	0	2048	2047	13	11	13	0	943	953	7	17	5	1	240	242	6	3	15	1	302	307	6	21	5	2	545	511	6
18	4	0	173	168	8	13	13	0	302	313	6	19	5	1	61	81	25	5	15	1	300	296	6	0	6	2	1264	1254	8
20	4	0	282	281	6	15	13	0	272	287	7	21	5	1	847	844	7	7	15	1	300	310	6	2	6	2	54	63	14
22	4	0	386	395	6	0	14	0	1555	1554	12	0	6	1	293	270	3	9	15	1	79	58	17	4	6	2	985	991	7
1	5	0	1543	1531	6	2	14	0	401	404	5	2	6	1	199	193	4	11	15	1	183	170	8	6	6	2	2438	2400	9
3	5	0	60	58	10	4	14	0	235	229	6	4	6	1	350	348	3	13	15	1	143	140	10	8	6	2	213	211	5
5	5	0	3255	3179	8	6	14	0	733	733	6	6	6	1	851	846	6	0	16	1	369	371	5	10	6	2	97	87	10
7	5	0	914	895	7	8	14	0	160	163	8	8	6	1	478	463	4	2	16	1	244	245	6	12	6	2	419	431	5
9	5	0	85	88	9	10	14	0	1413	1422	10	10	6	1	50	18	21	4	16	1	35	57	35	14	6	2	955	959	8
11	5	0	347	365	4	12	14	0	57	52	31	12	6	1	385	380	4	6	16	1	1265	1271	10	16	6	2	1484	1496	11
13	5	0	305	314	5	14	14	0	19	5	19	14	6	1	89	51	11	8	16	1	313	301	6	18	6	2	86	80	15
15	5	0	291	288	5	1	15	0	308	305	5	16	6	1	1087	1087	8	10	16	1	28	12	28	20	6	2	49	43	48
17	5	0	516	467	5	3	15	0	429	439	5	18	6	1	217	223	7	12	16	1	81	94	19	1	7	2	802	787	6
19	5	0	168	170	8	5	15	0	422	426	5	20	6	1	431	431	6	1	17	1	47	6	47	3	7	2	43	49	22
21	5	0	267	291	7	7	15	0	0	30	1	1	7	1	71	64	9	3	17	1	289	286	6	5	7	2	4675	4627	10
0	6	0	981	995	7	9	15	0	208	210	7	3	7	1	574	571	4	5	17	1	781	771	7	7	7	2	155	159	6
2	6	0	156	158	4	11	15	0	382	381	6	5	7	1	486	478	4	7	17	1	292	280	7	9	7	2	558	581	5
4	6	0	423	424	4	13	15	0	493	491	6	7	7	1	173	175	5	9	17	1	475	465	6	11	7	2	102	93	10
6	6	0	564	550	4	0	16	0	572	574	6	9	7	1	519	536	5	0	18	1	264	277	7	13	7	2	420	423	5
8	6	0	649	639	5	2	16	0	191	195	7	11	7	1	0	9	1	2	18	1	70	59	22	15	7	2	1000	1003	7
10	6	0	1433	1442	10	4	16	0	136	133	9	13	7	1	95	98	11	4	18	1	404	403	6	17	7	2	890	898	7
12	6	0	264	263	5	6	16	0	867	881	7	15	7	1	57	45	22	6	18	1	403	390	6	19	7	2	108	116	13
14	6	0	487	481	5	8	16	0	56	49	27	17	7	1	159	166	8	1	19	1	340	342	7	0	8	2	292	302	4
16	6	0	501	503	5	10	16	0	69	29	22	19	7	1	151	152	10	3	19	1	425	420	6	2	8	2	504	494	4
18	6	0	398	400	5	12	16	0	485	481	6	0	8	1	772	770	6	0	0	2	3699	3712	7	4	8	2	269	276	4
20	6	0	0	3	1	1	17	0	265	259	6	2	8	1	40	49	26	2	0	2	691	709	5	6	8	2	440	392	4
1	7	0	718	709	5	3	17	0	300	298	6	4	8	1	100	115	8	4	0	2	459	451	4	8	8	2	679	688	6
3	7	0	244	243	4	5	17	0	1861	1871	15	6	8	1	333	351	4	6	0	2	741	710	5	10	8	2	149	141	7
5	7	0	1638	1623	9	7	17	0	60	52	28	8	8	1	150	158	6	8	0	2	754	748	5	12	8	2	235	234	6
7	7	0	463	463	5	9	17	0	52	44	41	10	8	1	178	148	6	10	0	2	1575	1552	9	14	8	2	622	621	6
9	7	0	1292	1292	10	0	18	0	214	225	8	12	8	1	465	463	5	12	0	2	895	887	6	16	8	2	961	946	7
11	7	0	624	587	5	2	18	0	335	331	6	14	8	1	544	543	5	14	0	2	1396	1418	9	18	8	2	135	132	10
13	7	0	488	484	5	4	18	0	101	91	14	16	8	1	766	768	7	16	0	2	817	816	7	1	9	2	545	538	5
15	7	0	320	321	5	6	18	0	240	254	8	18	8	1	311	307	6	18	0	2	910	905	7	3	9	2	64	47	15
17	7	0	201	196	7	8	18	0	378	367	6	20	8	1	215	217	8	20	0	2	101	95	13	5	9	2	466	465	5
19	7	0	738	747	6	1	19	0	301	294	7	1	9	1	921	909	7	22	0	2	160	177	10	7	9	2	461	452	5
0	8	0	2699	2671	9	3	19	0	90	91	17	3	9	1	183	181	5	1	1	2	609	615	4	9	9	2	639	641	5

Observed and calculated structure factors for K14

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1598	1599	12	16	2	3	1132	1151	8	13	11	3	0	48	1	8	4	4	292	297	5	8	14	4	132	135	11
13	9	2	107	107	11	18	2	3	136	135	10	15	11	3	72	73	21	10	4	4	438	450	5	10	14	4	1116	1121	9
15	9	2	288	296	6	20	2	3	83	70	17	17	11	3	504	501	6	12	4	4	169	159	7	12	14	4	0	20	1
17	9	2	685	670	6	1	3	3	498	482	4	0	12	3	350	356	5	14	4	4	896	906	7	1	15	4	268	262	6
19	9	2	288	285	7	3	3	3	308	302	3	2	12	3	255	261	5	16	4	4	1454	1481	10	3	15	4	437	434	5
0	10	2	4511	4476	11	5	3	3	1184	1153	8	4	12	3	337	341	5	18	4	4	220	215	7	5	15	4	164	169	9
2	10	2	650	651	6	7	3	3	783	762	6	6	12	3	160	151	7	1	5	4	1055	1058	8	7	15	4	171	156	9
4	10	2	762	767	6	9	3	3	259	248	4	8	12	3	120	114	10	3	5	4	177	165	5	9	15	4	190	194	9
6	10	2	63	50	16	11	3	3	1352	1350	9	10	12	3	257	263	6	5	5	4	1528	1581	10	0	16	4	137	141	10
8	10	2	311	310	5	13	3	3	108	116	9	12	12	3	281	271	6	7	5	4	448	444	5	2	16	4	172	177	9
10	10	2	1897	1932	12	15	3	3	62	77	19	14	12	3	170	178	9	9	5	4	79	80	13	4	16	4	70	81	22
12	10	2	318	322	5	17	3	3	218	226	7	16	12	3	478	474	6	11	5	4	918	926	7	6	16	4	500	499	6
14	10	2	394	393	5	19	3	3	150	158	10	1	13	3	207	208	6	13	5	4	150	155	8	8	16	4	0	19	1
16	10	2	167	171	9	21	3	3	423	429	6	3	13	3	445	451	5	15	5	4	278	284	6	1	17	4	341	334	6
18	10	2	330	316	6	0	4	3	2108	2026	8	5	13	3	458	456	5	17	5	4	66	66	22	3	17	4	211	190	8
1	11	2	302	311	5	2	4	3	43	60	19	7	13	3	106	111	11	19	5	4	66	105	26	1	1	5	55	47	18
3	11	2	761	764	6	4	4	3	382	378	4	9	13	3	341	350	6	0	6	4	2174	2211	10	3	1	5	266	271	4
5	11	2	205	210	6	6	4	3	215	209	4	11	13	3	383	395	6	2	6	4	165	182	6	5	1	5	538	528	5
7	11	2	35	15	35	8	4	3	271	278	4	13	13	3	17	51	17	4	6	4	417	420	4	7	1	5	42	35	12
9	11	2	695	703	6	10	4	3	333	311	4	15	13	3	163	139	9	6	6	4	147	151	7	9	1	5	314	319	5
11	11	2	1809	1790	13	12	4	3	789	794	6	0	14	3	49	46	33	8	6	4	346	339	4	11	1	5	274	274	5
13	11	2	22	14	21	14	4	3	99	92	11	2	14	3	253	252	6	10	6	4	1321	1307	10	13	1	5	141	147	8
15	11	2	295	284	6	16	4	3	268	258	6	4	14	3	443	451	5	12	6	4	360	363	5	15	1	5	60	34	23
17	11	2	122	115	12	18	4	3	135	137	10	6	14	3	238	231	6	14	6	4	282	266	6	17	1	5	750	759	7
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2	12	2	46	42	31	1	5	3	78	84	9	10	14	3	47	37	46	18	6	4	307	295	6	0	2	5	546	545	5
4	12	2	146	142	8	3	5	3	421	428	4	12	14	3	0	12	1	1	7	4	273	268	5	2	2	5	68	56	13
6	12	2	929	917	8	5	5	3	1098	1080	7	1	15	3	200	202	7	3	7	4	301	297	4	4	2	5	394	402	4
8	12	2	185	185	7	7	5	3	860	855	6	3	15	3	216	221	7	5	7	4	1440	1456	11	6	2	5	471	475	5
10	12	2	794	804	6	9	5	3	364	366	4	5	15	3	499	484	5	7	7	4	394	382	4	8	2	5	408	400	4
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16	12	2	368	374	6	15	5	3	121	108	10	11	15	3	386	368	6	13	7	4	418	410	5	14	2	5	36	9	35
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3	13	2	105	98	10	19	5	3	129	120	11	2	16	3	96	70	14	17	7	4	319	323	6	18	2	5	149	147	10
5	13	2	1821	1828	13	0	6	3	687	700	6	4	16	3	167	171	9	0	8	4	1913	1960	11	1	3	5	90	93	10
7	13	2	47	46	37	2	6	3	110	94	7	6	16	3	1101	1111	8	2	8	4	73	43	13	3	3	5	186	184	5
9	13	2	130	135	9	4	6	3	564	546	5	8	16	3	239	240	7	4	8	4	295	300	5	5	3	5	441	439	4
11	13	2	93	103	14	6	6	3	1189	1181	8	10	16	3	159	165	10	6	8	4	579	584	5	7	3	5	129	122	8
13	13	2	78	86	18	8	6	3	332	332	4	1	17	3	79	81	18	8	8	4	396	401	5	9	3	5	165	163	7
15	13	2	549	551	6	10	6	3	69	62	14	3	17	3	295	297	6	10	8	4	1196	1218	9	11	3	5	256	263	6
0	14	2	563	554	5	12	6	3	336	331	5	5	17	3	494	488	6	12	8	4	193	192	7	13	3	5	350	342	5
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4	14	2	718	718	6	16	6	3	1152	1148	9	0	18	3	221	226	8	16	8	4	235	207	7	17	3	5	574	571	6
6	14	2	472	470	5	18	6	3	348	355	6	2	18	3	172	174	9	18	8	4	80	81	20	0	4	5	10	17	10
8	14	2	249	249	6	20	6	3	394	387	6	2	0	4	407	410	4	1	9	4	41	51	41	2	4	5	51	11	20
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12	14	2	68	56	22	3	7	3	260	273	4	6	0	4	438	426	4	5	9	4	1701	1730	12	6	4	5	685	678	6
14	14	2	188	403	6	5	7	3	1210	1198	8	8	0	4	315	321	4	7	9	4	489	483	5	8	4	5	364	367	5
1	15	2	644	643	6	7	7	3	202	204	5	10	0	4	2699	2761	11	9	9	4	38	8	37	10	4	5	99	93	10
3	15	2	267	273	6	9	7	3	516	522	5	12	0	4	881	893	7	11	9	4	204	197	7	12	4	5	486	487	5
5	15	2	1516	1507	11	11	7	3	804	800	6	14	0	4	481	472	5	13	9	4	113	97	11	14	4	5	257	259	6
7	15	2	582	577	6	13	7	3	115	116	9	16	0	4	101	107	12	15	9	4	383	387	6	16	4	5	665	677	6
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2	16	2	118	115	11	2	8	3	149	152	7	5	1	4	126	99	6	6	10	4	256	261	5	7	5	5	591	593	5
4	16	2	108	117	12	4	8	3	337	351	4	7	1	4	19	9	18	8	10	4	406	405	5	9	5	5	360	357	5
6	16	2	462	470	5	6	8	3	552	554	5	9	1	4	1308	1305	9	10	10	4	567	561	5	11	5	5	301	307	5
8	16	2	136	100	10	8	8	3	41	18	41	11	1	4	1653	1671	12	12	10	4	185	196	8	13	5	5	477	478	5
10	16	2	710	700	6	10	8	3	25	12	25	13	1	4	106	108	10	14	10	4	908	913	7	15	5	5	134	132	10
1	17	2	197	194	8	12	8	3	584	576	5	15	1	4	132	130	9	16	10	4	451	448	6	17	5	5	187	181	8
3	17	2	421	415	6	14	8	3	324	321	5	17	1	4	47	34	46	1	11	4	247	253	5	0	6	5	234	264	5
5	17	2	218	216	8	16	8	3	281	259	6	19	1	4	578	568	6	3	11	4	361	366	5	2	6	5	114	118	8
7	17	2	53	44	36	18	8	3	145	141	10	0	2	4	256	280	4	5	11	4	1183	1203	9	4	6	5	13	28	13
9	17	2	358	354	6	1	9	3	548	555	5	2	2	4	226	235	4	7	11	4	48	17	30	6	6	5	420	407	4
0	18	2	815	800	7	3	9	3	71	69	14	4	2	4	403	392	4	9	11	4	133	120	9	8	6	5	298	297	5
2	18	2	51	36	43	5	9	3	143	128	7	6	2	4	505	525	4	11	11	4	50	24	33	10	6	5	51	30	25
4	18	2	289	289	7	7	9	3	235	224	5	8	2	4	60	58	16	13	11	4	127	137	11	12	6	5	291	277	6
6	18	2	429	417	6	9	9	3	152	152	7	10	2	4	402	411	4	15	11	4	786	790	7	14	6	5	68	53	21
1	1	3	232	227	3	11	9	3	923	920	7	12	2	4	336	331	5	0	12	4	1023	875	8	16	6	5	740	745	7
3	1	3	716	703	5	13	9	3	0	40	1	14	2	4	631	625	5	2	12	4	274	269	5	1	7	5	44	33	28
5	1	3	359	366	3	15	9	3	61	40	21	16	2	4	753	755	6	4	12	4	192	192	7	3	7	5	462	476	5
7	1	3	262	258	4	17	9	3	534	544	6	18	2	4	40	43	40	6	12	4	322	323	5	5	7	5	83	60	12
9	1	3	344	347	4	0	10	3	925	937	7	20	2	4	106	113	14	8	12	4	278	284	6	7	7	5	292	292	5
11	1	3	1406	1416	11	2	10	3	794	805	6	1	3	4	291	296	4	10	12	4	374	382	6	9	7	5	376	367	5
13	1	3	401	396	4	4	10	3	483	490	5	3	3	4	457	444	4	12	12	4	377	373	6	11	7	5	383	381	5
15	1	3	65	52	17	6	10	3	145	149	7	5	3	4	3421	3474	10	14	12	4	46	58	45	13	7	5	206	203	7
17	1	3	350	348	5	8	10	3	184	190	6	7	3	4	194	188	5	1	13	4	293	295	6	15	7	5	54	37	32
19	1	3	428	449	6	10	10	3	113	94	10	9	3	4	858	869	6	3	13	4	119	127	10	17	7	5	97	94	15
21	1	3	907	890	7	12	10	3	157	163	8	11	3	4	79	80	13	5	13	4	294	297	6	0	8	5	871	862	7
0	2	3	2507	2479	8	14	10	3	690	688	6	13	3	4	386	383	5	7	13	4	320	314	6	2	8	5	134	109	8
2	2	3	540	521	4	16	10	3	82	98	17	15	3	4	789	799	6	9	13	4	440	443	5	4	8	5	0	15	1
4	2	3	133	117	5	1	11	3	362	369	4	17	3	4	700	689	6	11	13	4	767	757	6	6	8	5	574	571	5
6	2	3	1125	1102	7	3	11	3	176	179	6	19	3	4	231	246	8	13	13	4	166	171	9	8	8	5	130	130	9
8	2	3	821	813	6	5	11	3	724	721	6	0	4	4	709	748	5	0	14	4	1478	1497	11	10	8	5	77	81	15
10	2	3	457	466	5	7	11	3	191	183	6	2	4	4	458	450	4	2	14	4	240	238	6	12	8	5	334	336	6
12	2	3	735	733	6	9	11	3	434	435	5	4	4	4	697	713	6	4	14	4	344	343	6	14	8	5	472	468	6
14	2	3	278	271	5	11	11	3	114	110	11	6	4	4	1860	1850	10	6	14	4	488	494	5	16	8	5	805	790	7

Observed and calculated structure factors for K14

h	k	l	10Fo	10Fc	10s
1	9	5	649	658	6
3	9	5	83	94	13
5	9	5	625	626	6
7	9	5	330	324	5
9	9	5	103	96	11
11	9	5	1534	1550	11
13	9	5	83	70	16
15	9	5	59	46	31
0	10	5	1055	1059	8
2	10	5	510	522	5
4	10	5	214	217	6
6	10	5	435	418	5
8	10	5	73	78	17
10	10	5	288	285	6
12	10	5	0	15	1
14	10	5	530	529	6
1	11	5	132	131	9
3	11	5	181	184	5
5	11	5	458	460	5
7	11	5	490	504	5
9	11	5	248	253	7
11	11	5	420	419	6
13	11	5	208	206	8
0	12	5	1170	1196	9
2	12	5	478	480	5
4	12	5	82	81	15
6	12	5	700	703	6
8	12	5	127	116	10
10	12	5	149	148	10
12	12	5	200	216	8
1	13	5	269	271	6
3	13	5	243	250	7
5	13	5	1006	1008	8
7	13	5	194	202	8
9	13	5	166	361	6
11	13	5	1217	1206	9
0	14	5	902	895	8
2	14	5	251	242	7
4	14	5	414	418	6
6	14	5	370	374	6
8	14	5	169	185	9
1	15	5	51	73	45
3	15	5	241	257	7
5	15	5	103	118	14
7	15	5	305	293	7
0	16	5	123	313	6
2	16	5	276	272	7
4	16	5	156	160	10
0	0	6	2717	2729	12
2	0	6	136	134	7
4	0	6	678	684	5
6	0	6	717	710	5
8	0	6	474	478	5
10	0	6	944	965	7
12	0	6	718	715	6
14	0	6	816	819	7
16	0	6	883	894	7
1	1	6	197	200	6
3	1	6	134	130	8
5	1	6	1718	1770	12
7	1	6	93	93	11
9	1	6	411	416	5
11	1	6	235	229	6
13	1	6	0	18	1
15	1	6	479	470	5
17	1	6	275	287	7
0	2	6	1692	1695	11
2	2	6	223	220	5
4	2	6	223	216	5
6	2	6	506	497	5
8	2	6	259	260	6
10	2	6	797	803	6
12	2	6	278	284	6
14	2	6	0	2	1
16	2	6	393	385	6
1	3	6	209	200	6
3	3	6	0	39	1
5	3	6	926	933	7
7	3	6	82	76	13
9	3	6	1097	1122	8
11	3	6	1125	1134	8
13	3	6	308	312	6
15	3	6	127	125	11
17	3	6	336	327	7
0	4	6	2494	2526	12
2	4	6	45	55	10
4	4	6	435	437	5
6	4	6	467	466	5
8	4	6	162	158	7
10	4	6	1442	1443	11
12	4	6	219	212	7
14	4	6	127	118	11
16	4	6	231	231	7
1	5	6	272	277	5
3	5	6	373	365	5
5	5	6	410	405	5
7	5	6	80	84	14
9	5	6	236	237	6
11	5	6	373	369	5
13	5	6	24	19	24
15	5	6	214	217	8
0	6	6	83	74	13
2	6	6	27	25	26
4	6	6	481	492	5
6	6	6	871	876	7
8	6	6	264	268	6
10	6	6	102	39	12
12	6	6	190	198	8
14	6	6	843	842	7
1	7	6	607	630	6
3	7	6	149	150	8
5	7	6	2495	2549	13
7	7	6	68	76	18
9	7	6	463	462	5
11	7	6	437	442	5
13	7	6	261	261	7
15	7	6	680	664	6
0	8	6	219	201	6
2	8	6	220	217	6
4	8	6	353	353	5
6	8	6	261	274	6
8	8	6	415	413	5
10	8	6	71	47	19
12	8	6	233	221	7
14	8	6	448	438	6
1	9	6	391	391	5
3	9	6	108	109	11
5	9	6	11	27	11
7	9	6	520	521	5
9	9	6	436	440	5
11	9	6	742	730	7
13	9	6	65	53	24
0	10	6	2186	2211	14
2	10	6	309	313	6
4	10	6	132	138	6
6	10	6	537	545	6
8	10	6	126	108	10
10	10	6	1319	1325	9
12	10	6	157	164	10
1	11	6	74	56	17
3	11	6	177	172	6
5	11	6	138	142	6
7	11	6	93	95	15
9	11	6	532	521	6
11	11	6	732	737	6
0	12	6	560	553	6
2	12	6	74	83	18
4	12	6	127	140	11
6	12	6	952	951	7
8	12	6	0	47	1
10	12	6	452	432	6
1	13	6	0	13	1
3	13	6	68	58	21
5	13	6	1358	1365	9
7	13	6	176	176	9
0	14	6	85	57	17
2	14	6	188	195	6
4	14	6	315	316	7
6	14	6	148	139	10
1	1	7	70	62	16
3	1	7	265	264	5
5	1	7	48	34	29
7	1	7	260	255	6
9	1	7	188	187	7
11	1	7	755	756	6
13	1	7	292	307	7
15	1	7	84	91	18
0	2	7	782	779	6
2	2	7	315	305	5
4	2	7	29	31	28
6	2	7	461	454	5
8	2	7	327	325	6
10	2	7	180	165	7
12	2	7	540	535	6
14	2	7	120	120	12
1	3	7	179	174	7
3	3	7	0	14	1
5	3	7	440	445	5
7	3	7	450	448	5
9	3	7	202	209	7
11	3	7	790	771	6
13	3	7	0	12	1
0	4	7	941	942	7
2	4	7	120	108	9
4	4	7	268	260	6
6	4	7	63	84	21
8	4	7	216	221	7
10	4	7	198	204	7
12	4	7	482	488	6
14	4	7	114	120	13
1	5	7	0	6	1
3	5	7	230	221	6
5	5	7	417	420	5
7	5	7	510	517	5
9	5	7	277	264	6
11	5	7	75	73	19
13	5	7	325	331	6
0	6	7	311	311	6
2	6	7	108	111	11
4	6	7	257	253	6
6	6	7	672	665	6
8	6	7	229	233	7
10	6	7	85	81	16
12	6	7	231	224	7
1	7	7	47	49	35
3	7	7	258	264	6
5	7	7	720	711	6
7	7	7	137	131	10
9	7	7	394	378	6
11	7	7	485	486	6
0	8	7	455	453	5
2	8	7	102	117	12
4	8	7	270	267	6
6	8	7	322	318	6
8	8	7	82	58	17
10	8	7	21	17	21
1	9	7	347	353	6
3	9	7	29	23	29
5	9	7	126	130	11
7	9	7	143	128	10
9	9	7	59	49	27
0	10	7	637	626	6
2	10	7	448	437	5
4	10	7	236	237	7
6	10	7	165	157	9
8	10	7	82	83	18
1	11	7	190	197	8
3	11	7	124	116	11
5	11	7	513	507	6
7	11	7	123	143	12
0	12	7	141	142	10
2	12	7	182	170	8
4	12	7	228	226	7
0	0	8	2554	2574	14
2	0	8	163	161	8
4	0	8	328	317	6
6	0	8	718	722	6
8	0	8	29	29	29
10	0	8	1528	1504	11
12	0	8	471	454	6
1	1	8	85	100	15
3	1	8	102	87	12
5	1	8	406	404	6
7	1	8	201	200	7
9	1	8	722	716	6
11	1	8	498	511	6
0	2	8	25	32	24
2	2	8	106	101	12
4	2	8	255	244	6
6	2	8	551	527	5
8	2	8	33	14	32
10	2	8	225	219	8
1	3	8	172	159	8
3	3	8	294	304	6
5	3	8	1807	1837	12
7	3	8	35	5	35
9	3	8	479	484	6
11	3	8	125	133	12
0	4	8	112	128	11
2	4	8	301	298	6
4	4	8	286	282	6
6	4	8	597	598	6
8	4	8	90	88	16
10	4	8	234	223	8
1	5	8	568	567	6
3	5	8	157	153	9
5	5	8	457	456	5
7	5	8	0	41	1
9	5	8	124	112	12
0	6	8	1842	1886	15
2	6	8	194	190	8
4	6	8	358	351	6
6	6	8	452	456	6
8	6	8	145	146	10
1	7	8	87	70	15
3	7	8	197	195	8
5	7	8	991	985	8
7	7	8	210	215	8
0	8	8	964	975	8
2	8	8	62	38	26
4	8	8	97	78	14
6	8	8	404	408	6
1	9	8	19	18	18
3	9	8	165	170	9
5	9	8	1193	1213	9
0	10	8	1111	1102	8
2	10	8	113	95	12
1	1	9	53	32	34
3	1	9	219	210	7
5	1	9	214	212	8
0	2	9	22	17	22
2	2	9	36	41	36
4	2	9	181	173	8
6	2	9	0	11	1
1	3	9	123	124	12
3	3	9	46	49	45
5	3	9	0	20	1
0	4	9	387	391	6
2	4	9	30	47	30
4	4	9	83	70	18
1	5	9	45	6	45
3	5	9	119	118	12

Observed and calculated structure factors for K15

h	k	l	10Fo	10Fc	10s
2	0	0	614	628	3
4	0	0	1249	1249	5
6	0	0	749	771	5
8	0	0	860	851	6
10	0	0	4008	3868	10
12	0	0	1399	1433	10
14	0	0	178	173	5
16	0	0	315	329	5
18	0	0	554	546	5
20	0	0	281	277	6
22	0	0	1662	1690	12
1	1	0	666	714	3
3	1	0	159	157	3
5	1	0	580	587	4
7	1	0	523	523	4
9	1	0	1796	1762	8
11	1	0	2957	2913	10
13	1	0	307	312	4
15	1	0	289	294	5
17	1	0	313	318	5
19	1	0	637	642	6
21	1	0	812	816	7
0	2	0	1289	1327	4
2	2	0	230	232	2
4	2	0	708	718	4
6	2	0	150	168	4
8	2	0	300	306	3
10	2	0	675	682	5
12	2	0	297	299	4
14	2	0	868	878	7
16	2	0	712	721	6
18	2	0	0	7	1
20	2	0	172	171	8
22	2	0	306	305	6
1	3	0	269	271	3
3	3	0	543	550	4
7	3	0	516	489	4
9	3	0	1027	1013	7
11	3	0	454	458	4
13	3	0	354	360	4
15	3	0	899	903	6
17	3	0	974	959	7
19	3	0	199	202	7
21	3	0	330	327	6
0	4	0	2272	2359	6
2	4	0	535	544	4
4	4	0	1178	1179	6
6	4	0	3700	3711	8
8	4	0	495	492	4
10	4	0	499	505	4
12	4	0	259	256	4
14	4	0	952	940	7
16	4	0	2118	2073	12
18	4	0	114	111	9
20	4	0	212	209	7
22	4	0	429	432	6
1	5	0	1392	1421	6
3	5	0	46	46	11
5	5	0	3232	3203	8
7	5	0	800	796	6
9	5	0	139	137	5
11	5	0	314	321	4
13	5	0	334	336	4
15	5	0	290	297	5
17	5	0	498	502	5
19	5	0	227	229	6
21	5	0	307	326	6
0	6	0	1060	1077	7
2	6	0	151	157	4
4	6	0	381	395	3
6	6	0	454	437	4
8	6	0	651	634	5
10	6	0	1454	1439	10
12	6	0	273	269	4
14	6	0	444	442	5
16	6	0	438	439	5
18	6	0	376	369	5
20	6	0	32	15	31
1	7	0	706	694	5
3	7	0	84	88	7
5	7	0	1537	1525	8
7	7	0	432	419	4
9	7	0	1321	1302	10
11	7	0	659	628	5
13	7	0	332	334	4
15	7	0	248	247	5
17	7	0	256	257	6
19	7	0	690	700	6
21	7	0	644	645	6
0	8	0	2731	2752	9
2	8	0	138	140	5
4	8	0	426	423	4
6	8	0	537	538	4
8	8	0	498	500	4
10	8	0	1437	1410	9
12	8	0	157	153	6
14	8	0	123	133	8
16	8	0	253	253	5
18	8	0	18	12	17
20	8	0	352	332	6
1	9	0	213	198	4
3	9	0	389	389	4
5	9	0	1935	1956	10
7	9	0	918	904	6
9	9	0	60	73	16
11	9	0	511	496	5
13	9	0	267	265	5
15	9	0	581	589	5
17	9	0	502	510	5
19	9	0	292	287	6
0	10	0	466	490	4
2	10	0	113	110	7
4	10	0	486	498	4
6	10	0	246	219	4
8	10	0	227	239	5
10	10	0	585	585	5
12	10	0	133	142	7
14	10	0	1222	1220	9
16	10	0	287	289	6
18	10	0	492	488	5
1	11	0	285	271	4
3	11	0	309	307	4
5	11	0	1108	1079	7
7	11	0	154	163	6
9	11	0	102	118	9
11	11	0	369	383	5
13	11	0	206	209	6
15	11	0	892	902	7
17	11	0	381	401	6
0	12	0	1527	1570	11
2	12	0	248	249	5
4	12	0	309	311	4
6	12	0	687	683	5
8	12	0	170	174	6
10	12	0	651	649	5
12	12	0	547	535	5
14	12	0	116	119	10
16	12	0	71	77	19
1	13	0	511	508	5
3	13	0	98	103	9
5	13	0	533	532	5
7	13	0	469	471	5
9	13	0	528	524	5
11	13	0	1017	1012	8
13	13	0	281	282	6
15	13	0	229	230	7
0	14	0	1571	1611	12
2	14	0	157	161	5
4	14	0	238	240	5
6	14	0	604	604	5
8	14	0	92	84	11
10	14	0	1387	1394	9
12	14	0	72	90	20
14	14	0	73	38	17
1	15	0	283	274	5
3	15	0	403	406	5
5	15	0	439	450	5
7	15	0	76	6	14
9	15	0	164	162	8
11	15	0	367	369	6
13	15	0	403	408	6
0	16	0	610	625	5
2	16	0	146	139	8
4	16	0	211	213	6
6	16	0	928	924	7
8	16	0	30	11	30
10	16	0	46	39	45
12	16	0	434	442	6
1	17	0	197	190	7
3	17	0	256	250	6
5	17	0	1942	1971	16
7	17	0	58	22	23
9	17	0	77	72	17
0	18	0	182	195	8
2	18	0	235	245	7
4	18	0	126	126	10
6	18	0	216	214	7
8	18	0	293	283	6
1	19	0	223	210	7
3	19	0	40	11	39
1	1	1	180	166	2
3	1	1	444	443	3
5	1	1	669	676	4
7	1	1	45	15	12
9	1	1	340	343	3
11	1	1	957	967	6
13	1	1	336	330	4
15	1	1	41	30	31
17	1	1	720	731	6
19	1	1	384	397	5
21	1	1	965	944	7
0	2	1	258	215	3
2	2	1	508	535	4
4	2	1	438	444	3
6	2	1	138	128	4
8	2	1	600	608	4
10	2	1	409	424	4
12	2	1	992	1000	7
14	2	1	84	82	10
16	2	1	814	815	6
18	2	1	0	32	1
20	2	1	178	181	7
22	2	1	184	188	8
1	3	1	125	329	3
3	3	1	237	232	3
5	3	1	249	237	3
7	3	1	508	504	4
9	3	1	258	264	3
11	3	1	275	287	4
13	3	1	265	275	4
15	3	1	38	22	37
17	3	1	319	317	5
19	3	1	202	207	7
21	3	1	172	171	6
0	4	1	897	896	6
2	4	1	98	103	5
4	4	1	246	242	3
6	4	1	872	850	6
8	4	1	493	482	4
10	4	1	207	181	4
12	4	1	713	719	6
14	4	1	212	212	5
16	4	1	721	716	6
18	4	1	248	245	6
20	4	1	94	91	13
1	5	1	90	97	6
3	5	1	456	461	4
5	5	1	1769	1716	8
7	5	1	943	941	7
9	5	1	504	484	4
11	5	1	386	413	4
13	5	1	534	543	5
15	5	1	154	162	7
17	5	1	223	229	6
19	5	1	58	63	22
21	5	1	813	797	7
0	6	1	293	270	3
2	6	1	163	154	3
4	6	1	238	232	3
6	6	1	940	929	7
8	6	1	449	439	4
10	6	1	40	34	27
12	6	1	385	377	4
14	6	1	44	36	24
16	6	1	1116	1113	8
18	6	1	250	243	6
20	6	1	412	421	5
1	7	1	122	121	5
3	7	1	574	566	4
5	7	1	381	374	4
7	7	1	189	184	4
9	7	1	444	457	4
11	7	1	51	4	18
13	7	1	88	79	10
15	7	1	88	47	11
17	7	1	171	168	7
19	7	1	115	108	11
0	8	1	883	857	6
2	8	1	47	34	15
4	8	1	76	79	9
6	8	1	360	363	4
8	8	1	125	135	7
10	8	1	183	178	6
12	8	1	527	526	5
14	8	1	501	504	5
16	8	1	811	797	6
18	8	1	323	324	6
20	8	1	226	229	7
1	9	1	952	943	6
3	9	1	135	131	6
5	9	1	461	486	4
7	9	1	406	398	4
9	9	1	102	112	8
11	9	1	1761	1775	12
13	9	1	60	47	16
15	9	1	72	60	14
17	9	1	212	209	7
19	9	1	102	122	12
0	10	1	1253	1279	8
2	10	1	750	746	5
4	10	1	260	266	4
6	10	1	466	468	4
8	10	1	150	150	6
10	10	1	275	267	5
12	10	1	52	4	19
14	10	1	593	583	5
16	10	1	303	324	6
18	10	1	269	266	6
1	11	1	229	234	4
3	11	1	263	256	4
5	11	1	587	601	5
7	11	1	539	537	5
9	11	1	324	322	5
11	11	1	428	426	5
13	11	1	130	131	8
15	11	1	58	49	21
17	11	1	435	426	5
0	12	1	1190	1206	6
2	12	1	497	494	4
4	12	1	84	84	10
6	12	1	680	674	6
8	12	1	142	140	7
10	12	1	256	255	5
12	12	1	316	310	5
14	12	1	61	59	19
16	12	1	798	800	6
1	13	1	355	354	4
3	13	1	357	362	4
5	13	1	1004	1008	7
7	13	1	132	116	7
9	13	1	342	345	5
11	13	1	1116	1106	8
13	13	1	125	116	9
15	13	1	266	253	6
0	14	1	629	661	6
2	14	1	261	269	5
4	14	1	409	417	5
6	14	1	280	280	5
8	14	1	274	273	6
10	14	1	158	167	8
12	14	1	170	172	8
14	14	1	380	369	6
1	15	1	0	12	1
3	15	1	265	268	5
5	15	1	350	355	5
7	15	1	361	361	5
9	15	1	83	67	14
11	15	1	168	169	8
13	15	1	133	136	10
0	16	1	319	323	5
2	16	1	276	267	6
4	16	1	20	31	20
6	16	1	1287	1273	10
8	16	1	274	280	6
10	16	1	0	34	1
12	16	1	128	130	10
1	17	1	97	85	11
3	17	1	313	310	6
5	17	1	675	691	6
7	17	1	241	227	7
9	17	1	392	394	6
0	18	1	208	229	7
2	18	1	70	74	17
4	18	1	331	336	6
6	18	1	338	335	6
8	18	1	50	11	35
1	19	1	351	350	6
3	19	1	392	391	6
0	0	2	3534	3617	7
2	0	2	517	545	4
4	0	2	458	455	3
6	0	2	707	662	5
8	0	2	505	487	4
10	0	2	1499	1466	9
12	0	2	915	918	6
14	0	2	1334	1348	9
16	0	2	764	773	6
18	0	2	750	743	6
20	0	2	41	64	41
22	0	2	272	284	6
1	1	2	451	456	3
3	1	2	738	734	5
5	1	2	1243	1248	7
7	1	2	165	163	4
9	1	2	664	671	5
11	1	2	548	541	5
13	1	2	89	87	10
15	1	2	683	700	6
17	1	2	74	55	14
19	1	2	0	13	1
21	1	2	260	249	6
0	2	2	4248	4210	7
2	2	2	299	302	3
4	2	2	451	451	4
6	2	2	177	364	3
8	2	2	255	244	3
10	2	2	1377	1354	9
12	2	2	571	571	5
14	2	2	128	134	7
16	2	2	104	299	5
18	2	2	51	33	24
20	2	2	0	7	1
1	3	2	389	386	3
3	3	2	143	349	3
5	3	2	1216	1221	7
7	3	2	97	83	6
9	3	2	1676	1681	9
11	3	2	1451	1460	10
13	3	2	436	437	5
15	3	2	179	169	6
17	3	2	321	325	5
19	3	2	825	836	6
21	3	2	596	607	6
0	4	2	2211	2206	7
2	4	2	653	662	5
4	4	2	70	17	7
6	4	2	560	427	4
8	4	2	151	165	5
10	4	2	2176	2167	10
12	4	2	294	291	4
14	4	2	262	266	5
16	4	2	110	116	9
18	4	2	502	498	5
20	4	2	321	320	6
1	5	2	1051	1030	7
3	5	2	151	156	4
5	5	2	1849	1804	8
7	5	2	190	162	4
9	5	2	476	480	4
11	5	2	655	656	5
13	5	2	33	5	32
15	5	2	273	274	5
17	5	2	728	731	6
19	5	2	440	431	5
21	5	2	449	440	6
0	6	2	1211	1213	8
2	6	2	186	201	4
4	6	2	1105	1095	7
6	6	2	2449	2373	9
8	6	2	299	291	4
10	6	2	20	18	20
12	6	2	153	352	4
14	6	2	995	1004	7
16	6	2	1526	1518	10
18	6	2	61	35	20
20	6	2	105	112	12
1	7	2	623	621	5
3	7	2	55	13	12
5	7	2	4878	4691	11
7	7	2	227	224	4
9	7	2	516	524	5
11	7	2	57	49	17
13	7	2	327	327	5
15	7	2	969	979	7
17	7	2	972	974	7
19	7	2	60	41	23
0	8	2	311	311	3
2	8	2	193	190	4
4	8	2	246	261	4
6	8	2	426	411	4
8	8	2	572	565	5
10	8	2	88	79	10
12	8	2	165	159	6
14	8	2	632	628	5
16	8	2	903	914	7
18	8	2	95	71	13
1	9	2	497	481	4
3	9	2	31	32	30
5	9	2	451	454	4
7	9	2	408	402	4

Observed and calculated structure factors for K15

h	k	l	10Fo	10Fc	10s
9	9	2	700	705	5
11	9	2	1604	1604	12
13	9	2	101	105	10
15	9	2	312	314	5
17	9	2	631	636	5
19	9	2	291	283	6
0	10	2	4638	4592	11
2	10	2	691	685	5
4	10	2	753	749	6
6	10	2	54	26	17
8	10	2	236	239	5
10	10	2	1949	1944	12
12	10	2	354	350	5
14	10	2	353	358	5
16	10	2	143	151	9
18	10	2	264	245	6
1	11	2	337	339	4
3	11	2	670	663	5
5	11	2	216	210	5
7	11	2	33	31	33
9	11	2	734	727	6
11	11	2	1805	1814	13
13	11	2	38	26	38
15	11	2	203	203	7
17	11	2	62	50	21
0	12	2	1371	1383	9
2	12	2	27	26	26
4	12	2	82	52	11
6	12	2	834	826	6
8	12	2	153	161	7
10	12	2	829	833	6
12	12	2	223	220	6
14	12	2	521	520	5
16	12	2	374	370	6
1	13	2	121	123	8
3	13	2	79	78	11
5	13	2	1931	1953	12
7	13	2	76	63	13
9	13	2	121	128	9
11	13	2	46	20	33
13	13	2	116	116	10
15	13	2	537	539	5
0	14	2	491	488	5
2	14	2	255	255	5
4	14	2	777	792	6
6	14	2	484	485	5
8	14	2	146	152	8
10	14	2	154	160	8
12	14	2	69	77	19
14	14	2	443	462	6
1	15	2	537	536	5
3	15	2	316	316	5
5	15	2	1544	1550	11
7	15	2	473	465	5
9	15	2	117	112	10
11	15	2	359	350	6
13	15	2	144	143	10
0	16	2	1022	1036	8
2	16	2	136	127	8
4	16	2	93	96	12
6	16	2	376	366	5
8	16	2	77	87	16
10	16	2	744	738	6
1	17	2	216	207	7
3	17	2	344	341	6
5	17	2	225	223	7
7	17	2	41	18	41
9	17	2	414	406	6
0	18	2	846	843	7
2	18	2	36	38	36
4	18	2	247	264	7
6	18	2	439	436	6
1	1	3	266	260	3
3	1	3	623	620	5
5	1	3	338	344	3
7	1	3	347	348	3
9	1	3	294	304	4
11	1	3	1475	1473	10
13	1	3	406	413	4
15	1	3	119	99	8
17	1	3	140	352	5
19	1	3	374	389	5
21	1	3	916	902	7
0	2	3	2477	2435	8
2	2	3	610	598	4
4	2	3	92	79	6
6	2	3	1207	1189	8
8	2	3	702	693	5
10	2	3	429	436	4
12	2	3	758	754	6
14	2	3	282	281	5
16	2	3	1177	1181	9
18	2	3	202	208	7
20	2	3	113	114	11
1	3	3	533	532	4
3	3	3	246	246	3
5	3	3	1143	1116	8
7	3	3	757	748	6
9	3	3	218	206	4
11	3	3	1345	1359	9
13	3	3	77	66	11
15	3	3	88	102	11
17	3	3	251	250	6
19	3	3	143	138	9
21	3	3	435	430	6
0	4	3	2051	1983	8
2	4	3	51	41	12
4	4	3	363	363	3
6	4	3	168	166	5
8	4	3	262	269	4
10	4	3	338	318	4
12	4	3	773	787	6
14	4	3	71	69	13
16	4	3	289	294	5
18	4	3	145	155	9
20	4	3	30	38	29
1	5	3	98	92	6
3	5	3	307	307	3
5	5	3	1054	1038	7
7	5	3	912	919	7
9	5	3	379	379	4
11	5	3	219	209	5
13	5	3	407	402	5
15	5	3	124	75	8
17	5	3	294	296	5
19	5	3	108	95	11
0	6	3	668	662	5
2	6	3	122	114	5
4	6	3	461	445	4
6	6	3	1228	1225	8
8	6	3	101	105	4
10	6	3	96	99	9
12	6	3	334	334	4
14	6	3	66	53	15
16	6	3	1177	1183	8
18	6	3	366	367	5
20	6	3	388	381	6
1	7	3	177	159	5
3	7	3	261	273	4
5	7	3	1131	1106	8
7	7	3	174	183	5
9	7	3	456	459	4
11	7	3	790	790	6
13	7	3	117	116	8
15	7	3	144	156	8
17	7	3	586	588	5
19	7	3	67	77	21
0	8	3	699	689	5
2	8	3	94	92	8
4	8	3	330	322	4
6	8	3	537	535	5
8	8	3	35	24	35
10	8	3	35	27	35
12	8	3	619	621	5
14	8	3	303	305	5
16	8	3	299	281	6
18	8	3	174	162	8
1	9	3	571	571	5
3	9	3	83	84	10
5	9	3	244	237	5
7	9	3	296	297	4
9	9	3	150	125	6
11	9	3	936	956	7
13	9	3	25	15	25
15	9	3	70	76	16
17	9	3	548	555	5
0	10	3	815	834	7
2	10	3	722	736	6
4	10	3	364	363	4
6	10	3	222	206	5
8	10	3	200	203	6
10	10	3	83	62	12
12	10	3	125	113	9
14	10	3	557	560	5
16	10	3	92	101	14
1	11	3	334	339	4
3	11	3	189	189	6
5	11	3	650	643	5
7	11	3	235	232	5
9	11	3	379	376	5
11	11	3	158	164	7
13	11	3	48	37	10
15	11	3	100	92	13
17	11	3	523	517	6
0	12	3	335	325	4
2	12	3	285	285	5
4	12	3	338	335	5
6	12	3	163	174	7
8	12	3	57	63	19
10	12	3	247	247	6
12	12	3	308	305	6
14	12	3	135	151	9
16	12	3	522	508	5
1	13	3	238	242	5
3	13	3	452	454	5
5	13	3	393	401	5
7	13	3	75	87	14
9	13	3	274	273	6
11	13	3	391	390	5
13	13	3	27	15	26
15	13	3	158	158	9
0	14	3	26	19	26
2	14	3	218	220	6
4	14	3	347	354	5
6	14	3	166	170	7
8	14	3	315	316	6
10	14	3	34	4	34
12	14	3	65	42	19
1	15	3	178	180	7
3	15	3	207	209	7
5	15	3	547	560	5
7	15	3	229	222	6
9	15	3	112	108	11
11	15	3	395	385	6
0	16	3	199	195	7
2	16	3	118	111	10
4	16	3	186	187	7
6	16	3	1135	1135	9
8	16	3	243	240	7
10	16	3	153	134	9
1	17	3	149	159	9
3	17	3	329	321	6
5	17	3	429	426	6
7	17	3	37	23	37
0	18	3	261	268	7
2	18	3	170	181	8
4	18	3	167	159	9
0	0	4	6800	6819	11
2	0	4	353	361	4
4	0	4	688	700	5
6	0	4	291	284	4
8	0	4	240	251	4
10	0	4	2792	2779	11
12	0	4	952	962	7
14	0	4	333	340	5
16	0	4	71	83	16
18	0	4	539	520	5
20	0	4	164	164	9
1	1	4	230	229	4
3	1	4	123	115	5
5	1	4	203	181	4
7	1	4	88	80	9
9	1	4	1298	1325	8
11	1	4	1644	1656	11
13	1	4	157	158	7
15	1	4	222	206	6
17	1	4	43	9	42
19	1	4	572	578	6
0	2	4	312	337	4
2	2	4	146	146	5
4	2	4	447	448	4
6	2	4	440	460	4
8	2	4	120	121	7
10	2	4	437	464	5
12	2	4	317	312	4
14	2	4	649	655	5
16	2	4	727	728	6
18	2	4	0	7	1
20	2	4	135	120	10
1	3	4	192	182	4
3	3	4	456	454	4
5	3	4	3503	3522	10
7	3	4	163	162	5
9	3	4	763	782	6
11	3	4	168	170	6
13	3	4	116	120	5
15	3	4	781	773	6
17	3	4	734	736	6
19	3	4	166	178	8
0	4	4	646	683	5
2	4	4	362	351	4
4	4	4	697	719	5
6	4	4	1929	1882	10
8	4	4	206	217	5
10	4	4	345	353	4
12	4	4	154	155	7
14	4	4	893	897	7
16	4	4	1478	1497	11
18	4	4	158	159	8
1	5	4	964	968	7
3	5	4	151	138	5
5	5	4	1565	1600	10
7	5	4	366	365	4
9	5	4	144	138	6
11	5	4	875	878	7
13	5	4	157	172	7
15	5	4	297	294	5
17	5	4	98	109	11
19	5	4	162	160	9
0	6	4	2265	2281	10
2	6	4	169	179	5
4	6	4	383	382	4
6	6	4	246	248	4
8	6	4	351	346	4
10	6	4	1313	1311	9
12	6	4	363	370	5
14	6	4	255	246	6
16	6	4	119	122	10
18	6	4	271	269	6
1	7	4	287	259	4
3	7	4	159	153	6
5	7	4	1351	1388	11
7	7	4	347	341	4
9	7	4	1011	1022	7
11	7	4	805	792	6
13	7	4	275	275	5
15	7	4	218	233	6
17	7	4	365	375	6
0	8	4	1966	2035	11
2	8	4	0	8	1
4	8	4	193	190	5
6	8	4	494	484	5
8	8	4	373	389	4
10	8	4	1209	1225	9
12	8	4	82	83	12
14	8	4	120	110	9
16	8	4	183	196	8
18	8	4	70	47	19
1	9	4	125	114	7
3	9	4	270	267	4
5	9	4	1795	1810	12
7	9	4	504	516	5
9	9	4	38	7	37
11	9	4	166	117	7
13	9	4	102	110	11
15	9	4	417	415	5
17	9	4	599	592	6
0	10	4	981	992	7
2	10	4	125	128	7
4	10	4	539	543	5
6	10	4	261	258	5
8	10	4	262	255	5
10	10	4	506	502	5
12	10	4	178	191	7
14	10	4	929	933	7
16	10	4	427	420	6
1	11	4	148	145	7
3	11	4	350	350	5
5	11	4	1240	1263	9
7	11	4	62	65	17
9	11	4	78	72	13
11	11	4	56	60	21
13	11	4	136	130	9
15	11	4	773	755	6
0	12	4	973	974	7
2	12	4	251	252	5
4	12	4	182	193	6
6	12	4	325	324	5
8	12	4	215	215	6
10	12	4	421	422	5
12	12	4	361	354	6
14	12	4	49	39	36
1	13	4	280	279	5
3	13	4	47	51	27
5	13	4	356	352	5
7	13	4	267	270	6
9	13	4	509	498	5
11	13	4	786	792	7
13	13	4	140	154	9
0	14	4	1523	1520	11
2	14	4	202	204	6
4	14	4	337	342	5
6	14	4	404	398	5
8	14	4	90	64	13
10	14	4	1109	1094	8
12	14	4	62	51	22
1	15	4	234	229	6
3	15	4	397	395	5
5	15	4	192	185	7
7	15	4	130	118	10
9	15	4	153	156	9
0	16	4	194	181	7
2	16	4	138	139	9
4	16	4	152	145	9
6	16	4	540	533	6
8	16	4	63	40	22
1	17	4	275	279	6
3	17	4	162	155	9
5	17	4	1482	1468	11
1	1	5	78	72	9
3	1	5	212	213	5
5	1	5	552	544	5
7	1	5	28	32	27
9	1	5	300	300	4
11	1	5	329	328	5
13	1	5	164	179	7
15	1	5	0	5	1
17	1	5	723	734	6
19	1	5	294	307	6
0	2	5	574	563	5
2	2	5	122	111	7
4	2	5	425	433	4
6	2	5	393	389	4
8	2	5	312	307	4
10	2	5	166	172	6
12	2	5	773	787	6
14	2	5	29	13	29
16	2	5	361	349	5
18	2	5	81	73	16
1	3	5	107	125	7
3	3	5	210	205	5
5	3	5	475	484	4
7	3	5	117	124	7
9	3	5	108	103	8
11	3	5	250	248	5
13	3	5	281	283	5
15	3	5	0	37	1
17	3	5	530	514	5
0	4	5	19	9	19
2	4	5	73	69	11
4	4	5	106	111	8
6	4	5	715	703	6
8	4	5	332	345	4
10	4	5	107	88	9
12	4	5	475	491	5
14	4	5	223	215	6
16	4	5	710	713	6
18	4	5	254	262	7
1	5	5	150	145	6
3	5	5	246	254	5
5	5	5	850	847	6
7	5	5	636	638	6
9	5	5	349	354	5
11	5	5	342	339	5
13	5	5	349	357	5
15	5	5	116	108	10
17	5	5	167	161	8
0	6	5	255	282	4
2	6	5	89	80	9
4	6	5	55	42	16
6	6	5	461	457	4
8	6	5	297	302	5
10	6	5	0	13	1
12	6	5	280	270	5
14	6	5	59	49	20
16	6	5	766	776	6
1	7	5	85	76	9
3	7	5	462	466	5
5	7	5	43	8	28
7	7	5	300	302	5
9	7	5	297	302	5
11	7	5	368	369	5
13	7	5	196	175	6
15	7	5	43	41	43
17	7	5	76	79	18
0	8	5	918	918	7
2	8	5	156	149	6
4	8	5	57	36	17
6	8	5	585	576	5
8	8	5	112	117	9

Observed and calculated structure factors for K15

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
10	8	5	110	116	10	1	1	6	122	112	7	4	8	6	342	133	5	13	3	7	24	28	24	5	1	8	444	447	5
12	8	5	375	377	5	3	1	6	152	148	6	6	8	6	271	271	5	0	4	7	924	910	7	7	1	8	156	162	8
14	8	5	444	434	5	5	1	6	1747	1777	12	8	8	6	334	338	5	2	4	7	100	78	10	9	1	8	710	702	6
16	8	5	822	815	6	7	1	6	67	67	14	10	8	6	76	88	15	4	4	7	258	247	5	11	1	8	503	503	5
1	9	5	673	681	6	9	1	6	174	170	5	12	8	6	162	167	8	6	4	7	48	59	28	0	2	8	44	12	39
3	9	5	79	51	11	11	1	6	289	283	5	14	8	6	439	434	6	8	4	7	204	199	6	2	2	8	68	57	16
5	9	5	573	557	5	13	1	6	42	40	42	1	9	6	358	351	5	10	4	7	212	205	7	4	2	8	256	264	6
7	9	5	383	382	5	15	1	6	440	445	5	3	9	6	118	121	9	12	4	7	472	475	5	6	2	8	497	485	5
9	9	5	80	96	13	17	1	6	345	331	6	5	9	6	0	28	1	14	4	7	101	91	12	8	2	8	56	48	24
11	9	5	1555	1583	11	0	2	6	1724	1733	11	7	9	6	468	474	5	1	5	7	46	2	24	10	2	8	256	242	6
13	9	5	101	112	12	2	2	6	180	179	5	9	9	6	471	473	5	3	5	7	164	162	7	1	3	8	102	94	10
15	9	5	91	82	14	4	2	6	171	164	6	11	9	6	758	739	6	5	5	7	394	405	5	3	3	8	301	314	6
0	10	5	1002	1005	8	6	2	6	451	457	5	13	9	6	39	42	38	7	5	7	538	543	5	5	3	8	1859	1831	14
2	10	5	472	488	5	8	2	6	225	229	5	0	10	6	2276	2273	13	9	5	7	265	270	6	7	3	8	0	17	1
4	10	5	118	123	9	10	2	6	803	819	6	2	10	6	327	329	5	11	5	7	85	92	14	9	3	8	434	429	5
6	10	5	492	481	5	12	2	6	111	112	5	4	10	6	318	319	5	13	5	7	239	238	7	11	3	8	86	74	14
8	10	5	96	116	11	14	2	6	18	31	18	6	10	6	470	476	5	0	6	7	292	284	5	0	4	8	164	159	7
10	10	5	270	270	6	16	2	6	162	160	6	8	10	6	64	61	19	2	6	7	113	121	9	2	4	8	239	241	6
12	10	5	64	60	19	1	3	6	199	194	5	10	10	6	1324	1319	10	4	6	7	187	200	7	4	4	8	289	271	6
14	10	5	452	446	5	3	3	6	134	141	7	12	10	6	194	191	8	6	6	7	680	680	6	6	4	8	653	626	6
1	11	5	106	99	9	5	3	6	871	879	7	1	11	6	64	72	18	8	6	7	216	215	6	8	4	8	10	32	29
3	11	5	212	216	6	7	3	6	44	25	26	3	11	6	316	312	5	10	6	7	123	105	10	10	4	8	231	165	7
5	11	5	417	413	5	9	3	6	1106	1115	8	5	11	6	346	353	5	12	6	7	227	226	7	1	5	8	513	519	5
7	11	5	535	525	5	11	3	6	1116	1129	8	7	11	6	64	80	21	1	7	7	78	73	13	3	5	8	136	140	9
9	11	5	222	215	6	13	3	6	212	218	7	9	11	6	514	517	6	3	7	7	238	242	6	5	5	8	465	461	5
11	11	5	441	436	5	15	3	6	76	72	16	11	11	6	751	750	6	5	7	7	652	651	6	7	5	8	38	1	38
13	11	5	190	188	8	17	3	6	154	146	6	0	12	6	517	526	5	7	7	7	122	118	9	9	5	8	153	148	9
0	12	5	1128	1143	8	0	4	6	2496	2542	12	2	12	6	56	22	24	9	7	7	335	332	6	0	6	8	1884	1893	14
2	12	5	493	485	5	2	4	6	57	60	16	4	12	6	91	76	13	11	7	7	466	480	6	2	6	8	191	192	7
4	12	5	66	74	17	4	4	6	141	146	4	6	12	6	898	893	7	0	8	7	412	412	5	4	6	8	312	324	6
6	12	5	704	697	6	6	4	6	615	580	5	8	12	6	53	43	28	2	8	7	80	77	13	6	6	8	495	504	5
8	12	5	77	86	15	8	4	6	113	124	9	10	12	6	453	446	6	4	8	7	259	248	6	8	6	8	163	162	8
10	12	5	136	143	9	10	4	6	1430	1422	10	1	13	6	29	30	29	6	8	7	316	300	6	1	7	8	56	54	23
12	12	5	251	255	7	12	4	6	267	264	6	3	13	6	88	66	14	8	8	7	18	25	18	3	7	8	106	99	11
1	13	5	314	306	5	14	4	6	112	87	10	5	13	6	1479	1453	10	10	8	7	25	9	25	5	7	8	954	950	8
3	13	5	258	264	6	16	4	6	282	284	6	7	13	6	183	179	8	1	9	7	358	369	5	7	7	8	178	195	8
5	13	5	965	970	7	1	5	6	285	294	5	0	14	6	40	38	39	3	9	7	61	19	20	0	8	8	1014	1013	7
7	13	5	210	207	7	3	5	6	261	261	5	2	14	6	313	314	6	5	9	7	170	188	8	2	8	8	63	36	20
9	13	5	309	308	6	5	5	6	460	461	5	4	14	6	368	367	6	7	9	7	154	169	9	4	8	8	0	20	1
11	13	5	1196	1188	8	7	5	6	100	96	10	6	14	6	183	171	8	9	9	7	60	31	22	6	8	8	314	337	6
0	14	5	853	852	7	9	5	6	278	269	5	1	1	7	83	77	11	0	10	7	546	555	5	1	9	8	49	14	14
2	14	5	234	231	6	11	5	6	331	337	5	3	1	7	227	228	5	2	10	7	395	405	5	3	9	8	142	141	9
4	14	5	327	337	6	13	5	6	107	108	11	5	1	7	38	28	38	4	10	7	172	166	7	5	9	8	1248	1235	9
6	14	5	429	433	6	15	5	6	237	244	7	7	1	7	293	292	5	6	10	7	200	188	7	0	10	8	1084	1091	8
8	14	5	201	191	7	0	6	6	113	108	8	9	1	7	171	169	7	8	10	7	107	98	11	2	10	8	177	166	8
10	14	5	223	226	7	2	6	6	58	38	16	11	1	7	796	787	6	1	11	7	178	182	7	1	1	9	54	51	25
1	15	5	101	103	12	4	6	6	531	534	5	13	1	7	312	315	6	3	11	7	115	108	10	3	1	9	156	161	8
3	15	5	223	218	7	6	6	6	849	858	6	15	1	7	115	116	11	5	11	7	461	458	5	5	1	9	217	211	7
5	15	5	165	152	8	8	6	6	299	302	5	0	2	7	758	759	6	7	11	7	171	171	9	0	2	9	43	17	42
7	15	5	134	130	6	10	6	6	96	91	11	2	2	7	328	331	5	0	12	7	122	124	10	2	2	9	74	79	17
0	16	5	262	261	6	12	6	6	161	154	8	4	2	7	28	11	27	2	12	7	184	186	8	4	2	9	189	189	8
2	16	5	288	279	6	14	6	6	850	841	7	6	2	7	500	498	5	4	12	7	232	229	7	6	2	9	13	16	13
4	16	5	134	132	10	1	7	6	531	532	5	8	2	7	280	274	5	1	13	7	185	181	8	1	3	9	150	148	9
0	0	6	2620	2668	11	3	7	6	167	167	6	10	2	7	148	151	8	0	0	8	2523	2572	14	3	3	9	56	12	26
2	0	6	62	52	14	5	7	6	2524	2555	13	12	2	7	547	541	5	2	0	8	142	135	8	5	3	9	59	19	23
4	0	6	665	674	5	7	7	6	116	123	9	14	2	7	139	135	9	4	0	8	245	246	6	0	4	9	166	163	6
6	0	6	709	725	6	9	7	6	404	404	5	1	3	7	191	194	6	6	0	8	630	637	6	2	4	9	64	61	21
8	0	6	316	320	5	11	7	6	364	357	5	3	3	7	0	22	1	8	0	8	50	21	29	4	4	9	79	67	15
10	0	6	914	915	7	13	7	6	199	190	7	5	3	7	421	418	5	10	0	8	1494	1493	10	1	5	9	14	6	14
12	0	6	716	732	6	15	7	6	654	650	6	7	3	7	439	445	5	12	0	8	506	502	6	3	5	9	71	68	19
14	0	6	778	782	6	0	8	6	243	226	5	9	3	7	179	175	7	1	1	8	92	92	11						
16	0	6	853	860	7	2	8	6	170	161	6	11	3	7	779	771	6	3	1	8	135	132	8						

Observed and calculated structure factors for K16

h	k	l	10Fo	10Fc	10s
2	0	0	611	629	4
4	0	0	1458	1471	5
6	0	0	535	553	4
8	0	0	1112	1088	8
10	0	0	3737	3793	10
12	0	0	1326	1348	10
14	0	0	353	344	4
16	0	0	283	272	5
18	0	0	823	803	7
20	0	0	299	295	6
22	0	0	1472	1494	11
1	1	0	691	718	3
3	1	0	400	384	3
5	1	0	707	709	5
7	1	0	411	407	3
9	1	0	1722	1729	8
11	1	0	2875	2862	10
13	1	0	188	199	6
15	1	0	160	152	7
17	1	0	269	276	6
19	1	0	642	639	6
21	1	0	768	766	7
0	2	0	1150	1199	4
2	2	0	348	358	3
4	2	0	634	654	5
6	2	0	95	46	6
8	2	0	209	213	4
10	2	0	591	602	5
12	2	0	294	296	4
14	2	0	836	841	6
16	2	0	739	747	6
18	2	0	140	130	9
20	2	0	191	191	8
22	2	0	360	348	6
1	3	0	476	460	4
3	3	0	452	460	4
5	3	0	4884	4953	8
7	3	0	501	477	4
9	3	0	1179	1171	9
11	3	0	316	308	4
13	3	0	490	494	5
15	3	0	914	925	7
17	3	0	887	893	7
19	3	0	296	294	6
21	3	0	363	350	6
0	4	0	2486	2531	6
2	4	0	730	734	5
4	4	0	1239	1233	7
6	4	0	1580	1586	9
8	4	0	674	665	5
10	4	0	672	680	5
12	4	0	287	293	5
14	4	0	965	980	7
16	4	0	1974	1976	13
18	4	0	234	227	6
20	4	0	357	341	6
1	5	0	1602	1587	7
3	5	0	85	78	7
5	5	0	1238	1196	8
7	5	0	928	911	7
9	5	0	86	97	10
11	5	0	371	392	4
13	5	0	322	322	5
15	5	0	308	307	5
17	5	0	413	419	5
19	5	0	149	144	9
21	5	0	237	247	8
0	6	0	1017	1010	7
2	6	0	108	105	6
4	6	0	422	426	4
6	6	0	589	567	4
8	6	0	631	622	5
10	6	0	1429	1435	10
12	6	0	311	308	5
14	6	0	461	468	5
16	6	0	519	513	5
18	6	0	418	414	5
20	6	0	91	16	16
1	7	0	796	775	5
3	7	0	291	300	3
5	7	0	1694	1668	9
7	7	0	471	456	4
9	7	0	1334	1336	10
11	7	0	581	545	5
13	7	0	566	575	5
15	7	0	336	334	5
17	7	0	152	149	8
19	7	0	794	787	7
0	8	0	2697	2699	9
2	8	0	190	187	4
4	8	0	612	609	5
6	8	0	651	666	5
8	8	0	525	529	5
10	8	0	1436	1450	11
12	8	0	314	332	5
14	8	0	87	41	12
16	8	0	247	238	6
18	8	0	79	46	17
20	8	0	355	344	6
1	9	0	165	139	5
3	9	0	461	466	4
5	9	0	1759	1790	10
7	9	0	919	896	7
9	9	0	90	98	11
11	9	0	625	603	5
13	9	0	265	271	6
15	9	0	501	495	5
17	9	0	486	475	5
19	9	0	355	347	6
0	10	0	431	442	4
2	10	0	111	108	8
4	10	0	389	387	4
6	10	0	227	229	5
8	10	0	509	513	5
10	10	0	670	680	6
12	10	0	121	126	10
14	10	0	1207	1228	8
16	10	0	317	322	6
18	10	0	670	664	6
1	11	0	475	465	5
3	11	0	316	315	4
5	11	0	1007	1022	8
7	11	0	95	101	11
9	11	0	215	219	6
11	11	0	511	521	5
13	11	0	190	193	7
15	11	0	986	986	8
17	11	0	539	551	6
0	12	0	1310	1327	9
2	12	0	264	262	5
4	12	0	352	350	5
6	12	0	705	702	6
8	12	0	265	264	5
10	12	0	536	524	5
12	12	0	572	576	6
14	12	0	202	195	7
16	12	0	178	170	9
1	13	0	536	541	5
3	13	0	255	255	5
5	13	0	404	401	5
7	13	0	572	573	5
9	13	0	415	406	5
11	13	0	920	923	7
13	13	0	331	336	6
15	13	0	300	303	7
0	14	0	1542	1551	10
2	14	0	446	453	5
4	14	0	225	222	6
6	14	0	803	801	6
8	14	0	186	190	7
10	14	0	1440	1459	12
12	14	0	65	32	24
14	14	0	62	37	26
1	15	0	348	341	5
3	15	0	472	460	5
5	15	0	403	412	5
7	15	0	105	80	12
9	15	0	256	245	6
11	15	0	420	404	6
13	15	0	532	537	6
0	16	0	520	524	5
2	16	0	205	204	7
4	16	0	90	98	14
6	16	0	899	881	7
8	16	0	41	43	41
10	16	0	0	2	1
12	16	0	489	485	6
1	17	0	255	252	7
3	17	0	345	341	6
5	17	0	1868	1850	12
7	17	0	81	55	18
9	17	0	51	2	40
0	18	0	253	253	7
2	18	0	352	348	6
4	18	0	100	93	15
6	18	0	219	224	8
1	19	0	344	344	7
3	19	0	118	98	13
1	1	1	136	122	3
3	1	1	629	611	4
5	1	1	556	565	4
7	1	1	235	223	3
9	1	1	448	443	4
11	1	1	865	886	7
13	1	1	288	284	5
15	1	1	115	110	9
17	1	1	732	747	6
19	1	1	465	487	5
21	1	1	987	982	8
0	2	1	417	369	3
2	2	1	334	351	3
4	2	1	398	400	3
6	2	1	313	300	3
8	2	1	878	879	6
10	2	1	568	589	5
12	2	1	996	994	7
14	2	1	54	43	19
16	2	1	792	806	6
18	2	1	106	99	11
20	2	1	88	85	15
22	2	1	246	247	7
1	3	1	230	231	3
3	3	1	192	179	3
5	3	1	125	124	5
7	3	1	552	541	4
9	3	1	378	391	4
11	3	1	239	242	5
13	3	1	393	395	4
15	3	1	48	30	27
17	3	1	388	390	5
19	3	1	234	234	7
21	3	1	369	370	6
0	4	1	931	939	6
2	4	1	14	13	14
4	4	1	315	315	3
6	4	1	849	809	6
8	4	1	554	553	4
10	4	1	115	99	8
12	4	1	705	719	6
14	4	1	311	309	5
16	4	1	674	671	6
18	4	1	226	224	6
20	4	1	166	163	9
1	5	1	116	125	5
3	5	1	785	796	6
5	5	1	1846	1839	8
7	5	1	840	813	6
9	5	1	522	514	5
11	5	1	350	372	4
13	5	1	791	804	6
15	5	1	301	298	5
17	5	1	263	248	6
19	5	1	119	101	11
21	5	1	919	910	8
0	6	1	239	218	3
2	6	1	260	254	3
4	6	1	378	376	3
6	6	1	815	800	5
8	6	1	460	444	4
10	6	1	51	57	20
12	6	1	369	369	4
14	6	1	60	52	17
16	6	1	1077	1077	8
18	6	1	203	199	7
20	6	1	402	414	6
1	7	1	33	9	32
3	7	1	618	613	5
5	7	1	453	455	4
7	7	1	158	151	6
9	7	1	620	634	5
11	7	1	57	41	20
13	7	1	103	113	10
15	7	1	110	91	10
17	7	1	146	150	9
19	7	1	198	185	8
0	8	1	795	784	5
2	8	1	130	122	6
4	8	1	172	186	5
6	8	1	350	363	4
8	8	1	196	199	5
10	8	1	176	178	6
12	8	1	408	423	5
14	8	1	587	586	5
16	8	1	799	807	7
18	8	1	303	304	6
20	8	1	162	164	10
1	9	1	917	905	7
3	9	1	242	233	4
5	9	1	622	645	5
7	9	1	270	266	5
9	9	1	123	124	8
11	9	1	1673	1695	12
13	9	1	57	61	20
15	9	1	47	44	41
17	9	1	191	183	8
19	9	1	160	178	10
0	10	1	1357	1374	10
2	10	1	832	822	6
4	10	1	465	485	5
6	10	1	333	338	4
8	10	1	93	86	10
10	10	1	305	294	5
12	10	1	90	90	13
14	10	1	764	771	6
16	10	1	242	258	7
18	10	1	394	377	6
1	11	1	341	358	4
3	11	1	274	274	5
5	11	1	624	646	5
7	11	1	441	449	5
9	11	1	463	457	5
11	11	1	429	427	5
13	11	1	121	132	10
15	11	1	35	18	35
17	11	1	355	351	6
0	12	1	1280	1291	9
2	12	1	461	463	5
4	12	1	74	76	14
6	12	1	662	654	6
8	12	1	218	219	6
10	12	1	299	293	5
12	12	1	250	248	6
14	12	1	71	92	20
16	12	1	732	737	6
1	13	1	283	280	5
3	13	1	344	344	5
5	13	1	1039	1066	8
7	13	1	93	80	12
9	13	1	453	449	5
11	13	1	1092	1100	9
13	13	1	45	69	44
15	13	1	254	250	7
0	14	1	670	692	6
2	14	1	324	327	5
4	14	1	590	598	6
6	14	1	153	144	8
8	14	1	287	285	6
10	14	1	149	167	9
12	14	1	74	86	20
14	14	1	509	507	6
1	15	1	80	64	14
3	15	1	295	295	6
5	15	1	299	297	6
7	15	1	270	266	6
9	15	1	92	95	15
11	15	1	210	198	8
13	15	1	129	119	12
0	16	1	336	341	6
2	16	1	247	260	6
4	16	1	95	87	13
6	16	1	1252	1260	9
8	16	1	315	321	6
10	16	1	0	25	1
12	16	1	98	90	15
1	17	1	75	51	18
3	17	1	281	289	6
5	17	1	766	779	7
7	17	1	323	308	6
9	17	1	529	524	6
0	18	1	289	291	7
2	18	1	53	39	37
4	18	1	465	461	6
6	18	1	456	449	6
1	19	1	350	340	6
0	0	2	3808	3767	7
2	0	2	760	782	5
4	0	2	505	501	4
6	0	2	774	745	5
8	0	2	919	894	6
10	0	2	1596	1574	10
12	0	2	850	860	7
14	0	2	1447	1473	10
16	0	2	808	815	7
18	0	2	1044	1045	8
20	0	2	84	93	16
1	1	2	658	657	5
3	1	2	722	721	4
5	1	2	1235	1243	7
7	1	2	149	146	5
9	1	2	795	791	6
11	1	2	680	668	5
13	1	2	156	146	7
15	1	2	721	726	6
17	1	2	159	163	8
19	1	2	46	33	46
21	1	2	286	282	7
0	2	2	4243	4079	7
2	2	2	158	360	3
4	2	2	547	542	4
6	2	2	430	424	4
8	2	2	110	303	4
10	2	2	1271	1278	10
12	2	2	502	511	5
14	2	2	129	134	8
16	2	2	342	343	5
18	2	2	103	100	11
20	2	2	56	48	28
1	3	2	384	378	3
3	3	2	58	53	10
5	3	2	1311	1286	8
7	3	2	219	225	4
9	3	2	1701	1727	10
11	3	2	1404	1397	10
13	3	2	672	681	6
15	3	2	275	271	5
17	3	2	281	274	6
19	3	2	884	884	7
21	3	2	585	592	6
0	4	2	2155	2142	7
2	4	2	726	721	5
4	4	2	177	183	4
6	4	2	131	113	5
8	4	2	245	251	4
10	4	2	2181	2228	10
12	4	2	209	214	5
14	4	2	147	144	5
16	4	2	39	19	38
18	4	2	564	563	6
20	4	2	370	367	6
1	5	2	1027	1020	7
3	5	2	47	45	14
5	5	2	1658	1617	9
7	5	2	196	182	5
9	5	2	471	465	4
11	5	2	617	623	5
13	5	2	166	159	6
15	5	2	207	202	6
17	5	2	823	821	6
19	5	2	456	453	5
21	5	2	558	546	6
0	6	2	1247	1249	8
2	6	2	23	14	22
4	6	2	981	984	7
6	6	2	2417	2387	10
8	6	2	179	173	5
10	6	2	81	82	12
12	6	2	464	478	5
14	6	2	958	965	7
16	6	2	1395	1433	11
18	6	2	126	128	11
20	6	2	43	20	42
1	7	2	868	870	6
3	7	2	92	91	8
5	7	2	4617	4615	11
7	7	2	169	164	6
9	7	2	585	597	5
11	7	2	149	161	7
13	7	2	472	478	5
15	7	2	990	997	8
17	7	2	837	837	7
19	7	2	134	134	11
0	8	2	301	304	4
2	8	2	530	530	5
4	8	2	283	297	4
6	8	2	371	351	4
8	8	2	768	759	6
10	8	2	221	204	5
12	8	2	292	295	5
14	8	2	641	642	6
16	8	2	932	941	7
18	8	2	183	178	9
1	9	2	591	578	5
3	9	2	36	39	36
5	9	2	459	444	5
7	9	2	476	466	5
9	9	2	613	615	5
11	9	2	1595	1610	13
13	9	2	91	82	13
15	9	2	342	329	6
17	9	2	668	675	6

Observed and calculated structure factors for K16

h	k	l	10Fo	10Fc	10σ
19	9	2	263	260	7
0	10	2	4368	4440	12
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4	10	2	759	758	6
6	10	2	41	61	41
8	10	2	160	359	5
10	10	2	1897	1920	13
12	10	2	340	320	5
14	10	2	403	401	5
16	10	2	174	180	9
18	10	2	375	367	6
1	11	2	253	257	5
3	11	2	802	801	6
5	11	2	212	216	6
7	11	2	35	20	35
9	11	2	715	724	6
11	11	2	1715	1722	13
13	11	2	24	20	24
15	11	2	357	358	6
17	11	2	153	154	10
0	12	2	1435	1436	9
2	12	2	21	26	20
4	12	2	170	169	7
6	12	2	970	975	8
8	12	2	198	195	6
10	12	2	843	842	7
12	12	2	306	303	6
14	12	2	457	456	6
16	12	2	167	358	6
1	13	2	172	163	7
3	13	2	70	80	16
5	13	2	1785	1802	13
7	13	2	74	80	16
9	13	2	114	106	10
11	13	2	99	98	13
13	13	2	70	77	20
15	13	2	567	550	6
0	14	2	578	585	5
2	14	2	379	375	5
4	14	2	712	716	6
6	14	2	442	433	5
8	14	2	266	271	6
10	14	2	325	292	6
12	14	2	65	69	23
14	14	2	387	393	6
1	15	2	672	675	6
3	15	2	272	275	6
5	15	2	1509	1520	11
7	15	2	625	617	6
9	15	2	0	15	1
11	15	2	413	410	6
13	15	2	175	173	9
0	16	2	876	884	7
2	16	2	140	129	10
4	16	2	128	147	10
6	16	2	473	471	5
8	16	2	120	111	11
10	16	2	670	668	6
1	17	2	186	180	8
3	17	2	452	454	6
5	17	2	216	222	8
7	17	2	0	27	1
9	17	2	137	330	7
0	18	2	816	805	7
2	18	2	33	30	32
4	18	2	301	298	7
6	18	2	421	423	6
1	1	3	243	233	3
3	1	3	801	792	5
5	1	3	421	431	4
7	1	3	191	183	5
9	1	3	406	411	4
11	1	3	1414	1410	11
13	1	3	376	382	4
15	1	3	58	38	20
17	1	3	345	350	5
19	1	3	447	465	6
21	1	3	954	931	8
0	2	3	2633	2568	8
2	2	3	461	438	4
4	2	3	104	101	6
6	2	3	1108	1081	7
8	2	3	919	915	7
10	2	3	542	563	5
12	2	3	704	720	6
14	2	3	270	270	5
16	2	3	1137	1149	8
18	2	3	91	87	14
20	2	3	48	4	48
1	3	3	483	468	4
3	3	3	344	344	3
5	3	3	1213	1195	9
7	3	3	774	760	6
9	3	3	281	264	4
11	3	3	1311	1322	9
13	3	3	160	157	7
15	3	3	49	35	25
17	3	3	215	212	7
19	3	3	162	168	9
21	3	3	423	418	6
0	4	3	2072	1998	8
2	4	3	90	106	7
4	4	3	428	417	4
6	4	3	204	199	4
8	4	3	306	316	4
10	4	3	246	232	5
12	4	3	794	805	6
14	4	3	128	133	9
16	4	3	283	278	6
18	4	3	155	142	9
20	4	3	93	77	15
1	5	3	91	77	7
3	5	3	522	532	4
5	5	3	1167	1164	7
7	5	3	829	825	6
9	5	3	387	384	4
11	5	3	200	189	6
13	5	3	618	621	5
15	5	3	189	188	7
17	5	3	300	310	6
19	5	3	141	142	10
0	6	3	761	758	6
2	6	3	63	54	12
4	6	3	584	574	5
6	6	3	1158	1155	8
8	6	3	338	325	4
10	6	3	51	29	22
12	6	3	305	311	5
14	6	3	26	34	25
16	6	3	1131	1132	9
18	6	3	328	329	6
20	6	3	368	369	6
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5	7	3	1190	1179	8
7	7	3	220	221	5
9	7	3	587	595	5
11	7	3	769	771	6
13	7	3	105	108	11
15	7	3	174	185	8
17	7	3	599	603	6
19	7	3	171	168	9
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4	8	3	409	407	4
6	8	3	561	550	5
8	8	3	45	33	27
10	8	3	46	43	30
12	8	3	551	555	5
14	8	3	385	358	5
16	8	3	321	314	6
18	8	3	142	145	10
1	9	3	536	540	5
3	9	3	33	41	32
5	9	3	85	75	11
7	9	3	204	192	6
9	9	3	171	176	7
11	9	3	913	903	7
13	9	3	75	81	16
15	9	3	0	5	1
17	9	3	548	542	6
0	10	3	960	963	8
2	10	3	827	837	6
4	10	3	569	574	5
6	10	3	128	117	8
8	10	3	179	179	7
10	10	3	102	94	11
12	10	3	172	191	8
14	10	3	764	759	7
16	10	3	74	61	19
1	11	3	434	440	5
3	11	3	216	229	6
5	11	3	718	709	6
7	11	3	148	141	8
9	11	3	511	510	5
11	11	3	133	134	9
13	11	3	64	65	22
15	11	3	111	123	13
0	12	3	385	379	5
2	12	3	219	236	6
4	12	3	333	337	5
6	12	3	133	131	9
8	12	3	164	157	7
10	12	3	286	292	6
12	12	3	267	265	7
14	12	3	178	180	8
16	12	3	454	457	6
1	13	3	179	173	7
3	13	3	448	457	5
5	13	3	456	459	5
7	13	3	98	120	13
9	13	3	404	391	5
11	13	3	390	382	6
13	13	3	57	79	31
0	14	3	37	36	37
2	14	3	283	287	6
4	14	3	522	525	5
6	14	3	286	283	6
8	14	3	342	342	6
10	14	3	41	14	41
12	14	3	65	42	24
1	15	3	238	242	6
3	15	3	200	195	7
5	15	3	482	479	5
7	15	3	116	119	12
9	15	3	165	162	9
11	15	3	379	382	6
0	16	3	182	169	8
2	16	3	86	71	15
4	16	3	146	151	9
6	16	3	1093	1089	9
8	16	3	247	245	7
10	16	3	144	141	10
1	17	3	59	33	26
3	17	3	307	287	6
5	17	3	495	492	6
7	17	3	72	34	22
0	18	3	223	220	8
2	18	3	153	155	10
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4	0	4	855	884	6
6	0	4	496	483	4
8	0	4	376	377	4
10	0	4	2689	2739	12
12	0	4	868	870	7
14	0	4	517	509	5
16	0	4	123	119	10
18	0	4	744	733	6
20	0	4	152	147	10
1	1	4	232	225	4
3	1	4	32	12	32
5	1	4	120	89	7
7	1	4	18	5	18
9	1	4	1342	1343	9
11	1	4	1613	1627	12
13	1	4	58	66	20
15	1	4	108	107	11
17	1	4	78	62	16
19	1	4	582	574	6
0	2	4	248	270	4
2	2	4	248	253	4
4	2	4	395	386	4
6	2	4	534	552	5
8	2	4	42	37	34
10	2	4	406	409	4
12	2	4	321	321	5
14	2	4	616	615	5
16	2	4	743	747	6
18	2	4	112	102	12
20	2	4	136	126	11
1	3	4	324	332	4
3	3	4	426	409	4
5	3	4	3415	3463	11
7	3	4	164	161	6
9	3	4	905	912	7
11	3	4	29	43	28
13	3	4	439	437	5
15	3	4	786	787	6
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19	3	4	251	249	7
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2	4	4	489	481	4
4	4	4	738	762	6
6	4	4	1789	1784	10
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10	4	4	484	492	4
12	4	4	174	162	7
14	4	4	921	947	7
16	4	4	1439	1430	10
18	4	4	257	257	7
0	5	4	1103	1101	8
2	5	4	176	160	5
4	5	4	1576	1600	10
6	5	4	461	459	4
8	5	4	92	76	10
10	5	4	933	941	7
12	5	4	148	157	8
14	5	4	283	292	6
16	5	4	36	21	16
18	5	4	71	89	23
0	6	4	2202	2218	10
2	6	4	117	134	8
4	6	4	406	406	4
6	6	4	161	153	6
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10	6	4	1301	1299	10
12	6	4	411	414	5
14	6	4	239	243	6
16	6	4	203	197	8
18	6	4	324	318	6
1	7	4	322	311	4
3	7	4	346	346	4
5	7	4	1446	1477	11
7	7	4	377	381	5
9	7	4	1014	1027	7
11	7	4	716	720	6
13	7	4	491	487	5
15	7	4	311	313	6
17	7	4	280	283	6
0	8	4	1940	1980	11
2	8	4	49	21	21
4	8	4	312	315	5
6	8	4	607	604	5
8	8	4	426	433	5
10	8	4	1245	1264	9
12	8	4	235	230	6
14	8	4	80	50	16
16	8	4	180	186	8
18	8	4	128	105	11
1	9	4	81	70	12
3	9	4	319	326	5
5	9	4	1663	1691	12
7	9	4	503	503	5
9	9	4	12	28	12
11	9	4	193	192	7
13	9	4	96	101	13
15	9	4	336	338	6
17	9	4	587	579	6
0	10	4	947	966	7
2	10	4	67	40	15
4	10	4	447	462	5
6	10	4	267	256	5
8	10	4	490	484	5
10	10	4	578	570	5
12	10	4	181	187	8
14	10	4	915	927	7
16	10	4	430	441	6
1	11	4	304	298	5
3	11	4	393	394	5
5	11	4	1190	1214	9
7	11	4	51	22	26
9	11	4	132	127	9
11	11	4	85	60	15
13	11	4	141	125	10
15	11	4	839	840	7
0	12	4	805	802	6
2	12	4	287	287	5
4	12	4	205	206	7
6	12	4	339	344	5
8	12	4	313	318	6
10	12	4	320	322	6
12	12	4	388	383	6
14	12	4	80	79	18
1	13	4	302	301	5
3	13	4	152	158	8
5	13	4	262	259	6
7	13	4	333	337	6
9	13	4	420	420	6
11	13	4	731	735	7
13	13	4	184	187	9
0	14	4	1493	1494	11
2	14	4	277	270	6
4	14	4	343	342	6
6	14	4	539	549	6
8	14	4	136	149	11
10	14	4	1152	1145	9
12	14	4	28	7	27
1	15	4	298	287	6
3	15	4	456	454	6
5	15	4	161	155	9
7	15	4	200	195	8
9	15	4	230	217	8
0	16	4	101	95	14
2	16	4	181	181	9
4	16	4	80	55	18
6	16	4	500	494	6
8	16	4	0	25	1
1	17	4	339	332	6
3	17	4	214	220	8
1	1	5	52	50	19
3	1	5	341	339	4
5	1	5	483	471	5
7	1	5	73	88	14
9	1	5	362	361	5
11	1	5	282	277	5
13	1	5	113	126	10
15	1	5	102	103	13
17	1	5	765	762	6
19	1	5	378	396	6
0	2	5	497	487	5
2	2	5	32	15	32
4	2	5	404	408	4
6	2	5	511	508	5
8	2	5	487	488	5
10	2	5	306	291	5
12	2	5	805	805	6
14	2	5	0	12	1
16	2	5	164	353	6
18	2	5	181	178	8
1	3	5	81	78	10
3	3	5	161	156	6
5	3	5	394	397	4
7	3	5	124	124	8
9	3	5	194	186	6
11	3	5	279	269	5
13	3	5	190	389	5
15	3	5	68	72	19
17	3	5	592	583	6
0	4	5	0	23	1
2	4	5	13	8	13
4	4	5	172	175	6
6	4	5	708	689	5
8	4	5	391	394	4
10	4	5	49	38	27
12	4	5	479	485	5
14	4	5	103	298	6
16	4	5	674	671	6
18	4	5	244	246	8
1	5	5	149	141	6
3	5	5	443	444	4
5	5	5	908	916	7
7	5	5	569	558	5
9	5	5	373	379	5
11	5	5	300	294	5
13	5	5	546	552	5
15	5	5	216	204	7
17	5	5	190	187	8
0	6	5	207	243	5
2	6	5	141	152	7
4	6	5	57	48	18
6	6	5	384	369	4
8	6	5	276	280	5
10	6	5	59	55	20
12	6	5	277	277	6
14	6	5	78	50	16
16	6	5	737	735	6
1	7	5	24	10	23
3	7	5	480	487	5
5	7	5	53	52	22
7	7	5	283	287	5
9	7	5	432	430	5
11	7	5	397	399	5
13	7	5	222	226	7
15	7	5	40	5	39
17	7	5	99	104	15
0	8	5	885	888	7
2	8	5	63	53	16
4	8	5	40	37	39
6	8	5	601	587	5
8	8	5	160	161	7
10	8	5	101	111	11
12	8	5	298	294	6
14	8	5	496	500	6
16	8	5	825	814	7
1	9	5	638	645	6
3	9	5	119	118	9
5	9	5	652	651	6
7	9	5	299	298	5
9	9	5	99	104	12

Observed and calculated structure factors for K16

h	k	l	10Fo	10Fc	10s
11	9	5	1500	1515	12
13	9	5	40	41	40
15	9	5	54	7	14
0	10	5	1082	1062	8
2	10	5	522	527	5
4	10	5	282	274	5
6	10	5	390	379	5
8	10	5	51	54	28
10	10	5	280	283	6
12	10	5	0	7	1
14	10	5	586	579	6
1	11	5	193	193	7
3	11	5	201	216	7
5	11	5	436	432	5
7	11	5	465	469	5
9	11	5	307	306	6
11	11	5	468	454	6
13	11	5	208	203	8
0	12	5	1228	1232	9
2	12	5	476	474	5
4	12	5	94	86	13
6	12	5	701	703	6
8	12	5	127	136	10
10	12	5	161	170	9
12	12	5	192	198	8
1	13	5	232	246	7
3	13	5	242	255	7
5	13	5	982	1008	8
7	13	5	181	187	8
9	13	5	384	390	6
11	13	5	1207	1187	9
0	14	5	880	873	7
2	14	5	274	270	6
4	14	5	469	470	6
6	14	5	318	328	6
8	14	5	194	192	8
1	15	5	48	40	48
3	15	5	247	248	7
5	15	5	120	130	12
7	15	5	257	260	8
0	16	5	314	304	7
2	16	5	293	283	7
0	0	6	2737	2747	12
2	0	6	171	171	6
4	0	6	696	705	6
6	0	6	692	697	6
8	0	6	558	556	5
10	0	6	955	966	7
12	0	6	719	713	6
14	0	6	850	849	7
16	0	6	874	874	7
1	1	6	214	215	5
3	1	6	111	108	9
5	1	6	1748	1777	12
7	1	6	63	71	17
9	1	6	412	414	5
11	1	6	205	211	7
13	1	6	7	13	7
15	1	6	485	482	6
17	1	6	269	277	7
0	2	6	1672	1678	12
2	2	6	229	221	5
4	2	6	231	224	5
6	2	6	493	498	5
8	2	6	272	275	5
10	2	6	769	781	6
12	2	6	252	270	7
14	2	6	39	19	39
16	2	6	395	385	6
1	3	6	197	184	6
3	3	6	43	13	33
5	3	6	908	927	7
7	3	6	89	92	12
9	3	6	1157	1158	8
11	3	6	1093	1102	8
13	3	6	371	381	6
15	3	6	146	132	10
0	4	6	2523	2535	12
2	4	6	106	82	9
4	4	6	460	465	5
6	4	6	421	422	5
8	4	6	179	182	7
10	4	6	1448	1458	9
12	4	6	218	228	7
14	4	6	122	125	11
16	4	6	207	199	8
1	5	6	277	278	5
3	5	6	387	406	5
5	5	6	375	367	5
7	5	6	87	83	13
9	5	6	218	225	6
11	5	6	386	371	5
13	5	6	23	10	23
15	5	6	177	179	9
0	6	6	99	90	10
2	6	6	51	45	22
4	6	6	495	497	5
6	6	6	867	862	7
8	6	6	241	242	6
10	6	6	65	46	19
12	6	6	219	213	7
14	6	6	846	848	7
1	7	6	684	688	6
3	7	6	134	140	8
5	7	6	2521	2534	13
7	7	6	57	66	24
9	7	6	482	486	5
11	7	6	492	488	5
13	7	6	307	296	6
15	7	6	641	646	6
0	8	6	203	194	6
2	8	6	222	231	6
4	8	6	366	365	5
6	8	6	252	258	6
8	8	6	444	454	5
10	8	6	23	12	23
12	8	6	259	261	7
14	8	6	462	452	6
1	9	6	408	411	5
3	9	6	132	113	9
5	9	6	74	51	15
7	9	6	520	526	5
9	9	6	433	425	5
11	9	6	757	735	6
13	9	6	85	77	16
0	10	6	2181	2179	14
2	10	6	291	295	6
4	10	6	337	336	5
6	10	6	570	566	6
8	10	6	149	150	9
10	10	6	1307	1318	9
12	10	6	138	149	11
1	11	6	5	16	5
3	11	6	347	388	5
5	11	6	342	344	6
7	11	6	75	81	18
9	11	6	550	547	6
11	11	6	690	692	6
0	12	6	587	592	6
2	12	6	50	75	40
4	12	6	167	163	9
6	12	6	985	987	8
8	12	6	67	53	21
10	12	6	463	464	6
1	13	6	33	1	33
3	13	6	42	31	42
5	13	6	1337	1343	10
7	13	6	196	210	8
0	14	6	50	65	50
2	14	6	431	423	6
4	14	6	315	310	7
1	1	7	69	64	16
3	1	7	303	306	5
5	1	7	90	74	12
7	1	7	222	217	6
9	1	7	220	216	7
11	1	7	757	753	6
13	1	7	284	297	7
15	1	7	0	35	1
0	2	7	822	818	6
2	2	7	289	277	5
4	2	7	53	18	23
6	2	7	429	426	5
8	2	7	187	168	5
10	2	7	213	217	7
12	2	7	551	539	5
14	2	7	101	103	14
1	3	7	174	162	7
3	3	7	0	7	1
5	3	7	464	466	5
7	3	7	457	451	5
9	3	7	216	226	7
11	3	7	760	754	6
13	3	7	68	16	22
0	4	7	941	910	7
2	4	7	172	149	7
4	4	7	300	299	6
6	4	7	59	64	21
8	4	7	255	257	6
10	4	7	143	146	9
12	4	7	481	480	6
14	4	7	147	159	11
1	5	7	100	3	11
3	5	7	281	282	6
5	5	7	468	478	5
7	5	7	490	492	5
9	5	7	283	277	6
11	5	7	77	75	18
13	5	7	198	192	6
0	6	7	156	145	5
2	6	7	101	92	11
4	6	7	267	272	6
6	6	7	654	650	6
8	6	7	222	229	7
10	6	7	67	60	20
12	6	7	212	214	8
1	7	7	0	21	1
3	7	7	278	289	6
5	7	7	711	702	6
7	7	7	160	142	8
9	7	7	430	429	6
11	7	7	463	471	6
0	8	7	429	426	5
2	8	7	185	171	7
4	8	7	311	310	6
6	8	7	301	304	6
8	8	7	102	102	13
10	8	7	0	21	1
1	9	7	345	348	6
3	9	7	18	15	17
5	9	7	94	91	13
7	9	7	96	99	14
9	9	7	31	58	30
0	10	7	652	651	6
2	10	7	441	448	6
4	10	7	278	280	7
6	10	7	164	145	9
8	10	7	75	65	19
1	11	7	209	233	8
3	11	7	134	143	11
5	11	7	514	508	6
7	11	7	106	122	14
0	12	7	166	162	9
2	12	7	140	142	10
4	12	7	214	224	8
0	0	8	2561	2551	14
2	0	8	151	151	8
4	0	8	161	155	6
6	0	8	767	767	6
8	0	8	77	65	19
10	0	8	1457	1482	11
1	1	8	84	89	14
3	1	8	91	67	14
5	1	8	389	401	6
7	1	8	210	203	7
9	1	8	737	731	6
11	1	8	500	495	6
0	2	8	71	32	19
2	2	8	107	111	11
4	2	8	241	234	7
6	2	8	551	543	6
8	2	8	39	4	39
10	2	8	236	223	7
1	3	8	191	185	7
3	3	8	283	286	6
5	3	8	1815	1817	12
7	3	8	29	17	28
9	3	8	509	508	6
11	3	8	168	160	9
0	4	8	116	135	11
2	4	8	332	317	6
4	4	8	298	304	6
6	4	8	565	559	6
8	4	8	125	128	11
10	4	8	231	240	8
1	5	8	589	590	6
3	5	8	133	143	10
5	5	8	476	470	5
7	5	8	43	47	42
9	5	8	95	110	15
0	6	8	1880	1878	15
2	6	8	161	168	9
4	6	8	338	344	6
6	6	8	455	459	6
8	6	8	137	139	11
1	7	8	103	94	13
3	7	8	227	224	7
5	7	8	978	981	7
7	7	8	205	213	8
0	8	8	983	974	8
2	8	8	68	55	22
4	8	8	91	81	16
6	8	8	415	425	6
1	9	8	24	7	24
3	9	8	189	185	8
5	9	8	1166	1188	9
0	10	8	1100	1092	8
2	10	8	76	77	20
1	1	9	29	41	28
3	1	9	264	257	7
5	1	9	175	174	9
0	2	9	43	48	43
2	2	9	0	6	1
4	2	9	183	178	8
6	2	9	41	23	40
1	3	9	132	135	11
3	3	9	87	81	16
5	3	9	47	17	47
0	4	9	395	383	6
2	4	9	44	34	44
4	4	9	88	87	17
1	5	9	0	16	1
3	5	9	159	161	10

Observed and calculated structure factors for K17

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	661	672	4	2	8	0	157	168	5	1	1	1	177	160	2	5	9	1	500	526	5	3	1	2	760	755	5
4	0	0	1311	1318	5	4	8	0	459	470	4	3	1	1	471	460	3	7	9	1	382	373	4	5	1	2	1243	1237	7
6	0	0	688	709	5	6	8	0	567	565	5	5	1	1	638	650	4	9	9	1	109	115	8	7	1	2	158	154	4
8	0	0	854	851	6	8	8	0	483	487	5	7	1	1	73	65	7	11	9	1	1743	1762	12	9	1	2	733	710	5
10	0	0	1901	3852	10	10	8	0	1410	1411	11	9	1	1	367	361	4	13	9	1	26	30	26	11	1	2	579	574	5
12	0	0	1354	1401	10	12	8	0	186	195	6	11	1	1	952	956	7	15	9	1	38	34	38	13	1	2	102	92	9
14	0	0	227	214	5	14	8	0	103	106	10	13	1	1	344	336	4	17	9	1	204	201	7	15	1	2	708	702	6
16	0	0	314	307	5	16	8	0	238	248	6	15	1	1	24	5	24	19	9	1	107	125	12	17	1	2	66	75	16
18	0	0	594	593	5	18	8	0	47	3	40	17	1	1	727	731	6	0	10	1	1283	1296	8	19	1	2	11	6	11
20	0	0	315	283	6	20	8	0	149	131	6	19	1	1	396	411	5	2	10	1	778	769	6	21	1	2	265	252	7
22	0	0	1635	1647	11	1	9	0	174	164	5	21	1	1	971	962	7	4	10	1	295	306	4	0	2	2	4236	4169	7
1	1	0	683	723	3	3	9	0	411	426	4	0	2	1	309	252	3	6	10	1	450	450	5	2	2	2	332	330	3
3	1	0	201	196	2	5	9	0	1860	1909	10	2	2	1	493	517	4	8	10	1	131	139	8	4	2	2	484	484	4
5	1	0	607	615	4	7	9	0	872	882	7	4	2	1	426	431	3	10	10	1	277	275	5	6	2	2	400	389	3
7	1	0	503	499	4	9	9	0	57	60	18	6	2	1	170	159	4	12	10	1	32	27	32	8	2	2	275	267	4
9	1	0	1759	1753	9	11	9	0	536	527	5	8	2	1	630	642	5	14	10	1	622	624	6	10	2	2	1335	1331	10
11	1	0	2938	2899	10	13	9	0	262	269	5	10	2	1	442	467	4	16	10	1	302	311	6	12	2	2	559	553	5
13	1	0	293	299	4	15	9	0	550	558	5	12	2	1	996	1002	7	18	10	1	295	291	6	14	2	2	128	131	7
15	1	0	251	257	5	17	9	0	495	491	5	14	2	1	68	63	13	1	11	1	250	256	5	16	2	2	312	309	5
17	1	0	311	310	5	19	9	0	290	287	7	16	2	1	816	816	6	3	11	1	268	262	5	18	2	2	48	49	29
19	1	0	646	655	6	0	10	0	463	489	4	18	2	1	0	5	1	5	11	1	592	600	5	20	2	2	174	12	8
21	1	0	796	806	7	2	10	0	74	72	12	20	2	1	155	159	9	7	11	1	519	521	5	1	3	2	421	387	3
0	2	0	1261	1290	4	4	10	0	473	486	5	22	2	1	192	198	8	9	11	1	333	339	5	3	3	2	316	309	3
2	2	0	247	263	3	6	10	0	227	218	5	1	3	1	316	316	3	11	11	1	435	430	5	5	3	2	1256	1239	8
4	2	0	696	704	5	8	10	0	265	278	5	3	3	1	238	228	3	13	11	1	103	122	11	7	3	2	98	106	7
6	2	0	127	141	4	10	10	0	595	619	5	5	3	1	223	212	3	15	11	1	57	39	26	9	3	2	1690	1702	9
8	2	0	288	284	3	12	10	0	135	126	8	7	3	1	522	518	4	17	11	1	411	416	6	11	3	2	1400	1443	11
10	2	0	653	664	5	14	10	0	1221	1239	8	9	3	1	292	293	4	0	12	1	1220	1265	9	13	3	2	486	474	5
12	2	0	289	296	4	16	10	0	294	292	6	11	3	1	281	280	4	2	12	1	485	490	5	15	3	2	199	202	6
14	2	0	860	871	7	18	10	0	519	523	6	13	3	1	299	305	4	4	12	1	89	73	11	17	3	2	317	307	5
16	2	0	725	724	6	1	11	0	323	321	4	15	3	1	61	11	17	6	12	1	664	665	5	19	3	2	863	859	7
18	2	0	60	34	19	3	11	0	286	284	5	17	3	1	327	332	5	8	12	1	150	156	7	21	3	2	594	597	6
20	2	0	177	186	8	5	11	0	1065	1068	8	19	3	1	226	226	7	10	12	1	279	281	6	0	4	2	2225	2184	7
22	2	0	320	317	7	7	11	0	147	143	7	21	3	1	369	370	6	12	12	1	289	299	6	2	4	2	660	645	4
1	3	0	342	329	3	9	11	0	151	154	7	0	4	1	886	896	6	14	12	1	85	77	15	4	4	2	0	42	1
3	3	0	550	569	4	11	11	0	195	412	5	2	4	1	101	92	5	16	12	1	787	781	7	6	4	2	351	339	3
7	3	0	527	504	4	13	11	0	184	191	7	4	4	1	260	259	3	1	13	1	353	342	5	8	4	2	139	155	6
9	3	0	1079	1066	7	15	11	0	917	920	7	6	4	1	892	842	6	3	13	1	358	365	5	10	4	2	2125	2177	10
11	3	0	411	418	4	17	11	0	410	419	6	8	4	1	506	501	4	5	13	1	1007	1022	8	12	4	2	270	277	5
13	3	0	376	372	4	0	12	0	1468	1507	11	10	4	1	186	157	5	7	13	1	114	111	9	14	4	2	304	301	5
15	3	0	917	915	7	2	12	0	261	257	5	12	4	1	721	721	6	9	13	1	358	368	5	16	4	2	125	94	8
17	3	0	940	939	7	4	12	0	329	308	5	14	4	1	219	218	6	11	13	1	1108	1110	8	18	4	2	493	497	5
19	3	0	228	234	7	6	12	0	660	677	6	16	4	1	711	711	6	13	13	1	118	110	11	20	4	2	345	337	6
21	3	0	350	335	6	8	12	0	180	190	7	18	4	1	227	235	6	15	13	1	250	248	7	1	5	2	1029	1008	8
0	4	0	2384	2403	6	10	12	0	626	620	6	20	4	1	96	107	13	0	14	1	643	659	6	3	5	2	110	112	6
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4	4	0	1188	1190	7	14	12	0	121	132	10	3	5	1	504	514	4	4	14	1	432	442	5	7	5	2	185	174	5
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8	4	0	525	507	4	1	13	0	510	507	5	7	5	1	951	922	6	8	14	1	288	283	6	11	5	2	655	642	5
10	4	0	539	546	5	3	13	0	125	123	8	9	5	1	488	482	4	10	14	1	152	160	8	13	5	2	34	34	34
12	4	0	291	269	4	5	13	0	516	509	5	11	5	1	379	405	4	12	14	1	148	154	9	15	5	2	258	261	6
14	4	0	962	963	7	7	13	0	488	482	5	13	5	1	588	592	5	14	14	1	412	388	6	17	5	2	745	746	6
16	4	0	2047	2046	13	9	13	0	523	518	5	15	5	1	215	204	6	1	15	1	0	7	1	19	5	2	438	435	6
18	4	0	120	118	9	11	13	0	983	989	7	17	5	1	242	235	6	3	15	1	279	274	6	21	5	2	472	463	6
20	4	0	273	249	6	13	13	0	278	281	6	19	5	1	91	82	13	5	15	1	349	360	5	0	6	2	1242	1226	8
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1	5	0	1470	1453	7	0	14	0	1624	1609	13	0	6	1	285	262	3	9	15	1	71	60	18	4	6	2	1070	1079	7
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7	5	0	830	825	6	6	14	0	642	655	6	6	6	1	902	904	6	0	16	1	139	335	6	10	6	2	16	32	16
9	5	0	131	139	6	8	14	0	92	87	12	8	6	1	460	456	4	2	16	1	274	274	6	12	6	2	172	175	4
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13	5	0	333	343	5	12	14	0	74	77	20	12	6	1	373	367	4	6	16	1	1267	1270	9	16	6	2	1476	1495	11
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17	5	0	490	489	5	1	15	0	282	274	6	16	6	1	1104	1129	8	10	16	1	0	33	1	20	6	2	78	85	17
19	5	0	196	211	7	3	15	0	409	413	5	18	6	1	252	243	6	12	16	1	115	125	12	1	7	2	708	690	5
21	5	0	296	302	7	5	15	0	424	431	5	20	6	1	416	422	6	1	17	1	60	61	24	3	7	2	13	27	13
0	6	0	1064	1053	7	7	15	0	40	13	39	1	7	1	116	106	6	3	17	1	320	309	6	5	7	2	4685	4676	10
2	6	0	190	172	4	9	15	0	173	179	8	3	7	1	592	582	4	5	17	1	703	710	6	7	7	2	189	194	5
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6	6	0	489	483	4	13	15	0	435	431	6	7	7	1	189	177	5	9	17	1	431	421	6	11	7	2	33	17	33
8	6	0	656	643	5	0	16	0	603	604	6	9	7	1	468	485	4	0	18	1	227	230	7	13	7	2	331	338	5
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14	6	0	464	470	5	6	16	0	906	916	7	15	7	1	70	59	15	6	18	1	363	356	6	19	7	2	72	70	18
16	6	0	438	454	5	8	16	0	0	24	1	17	7	1	172	159	8	1	19	1	346	341	6	0	8	2	317	313	4
18	6	0	382	372	5	10	16	0	26	30	25	19	7	1	115	119	12	3	19	1	402	402	6	2	8	2	422	415	4
20	6	0	53	17	32	12	16	0	444	442	6	0	8	1	873	855	6	0	0	2	3533	3645	6	4	8	2	260	260	4
1	7	0	734	713	5	1	17	0	222	219	7	2	8	1	14	1	33	2	0	2	560	580	4	6	8	2	417	409	4
3	7	0	108	110	6	3	17	0	250	248	7	4	8	1	83	98	9	4	0	2	477	470	4	8	8	2	582	590	5
5	7	0	1575	1569	9	5	17	0	1924	1947	15	6	8	1	356	365	4	6	0	2	712	678	5	10	8	2	106	111	9
7	7	0	421	421	4	7	17	0	61	46	25	8	8	1	135	138	7	8	0	2	559	542	4	12	8	2	192	190	6
9	7	0	1315	1318	10	9	17	0	67	71	22	10	8	1	201	192	5	10	0	2	1533	1499	10	14	8	2	637	637	6
11	7	0	646	606	6	0	18	0	181	194	9	12	8	1	507	504	5	12	0	2	894	895	7	16	8	2	933	922	7
13	7	0	374	370	5	2	18	0	260	270	7	14	8	1	512	514	5	14	0	2	1388	1380	10	18	8	2	84	87	16
15	7	0	263	266	6	4	18	0	99	114	14	16	8	1	804	804	6	16	0	2	777	775	6	1	9	2	508	495	4
17	7	0	250	235	6	6	18	0	214	229	8	18	8	1	323	321	6	18	0	2	816	801	7	3	9	2	51	32	19
19	7	0	726	725	6	8	18	0	316	101	7	20	8	1	222	216	8	20	0	2	72	66	17	5	9	2	460	449	4
21	7	0	671	659	6	1	19	0	232	237	8	1	9	1	955	939	7	22	0	2	217	251	8	7	9	2	413	405	4
0	8	0	2779	2726	9	3	19	0	29	35	28	3	9	1	137	139	6	1	1	2	509	511	4	9	9	2	690	696	5

Observed and calculated structure factors for K17

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1609	1602	12	16	2	3	1181	1179	8	13	11	3	55	48	26	6	4	4	1864	1859	10	6	14	4	432	439	5
13	9	2	95	94	11	18	2	3	180	182	7	15	11	3	118	103	11	8	4	4	225	228	5	8	14	4	81	69	16
15	9	2	334	324	6	20	2	3	70	83	20	17	11	3	510	512	6	10	4	4	376	385	4	10	14	4	1110	1110	8
17	9	2	634	633	6	1	3	3	534	526	4	0	12	3	353	358	5	12	4	4	152	162	7	12	14	4	63	40	24
19	9	2	299	289	7	3	3	3	271	264	3	2	12	3	271	281	5	14	4	4	914	922	7	1	15	4	223	229	7
0	10	2	4587	4558	11	5	3	3	1149	1136	9	4	12	3	320	326	5	16	4	4	1455	1479	10	3	15	4	411	406	6
2	10	2	693	692	6	7	3	3	764	755	6	6	12	3	162	161	7	18	4	4	175	166	8	5	15	4	176	172	8
4	10	2	769	771	6	9	3	3	218	215	5	8	12	3	85	76	13	1	5	4	996	999	7	7	15	4	124	133	11
6	10	2	47	7	21	11	3	3	1349	1353	9	10	12	3	250	273	6	3	5	4	157	156	6	9	15	4	178	166	9
8	10	2	236	241	5	13	3	3	90	87	10	12	12	3	304	299	6	5	5	4	1569	1594	10	0	16	4	161	162	8
10	10	2	1908	1944	13	15	3	3	77	82	13	14	12	3	173	168	8	7	5	4	389	392	4	2	16	4	155	141	9
12	10	2	318	330	5	17	3	3	243	241	6	16	12	3	499	493	6	9	5	4	131	124	7	4	16	4	130	129	11
14	10	2	388	381	5	19	3	3	160	154	8	1	13	3	225	232	6	11	5	4	884	892	7	6	16	4	523	527	6
16	10	2	163	163	8	21	3	3	425	430	6	3	13	3	457	463	5	13	5	4	182	180	7	8	16	4	42	34	42
18	10	2	274	270	7	0	4	3	2052	1977	8	5	13	3	411	413	5	15	5	4	279	289	6	1	17	4	322	305	6
1	11	2	319	326	5	2	4	3	46	50	15	7	13	3	85	92	14	17	5	4	117	97	11	3	17	4	151	149	10
3	11	2	682	683	6	4	4	3	369	369	4	9	13	3	312	304	6	19	5	4	157	142	9	5	17	4	1475	1453	10
5	11	2	213	221	5	6	4	3	181	174	5	11	13	3	408	398	6	0	6	4	2249	2266	10	1	1	5	145	75	6
7	11	2	52	28	20	8	4	3	275	281	4	13	13	3	18	25	17	2	6	4	168	187	6	3	1	5	226	233	5
9	11	2	732	729	6	10	4	3	312	297	4	15	13	3	178	161	8	4	6	4	408	404	4	5	1	5	532	523	5
11	11	2	1810	1796	13	12	4	3	775	792	6	0	14	3	42	15	42	6	6	4	209	209	5	7	1	5	26	7	25
13	11	2	70	17	16	14	4	3	88	67	11	2	14	3	233	241	6	8	6	4	345	349	4	9	1	5	310	311	5
15	11	2	252	247	7	16	4	3	294	294	6	4	14	3	377	384	5	10	6	4	1305	1308	10	11	1	5	319	324	5
17	11	2	52	61	32	18	4	3	144	147	9	6	14	3	182	190	7	12	6	4	374	375	5	13	1	5	161	174	7
0	12	2	1406	1393	10	20	4	3	47	42	47	8	14	3	322	331	6	14	6	4	261	263	6	15	1	5	68	24	17
2	12	2	15	7	15	1	5	3	72	86	9	10	14	3	35	9	14	16	6	4	140	137	9	17	1	5	740	737	6
4	12	2	66	70	17	3	5	3	341	343	4	12	14	3	42	22	42	18	6	4	281	273	7	19	1	5	313	322	7
6	12	2	862	860	6	5	5	3	1088	1079	8	1	15	3	188	187	7	1	7	4	278	266	4	0	2	5	555	543	5
8	12	2	150	156	8	7	5	3	911	904	7	3	15	3	210	209	7	3	7	4	176	178	6	2	2	5	105	94	8
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14	12	2	527	510	5	13	5	3	452	446	5	9	15	3	134	112	10	9	7	4	1010	1027	8	8	2	5	339	332	4
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1	13	2	164	153	7	17	5	3	290	300	6	0	16	3	200	199	8	13	7	4	320	308	5	12	2	5	800	794	6
3	13	2	89	97	11	19	5	3	107	113	12	2	16	3	107	110	13	15	7	4	250	255	6	14	2	5	27	4	26
5	13	2	1906	1919	13	0	6	3	682	683	5	4	16	3	173	182	8	17	7	4	345	355	6	16	2	5	357	356	6
7	13	2	41	50	41	2	6	3	126	107	6	6	16	3	1129	1129	9	0	8	4	1973	2017	11	18	2	5	65	97	23
9	13	2	168	150	7	4	6	3	487	469	4	8	16	3	243	245	7	2	8	4	25	22	25	1	3	5	121	122	7
11	13	2	43	44	42	6	6	3	1192	1212	8	10	16	3	126	139	12	4	8	4	210	224	6	3	3	5	198	195	5
13	13	2	109	99	12	8	6	3	117	119	4	1	17	3	111	135	13	6	8	4	516	508	5	5	3	5	463	464	5
15	13	2	535	540	6	10	6	3	100	85	9	3	17	3	318	324	6	8	8	4	367	381	5	7	3	5	120	119	8
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8	14	2	155	169	8	20	6	3	183	180	6	4	18	3	169	175	9	18	8	4	82	56	17	17	3	5	528	529	6
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14	14	2	452	458	6	5	7	3	1120	1112	8	6	0	4	348	334	4	5	9	4	1733	1776	12	4	4	5	120	123	8
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3	15	2	294	299	6	9	7	3	470	476	5	10	0	4	2729	2768	11	9	9	4	26	3	25	8	4	5	344	355	5
5	15	2	1511	1545	11	11	7	3	800	792	6	12	0	4	928	933	7	11	9	4	157	139	7	10	4	5	91	72	10
7	15	2	502	501	5	13	7	3	125	118	9	14	0	4	384	383	5	13	9	4	110	112	11	12	4	5	486	490	5
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13	15	2	155	145	10	19	7	3	102	90	13	20	0	4	151	159	10	0	10	4	992	992	7	18	4	5	255	258	7
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8	16	2	97	93	13	8	8	3	22	23	21	9	1	4	1310	1335	9	10	10	4	537	529	5	9	5	5	354	357	5
10	16	2	724	717	6	10	8	3	0	37	1	11	1	4	1635	1649	12	12	10	4	175	177	7	11	5	5	331	333	5
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5	17	2	233	232	7	16	8	3	318	294	6	17	1	4	27	19	26	1	11	4	186	184	6	17	5	5	169	169	9
7	17	2	35	8	34	18	8	3	169	161	8	19	1	4	595	591	6	3	11	4	334	345	5	0	6	5	243	275	5
9	17	2	412	408	6	1	9	3	576	565	5	0	2	4	299	322	4	5	11	4	1231	1261	9	2	6	5	76	92	12
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9	1	3	322	327	4	0	10	3	855	855	6	18	2	4	71	17	18	6	12	4	316	319	5	3	7	5	461	478	5
11	1	3	1458	1465	11	2	10	3	753	762	6	20	2	4	137	128	10	8	12	4	226	235	6	5	7	5	0	4	1
13	1	3	422	419	5	4	10	3	394	406	5	1	3	4	227	232	4	10	12	4	395	396	5	7	7	5	297	296	5
15	1	3	55	68	20	6	10	3	199	196	6	3	3	4	484	475	4	12	12	4	365	354	6	9	7	5	334	323	5
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19	1	3	186	401	6	10	10	3	77	66	13	7	3	4	177	177	5	1	13	4	282	275	6	13	7	5	180	184	8
21	1	3	942	919	7	12	10	3	136	135	9	9	3	4	801	827	6	3	13	4	70	63	16	15	7	5	44	29	44
0	2	3	2527	2469	8	14	10	3	601	605	6	11	3	4	145	135	7	5	13	4	354	335	5	17	7	5	86	89	16
2	2	3	594	578	4	16	10	3	102	94	12	13	3	4	323	330	5	7	13	4	268	273	6	0	8	5	903	924	7
4	2	3	88	79	7	1	11	3	358	358	5	15	3	4	803	781	6	9	13	4	492	499	5	2	8	5	137	136	8
6	2	3	1192	1172	9	3	11	3	189	197	6	17	3	4	714	719	6	11	13	4	775	774	7	4	8	5	29	23	28
8	2	3	739	723	5	5	11	3	641	648	5	19	3	4	198	205	8	13	13	4	146	152	10	6	8	5	580	581	5
10	2	3	459	474	5	7	11	3	212	215	6	0	4	4	676	714	5	0	14	4	1531	1524	11	8	8	5	121	118	9
12	2	3	731	750	6	9	11	3	391	394	5	2	4	4	387	364	4	2	14	4	199	202	7	10	8	5	120	124	10
14	2	3	267	273	5	11	11	3	167	163	7	4	4	4	712	731	6	4	14	4	351	348	6	12	8	5	369	364	5

Observed and calculated structure factors for K17

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
14	8	5	446	443	6	3	1	6	149	150	7	4	8	6	334	337	5	11	3	7	772	773	6	5	1	8	437	439	5
16	8	5	829	818	7	5	1	6	1750	1779	12	6	8	6	286	278	6	13	3	7	0	27	-1	7	1	8	166	170	8
1	9	5	674	678	6	7	1	6	68	69	14	8	8	6	354	354	5	0	4	7	935	904	7	9	1	8	721	718	6
3	9	5	53	59	22	9	1	6	395	390	5	10	8	6	82	69	15	2	4	7	115	97	9	11	1	8	489	501	6
5	9	5	603	586	5	11	1	6	268	262	6	12	8	6	192	190	8	4	4	7	259	256	6	0	2	8	54	9	24
7	9	5	171	365	5	13	1	6	50	40	27	14	8	6	445	442	6	6	4	7	36	61	35	2	2	8	55	68	26
9	9	5	97	96	12	15	1	6	466	457	6	1	9	6	364	363	5	8	4	7	216	213	6	4	2	8	252	260	6
11	9	5	1566	1576	11	17	1	6	328	322	6	3	9	6	114	121	10	10	4	7	177	187	8	6	2	8	506	506	6
13	9	5	99	101	13	0	2	6	1710	1712	12	5	9	6	33	37	33	12	4	7	479	475	6	8	2	8	56	40	27
15	9	5	49	59	48	2	2	6	203	193	5	7	9	6	474	478	5	14	4	7	101	97	13	10	2	8	261	239	7
0	10	5	1036	1013	7	4	2	6	190	190	6	9	9	6	482	473	5	1	5	7	36	8	36	1	3	8	135	126	9
2	10	5	509	506	5	6	2	6	476	471	5	11	9	6	812	742	6	3	5	7	182	183	7	3	3	8	320	325	6
4	10	5	157	153	7	8	2	6	244	245	5	13	9	6	51	52	36	5	5	7	431	431	5	5	3	8	1840	1837	14
6	10	5	476	463	5	10	2	6	799	807	6	0	10	6	2245	2255	14	7	5	7	533	535	5	7	3	8	0	10	1
8	10	5	111	111	10	12	2	6	280	302	6	2	10	6	335	338	6	9	5	7	279	272	6	9	3	8	458	457	6
10	10	5	271	274	6	14	2	6	36	22	36	4	10	6	324	341	6	11	5	7	113	98	11	11	3	8	112	100	11
12	10	5	50	39	33	16	2	6	373	367	6	6	10	6	503	502	5	13	5	7	272	269	6	0	4	8	138	144	9
14	10	5	477	476	6	1	3	6	197	190	6	8	10	6	71	59	18	0	6	7	297	301	6	2	4	8	242	250	6
1	11	5	115	112	9	3	3	6	125	126	8	10	10	6	1311	1322	9	2	6	7	120	122	9	4	4	8	282	280	6
3	11	5	217	217	6	5	3	6	891	893	7	12	10	6	176	173	9	4	6	7	214	217	6	6	4	8	601	609	6
5	11	5	416	407	5	7	3	6	37	31	36	1	11	6	42	60	41	6	6	7	682	679	6	8	4	8	65	43	19
7	11	5	516	517	5	9	3	6	1125	1132	8	3	11	6	320	320	6	8	6	7	201	225	7	10	4	8	204	186	8
9	11	5	230	226	7	11	3	6	1120	1121	8	5	11	6	335	342	6	10	6	7	110	97	11	1	5	8	535	535	6
11	11	5	440	441	6	13	3	6	238	244	7	7	11	6	90	81	14	12	6	7	220	221	7	3	5	8	133	147	9
13	11	5	185	184	8	15	3	6	98	89	12	9	11	6	541	532	6	1	7	7	74	67	16	5	5	8	458	459	6
0	12	5	1163	1178	9	17	3	6	316	332	7	11	11	6	747	740	6	3	7	7	256	255	6	7	5	8	0	13	1
2	12	5	476	482	5	0	4	6	2520	2550	12	0	12	6	541	540	5	5	7	7	664	658	6	9	5	8	153	136	9
4	12	5	74	83	16	2	4	6	60	52	16	2	12	6	57	41	23	7	7	7	126	129	10	0	6	8	1892	1901	15
6	12	5	702	701	6	4	4	6	370	381	5	4	12	6	95	92	13	9	7	7	350	345	6	2	6	8	188	198	8
8	12	5	111	96	10	6	4	6	524	531	5	6	12	6	920	916	7	11	7	7	486	483	6	4	6	8	344	342	6
10	12	5	170	161	9	8	4	6	108	122	10	8	12	6	25	38	25	0	8	7	408	409	5	6	6	8	488	481	6
12	12	5	238	243	7	10	4	6	1434	1438	9	10	12	6	468	448	6	2	8	7	76	97	17	8	6	8	168	164	8
1	13	5	294	296	6	12	4	6	256	262	6	1	13	6	0	9	1	4	8	7	265	267	6	1	7	8	64	57	23
3	13	5	271	268	6	14	4	6	112	106	11	3	13	6	88	72	15	6	8	7	307	296	6	3	7	8	114	113	12
5	13	5	966	980	8	16	4	6	270	267	7	5	13	6	1413	1436	10	8	8	7	39	43	39	5	7	8	960	963	8
7	13	5	211	208	7	1	5	6	285	277	5	7	13	6	176	173	9	10	8	7	36	16	36	7	7	8	186	187	8
9	13	5	345	326	6	3	5	6	295	293	5	0	14	6	80	56	16	1	9	7	368	366	6	0	8	8	1020	1006	8
11	13	5	1210	1193	9	5	5	6	440	440	5	2	14	6	318	327	7	3	9	7	53	34	31	2	8	8	32	18	31
0	14	5	852	849	7	7	5	6	90	95	12	4	14	6	353	356	6	5	9	7	148	156	9	4	8	8	61	40	23
2	14	5	249	243	7	9	5	6	252	252	6	6	14	6	171	161	9	7	9	7	149	153	9	6	8	8	147	356	6
4	14	5	357	355	6	11	5	6	356	350	5	1	1	7	63	79	17	9	9	7	33	37	32	1	9	8	0	1	1
6	14	5	415	416	6	13	5	6	88	89	14	3	1	7	241	239	6	0	10	7	581	573	5	3	9	8	139	151	11
8	14	5	185	198	8	15	5	6	224	228	7	5	1	7	0	43	1	2	10	7	419	415	6	5	9	8	1230	1223	9
10	14	5	221	219	8	0	6	6	93	100	11	7	1	7	290	280	6	4	10	7	192	189	8	0	10	8	1097	1098	9
1	15	5	96	94	14	2	6	6	43	33	38	9	1	7	173	177	7	6	10	7	184	187	8	2	10	8	159	157	9
3	15	5	216	223	8	4	6	6	529	536	5	11	1	7	781	788	6	8	10	7	99	92	14	1	1	9	77	56	17
5	15	5	146	158	10	6	6	6	852	854	7	13	1	7	320	319	6	1	11	7	185	191	8	3	1	9	189	181	8
7	15	5	329	314	6	8	6	6	295	297	5	15	1	7	97	98	14	3	11	7	120	116	11	5	1	9	189	198	8
0	16	5	299	282	7	10	6	6	94	84	12	0	2	7	787	781	6	5	11	7	473	462	6	0	2	9	13	20	12
2	16	5	302	287	7	12	6	6	165	162	8	2	2	7	336	331	5	7	11	7	145	159	10	2	2	9	85	65	15
4	16	5	135	147	11	14	6	6	867	860	7	4	2	7	0	16	1	0	12	7	145	144	10	4	2	9	192	195	8
0	0	6	2665	2684	12	1	7	6	566	576	5	6	2	7	488	491	5	2	12	7	175	180	9	6	2	9	42	28	42
2	0	6	83	64	11	3	7	6	197	183	6	8	2	7	282	281	6	4	12	7	220	225	8	1	3	9	147	148	10
4	0	6	670	678	5	5	7	6	2527	2552	13	10	2	7	185	168	7	0	0	8	2527	2566	14	3	3	9	43	30	42
6	0	6	723	726	6	7	7	6	104	99	10	12	2	7	550	544	6	2	0	8	160	152	8	5	3	9	44	27	44
8	0	6	351	355	5	9	7	6	429	434	5	14	2	7	131	125	10	4	0	8	286	277	6	0	4	9	369	363	6
10	0	6	932	936	7	11	7	6	384	391	6	1	3	7	184	187	7	6	0	8	666	666	6	2	4	9	27	53	26
12	0	6	724	716	6	13	7	6	210	200	7	3	3	7	0	22	1	8	0	8	0	19	1	4	4	9	72	64	19
14	0	6	798	797	7	15	7	6	645	649	6	5	3	7	421	410	5	10	0	8	1485	1495	11	1	5	9	44	8	44
16	0	6	862	864	7	0	8	6	226	221	6	7	3	7	452	449	5	1	1	8	79	90	16	3	5	9	87	80	16
1	1	6	160	146	6	2	8	6	177	176	7	9	3	7	214	189	6	3	1	8	126	125	10						

Observed and calculated structure factors for K18

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	647	668	4	2	8	0	175	174	5	1	1	1	161	146	3	5	9	1	450	469	4	3	1	2	753	757	5
4	0	0	1279	1297	6	4	8	0	462	456	4	3	1	1	463	462	4	7	9	1	345	348	5	5	1	2	1164	1160	8
6	0	0	638	645	4	6	8	0	586	576	5	5	1	1	745	756	5	9	9	1	87	88	11	7	1	2	148	148	5
8	0	0	902	887	6	8	8	0	480	480	5	7	1	1	98	80	6	11	9	1	1720	1724	13	9	1	2	693	690	5
10	0	0	3629	3746	11	10	8	0	1361	1362	10	9	1	1	416	398	4	13	9	1	36	48	36	11	1	2	608	606	5
12	0	0	1393	1392	9	12	8	0	194	200	6	11	1	1	900	904	7	15	9	1	92	63	13	13	1	2	108	92	8
14	0	0	234	224	5	14	8	0	113	123	10	13	1	1	350	350	5	17	9	1	190	189	8	15	1	2	664	681	6
16	0	0	269	261	6	16	8	0	256	269	6	15	1	1	68	37	14	19	9	1	153	164	10	17	1	2	100	80	11
18	0	0	608	587	6	18	8	0	0	11	1	17	1	1	732	736	6	0	10	1	1287	1285	9	19	1	2	0	17	1
20	0	0	271	260	7	20	8	0	329	318	7	19	1	1	445	453	6	2	10	1	769	773	6	21	1	2	292	286	7
22	0	0	1669	1655	12	1	9	0	104	99	8	21	1	1	916	907	8	4	10	1	296	305	5	0	2	2	4124	4127	8
1	1	0	676	715	3	3	9	0	421	420	4	0	2	1	152	103	3	6	10	1	440	430	5	2	2	2	335	341	3
3	1	0	213	195	3	5	9	0	1849	1882	11	2	2	1	476	505	3	8	10	1	148	146	7	4	2	2	502	497	4
5	1	0	540	536	4	7	9	0	882	875	6	4	2	1	439	444	3	10	10	1	269	270	6	6	2	2	433	419	4
7	1	0	497	496	4	9	9	0	57	34	18	6	2	1	234	216	3	12	10	1	37	9	36	8	2	2	278	263	4
9	1	0	1737	1726	9	11	9	0	600	584	5	8	2	1	637	642	5	14	10	1	636	632	6	10	2	2	1307	1302	9
11	1	0	2922	2890	11	13	9	0	274	268	6	10	2	1	345	367	4	16	10	1	284	296	7	12	2	2	531	548	5
13	1	0	319	318	4	15	9	0	539	545	6	12	2	1	992	983	7	18	10	1	285	280	7	14	2	2	125	123	9
15	1	0	263	273	5	17	9	0	479	486	6	14	2	1	112	104	8	1	11	1	215	224	5	16	2	2	331	325	5
17	1	0	314	300	5	19	9	0	269	270	7	16	2	1	748	754	6	3	11	1	247	244	5	18	2	2	61	48	22
19	1	0	626	630	6	0	10	0	391	400	4	18	2	1	0	24	1	5	11	1	653	665	6	20	2	2	48	23	47
21	1	0	775	780	7	2	10	0	74	44	12	20	2	1	169	177	9	7	11	1	541	538	5	1	3	2	379	385	3
0	2	0	1299	1325	4	4	10	0	456	465	5	22	2	1	208	203	8	9	11	1	337	332	5	3	3	2	275	276	3
2	2	0	242	258	3	6	10	0	251	238	5	1	3	1	317	313	3	11	11	1	389	392	5	5	3	2	1165	1145	8
4	2	0	696	713	5	8	10	0	304	306	5	3	3	1	236	227	3	13	11	1	133	134	9	7	3	2	121	119	6
6	2	0	139	150	4	10	10	0	562	569	5	5	3	1	272	261	3	15	11	1	77	85	17	9	3	2	1650	1673	10
8	2	0	294	294	3	12	10	0	137	131	8	7	3	1	502	502	4	17	11	1	432	432	6	11	3	2	1411	1416	9
10	2	0	670	680	5	14	10	0	1200	1217	9	9	3	1	278	273	4	0	12	1	1164	1188	8	13	3	2	475	472	5
12	2	0	301	296	4	16	10	0	254	265	7	11	3	1	265	264	4	2	12	1	477	480	5	15	3	2	177	177	7
14	2	0	875	869	6	18	10	0	525	530	6	13	3	1	277	292	5	4	12	1	82	88	13	17	3	2	298	305	6
16	2	0	716	727	6	1	11	0	309	306	5	15	3	1	0	28	1	6	12	1	659	654	6	19	3	2	851	849	7
18	2	0	46	23	36	3	11	0	291	293	5	17	3	1	321	324	6	8	12	1	159	165	8	21	3	2	566	563	6
20	2	0	179	185	9	5	11	0	986	989	8	19	3	1	216	209	7	10	12	1	226	228	7	0	4	2	2051	2042	8
22	2	0	349	331	7	7	11	0	139	142	8	21	3	1	347	355	7	12	12	1	296	283	6	2	4	2	649	639	5
1	3	0	339	335	3	9	11	0	124	121	9	0	4	1	973	980	6	14	12	1	42	55	42	4	4	2	45	40	15
3	3	0	535	540	4	11	11	0	427	437	5	2	4	1	70	94	8	16	12	1	764	753	7	6	4	2	316	298	3
5	3	0	4892	4904	9	13	11	0	196	197	7	4	4	1	248	243	3	1	13	1	145	142	5	8	4	2	141	152	6
7	3	0	519	503	4	15	11	0	907	904	7	6	4	1	839	801	6	3	13	1	150	364	5	10	4	2	2037	2111	11
9	3	0	1040	1041	8	17	11	0	429	436	6	8	4	1	498	495	4	5	13	1	995	1001	8	12	4	2	259	257	5
11	3	0	381	373	4	0	12	0	1488	1519	10	10	4	1	224	215	5	7	13	1	101	91	11	14	4	2	276	284	6
13	3	0	371	381	4	2	12	0	248	247	5	12	4	1	722	727	6	9	13	1	346	353	6	16	4	2	55	14	22
15	3	0	884	876	7	4	12	0	277	276	5	14	4	1	249	245	5	11	13	1	1082	1098	9	18	4	2	498	501	6
17	3	0	962	949	7	6	12	0	646	650	6	16	4	1	680	679	6	13	13	1	136	129	10	20	4	2	129	320	6
19	3	0	242	240	7	8	12	0	183	181	7	18	4	1	249	253	7	15	13	1	260	258	7	1	5	2	1013	984	6
21	3	0	396	381	6	10	12	0	640	632	6	20	4	1	80	87	17	0	14	1	680	686	6	3	5	2	106	97	6
0	4	0	2244	2262	6	12	12	0	546	532	6	1	5	1	119	108	5	2	14	1	285	277	6	5	5	2	1791	1768	9
2	4	0	559	570	4	14	12	0	114	119	12	3	5	1	521	544	4	4	14	1	437	434	5	7	5	2	191	191	5
4	4	0	1168	1178	7	16	12	0	119	109	12	5	5	1	1659	1633	8	6	14	1	263	262	6	9	5	2	441	443	4
6	4	0	1693	1657	9	1	13	0	468	484	5	7	5	1	927	900	6	8	14	1	294	291	6	11	5	2	635	632	5
8	4	0	492	490	4	3	13	0	141	143	8	9	5	1	530	519	5	10	14	1	179	191	8	13	5	2	78	42	13
10	4	0	486	488	4	5	13	0	452	443	5	11	5	1	330	358	4	12	14	1	160	167	9	15	5	2	255	256	6
12	4	0	256	247	5	7	13	0	459	473	5	13	5	1	582	595	5	14	14	1	391	388	7	17	5	2	749	751	6
14	4	0	929	934	7	9	13	0	529	514	5	15	5	1	161	143	7	1	15	1	0	18	1	19	5	2	425	420	6
16	4	0	2028	2010	14	11	13	0	952	950	8	17	5	1	214	225	7	3	15	1	282	292	6	21	5	2	542	474	6
18	4	0	121	100	10	13	13	0	278	289	7	19	5	1	46	52	46	5	15	1	285	287	6	0	6	2	1175	1159	9
20	4	0	245	238	7	15	13	0	253	233	7	21	5	1	789	782	7	7	15	1	352	349	6	2	6	2	146	156	5
22	4	0	396	407	7	0	14	0	1517	1547	11	0	6	1	396	367	3	9	15	1	71	64	19	4	6	2	1081	1081	8
1	5	0	1452	1440	7	2	14	0	378	387	5	2	6	1	167	167	4	11	15	1	172	147	9	6	6	2	2351	2350	10
3	5	0	50	55	12	4	14	0	220	226	6	4	6	1	268	260	3	13	15	1	146	148	11	8	6	2	275	269	4
5	5	0	1234	1177	9	6	14	0	681	686	6	6	6	1	866	877	7	0	16	1	304	319	6	10	6	2	39	9	38
7	5	0	845	822	6	8	14	0	139	118	8	8	6	1	506	489	4	2	16	1	258	246	6	12	6	2	357	368	5
9	5	0	142	155	6	10	14	0	1378	1377	11	10	6	1	71	66	13	4	16	1	30	26	29	14	6	2	991	1001	7
11	5	0	314	338	4	12	14	0	90	82	17	12	6	1	375	362	5	6	16	1	1280	1275	10	16	6	2	1453	1467	10
13	5	0	317	325	5	14	14	0	57	7	30	14	6	1	0	10	1	8	16	1	294	294	7	18	6	2	69	17	19
15	5	0	291	287	5	1	15	0	267	261	6	16	6	1	1080	1082	8	10	16	1	71	36	20	20	6	2	103	87	14
17	5	0	499	499	6	3	15	0	406	409	5	18	6	1	276	263	6	12	16	1	109	97	13	1	7	2	732	709	6
19	5	0	214	211	7	5	15	0	478	480	5	20	6	1	439	435	6	1	17	1	50	61	35	3	7	2	34	6	34
21	5	0	303	307	7	7	15	0	0	8	1	1	7	1	137	123	5	3	17	1	304	308	7	5	7	2	4581	4582	12
0	6	0	974	976	6	9	15	0	163	156	9	3	7	1	574	570	4	5	17	1	719	723	6	7	7	2	193	195	5
2	6	0	163	172	4	11	15	0	374	373	7	5	7	1	434	431	4	7	17	1	246	244	8	9	7	2	516	526	5
4	6	0	419	434	4	13	15	0	443	432	6	7	7	1	215	200	5	9	17	1	420	417	7	11	7	2	47	58	27
6	6	0	546	522	5	0	16	0	599	607	6	9	7	1	461	475	5	0	18	1	281	281	7	13	7	2	355	359	5
8	6	0	652	636	5	2	16	0	164	166	8	11	7	1	17	2	36	2	18	1	78	81	19	15	7	2	935	951	8
10	6	0	1385	1397	9	4	16	0	223	215	7	13	7	1	79	81	13	4	18	1	344	350	7	17	7	2	949	950	7
12	6	0	267	265	5	6	16	0	868	877	7	15	7	1	0	32	1	6	18	1	351	345	7	19	7	2	77	72	18
14	6	0	477	470	5	8	16	0	34	42	33	17	7	1	194	186	8	1	19	1	311	330	7	0	8	2	434	395	4
16	6	0	500	505	6	10	16	0	57	28	30	19	7	1	125	132	12	3	19	1	399	401	7	2	8	2	426	428	4
18	6	0	384	383	6	12	16	0	442	442	6	0	8	1	763	751	6	0	0	2	3626	3509	7	4	8	2	238	241	5
20	6	0	23	25	23	1	17	0	255	244	7	2	8	1	27	7	27	2	0	2	559	593	4	6	8	2	428	404	4
1	7	0	711	708	5	3	17	0	264	276	7	4	8	1	92	105	9	4	0	2	467	449	4	8	8	2	578	587	5
3	7	0	137	142	5	5	17	0	1881	1897	13	6	8	1	326	341	4	6	0	2	754	718	5	10	8	2	62	63	17
5	7	0	1492	1487	10	7	17	0	52	44	16	8	8	1	141	138	7	8	0	2	569	563	5	12	8	2	202	196	6
7	7	0	440	434	4	9	17	0	47	64	47	10	8	1	133	114	8	10	0	2	1447	1416	10	14	8	2	607	608	5
9	7	0	1275	1285	9	0	18	0	245	263	7	12	8	1	497	505	5	12	0	2	905	895	7	16	8	2	902	909	7
11	7	0	616	583	6	2	18	0	285	288	7	14	8	1	550	549	5	14	0	2	1368	1379	10	18	8	2	74	73	19
13	7	0	384	378	5	4	18	0	91	82	16	16	8	1	758	760	7	16	0	2	736	744	6	1	9	2	468	456	4
15	7	0	236	245	6	6	18	0	232	248	8	18	8	1	344	338	6	18	0	2	809	794	7	3	9	2	38	37	38
17	7	0	235	234	7	8	18	0	329	316	7	20	8	1	246	244	8	20	0	2	65	58	21	5	9	2	459	447	5
19	7	0	712	717	6	1	19	0	215	225	8	1	9	1	952	928	7	22	0	2	221	233	8	7	9	2	411	406	5
0	8	0	2701	2651	9	3	19	0	60	63	10	1	9	1	150	145	6	1	1	2	521	525	4	9	9	2	705	716	6

Observed and calculated structure factors for K18

h	k	l	10Fo	10Fc	10s
11	9	2	1585	1585	11
13	9	2	115	112	10
15	9	2	327	329	6
17	9	2	625	632	6
19	9	2	288	296	7
0	10	2	4520	4483	12
2	10	2	663	678	6
4	10	2	770	762	6
6	10	2	14	32	33
8	10	2	263	271	5
10	10	2	1892	1892	14
12	10	2	330	332	6
14	10	2	368	368	6
16	10	2	186	198	8
18	10	2	281	274	7
1	11	2	371	348	5
3	11	2	693	700	6
5	11	2	147	147	8
7	11	2	21	25	20
9	11	2	697	693	6
11	11	2	1773	1795	12
13	11	2	32	41	32
15	11	2	235	232	7
17	11	2	81	82	18
0	12	2	1377	1369	10
2	12	2	0	6	1
4	12	2	67	53	16
6	12	2	863	862	7
8	12	2	151	158	8
10	12	2	805	810	7
12	12	2	234	236	7
14	12	2	522	518	6
16	12	2	162	180	7
1	13	2	171	177	7
3	13	2	86	87	13
5	13	2	1891	1874	14
7	13	2	33	16	32
9	13	2	166	152	8
11	13	2	73	82	17
13	13	2	117	107	11
15	13	2	513	520	6
0	14	2	479	486	5
2	14	2	305	301	6
4	14	2	743	753	6
6	14	2	482	476	5
8	14	2	179	191	8
10	14	2	171	170	9
12	14	2	56	65	32
14	14	2	415	421	6
1	15	2	552	560	6
3	15	2	289	294	6
5	15	2	1514	1511	11
7	15	2	510	507	6
9	15	2	117	102	11
11	15	2	374	370	7
13	15	2	153	144	10
0	16	2	1006	1005	8
2	16	2	122	125	10
4	16	2	89	69	14
6	16	2	441	448	6
8	16	2	125	76	10
10	16	2	725	719	7
1	17	2	219	215	7
3	17	2	382	374	6
5	17	2	180	188	9
7	17	2	56	17	32
9	17	2	405	393	7
0	18	2	832	800	7
2	18	2	55	31	31
4	18	2	248	251	8
6	18	2	414	411	7
1	1	3	251	250	3
3	1	3	643	651	5
5	1	3	285	286	4
7	1	3	297	296	4
9	1	3	340	356	4
11	1	3	1426	1425	10
13	1	3	430	432	5
15	1	3	124	103	9
17	1	3	354	354	6
19	1	3	424	441	6
21	1	3	896	868	7
0	2	3	2411	2350	8
2	2	3	575	567	4
4	2	3	81	71	8
6	2	3	1160	1124	8
8	2	3	743	726	5
10	2	3	377	390	4
12	2	3	730	740	6
14	2	3	310	310	5
16	2	3	1123	1131	8
18	2	3	189	207	8
20	2	3	96	105	15
1	3	3	541	530	4
3	3	3	268	270	3
5	3	3	1147	1104	8
7	3	3	754	743	6
9	3	3	203	201	5
11	3	3	1354	1345	10
13	3	3	79	77	13
15	3	3	125	104	9
17	3	3	235	247	7
19	3	3	129	137	11
21	3	3	410	416	7
0	4	3	2108	2042	9
2	4	3	51	48	14
4	4	3	165	164	4
6	4	3	201	200	5
8	4	3	272	274	4
10	4	3	365	347	4
12	4	3	791	795	6
14	4	3	97	92	11
16	4	3	262	262	6
18	4	3	162	161	9
20	4	3	44	27	44
1	5	3	88	84	8
3	5	3	358	358	4
5	5	3	986	978	7
7	5	3	881	888	7
9	5	3	413	404	4
11	5	3	168	170	6
13	5	3	440	446	5
15	5	3	52	54	27
17	5	3	281	290	6
19	5	3	101	87	13
0	6	3	594	610	5
2	6	3	122	107	7
4	6	3	493	468	5
6	6	3	1193	1197	9
8	6	3	354	349	4
10	6	3	118	123	9
12	6	3	318	320	5
14	6	3	64	77	17
16	6	3	1136	1144	9
18	6	3	378	390	6
20	6	3	386	394	7
1	7	3	174	164	5
3	7	3	262	273	5
5	7	3	1180	1166	9
7	7	3	167	172	6
9	7	3	478	473	5
11	7	3	811	805	6
13	7	3	122	118	9
15	7	3	128	140	10
17	7	3	616	614	6
19	7	3	118	101	12
0	8	3	790	781	6
2	8	3	118	121	8
4	8	3	334	340	4
6	8	3	552	557	5
8	8	3	35	28	35
10	8	3	51	35	21
12	8	3	598	601	6
14	8	3	343	337	6
16	8	3	259	245	7
18	8	3	170	170	9
1	9	3	563	562	5
3	9	3	105	89	9
5	9	3	238	243	6
7	9	3	262	257	5
9	9	3	110	115	10
11	9	3	915	916	7
13	9	3	53	16	24
15	9	3	64	84	23
17	9	3	530	538	6
0	10	3	852	860	7
2	10	3	755	767	6
4	10	3	403	403	5
6	10	3	184	186	6
8	10	3	195	209	7
10	10	3	64	68	18
12	10	3	113	113	11
14	10	3	615	615	6
16	10	3	84	84	16
1	11	3	325	325	5
3	11	3	184	188	6
5	11	3	715	717	6
7	11	3	228	227	6
9	11	3	389	391	5
11	11	3	114	117	10
13	11	3	45	40	44
15	11	3	65	62	23
17	11	3	532	533	6
0	12	3	282	292	5
2	12	3	274	274	5
4	12	3	340	341	5
6	12	3	161	145	7
8	12	3	101	84	11
10	12	3	213	217	7
12	12	3	291	284	6
14	12	3	144	149	10
16	12	3	466	456	6
1	13	3	238	232	6
3	13	3	458	463	5
5	13	3	385	392	6
7	13	3	108	116	11
9	13	3	293	288	6
11	13	3	396	380	6
13	13	3	40	8	39
15	13	3	171	165	10
0	14	3	32	13	32
2	14	3	231	239	6
4	14	3	367	373	6
6	14	3	170	183	8
8	14	3	355	344	6
10	14	3	56	21	28
12	14	3	0	18	1
1	15	3	169	169	8
3	15	3	226	222	7
5	15	3	486	483	6
7	15	3	207	213	8
9	15	3	127	117	11
11	15	3	364	350	7
0	16	3	180	171	8
2	16	3	87	80	16
4	16	3	190	196	8
6	16	3	1138	1124	9
8	16	3	236	245	8
10	16	3	137	128	11
1	17	3	125	134	11
3	17	3	332	322	7
5	17	3	451	444	6
7	17	3	14	11	13
0	18	3	229	227	8
2	18	3	194	191	9
4	18	3	178	171	10
2	0	4	388	402	4
4	0	4	729	747	6
6	0	4	388	374	4
8	0	4	255	262	5
10	0	4	2678	2696	12
12	0	4	920	938	7
14	0	4	380	387	5
16	0	4	137	142	9
18	0	4	566	564	6
20	0	4	152	147	10
1	1	4	238	233	4
3	1	4	100	91	7
5	1	4	252	211	4
7	1	4	72	59	12
9	1	4	1304	1314	10
11	1	4	1613	1644	13
13	1	4	175	166	7
15	1	4	192	193	7
17	1	4	0	25	1
19	1	4	580	573	6
0	2	4	319	340	4
2	2	4	175	177	5
4	2	4	436	437	4
6	2	4	463	480	4
8	2	4	97	107	10
10	2	4	440	462	5
12	2	4	313	310	5
14	2	4	653	647	6
16	2	4	731	738	7
18	2	4	19	7	39
20	2	4	148	130	10
1	3	4	235	240	4
3	3	4	468	457	4
5	3	4	3394	3436	11
7	3	4	171	178	6
9	3	4	804	810	6
11	3	4	91	98	11
13	3	4	332	339	5
15	3	4	751	754	6
17	3	4	730	730	7
19	3	4	204	210	8
0	4	4	605	619	5
2	4	4	396	373	4
4	4	4	692	721	6
6	4	4	1822	1852	11
8	4	4	218	220	5
10	4	4	337	342	5
12	4	4	149	153	8
14	4	4	900	899	7
16	4	4	1404	1446	11
18	4	4	163	157	9
1	5	4	986	991	7
3	5	4	159	147	6
5	5	4	1514	1577	11
7	5	4	397	390	4
9	5	4	148	144	7
11	5	4	885	903	7
13	5	4	161	168	8
15	5	4	296	283	6
17	5	4	107	105	12
19	5	4	136	140	11
0	6	4	2189	2221	11
2	6	4	186	184	5
4	6	4	410	413	4
6	6	4	186	179	6
8	6	4	342	340	5
10	6	4	1274	1287	9
12	6	4	373	367	5
14	6	4	257	265	6
16	6	4	177	177	8
18	6	4	300	280	7
1	7	4	274	268	5
3	7	4	210	202	5
5	7	4	1363	1356	10
7	7	4	356	354	5
9	7	4	998	1005	7
11	7	4	769	758	6
13	7	4	316	317	6
15	7	4	231	235	7
17	7	4	346	354	7
0	8	4	1888	1960	12
2	8	4	30	24	30
4	8	4	200	210	6
6	8	4	534	522	5
8	8	4	379	381	5
10	8	4	1184	1191	8
12	8	4	125	120	9
14	8	4	111	108	11
16	8	4	209	216	8
18	8	4	68	51	22
1	9	4	48	47	25
3	9	4	281	287	5
5	9	4	1765	1774	13
7	9	4	490	498	5
9	9	4	40	25	39
11	9	4	169	177	8
13	9	4	111	113	12
15	9	4	378	382	6
17	9	4	582	580	6
0	10	4	927	929	7
2	10	4	72	79	15
4	10	4	512	519	5
6	10	4	246	245	6
8	10	4	317	314	6
10	10	4	491	490	5
12	10	4	168	179	9
14	10	4	930	929	8
16	10	4	414	407	6
1	11	4	172	175	7
3	11	4	155	155	5
5	11	4	1163	1201	9
7	11	4	27	53	26
9	11	4	29	68	29
11	11	4	48	13	38
13	11	4	118	125	12
15	11	4	776	766	7
0	12	4	931	950	7
2	12	4	251	255	6
4	12	4	154	160	8
6	12	4	104	103	6
8	12	4	225	230	7
10	12	4	410	413	6
12	12	4	351	358	6
14	12	4	0	12	1
1	13	4	355	263	5
3	13	4	73	80	18
5	13	4	287	289	6
7	13	4	275	270	6
9	13	4	506	497	6
11	13	4	764	752	7
13	13	4	153	160	10
0	14	4	1459	1483	10
2	14	4	239	226	7
4	14	4	331	336	6
6	14	4	451	463	6
8	14	4	117	95	12
10	14	4	1087	1087	8
12	14	4	61	45	30
1	15	4	208	217	7
3	15	4	404	405	6
5	15	4	218	210	8
7	15	4	139	130	11
9	15	4	144	147	11
0	16	4	167	166	9
2	16	4	165	158	9
4	16	4	148	147	11
6	16	4	499	497	6
8	16	4	57	19	29
1	17	4	327	326	7
3	17	4	185	173	9
1	1	5	78	61	11
3	1	5	237	235	5
5	1	5	595	592	5
7	1	5	46	8	26
9	1	5	321	333	5
11	1	5	290	283	5
13	1	5	181	188	7
15	1	5	0	5	1
17	1	5	736	747	6
19	1	5	343	356	7
0	2	5	648	637	5
2	2	5	106	93	8
4	2	5	430	435	4
6	2	5	443	447	5
8	2	5	327	329	5
10	2	5	133	133	8
12	2	5	782	786	6
14	2	5	46	31	40
16	2	5	319	305	6
18	2	5	71	82	21
1	3	5	127	120	7
3	3	5	208	201	5
5	3	5	494	495	5
7	3	5	96	115	11
9	3	5	127	115	8
11	3	5	262	264	6
13	3	5	297	298	6
15	3	5	50	28	31
17	3	5	529	528	6
0	4	5	59	45	16
2	4	5	59	48	18
4	4	5	118	121	8
6	4	5	699	680	6
8	4	5	343	357	5
10	4	5	128	114	9
12	4	5	482	497	5
14	4	5	230	246	7
16	4	5	676	685	6
18	4	5	271	274	7
1	5	5	143	148	7
3	5	5	297	297	5
5	5	5	793	788	7
7	5	5	620	618	6
9	5	5	374	387	5
11	5	5	288	296	6
13	5	5	400	397	6
15	5	5	99	90	14
17	5	5	170	165	9
0	6	5	297	335	5
2	6	5	102	96	9
4	6	5	31	25	30
6	6	5	430	423	5
8	6	5	120	128	5
10	6	5	0	30	1
12	6	5	261	261	6
14	6	5	62	28	22
16	6	5	730	737	7
1	7	5	82	73	12
3	7	5	461	477	5
5	7	5	46	30	29
7	7	5	103	111	5
9	7	5	141	122	5
11	7	5	173	173	6
13	7	5	184	184	8
15	7	5	49	49	48
17	7	5	86	71	17
0	8	5	857	852	7
2	8	5	130	128	8
4	8	5	0	17	1
6	8	5	570	564	5
8	8	5	111	119	10
10	8	5	83	65	14
12	8	5	373	367	6
14	8	5	470	475	6

Observed and calculated structure factors for K18

h	k	l	10Fo	10Fc	10s
16	8	5	795	784	7
1	9	5	683	673	6
3	9	5	79	67	14
5	9	5	559	545	5
7	9	5	363	345	5
9	9	5	83	74	14
11	9	5	1534	1549	11
13	9	5	115	113	12
15	9	5	79	82	20
0	10	5	1010	1007	8
2	10	5	500	507	5
4	10	5	158	149	8
6	10	5	472	451	5
8	10	5	113	112	10
10	10	5	270	268	7
12	10	5	70	54	20
14	10	5	486	481	6
1	11	5	101	94	11
3	11	5	202	204	7
5	11	5	465	457	5
7	11	5	533	534	5
9	11	5	218	222	8
11	11	5	413	417	6
13	11	5	202	196	8
0	12	5	1138	1139	9
2	12	5	476	478	6
4	12	5	81	71	16
6	12	5	693	695	6
8	12	5	111	102	12
10	12	5	118	118	12
12	12	5	248	231	8
1	13	5	303	300	6
3	13	5	256	266	7
5	13	5	973	968	8
7	13	5	182	191	8
9	13	5	311	311	7
11	13	5	1200	1191	9
0	14	5	874	875	7
2	14	5	228	234	7
4	14	5	354	351	6
6	14	5	413	419	6
8	14	5	193	201	9
1	15	5	89	106	16
3	15	5	227	243	8
5	15	5	98	103	16
7	15	5	328	324	7
0	16	5	266	271	7
2	16	5	273	269	7
4	16	5	143	134	11
0	0	6	2645	2634	12
2	0	6	85	81	11
4	0	6	647	664	6
6	0	6	696	716	6
8	0	6	370	374	5
10	0	6	898	898	7
12	0	6	710	724	6
14	0	6	782	795	7
16	0	6	843	858	7
1	1	6	140	149	8
3	1	6	152	148	7
5	1	6	1756	1753	13
7	1	6	76	72	13
9	1	6	375	382	5
11	1	6	247	245	6
13	1	6	51	35	29
15	1	6	447	443	6
17	1	6	120	320	7
0	2	6	1698	1707	12
2	2	6	207	203	6
4	2	6	208	195	6
6	2	6	494	490	5
8	2	6	250	247	6
10	2	6	793	794	7
12	2	6	314	302	6
14	2	6	19	18	18
16	2	6	387	383	6
1	3	6	203	195	6
3	3	6	93	110	12
5	3	6	846	851	7
7	3	6	31	42	31
9	3	6	1121	1123	9
11	3	6	1111	1116	8
13	3	6	236	246	7
15	3	6	76	74	18
17	3	6	139	337	7
0	4	6	2469	2497	13
2	4	6	41	56	41
4	4	6	374	374	5
6	4	6	509	516	5
8	4	6	126	129	9
10	4	6	1411	1412	10
12	4	6	251	251	7
14	4	6	71	92	21
16	4	6	220	232	8
1	5	6	269	265	5
3	5	6	295	303	5
5	5	6	455	449	5
7	5	6	69	84	17
9	5	6	235	240	7
11	5	6	352	361	6
13	5	6	89	83	15
15	5	6	220	232	8
0	6	6	123	135	9
2	6	6	0	24	1
4	6	6	543	543	5
6	6	6	847	849	7
8	6	6	104	301	6
10	6	6	114	101	10
12	6	6	153	165	9
14	6	6	867	859	7
1	7	6	592	584	5
3	7	6	170	168	7
5	7	6	2480	2513	14
7	7	6	104	103	11
9	7	6	416	416	6
11	7	6	416	424	6
13	7	6	229	215	7
15	7	6	625	630	6
0	8	6	283	269	6
2	8	6	176	182	8
4	8	6	326	324	6
6	8	6	280	280	6
8	8	6	345	352	6
10	8	6	72	98	20
12	8	6	197	195	8
14	8	6	425	426	6
1	9	6	140	141	6
3	9	6	112	116	11
5	9	6	51	41	29
7	9	6	488	486	5
9	9	6	482	484	6
11	9	6	729	727	7
13	9	6	0	41	1
0	10	6	2211	2212	15
2	10	6	337	332	6
4	10	6	134	133	6
6	10	6	521	526	6
8	10	6	91	79	15
10	10	6	1307	1287	9
12	10	6	190	180	9
1	11	6	52	75	31
3	11	6	333	333	6
5	11	6	396	399	6
7	11	6	79	86	19
9	11	6	500	507	6
11	11	6	736	737	7
0	12	6	519	524	6
2	12	6	45	53	44
4	12	6	114	81	12
6	12	6	924	922	7
8	12	6	52	34	40
10	12	6	447	431	6
1	13	6	10	8	29
3	13	6	69	59	22
5	13	6	1404	1405	10
7	13	6	159	169	10
0	14	6	39	17	38
2	14	6	355	354	7
4	14	6	359	342	7
6	14	6	148	152	11
1	1	7	71	70	15
3	1	7	252	244	6
5	1	7	103	14	10
7	1	7	285	272	6
9	1	7	202	199	7
11	1	7	766	758	7
13	1	7	133	133	7
15	1	7	107	120	14
0	2	7	717	714	6
2	2	7	316	321	6
4	2	7	0	6	1
6	2	7	467	469	5
8	2	7	281	285	6
10	2	7	99	114	14
12	2	7	543	535	6
14	2	7	149	156	10
1	3	7	192	191	7
3	3	7	37	21	36
5	3	7	417	408	5
7	3	7	450	446	5
9	3	7	175	175	8
11	3	7	770	766	7
13	3	7	22	34	21
0	4	7	968	950	8
2	4	7	104	91	11
4	4	7	258	251	6
6	4	7	126	80	10
8	4	7	214	208	7
10	4	7	224	222	7
12	4	7	478	489	6
14	4	7	115	112	13
1	5	7	0	6	1
3	5	7	183	189	7
5	5	7	162	167	6
7	5	7	531	531	6
9	5	7	298	295	6
11	5	7	94	69	14
13	5	7	268	270	7
0	6	7	254	261	6
2	6	7	121	120	10
4	6	7	212	216	7
6	6	7	688	671	6
8	6	7	226	245	7
10	6	7	114	121	13
12	6	7	210	216	8
1	7	7	82	75	15
3	7	7	254	252	7
5	7	7	707	690	6
7	7	7	130	114	10
9	7	7	344	345	6
11	7	7	502	492	6
0	8	7	470	470	6
2	8	7	100	99	12
4	8	7	265	264	7
6	8	7	325	320	6
8	8	7	13	36	12
10	8	7	21	34	20
1	9	7	377	365	6
3	9	7	18	38	18
5	9	7	184	191	9
7	9	7	147	143	10
9	9	7	34	23	33
0	10	7	560	578	6
2	10	7	421	423	6
4	10	7	192	189	8
6	10	7	180	182	9
8	10	7	122	102	12
1	11	7	166	170	9
3	11	7	97	112	15
5	11	7	527	511	6
7	11	7	163	169	10
0	12	7	87	96	17
2	12	7	173	180	9
4	12	7	242	237	8
0	0	8	2540	2540	15
2	0	8	165	158	8
4	0	8	268	271	7
6	0	8	680	689	6
8	0	8	40	12	40
10	0	8	1446	1462	10
1	1	8	92	88	14
3	1	8	129	127	10
5	1	8	474	471	6
7	1	8	181	172	9
9	1	8	718	716	7
11	1	8	493	496	6
0	2	8	0	4	1
2	2	8	83	75	16
4	2	8	267	259	7
6	2	8	518	508	6
8	2	8	16	40	35
10	2	8	265	246	7
1	3	8	150	128	9
3	3	8	315	318	6
5	3	8	1846	1814	13
7	3	8	42	12	42
9	3	8	458	449	6
11	3	8	141	123	11
0	4	8	186	193	8
2	4	8	254	260	7
4	4	8	284	277	7
6	4	8	599	611	6
8	4	8	0	40	1
10	4	8	180	160	9
1	5	8	540	543	6
3	5	8	138	153	10
5	5	8	444	444	6
7	5	8	25	20	24
9	5	8	149	145	10
0	6	8	1902	1895	13
2	6	8	190	190	8
4	6	8	344	344	6
6	6	8	473	471	6
8	6	8	147	153	10
1	7	8	56	53	30
3	7	8	141	138	10
5	7	8	939	934	8
7	7	8	210	207	8
0	8	8	980	974	8
2	8	8	51	19	50
4	8	8	0	28	1
6	8	8	376	372	7
1	9	8	10	17	10
3	9	8	157	150	10
5	9	8	1237	1243	10
0	10	8	1082	1068	8
2	10	8	150	138	10
1	1	9	72	46	20
3	1	9	192	184	9
5	1	9	237	237	8
0	2	9	34	44	34
2	2	9	48	60	47
4	2	9	204	203	8
6	2	9	56	8	31
1	3	9	146	151	10
3	3	9	32	28	32
5	3	9	0	39	1
0	4	9	399	404	6
2	4	9	65	56	25
4	4	9	55	63	15
1	5	9	37	6	16
3	5	9	98	86	16

Observed and calculated structure factors for K19

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	671	678	4	4	8	0	494	485	4	3	1	1	518	510	4	7	9	1	261	263	5	9	1	2	725	717	5
4	0	0	1363	1333	6	6	8	0	621	624	5	5	1	1	755	751	5	9	9	1	61	65	14	11	1	2	691	691	5
6	0	0	542	561	4	8	8	0	449	456	4	7	1	1	208	200	3	11	9	1	1668	1681	12	13	1	2	63	58	13
8	0	0	936	911	6	10	8	0	1399	1400	9	9	1	1	488	486	4	13	9	1	50	17	21	15	1	2	703	708	6
10	0	0	3835	3736	11	12	8	0	262	264	5	11	1	1	833	849	6	15	9	1	0	4	1	17	1	2	125	118	8
12	0	0	1385	1386	10	14	8	0	121	115	8	13	1	1	356	347	4	17	9	1	166	162	8	19	1	2	46	33	13
14	0	0	281	267	5	16	8	0	263	267	6	15	1	1	51	54	19	19	9	1	154	175	9	21	1	2	339	320	6
16	0	0	230	219	5	18	8	0	0	18	1	17	1	1	719	734	6	0	10	1	1264	1292	8	0	2	2	4097	4059	8
18	0	0	699	687	6	20	8	0	378	358	6	19	1	1	462	474	5	2	10	1	824	813	6	2	2	2	363	357	3
20	0	0	294	296	6	1	9	0	115	103	7	21	1	1	962	937	7	4	10	1	355	362	4	4	2	2	544	529	4
22	0	0	1564	1574	11	3	9	0	427	447	4	0	2	1	161	116	3	6	10	1	395	405	4	6	2	2	439	430	4
1	1	0	765	784	3	5	9	0	1792	1820	10	2	2	1	389	410	3	8	10	1	130	135	7	8	2	2	328	320	4
3	1	0	307	294	3	7	9	0	901	892	7	4	2	1	520	522	4	10	10	1	273	265	5	10	2	2	1303	1280	8
5	1	0	569	574	4	9	9	0	69	68	13	6	2	1	271	259	3	12	10	1	29	35	28	12	2	2	515	518	5
7	1	0	397	398	3	11	9	0	627	617	5	8	2	1	727	737	5	14	10	1	702	696	6	14	2	2	127	132	7
9	1	0	1704	1672	9	13	9	0	259	268	6	10	2	1	450	467	4	16	10	1	248	262	6	16	2	2	354	348	5
11	1	0	2899	2845	11	15	9	0	513	520	5	12	2	1	947	951	7	18	10	1	347	339	6	18	2	2	88	69	12
13	1	0	253	256	5	17	9	0	468	472	5	14	2	1	116	104	8	1	11	1	318	318	4	20	2	2	62	17	21
15	1	0	231	213	5	19	9	0	315	317	6	16	2	1	742	739	6	3	11	1	279	277	5	1	3	2	418	413	4
17	1	0	316	316	5	0	10	0	316	335	4	18	2	1	67	40	15	5	11	1	613	634	5	3	3	2	194	185	3
19	1	0	624	628	6	2	10	0	55	59	16	20	2	1	93	94	13	7	11	1	462	457	5	5	3	2	1121	1111	8
21	1	0	766	760	7	4	10	0	391	388	4	22	2	1	235	236	7	9	11	1	411	416	5	7	3	2	221	222	4
0	2	0	1183	1227	4	6	10	0	262	266	5	1	3	1	307	304	3	11	11	1	409	406	5	9	3	2	1628	1654	10
2	2	0	335	349	3	8	10	0	400	413	4	3	3	1	242	231	3	13	11	1	112	112	9	11	3	2	1356	1347	9
4	2	0	620	631	4	10	10	0	586	603	5	5	3	1	251	244	3	15	11	1	26	25	26	13	3	2	579	573	5
6	2	0	53	59	10	12	10	0	154	155	7	7	3	1	523	526	4	17	11	1	383	381	6	15	3	2	236	221	5
8	2	0	230	234	3	14	10	0	1186	1216	10	9	3	1	310	317	3	0	12	1	1193	1182	8	17	3	2	319	320	5
10	2	0	621	634	5	16	10	0	249	243	6	11	3	1	229	235	4	2	12	1	509	501	5	19	3	2	876	881	7
12	2	0	315	318	4	18	10	0	619	619	6	13	3	1	311	327	4	4	12	1	108	94	9	21	3	2	538	544	6
14	2	0	851	849	7	1	11	0	392	389	4	15	3	1	0	2	1	6	12	1	633	639	5	0	4	2	2001	1949	7
16	2	0	740	734	6	3	11	0	270	271	4	17	3	1	363	357	5	8	12	1	167	155	7	2	4	2	697	691	5
18	2	0	127	116	8	5	11	0	909	921	7	19	3	1	228	225	6	10	12	1	243	244	6	4	4	2	22	42	21
20	2	0	198	196	7	7	11	0	118	131	8	21	3	1	340	346	6	12	12	1	266	260	6	6	4	2	186	170	4
22	2	0	358	339	6	9	11	0	145	140	7	0	4	1	1002	999	6	14	12	1	75	95	17	8	4	2	134	137	5
1	3	0	413	410	3	11	11	0	529	537	5	2	4	1	30	31	29	16	12	1	700	702	6	10	4	2	2133	2139	11
3	3	0	603	608	4	13	11	0	123	132	9	4	4	1	326	321	3	1	13	1	358	353	5	12	4	2	284	282	4
5	3	0	4753	4790	9	15	11	0	956	966	8	6	4	1	822	787	5	3	13	1	363	374	5	14	4	2	287	287	5
7	3	0	506	476	4	17	11	0	495	497	6	8	4	1	525	523	4	5	13	1	997	998	8	16	4	2	68	43	14
9	3	0	1093	1101	7	0	12	0	1379	1406	9	10	4	1	176	147	5	7	13	1	53	56	21	18	4	2	504	500	5
11	3	0	280	270	4	2	12	0	273	266	5	12	4	1	710	719	6	9	13	1	366	373	5	20	4	2	378	375	6
13	3	0	367	371	4	4	12	0	267	266	5	14	4	1	296	295	5	11	13	1	1102	1107	8	1	5	2	1002	972	6
15	3	0	889	899	7	6	12	0	643	652	6	16	4	1	649	657	6	13	13	1	103	111	12	3	5	2	56	18	11
17	3	0	924	931	7	8	12	0	226	228	6	18	4	1	222	235	6	15	13	1	267	259	7	5	5	2	1754	1723	9
19	3	0	266	268	6	10	12	0	576	568	5	20	4	1	143	148	9	0	14	1	652	660	6	7	5	2	206	194	4
21	3	0	418	412	6	12	12	0	546	532	5	1	5	1	158	159	4	2	14	1	313	307	5	9	5	2	404	410	4
0	4	0	2236	2313	7	14	12	0	120	138	10	3	5	1	643	645	4	4	14	1	509	515	5	11	5	2	654	646	5
2	4	0	709	706	5	16	12	0	166	148	9	5	5	1	1665	1648	8	6	14	1	203	195	6	13	5	2	113	110	8
4	4	0	1086	1077	7	1	13	0	520	519	5	7	5	1	867	834	6	8	14	1	310	309	6	15	5	2	237	227	5
6	4	0	1646	1617	9	3	13	0	249	252	5	9	5	1	566	560	5	10	14	1	142	159	9	17	5	2	784	784	6
8	4	0	580	575	5	5	13	0	396	388	5	11	5	1	296	323	4	12	14	1	134	131	9	19	5	2	454	448	6
10	4	0	574	582	5	7	13	0	561	566	5	13	5	1	693	698	6	14	14	1	445	438	6	21	5	2	529	513	6
12	4	0	339	338	4	9	13	0	427	428	5	15	5	1	258	250	5	1	15	1	85	46	12	0	6	2	1166	1152	8
14	4	0	920	921	7	11	13	0	895	901	7	17	5	1	243	240	6	3	15	1	307	301	5	2	6	2	52	56	12
16	4	0	1974	1963	13	13	13	0	330	344	6	19	5	1	84	91	14	5	15	1	290	290	6	4	6	2	980	982	7
18	4	0	169	163	7	15	13	0	298	294	6	21	5	1	848	829	7	7	15	1	277	275	6	6	6	2	2407	2351	10
20	4	0	328	314	6	0	14	0	1419	1456	10	0	6	1	396	362	3	9	15	1	101	81	11	8	6	2	206	209	5
1	5	0	1531	1531	7	2	14	0	417	415	5	2	6	1	248	238	3	11	15	1	180	175	8	10	6	2	42	32	24
3	5	0	31	16	31	4	14	0	217	217	6	4	6	1	236	237	3	13	15	1	134	125	10	12	6	2	453	466	5
5	5	0	3122	3130	9	6	14	0	807	815	7	6	6	1	861	863	6	0	16	1	277	272	6	14	6	2	974	975	7
7	5	0	921	899	7	8	14	0	105	120	10	8	6	1	519	503	4	2	16	1	269	272	6	16	6	2	1400	1427	10
9	5	0	198	132	4	10	14	0	1382	1391	10	10	6	1	27	28	26	4	16	1	53	54	25	18	6	2	108	101	11
11	5	0	368	390	4	12	14	0	66	50	22	12	6	1	332	316	4	6	16	1	1269	1252	9	20	6	2	26	46	25
13	5	0	346	364	4	14	14	0	57	41	28	14	6	1	4	3	3	8	16	1	361	358	6	1	7	2	834	811	6
15	5	0	301	298	5	1	15	0	289	275	5	16	6	1	1046	1060	8	10	16	1	82	62	15	3	7	2	33	8	31
17	5	0	425	437	5	3	15	0	458	447	5	18	6	1	228	239	7	12	16	1	66	79	21	5	7	2	4505	4483	12
19	5	0	177	193	8	5	15	0	467	465	5	20	6	1	406	410	6	1	17	1	0	32	1	7	7	2	184	181	5
21	5	0	268	280	7	7	15	0	48	25	30	1	7	1	50	34	13	3	17	1	298	296	6	9	7	2	531	531	5
0	6	0	892	906	6	9	15	0	159	154	8	3	7	1	647	642	5	5	17	1	744	740	7	11	7	2	187	193	6
2	6	0	159	157	4	11	15	0	402	405	6	5	7	1	401	406	4	7	17	1	269	268	7	13	7	2	377	374	5
4	6	0	412	418	4	13	15	0	488	488	6	7	7	1	164	155	5	9	17	1	442	440	6	15	7	2	962	979	8
6	6	0	580	575	5	0	16	0	566	564	5	9	7	1	554	570	5	0	18	1	256	268	7	17	7	2	880	881	7
8	6	0	696	693	5	2	16	0	226	216	6	11	7	1	53	29	18	2	18	1	20	44	20	19	7	2	74	98	17
10	6	0	1161	1186	11	4	16	0	151	144	8	13	7	1	79	65	11	4	18	1	403	408	6	0	8	2	408	415	4
12	6	0	315	316	4	6	16	0	842	853	7	15	7	1	107	95	9	6	18	1	419	413	6	2	8	2	533	529	4
14	6	0	473	476	5	8	16	0	78	80	15	17	7	1	187	180	7	1	19	1	357	344	6	4	8	2	179	189	5
16	6	0	563	559	5	10	16	0	17	21	37	19	7	1	159	165	8	0	0	2	3465	3504	7	6	8	2	386	378	4
18	6	0	387	382	5	12	16	0	462	468	6	0	8	1	703	680	5	2	0	2	703	715	5	8	8	2	686	692	6
20	6	0	38	9	37	1	17	0	281	273	6	2	8	1	61	70	12	4	0	2	368	367	3	10	8	2	127	126	7
1	7	0	723	711	5	3	17	0	321	315	6	4	8	1	162	175	5	6	0	2	749	721	5	12	8	2	219	218	6
3	7	0	194	196	4	5	17	0	1829	1832	12	6	8	1	310	327	4	8	0	2	719	710	5	14	8	2	573	579	5
5	7	0	1497	1508	9	7	17	0	45	49	44	8	8	1	135	138	6	10	0	2	1517	1468	10	16	8	2	895	907	7
7	7	0	493	476	4	9	17	0	0	7	1	10	8	1	133	128	7	12	0	2	933	937	7	18	8	2	143	135	9
9	7	0	1235	1254	9	0	18	0	304	315	6	12	8	1	442	444	5	14	0	2	1404	1408	10	1	9	2	554	543	5
11	7	0	530	503	5	2	18	0	339	339	6	14	8	1	569	570	5	16	0	2	725	728	6	3	9	2	80	63	10
13	7	0	465	470	5	4	18	0	61	63	24	16	8	1	764	763	6	18	0	2	966	961	7	5	9	2	476	482	5
15	7	0	293	294	5	6	18	0	222	223	7	18	8	1	326	324	6	20	0	2	116	90	10	7	9	2	465	464	5
17	7	0	207	206	7	8	18	0	368	362	6	20	8	1	181	180	8	1	1	2	567	577	4	9	9	2	634	649	5
19	7	0	783	773	6	1	19	0	281	281	7	1	9	1	967	958	7	3	1	2	809	800	5	11	9	2	1628	1610	13
0	8	0	2548	2597	10	3	19	0	105	98	13	3	9	1	165	157	5	5	1	2	1133	1108	7	13	9	2	47	57	30
2	8	0	174	177	4	1	1	1	192	174	2	5	9	1	497	517	4	7	1	2	181	167	4	15	9	2	326	331	6

Observed and calculated structure factors for K19

h	k	l	10Fo	10Fc	10s
17	9	2	669	672	6
19	9	2	283	280	7
0	10	2	4346	4355	13
2	10	2	672	659	5
4	10	2	756	756	6
6	10	2	94	97	9
8	10	2	282	277	5
10	10	2	1854	1886	13
12	10	2	325	321	5
14	10	2	395	380	5
16	10	2	231	229	7
18	10	2	312	304	6
1	11	2	323	323	4
3	11	2	772	768	6
5	11	2	121	124	8
7	11	2	34	13	33
9	11	2	640	655	6
11	11	2	1681	1715	14
13	11	2	36	35	36
15	11	2	324	315	6
17	11	2	107	103	12
0	12	2	1358	1365	10
2	12	2	61	23	16
4	12	2	127	95	8
6	12	2	932	931	7
8	12	2	154	158	7
10	12	2	819	818	7
12	12	2	269	275	6
14	12	2	514	514	5
16	12	2	376	379	6
1	13	2	177	176	6
3	13	2	78	88	13
5	13	2	1760	1809	13
7	13	2	77	71	14
9	13	2	135	127	8
11	13	2	91	114	13
13	13	2	89	76	13
15	13	2	566	560	6
0	14	2	486	496	5
2	14	2	348	353	5
4	14	2	704	701	6
6	14	2	427	417	5
8	14	2	218	225	7
10	14	2	230	230	6
12	14	2	41	54	41
14	14	2	389	387	6
1	15	2	598	609	6
3	15	2	257	261	6
5	15	2	1472	1491	10
7	15	2	563	567	6
9	15	2	49	70	35
11	15	2	408	403	6
13	15	2	149	132	9
0	16	2	910	924	8
2	16	2	130	125	10
4	16	2	99	96	12
6	16	2	481	495	6
8	16	2	102	99	12
10	16	2	696	689	6
1	17	2	195	196	7
3	17	2	437	434	6
5	17	2	195	196	8
7	17	2	42	39	42
9	17	2	143	134	6
0	18	2	771	751	7
2	18	2	65	47	21
4	18	2	273	270	7
6	18	2	428	426	6
1	1	3	279	276	3
3	1	3	700	695	5
5	1	3	287	290	3
7	1	3	200	198	4
9	1	3	425	438	4
11	1	3	1373	1379	9
13	1	3	428	429	4
15	1	3	17	16	16
17	1	3	330	344	5
19	1	3	455	461	5
21	1	3	915	896	7
0	2	3	2382	2358	8
2	2	3	501	475	4
4	2	3	42	9	15
6	2	3	1124	1097	7
8	2	3	817	803	6
10	2	3	465	478	4
12	2	3	688	700	6
14	2	3	319	318	5
16	2	3	1118	1114	8
18	2	3	147	145	8
20	2	3	29	15	29
1	3	3	527	524	4
3	3	3	272	275	3
5	3	3	1133	1107	9
7	3	3	748	748	6
9	3	3	228	220	4
11	3	3	1308	1320	9
13	3	3	97	109	9
15	3	3	97	66	10
17	3	3	231	231	6
19	3	3	150	147	8
21	3	3	406	409	6
0	4	3	2109	2048	9
2	4	3	91	86	6
4	4	3	423	416	4
6	4	3	209	212	4
8	4	3	286	290	4
10	4	3	302	286	4
12	4	3	784	795	6
14	4	3	134	126	7
16	4	3	265	247	6
18	4	3	151	150	8
20	4	3	78	72	16
1	5	3	66	37	9
3	5	3	423	423	4
5	5	3	1018	1006	8
7	5	3	840	833	6
9	5	3	423	430	4
11	5	3	155	145	6
13	5	3	515	528	5
15	5	3	154	147	7
17	5	3	307	303	6
19	5	3	137	130	9
0	6	3	620	624	5
2	6	3	81	64	8
4	6	3	476	451	4
6	6	3	1201	1194	8
8	6	3	367	374	4
10	6	3	84	86	10
12	6	3	273	274	5
14	6	3	78	76	13
16	6	3	1112	1127	8
18	6	3	370	369	6
20	6	3	357	370	6
1	7	3	110	102	7
3	7	3	331	337	4
5	7	3	1164	1150	8
7	7	3	200	207	5
9	7	3	543	549	5
11	7	3	794	786	6
13	7	3	141	136	8
15	7	3	189	190	7
17	7	3	624	620	6
19	7	3	134	135	10
0	8	3	844	825	6
2	8	3	166	171	5
4	8	3	395	396	4
6	8	3	574	568	5
8	8	3	46	27	22
10	8	3	8	19	8
12	8	3	551	558	5
14	8	3	350	349	5
16	8	3	264	252	6
18	8	3	153	160	9
1	9	3	584	586	5
3	9	3	89	97	10
5	9	3	192	190	5
7	9	3	199	191	5
9	9	3	115	112	8
11	9	3	877	883	7
13	9	3	37	13	16
15	9	3	51	38	30
17	9	3	511	518	6
0	10	3	866	884	6
2	10	3	808	819	6
4	10	3	459	459	5
6	10	3	176	175	6
8	10	3	217	219	5
10	10	3	81	69	12
12	10	3	134	139	8
14	10	3	689	688	6
16	10	3	62	61	23
1	11	3	395	400	5
3	11	3	230	234	5
5	11	3	713	703	6
7	11	3	153	154	7
9	11	3	473	474	5
11	11	3	99	118	11
13	11	3	83	73	14
15	11	3	112	115	11
17	11	3	495	494	6
0	12	3	286	285	5
2	12	3	273	278	5
4	12	3	353	347	5
6	12	3	133	126	8
8	12	3	101	92	10
10	12	3	236	232	6
12	12	3	285	266	6
14	12	3	176	178	8
16	12	3	407	405	6
1	13	3	243	236	6
3	13	3	481	477	5
5	13	3	376	387	5
7	13	3	126	140	9
9	13	3	310	315	6
11	13	3	379	384	6
13	13	3	23	26	23
0	14	3	23	6	22
2	14	3	276	270	6
4	14	3	453	448	5
6	14	3	220	216	6
8	14	3	365	366	6
10	14	3	38	1	38
12	14	3	36	4	36
1	15	3	232	224	6
3	15	3	206	205	7
5	15	3	473	476	5
7	15	3	143	133	9
9	15	3	153	148	8
11	15	3	381	366	6
0	16	3	121	111	11
2	16	3	82	91	15
4	16	3	162	172	9
6	16	3	1075	1088	9
8	16	3	285	285	6
10	16	3	82	95	17
1	17	3	88	104	14
3	17	3	304	293	6
5	17	3	461	453	6
7	17	3	35	6	34
0	18	3	237	244	7
2	18	3	183	156	8
0	0	4	6670	6597	12
2	0	4	396	403	4
4	0	4	777	786	6
6	0	4	450	445	4
8	0	4	265	263	4
10	0	4	2690	2679	12
12	0	4	897	917	7
14	0	4	421	432	5
16	0	4	186	176	7
18	0	4	645	637	6
20	0	4	153	161	9
1	1	4	259	251	4
3	1	4	65	43	11
5	1	4	201	191	4
7	1	4	18	7	18
9	1	4	1296	1288	9
11	1	4	1572	1610	12
13	1	4	130	118	7
15	1	4	156	156	7
17	1	4	38	19	38
19	1	4	560	569	6
0	2	4	278	300	4
2	2	4	239	235	4
4	2	4	388	380	4
6	2	4	512	534	4
8	2	4	43	59	23
10	2	4	408	430	4
12	2	4	324	334	5
14	2	4	623	625	5
16	2	4	740	741	6
18	2	4	94	89	12
20	2	4	135	133	10
1	3	4	285	289	4
3	3	4	505	489	4
5	3	4	3411	3356	11
7	3	4	152	156	6
9	3	4	832	850	6
11	3	4	55	22	17
13	3	4	320	336	5
15	3	4	761	768	6
17	3	4	710	713	6
19	3	4	228	227	7
0	4	4	612	639	5
2	4	4	475	455	4
4	4	4	647	666	5
6	4	4	1834	1812	11
8	4	4	275	284	4
10	4	4	388	402	4
12	4	4	196	208	6
14	4	4	888	891	7
16	4	4	1421	1404	10
18	4	4	213	203	7
1	5	4	1078	1065	8
3	5	4	177	179	5
5	5	4	1504	1545	11
7	5	4	454	453	4
9	5	4	123	116	7
11	5	4	911	937	7
13	5	4	205	199	6
15	5	4	279	285	6
17	5	4	35	46	34
19	5	4	119	126	11
0	6	4	2106	2148	11
2	6	4	155	169	6
4	6	4	395	394	4
6	6	4	143	142	6
8	6	4	375	375	4
10	6	4	1279	1276	9
12	6	4	413	418	5
14	6	4	253	256	6
16	6	4	221	222	7
18	6	4	289	290	6
1	7	4	264	262	4
3	7	4	266	266	4
5	7	4	1347	1365	9
7	7	4	401	397	4
9	7	4	956	966	7
11	7	4	687	692	6
13	7	4	404	400	5
15	7	4	277	279	6
17	7	4	343	334	6
0	8	4	1877	1908	11
2	8	4	46	21	22
4	8	4	235	233	5
6	8	4	579	566	5
8	8	4	372	372	5
10	8	4	1222	1217	9
12	8	4	167	172	7
14	8	4	105	111	10
16	8	4	212	214	7
18	8	4	47	49	47
1	9	4	42	47	32
3	9	4	311	321	5
5	9	4	1685	1714	12
7	9	4	506	508	5
9	9	4	63	2	15
11	9	4	208	206	6
13	9	4	87	106	11
15	9	4	367	361	6
17	9	4	574	568	6
0	10	4	876	878	7
2	10	4	0	11	1
4	10	4	436	449	4
6	10	4	234	224	5
8	10	4	398	403	5
10	10	4	523	521	5
12	10	4	210	209	7
14	10	4	923	920	7
16	10	4	383	385	6
1	11	4	237	237	5
3	11	4	342	346	5
5	11	4	1121	1137	8
7	11	4	35	47	35
9	11	4	57	69	20
11	11	4	81	74	14
13	11	4	87	75	14
15	11	4	849	822	7
0	12	4	857	859	7
2	12	4	285	285	5
4	12	4	142	141	8
6	12	4	291	302	6
8	12	4	275	283	6
10	12	4	355	357	6
12	12	4	353	347	6
14	12	4	52	34	34
1	13	4	287	290	6
3	13	4	158	158	7
5	13	4	252	246	6
7	13	4	343	341	5
9	13	4	443	432	5
11	13	4	704	710	6
13	13	4	198	201	8
0	14	4	1396	1403	10
2	14	4	253	243	6
4	14	4	328	327	6
6	14	4	568	569	6
8	14	4	90	89	13
10	14	4	1100	1095	9
12	14	4	0	18	1
1	15	4	239	226	7
3	15	4	449	437	5
5	15	4	197	200	8
7	15	4	151	141	9
9	15	4	165	142	8
0	16	4	132	132	10
2	16	4	208	196	7
4	16	4	108	93	12
6	16	4	478	474	6
8	16	4	49	11	19
1	17	4	351	349	6
3	17	4	196	200	8
1	1	5	77	79	10
3	1	5	266	275	4
5	1	5	585	585	5
7	1	5	69	77	13
9	1	5	394	395	4
11	1	5	242	244	5
13	1	5	172	176	7
15	1	5	65	64	17
17	1	5	745	747	6
19	1	5	371	378	6
0	2	5	629	629	5
2	2	5	42	18	24
4	2	5	482	489	5
6	2	5	476	476	4
8	2	5	397	393	4
10	2	5	206	204	6
12	2	5	765	763	6
14	2	5	43	32	42
16	2	5	289	288	6
18	2	5	126	135	10
1	3	5	112	116	7
3	3	5	212	199	5
5	3	5	469	481	4
7	3	5	103	114	9
9	3	5	143	137	7
11	3	5	273	281	5
13	3	5	330	330	5
15	3	5	63	54	17
17	3	5	549	554	6
0	4	5	74	67	11
2	4	5	37	12	37
4	4	5	170	166	6
6	4	5	682	666	6
8	4	5	370	378	4
10	4	5	100	71	9
12	4	5	483	492	5
14	4	5	286	288	6
16	4	5	671	665	6
18	4	5	255	260	7
1	5	5	169	172	6
3	5	5	364	365	4
5	5	5	792	796	6
7	5	5	561	565	5
9	5	5	406	417	5
11	5	5	267	261	5
13	5	5	470	474	5
15	5	5	184	169	7
17	5	5	181	179	8
0	6	5	309	345	4
2	6	5	130	135	7
4	6	5	33	17	32
6	6	5	407	403	4
8	6	5	327	331	5
10	6	5	26	12	26
12	6	5	240	234	6
14	6	5	47	18	32
16	6	5	714	710	6
1	7	5	34	27	34
3	7	5	493	508	5
5	7	5	36	18	35
7	7	5	289	294	5
9	7	5	180	180	5
11	7	5	403	395	5
13	7	5	190	186	7
15	7	5	33	5	33
17	7	5	85	78	16
0	8	5	820	824	6
2	8	5	96	81	9
4	8	5	52	35	20
6	8	5	568	563	5
8	8	5	133	129	8
10	8	5	81	79	13
12	8	5	111	116	6
14	8	5	490	495	6
16	8	5	800	788	6
1	9	5	682	680	6
3	9	5	79	69	12
5	9	5	576	561	5

Observed and calculated structure factors for K19

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	9	5	296	296	5	13	1	6	52	53	24	12	8	6	206	209	7	2	4	7	139	132	8	7	1	8	196	208	7
9	9	5	67	61	16	15	1	6	469	468	5	14	8	6	420	406	6	4	4	7	297	299	5	9	1	8	690	690	6
11	9	5	1468	1504	10	17	1	6	308	304	6	1	9	6	384	385	5	6	4	7	94	76	12	11	1	8	475	479	6
13	9	5	88	89	13	0	2	6	1653	1661	12	3	9	6	96	94	11	8	4	7	231	231	6	0	2	8	73	21	16
15	9	5	61	44	21	2	2	6	224	223	5	5	9	6	52	28	24	10	4	7	177	175	8	2	2	8	115	105	10
0	10	5	1010	1000	7	4	2	6	229	222	5	7	9	6	516	519	6	12	4	7	472	474	6	4	2	8	222	231	7
2	10	5	526	522	5	6	2	6	494	498	5	9	9	6	427	443	6	14	4	7	152	147	9	6	2	8	534	534	5
4	10	5	195	188	6	8	2	6	294	288	5	11	9	6	724	738	7	1	5	7	35	29	35	8	2	8	0	12	1
6	10	5	435	426	5	10	2	6	759	776	7	13	9	6	100	84	13	3	5	7	222	227	6	10	2	8	235	230	7
8	10	5	95	93	12	12	2	6	279	279	6	0	10	6	2118	2126	14	5	5	7	379	389	5	1	3	8	150	155	8
10	10	5	255	259	6	14	2	6	26	20	25	2	10	6	313	314	6	7	5	7	490	494	5	3	3	8	329	327	6
12	10	5	0	37	1	16	2	6	392	395	6	4	10	6	334	334	5	9	5	7	311	309	6	5	3	8	1767	1758	12
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1	11	5	164	167	7	3	3	6	68	62	13	8	10	6	95	92	13	13	5	7	331	325	6	9	3	8	468	466	6
3	11	5	212	220	6	5	3	6	835	839	6	10	10	6	1268	1280	9	0	6	7	281	281	6	11	3	8	178	171	8
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7	11	5	466	476	5	9	3	6	1092	1106	8	1	11	6	57	56	23	4	6	7	208	209	7	2	4	8	307	303	6
9	11	5	277	279	6	11	3	6	1070	1071	8	3	11	6	377	373	5	6	6	7	692	676	6	4	4	8	257	246	6
11	11	5	431	441	6	13	3	6	311	314	6	5	11	6	416	413	5	8	6	7	242	256	7	6	4	8	573	578	6
13	11	5	176	185	8	15	3	6	104	102	12	7	11	6	107	104	11	10	6	7	105	102	12	8	4	8	92	83	14
0	12	5	1157	1150	9	0	4	6	2372	2424	12	9	11	6	505	486	6	12	6	7	193	188	8	10	4	8	192	184	8
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6	12	5	699	694	6	6	4	6	427	441	5	2	12	6	57	71	25	5	7	7	696	689	6	5	5	8	437	429	6
8	12	5	106	92	11	8	4	6	103	111	10	4	12	6	102	110	12	7	7	7	152	141	8	7	5	8	51	43	33
10	12	5	126	135	10	10	4	6	1419	1415	9	6	12	6	955	962	7	9	7	7	403	396	6	9	5	8	122	137	11
12	12	5	215	209	7	12	4	6	265	268	6	8	12	6	5	26	5	11	7	7	499	490	6	0	6	8	1825	1843	12
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7	13	5	179	167	8	3	5	6	364	361	5	5	13	6	1333	1348	10	6	8	7	312	320	6	8	6	8	164	168	8
9	13	5	328	328	6	5	5	6	423	419	5	7	13	6	199	197	8	8	8	7	56	54	26	1	7	8	45	59	44
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4	14	5	411	408	6	13	5	6	39	32	19	1	1	7	81	81	13	5	9	7	140	158	9	0	8	8	939	923	7
6	14	5	362	365	6	15	5	6	194	197	8	3	1	7	274	269	5	7	9	7	93	94	13	2	8	8	64	50	20
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3	15	5	251	256	7	4	6	6	489	491	5	9	1	7	237	241	6	2	10	7	448	445	6	1	9	8	0	16	1
5	15	5	120	120	11	6	6	6	844	849	7	11	1	7	736	734	6	4	10	7	224	215	7	3	9	8	187	179	8
7	15	5	243	266	7	8	6	6	270	262	5	13	1	7	324	329	6	6	10	7	199	187	7	5	9	8	1204	1206	9
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2	16	5	305	291	7	12	6	6	229	221	7	0	2	7	720	721	6	1	11	7	206	208	8	2	10	8	103	86	12
0	0	6	2583	2615	12	14	6	6	842	844	7	2	2	7	298	289	5	3	11	7	134	139	10	1	1	9	75	62	17
2	0	6	157	151	6	1	7	6	645	644	6	4	2	7	30	15	29	5	11	7	514	515	6	3	1	9	222	214	7
4	0	6	607	616	5	3	7	6	175	183	7	6	2	7	443	445	5	7	11	7	122	123	11	5	1	9	238	234	7
6	0	6	691	707	6	5	7	6	2449	2448	14	8	2	7	320	318	5	0	12	7	79	85	16	0	2	9	65	48	20
8	0	6	454	453	5	7	7	6	69	88	16	10	2	7	159	156	8	2	12	7	151	167	10	2	2	9	0	14	1
10	0	6	915	920	7	9	7	6	417	429	5	12	2	7	528	524	6	4	12	7	241	245	7	4	2	9	233	233	7
12	0	6	752	758	6	11	7	6	508	511	5	14	2	7	157	152	9	0	0	8	2443	2468	15	6	2	9	0	14	1
14	0	6	802	807	7	13	7	6	228	221	7	1	3	7	180	182	6	2	0	8	154	156	8	1	3	9	171	161	8
16	0	6	831	834	7	15	7	6	641	638	6	3	3	7	0	22	1	4	0	8	295	296	6	3	3	9	56	43	26
1	1	6	178	176	6	0	8	6	315	274	5	5	3	7	421	416	5	6	0	8	741	733	6	5	3	9	61	31	22
3	1	6	175	166	6	2	8	6	232	236	6	7	3	7	439	452	5	8	0	8	8	12	8	0	4	9	414	408	6
5	1	6	1679	1709	12	4	8	6	295	292	5	9	3	7	193	194	7	10	0	8	1450	1440	10	2	4	9	46	38	45
7	1	6	54	56	19	6	8	6	266	265	6	11	3	7	764	758	6	1	1	8	115	108	10	4	4	9	84	82	16
9	1	6	382	382	5	8	8	6	409	410	5	13	3	7	44	20	44	3	1	8	91	91	12	1	5	9	41	8	40
11	1	6	194	196	7	10	8	6	0	56	1	0	4	7	954	945	7	5	1	8	465	455	5	3	5	9	112	122	12

Observed and calculated structure factors for K20

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	629	656	4	6	8	0	646	650	6	5	1	1	625	624	5	9	9	1	77	71	17	11	1	2	702	696	6
4	0	0	1395	1415	6	8	8	0	488	495	5	7	1	1	267	262	4	11	9	1	1641	1675	12	13	1	2	112	108	11
6	0	0	530	536	4	10	8	0	1428	1431	11	9	1	1	510	497	4	13	9	1	30	46	30	15	1	2	733	729	6
8	0	0	1039	1034	8	12	8	0	305	316	6	11	1	1	846	851	7	15	9	1	61	50	27	17	1	2	156	150	10
10	0	0	1682	1781	12	14	8	0	80	68	18	13	1	1	303	304	6	17	9	1	165	164	11	19	1	2	64	36	27
12	0	0	1351	1354	10	16	8	0	236	247	8	15	1	1	113	120	11	19	9	1	176	188	11	21	1	2	321	301	8
14	0	0	314	318	6	18	8	0	9	27	8	17	1	1	726	730	7	0	10	1	1340	1362	10	0	2	2	4157	4058	9
16	0	0	236	248	7	20	8	0	379	354	8	19	1	1	488	498	6	2	10	1	834	830	7	2	2	2	360	368	4
18	0	0	811	776	7	1	9	0	119	120	9	21	1	1	967	958	8	4	10	1	437	451	5	4	2	2	557	548	5
20	0	0	305	309	8	3	9	0	443	448	5	0	2	1	329	273	3	6	10	1	136	151	6	6	2	2	454	437	4
22	0	0	1494	1500	12	5	9	0	1780	1802	12	2	2	1	321	349	3	8	10	1	101	104	13	8	2	2	315	316	4
1	1	0	743	793	4	7	9	0	891	897	7	4	2	1	481	486	4	10	10	1	285	282	7	10	2	2	1290	1277	10
3	1	0	392	389	3	9	9	0	108	93	12	6	2	1	300	286	3	12	10	1	89	78	16	12	2	2	502	504	5
5	1	0	667	686	5	11	9	0	643	624	6	8	2	1	826	845	6	14	10	1	768	757	7	14	2	2	125	130	10
7	1	0	373	368	4	13	9	0	285	279	7	10	2	1	536	567	5	16	10	1	244	250	9	16	2	2	330	349	6
9	1	0	1683	1673	10	15	9	0	500	511	6	12	2	1	954	955	7	18	10	1	382	369	7	18	2	2	54	93	45
11	1	0	2810	2856	12	17	9	0	469	470	7	14	2	1	86	83	14	1	11	1	367	363	5	20	2	2	77	48	25
13	1	0	219	208	6	19	9	0	335	335	8	16	2	1	776	764	7	3	11	1	279	289	6	1	3	2	447	425	4
15	1	0	162	161	8	0	10	0	386	398	5	18	2	1	89	98	18	5	11	1	616	629	6	3	3	2	84	66	10
17	1	0	293	292	7	2	10	0	126	125	9	20	2	1	77	52	23	7	11	1	424	432	6	5	3	2	1244	1230	9
19	1	0	635	621	6	4	10	0	349	360	5	22	2	1	241	252	10	9	11	1	454	463	6	7	3	2	267	263	4
21	1	0	767	760	7	6	10	0	228	240	7	1	3	1	270	278	4	11	11	1	416	418	6	9	3	2	1643	1667	12
0	2	0	1151	1170	5	8	10	0	502	502	6	3	3	1	215	189	4	13	11	1	104	109	14	11	3	2	1363	1375	10
2	2	0	372	394	3	10	10	0	664	669	6	5	3	1	187	166	5	15	11	1	34	6	34	13	3	2	672	661	6
4	2	0	594	611	4	12	10	0	153	152	10	7	3	1	544	528	4	17	11	1	361	358	7	15	3	2	285	278	6
6	2	0	0	22	1	14	10	0	1194	1209	9	9	3	1	146	357	4	0	12	1	1266	1262	10	17	3	2	286	294	7
8	2	0	194	198	5	16	10	0	282	291	8	11	3	1	226	237	6	2	12	1	463	469	6	19	3	2	870	877	8
10	2	0	587	594	5	18	10	0	685	678	7	13	3	1	365	378	5	4	12	1	112	95	12	21	3	2	583	572	7
12	2	0	306	316	5	1	11	0	450	436	5	15	3	1	47	29	47	6	12	1	651	641	6	0	4	2	2123	2049	9
14	2	0	805	830	7	3	11	0	279	290	6	17	3	1	374	382	6	8	12	1	207	209	8	2	4	2	740	717	5
16	2	0	745	746	7	5	11	0	944	965	8	19	3	1	243	232	8	10	12	1	294	295	7	4	4	2	94	112	9
18	2	0	145	145	11	7	11	0	117	120	11	21	3	1	160	357	8	12	12	1	255	246	8	6	4	2	140	116	7
20	2	0	196	194	10	9	11	0	183	182	9	0	4	1	963	950	6	14	12	1	96	92	18	8	4	2	183	202	6
22	2	0	355	348	8	11	11	0	535	547	6	2	4	1	49	8	19	16	12	1	711	709	7	10	4	2	2181	2201	13
1	3	0	456	440	4	13	11	0	164	162	10	4	4	1	343	346	4	1	13	1	307	312	6	12	4	2	242	250	6
3	3	0	502	521	4	15	11	0	969	990	8	6	4	1	833	802	6	3	13	1	349	345	6	14	4	2	321	312	6
5	3	0	4691	4876	10	17	11	0	523	538	7	8	4	1	550	558	5	5	13	1	1041	1047	9	16	4	2	37	32	36
7	3	0	477	460	4	0	12	0	1327	1353	10	10	4	1	114	104	10	7	13	1	56	57	35	18	4	2	551	545	6
9	3	0	1149	1141	7	2	12	0	266	253	6	12	4	1	719	719	6	9	13	1	417	419	6	20	4	2	392	390	7
11	3	0	277	278	5	4	12	0	306	313	6	14	4	1	322	320	6	11	13	1	1092	1102	9	1	5	2	1020	985	7
13	3	0	448	453	5	6	12	0	664	678	6	16	4	1	653	658	6	13	13	1	101	82	17	3	5	2	0	39	1
15	3	0	935	932	8	8	12	0	246	248	7	18	4	1	216	219	9	15	13	1	244	239	9	5	5	2	1681	1650	10
17	3	0	912	902	7	10	12	0	544	542	6	20	4	1	199	174	10	0	14	1	656	669	6	7	5	2	204	190	6
19	3	0	277	286	7	12	12	0	563	558	6	1	5	1	162	162	5	2	14	1	338	331	6	9	5	2	422	428	5
21	3	0	188	178	7	14	12	0	164	177	11	3	5	1	760	771	5	4	14	1	573	583	6	11	5	2	636	630	6
0	4	0	2448	2463	7	16	12	0	171	164	11	5	5	1	1780	1774	10	6	14	1	159	151	10	13	5	2	164	151	8
2	4	0	768	762	5	1	13	0	537	541	6	7	5	1	817	795	6	8	14	1	329	310	7	15	5	2	202	205	8
4	4	0	1098	1121	8	3	13	0	285	284	6	9	5	1	565	556	5	10	14	1	155	153	11	17	5	2	813	810	7
6	4	0	3544	3602	10	5	13	0	392	389	6	11	5	1	315	344	5	12	14	1	98	96	18	19	5	2	451	446	7
8	4	0	656	647	5	7	13	0	583	591	6	13	5	1	786	791	6	14	14	1	506	487	7	21	5	2	566	542	7
10	4	0	651	670	6	9	13	0	393	394	6	15	5	1	326	317	6	1	15	1	81	68	19	0	6	2	1235	1229	8
12	4	0	340	331	5	11	13	0	913	905	8	17	5	1	243	248	8	3	15	1	282	288	7	2	6	2	0	11	1
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20	4	0	349	347	7	2	14	0	448	445	6	2	6	1	281	273	4	11	15	1	201	188	10	10	6	2	82	86	15
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5	5	0	3176	3164	10	6	14	0	821	825	7	6	6	1	822	825	6	0	16	1	311	315	7	14	6	2	944	954	7
7	5	0	934	927	7	8	14	0	155	175	11	8	6	1	482	471	5	2	16	1	251	255	8	16	6	2	1411	1426	10
9	5	0	78	99	14	10	14	0	1415	1441	11	10	6	1	33	40	33	4	16	1	69	68	26	18	6	2	133	133	12
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13	5	0	331	342	6	14	14	0	50	56	50	14	6	1	45	19	44	8	16	1	338	340	8	1	7	2	869	854	7
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17	5	0	420	411	6	3	15	0	449	453	6	18	6	1	214	213	9	12	16	1	82	75	25	5	7	2	4588	4560	13
19	5	0	168	160	10	5	15	0	442	440	6	20	6	1	409	397	7	1	17	1	18	29	18	7	7	2	163	170	8
21	5	0	250	256	9	7	15	0	75	64	24	1	7	1	31	13	31	3	17	1	289	291	8	9	7	2	549	562	5
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6	6	0	585	574	5	0	16	0	555	550	6	9	7	1	615	626	6	0	18	1	277	287	8	17	7	2	851	841	7
8	6	0	664	646	6	2	16	0	237	228	8	11	7	1	67	45	19	2	18	1	0	28	1	19	7	2	128	121	14
10	6	0	1429	1428	10	4	16	0	98	99	17	13	7	1	76	82	17	4	18	1	447	454	7	0	8	2	362	353	4
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14	6	0	467	468	6	8	16	0	82	83	23	17	7	1	173	165	10	1	19	1	339	343	8	4	8	2	245	237	6
16	6	0	550	543	6	10	16	0	34	17	34	19	7	1	180	188	11	0	0	2	3789	3686	8	6	8	2	396	369	5
18	6	0	416	417	7	12	16	0	477	482	7	0	8	1	763	731	6	2	0	2	786	802	5	8	8	2	752	746	7
20	6	0	31	5	30	1	17	0	275	273	8	2	8	1	114	127	9	4	0	2	409	399	4	10	8	2	179	180	8
1	7	0	742	731	5	3	17	0	347	345	7	4	8	1	198	201	6	6	0	2	765	713	6	12	8	2	266	268	7
3	7	0	277	276	4	5	17	0	1848	1843	12	6	8	1	355	347	5	8	0	2	866	865	7	14	8	2	606	603	6
5	7	0	1624	1622	11	7	17	0	58	54	50	8	8	1	191	184	7	10	0	2	1559	1563	12	16	8	2	912	928	8
7	7	0	484	484	5	9	17	0	54	7	54	10	8	1	193	173	7	12	0	2	904	910	7	18	8	2	189	171	10
9	7	0	1278	1279	9	0	18	0	274	287	8	12	8	1	424	416	6	14	0	2	1418	1432	10	1	9	2	585	580	5
11	7	0	556	517	6	2	18	0	369	362	7	14	8	1	591	593	6	16	0	2	773	783	7	3	9	2	83	67	15
13	7	0	564	564	5	4	18	0	69	70	32	16	8	1	797	780	7	18	0	2	1072	1049	8	5	9	2	479	480	5
15	7	0	326	340	6	6	18	0	218	232	10	18	8	1	330	311	7	20	0	2	128	111	13	7	9	2	487	480	5
17	7	0	171	169	10	8	18	0	398	393	8	20	8	1	158	141	12	1	1	2	624	633	5	9	9	2	618	615	6
19	7	0	784	775	7	1	19	0	327	337	8	1	9	1	966	943	7	3	1	2	755	760	6	11	9	2	1592	1614	12
0	8	0	2679	2647	11	3	19	0	135	123	15	3	9	1	214	220	6	5	1	2	1188	1176	9	13	9	2	61	52	27
2	8	0	173	180	6	1	1	1	177	175	4	5	9	1	596	618	5	7	1	2	167	157	5	15	9	2	325	324	7
4	8	0	565	559	5	3	1	1	596	595	5	7	9	1	244	237	6	9	1	2	752	757	6	17	9	2	670	678	7

Observed and calculated structure factors for K20

h	k	l	10Fo	10Fc	10s
19	9	2	252	261	9
0	10	2	4399	4400	14
2	10	2	621	622	6
4	10	2	742	750	7
6	10	2	89	83	14
8	10	2	337	340	6
10	10	2	1887	1919	12
12	10	2	332	321	6
14	10	2	389	391	7
16	10	2	182	200	11
18	10	2	383	358	7
1	11	2	294	294	6
3	11	2	803	800	7
5	11	2	172	176	9
7	11	2	47	6	46
9	11	2	669	678	6
11	11	2	1704	1711	13
13	11	2	19	22	18
15	11	2	358	353	7
17	11	2	142	140	13
0	12	2	1390	1397	10
2	12	2	0	46	1
4	12	2	149	153	10
6	12	2	970	972	8
8	12	2	180	171	9
10	12	2	810	821	7
12	12	2	318	306	7
14	12	2	475	470	7
16	12	2	157	173	8
1	13	2	166	171	9
3	13	2	79	78	19
5	13	2	1825	1797	13
7	13	2	86	88	18
9	13	2	133	115	12
11	13	2	111	115	15
13	13	2	65	80	32
15	13	2	571	570	7
0	14	2	571	569	6
2	14	2	193	186	6
4	14	2	680	682	7
6	14	2	428	430	6
8	14	2	273	276	8
10	14	2	279	288	8
12	14	2	48	54	48
14	14	2	165	169	8
1	15	2	672	669	6
3	15	2	254	253	8
5	15	2	1492	1497	12
7	15	2	610	617	7
9	15	2	0	8	1
11	15	2	423	418	7
13	15	2	150	154	13
0	16	2	903	895	7
2	16	2	146	131	12
4	16	2	140	130	13
6	16	2	498	495	7
8	16	2	114	99	15
10	16	2	675	681	7
1	17	2	189	178	10
3	17	2	457	465	7
5	17	2	226	226	9
7	17	2	23	46	23
9	17	2	115	115	8
0	18	2	781	772	8
2	18	2	0	36	1
4	18	2	288	292	9
6	18	2	431	423	8
1	1	3	268	268	4
3	1	3	786	766	6
5	1	3	384	388	4
7	1	3	163	159	6
9	1	3	453	450	5
11	1	3	1384	1381	11
13	1	3	194	199	5
15	1	3	51	45	33
17	1	3	136	140	7
19	1	3	459	479	7
21	1	3	947	914	8
0	2	3	2577	2501	9
2	2	3	449	420	4
4	2	3	25	15	25
6	2	3	1109	1091	7
8	2	3	901	894	7
10	2	3	548	560	5
12	2	3	698	702	6
14	2	3	312	305	6
16	2	3	1117	1130	9
18	2	3	96	100	17
20	2	3	40	29	39
1	3	3	509	486	4
3	3	3	126	311	4
5	3	3	1179	1159	9
7	3	3	770	766	6
9	3	3	249	249	6
11	3	3	1290	1317	9
13	3	3	139	141	10
15	3	3	38	41	37
17	3	3	199	208	9
19	3	3	163	161	11
21	3	3	414	412	8
0	4	3	2120	2026	10
2	4	3	97	101	9
4	4	3	444	429	4
6	4	3	218	209	6
8	4	3	311	309	5
10	4	3	256	247	6
12	4	3	797	797	6
14	4	3	142	140	10
16	4	3	245	256	8
18	4	3	120	131	14
20	4	3	94	89	19
1	5	3	43	18	32
3	5	3	513	524	5
5	5	3	1126	1127	8
7	5	3	799	792	6
9	5	3	418	430	5
11	5	3	183	175	8
13	5	3	608	615	6
15	5	3	226	210	8
17	5	3	309	306	7
19	5	3	144	133	12
0	6	3	712	700	5
2	6	3	85	52	12
4	6	3	527	517	5
6	6	3	1179	1163	9
8	6	3	350	357	5
10	6	3	54	36	27
12	6	3	287	284	6
14	6	3	51	58	50
16	6	3	1113	1118	9
18	6	3	329	348	8
20	6	3	361	359	8
1	7	3	71	71	17
3	7	3	333	328	5
5	7	3	1170	1176	9
7	7	3	213	219	7
9	7	3	582	588	6
11	7	3	772	781	7
13	7	3	135	127	11
15	7	3	199	195	9
17	7	3	595	613	7
19	7	3	161	162	12
0	8	3	805	783	6
2	8	3	224	225	6
4	8	3	426	426	5
6	8	3	564	551	5
8	8	3	13	23	13
10	8	3	40	33	39
12	8	3	528	531	6
14	8	3	156	166	7
16	8	3	284	280	8
18	8	3	144	140	13
1	9	3	565	575	6
3	9	3	107	60	12
5	9	3	107	101	12
7	9	3	172	165	8
9	9	3	134	130	10
11	9	3	875	882	7
13	9	3	128	66	12
15	9	3	63	9	29
17	9	3	529	518	7
0	10	3	934	938	7
2	10	3	839	840	7
4	10	3	530	537	6
6	10	3	167	136	9
8	10	3	189	198	8
10	10	3	91	89	17
12	10	3	182	172	9
14	10	3	732	750	7
16	10	3	53	59	53
1	11	3	434	434	5
3	11	3	262	247	7
5	11	3	708	709	6
7	11	3	124	132	11
9	11	3	506	517	6
11	11	3	95	120	18
13	11	3	86	80	19
15	11	3	125	134	15
17	11	3	472	483	7
0	12	3	145	149	6
2	12	3	240	245	7
4	12	3	353	352	6
6	12	3	131	120	11
8	12	3	150	144	11
10	12	3	273	282	8
12	12	3	260	257	8
14	12	3	165	177	12
16	12	3	438	416	7
1	13	3	207	200	8
3	13	3	450	463	6
5	13	3	427	430	6
7	13	3	126	142	13
9	13	3	171	165	7
11	13	3	176	178	7
13	13	3	61	61	40
0	14	3	54	18	42
2	14	3	284	290	7
4	14	3	506	507	6
6	14	3	275	273	8
8	14	3	179	170	7
10	14	3	0	2	1
12	14	3	0	23	1
1	15	3	225	241	9
3	15	3	182	182	10
5	15	3	479	477	7
7	15	3	99	109	18
9	15	3	159	167	12
11	15	3	176	171	8
0	16	3	154	137	12
2	16	3	91	73	20
4	16	3	174	162	11
6	16	3	1064	1077	9
8	16	3	259	264	9
10	16	3	108	122	18
1	17	3	33	48	32
3	17	3	279	288	9
5	17	3	491	479	7
7	17	3	64	29	39
0	18	3	230	232	9
2	18	3	143	142	14
0	0	4	6867	6703	14
2	0	4	381	373	4
4	0	4	819	825	6
6	0	4	481	461	5
8	0	4	347	345	5
10	0	4	2716	2731	14
12	0	4	882	902	7
14	0	4	483	484	6
16	0	4	139	144	11
18	0	4	733	721	7
20	0	4	181	164	11
1	1	4	257	242	5
3	1	4	15	20	15
5	1	4	141	128	8
7	1	4	14	8	14
9	1	4	1287	1313	9
11	1	4	1606	1614	11
13	1	4	100	79	13
15	1	4	113	118	13
17	1	4	58	42	34
19	1	4	566	566	7
0	2	4	254	277	5
2	2	4	256	251	5
4	2	4	372	378	5
6	2	4	530	548	5
8	2	4	46	38	45
10	2	4	391	410	5
12	2	4	322	327	6
14	2	4	604	610	6
16	2	4	741	747	7
18	2	4	112	109	16
20	2	4	141	132	13
1	3	4	310	308	5
3	3	4	448	434	5
5	3	4	3422	3423	13
7	3	4	154	142	8
9	3	4	877	885	7
11	3	4	0	26	1
13	3	4	407	405	6
15	3	4	791	796	7
17	3	4	705	687	7
19	3	4	251	244	9
0	4	4	707	724	6
2	4	4	504	489	5
4	4	4	672	700	6
6	4	4	1809	1796	13
8	4	4	333	331	6
10	4	4	468	472	5
12	4	4	201	198	8
14	4	4	920	914	7
16	4	4	1429	1409	10
18	4	4	253	252	8
1	5	4	1102	1096	8
3	5	4	187	181	7
5	5	4	1512	1569	10
7	5	4	477	467	5
9	5	4	69	82	20
11	5	4	943	949	8
13	5	4	169	177	9
15	5	4	273	284	8
17	5	4	46	25	46
19	5	4	92	98	21
0	6	4	2153	2192	13
2	6	4	118	139	10
4	6	4	397	396	5
6	6	4	141	138	9
8	6	4	343	337	6
10	6	4	1300	1303	9
12	6	4	415	423	6
14	6	4	243	244	8
16	6	4	223	215	9
18	6	4	329	312	8
1	7	4	277	278	6
3	7	4	348	338	5
5	7	4	1440	1450	11
7	7	4	400	401	5
9	7	4	982	982	8
11	7	4	702	701	7
13	7	4	464	475	6
15	7	4	334	318	7
17	7	4	304	298	8
0	8	4	1913	1932	13
2	8	4	40	29	40
4	8	4	287	294	6
6	8	4	593	602	6
8	8	4	400	401	6
10	8	4	1216	1240	10
12	8	4	227	221	8
14	8	4	62	72	33
16	8	4	199	203	10
18	8	4	85	84	23
1	9	4	46	53	45
3	9	4	114	324	6
5	9	4	1678	1706	12
7	9	4	509	504	6
9	9	4	48	17	47
11	9	4	206	208	8
13	9	4	118	109	13
15	9	4	340	354	8
17	9	4	565	572	7
0	10	4	946	946	8
2	10	4	74	65	18
4	10	4	421	429	6
6	10	4	262	256	7
8	10	4	486	484	6
10	10	4	564	576	6
12	10	4	206	206	9
14	10	4	918	908	8
16	10	4	420	428	7
1	11	4	289	287	7
3	11	4	371	370	6
5	11	4	1153	1170	9
7	11	4	78	27	20
9	11	4	104	101	15
11	11	4	82	85	21
13	11	4	68	96	11
15	11	4	840	844	8
0	12	4	818	819	7
2	12	4	290	286	7
4	12	4	195	174	9
6	12	4	336	322	7
8	12	4	311	312	7
10	12	4	345	337	7
12	12	4	381	372	7
14	12	4	54	57	54
1	13	4	306	314	7
3	13	4	181	182	10
5	13	4	265	260	8
7	13	4	363	364	7
9	13	4	403	408	7
11	13	4	730	727	7
13	13	4	184	206	12
0	14	4	1456	1465	11
2	14	4	276	265	8
4	14	4	326	323	7
6	14	4	549	571	7
8	14	4	144	136	12
10	14	4	1148	1142	9
12	14	4	28	11	28
1	15	4	282	263	8
3	15	4	449	451	7
5	15	4	179	173	11
7	15	4	187	180	11
9	15	4	188	187	11
0	16	4	104	114	18
2	16	4	206	199	10
4	16	4	14	58	13
6	16	4	495	485	7
8	16	4	0	4	1
1	17	4	373	345	7
3	17	4	233	218	10
1	1	5	68	74	19
3	1	5	327	330	5
5	1	5	519	511	5
7	1	5	107	109	12
9	1	5	398	402	6
11	1	5	239	251	7
13	1	5	138	143	11
15	1	5	129	112	12
17	1	5	744	748	7
19	1	5	396	405	8
0	2	5	553	540	5
2	2	5	0	24	1
4	2	5	466	469	5
6	2	5	491	492	5
8	2	5	464	469	5
10	2	5	269	272	7
12	2	5	762	776	6
14	2	5	32	22	32
16	2	5	317	316	8
18	2	5	180	178	11
1	3	5	93	96	13
3	3	5	165	169	8
5	3	5	426	433	5
7	3	5	122	119	10
9	3	5	156	161	9
11	3	5	268	276	7
13	3	5	366	375	6
15	3	5	62	73	32
17	3	5	559	574	7
0	4	5	44	47	43
2	4	5	33	6	32
4	4	5	165	184	8
6	4	5	674	675	6
8	4	5	383	392	6
10	4	5	71	45	19
12	4	5	484	494	6
14	4	5	306	304	7
16	4	5	669	664	7
18	4	5	241	249	9
1	5	5	184	178	7
3	5	5	416	419	5
5	5	5	880	879	7
7	5	5	531	542	6
9	5	5	420	419	6
11	5	5	294	280	7
13	5	5	535	542	6
15	5	5	217	220	9
17	5	5	197	188	10
0	6	5	263	291	6
2	6	5	156	152	9
4	6	5	18	11	18
6	6	5	391	375	6
8	6	5	293	307	6
10	6	5	44	35	44
12	6	5	256	249	7
14	6	5	0	27	1
16	6	5	712	709	7
1	7	5	34	4	33
3	7	5	487	497	6
5	7	5	48	40	48
7	7	5	289	291	7
9	7	5	431	415	6
11	7	5	191	199	6
13	7	5	215	208	9
15	7	5	14	3	14
17	7	5	80	87	25
0	8	5	844	861	7
2	8	5	109	47	12
4	8	5	64	54	24
6	8	5	580	580	6
8	8	5	153	152	10
10	8	5	112	112	14
12	8	5	297	293	7
14	8	5	520	508	7
16	8	5	816	801	7
1	9	5	677	669	6
3	9	5	107	102	14
5	9	5	643	628	6
7	9	5	289	285	7

Observed and calculated structure factors for K20

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
9	9	5	0	70	1	15	1	6	485	486	7	14	8	6	431	426	7	4	4	7	314	314	7	9	1	8	697	706	7
11	9	5	1490	1502	11	17	1	6	271	282	9	1	9	6	405	407	6	6	4	7	74	70	22	11	1	8	486	491	7
13	9	5	72	56	26	0	2	6	1687	1675	11	3	9	6	105	94	15	8	4	7	253	259	8	0	2	8	23	39	23
15	9	5	29	7	28	2	2	6	230	228	7	5	9	6	75	33	22	10	4	7	138	152	13	2	2	8	111	113	15
0	10	5	1053	1040	8	4	2	6	234	229	7	7	9	6	531	534	6	12	4	7	490	482	7	4	2	8	224	226	9
2	10	5	534	535	6	6	2	6	507	504	5	9	9	6	430	425	7	14	4	7	180	171	11	6	2	8	553	546	7
4	10	5	247	249	7	8	2	6	289	286	7	11	9	6	751	735	7	1	5	7	43	27	42	8	2	8	56	3	45
6	10	5	400	391	6	10	2	6	775	782	7	13	9	6	87	95	21	3	5	7	277	272	7	10	2	8	216	218	10
8	10	5	74	70	22	12	2	6	280	277	7	0	10	6	2155	2158	17	5	5	7	440	444	6	1	3	8	183	177	10
10	10	5	269	273	8	14	2	6	0	17	1	2	10	6	295	292	7	7	5	7	481	484	6	3	3	8	302	304	8
12	10	5	0	5	1	16	2	6	392	392	7	4	10	6	328	334	7	9	5	7	320	304	7	5	3	8	1818	1803	12
14	10	5	569	567	7	1	3	6	207	215	7	6	10	6	575	573	6	11	5	7	71	69	28	7	3	8	4	27	4
1	11	5	211	196	8	3	3	6	0	16	1	8	10	6	131	135	14	13	5	7	379	378	8	9	3	8	503	499	7
3	11	5	201	220	9	5	3	6	913	908	7	10	10	6	1312	1312	10	0	6	7	322	322	7	11	3	8	176	170	11
5	11	5	438	420	6	7	3	6	123	117	11	12	10	6	168	165	12	2	6	7	103	97	14	0	4	8	164	149	11
7	11	5	444	462	6	9	3	6	1120	1129	8	1	11	6	0	38	1	4	6	7	249	244	8	2	4	8	317	325	7
9	11	5	296	308	8	11	3	6	1083	1096	8	3	11	6	395	384	7	6	6	7	667	658	7	4	4	8	279	270	8
11	11	5	456	450	7	13	3	6	384	369	7	5	11	6	370	375	7	8	6	7	241	254	8	6	4	8	572	573	7
13	11	5	191	187	11	15	3	6	147	140	13	7	11	6	74	101	26	10	6	7	69	71	29	8	4	8	117	121	14
0	12	5	1213	1213	9	0	4	6	2478	2498	15	9	11	6	528	515	7	12	6	7	186	195	11	10	4	8	246	229	9
2	12	5	473	479	6	2	4	6	78	79	18	11	11	6	676	679	7	1	7	7	25	27	24	1	5	8	577	591	7
4	12	5	77	68	23	4	4	6	412	426	6	0	12	6	574	565	6	3	7	7	296	305	7	1	5	8	138	146	11
6	12	5	700	701	7	6	4	6	416	419	6	2	12	6	91	83	19	5	7	7	696	701	7	5	5	8	442	449	7
8	12	5	137	126	13	8	4	6	143	151	10	4	12	6	143	146	13	7	7	7	156	141	11	7	5	8	53	46	52
10	12	5	182	172	11	10	4	6	1484	1460	11	6	12	6	994	984	8	9	7	7	422	432	7	9	5	8	112	121	17
12	12	5	199	198	10	12	4	6	243	245	8	8	12	6	0	34	1	11	7	7	478	483	7	0	6	8	1865	1881	13
1	13	5	263	269	8	14	4	6	110	108	15	10	12	6	476	453	7	0	8	7	468	457	6	2	6	8	183	173	10
3	13	5	271	265	8	16	4	6	184	182	11	1	13	6	56	14	47	2	8	7	194	179	9	4	6	8	337	341	8
5	13	5	1007	997	8	1	5	6	272	260	6	3	13	6	37	24	36	4	8	7	332	327	7	6	6	8	439	451	7
7	13	5	178	175	11	3	5	6	399	398	6	5	13	6	1343	1341	10	6	8	7	301	308	8	8	6	8	148	153	13
9	13	5	368	371	8	5	5	6	393	381	6	7	13	6	211	212	10	8	8	7	81	94	24	1	7	8	62	79	17
11	13	5	1212	1192	9	7	5	6	71	81	21	0	14	6	63	51	16	10	8	7	0	15	-1	3	7	8	207	214	10
0	14	5	875	859	8	9	5	6	201	205	8	2	14	6	430	426	7	1	9	7	167	171	7	5	7	8	967	969	8
2	14	5	267	270	9	11	5	6	361	369	7	4	14	6	307	292	8	3	9	7	51	11	51	7	7	8	212	222	10
4	14	5	461	459	7	13	5	6	39	15	19	1	1	7	82	83	17	5	9	7	103	107	17	0	8	8	945	951	8
6	14	5	336	335	8	15	5	6	189	181	10	3	1	7	301	295	6	7	9	7	95	89	19	2	8	8	58	55	44
8	14	5	218	210	10	0	6	6	97	91	14	5	1	7	52	51	38	9	9	7	0	24	1	4	8	8	71	67	31
1	15	5	6	32	6	2	6	6	69	56	21	7	1	7	203	204	8	0	10	7	642	636	7	6	8	8	432	425	7
3	15	5	251	245	9	4	6	6	463	476	6	9	1	7	245	244	8	2	10	7	461	456	7	1	9	8	23	11	23
5	15	5	132	130	14	6	6	6	868	870	7	11	1	7	729	740	7	4	10	7	281	263	8	1	9	8	182	189	11
7	15	5	242	243	9	8	6	6	239	240	8	13	1	7	299	311	8	6	10	7	179	162	11	5	9	8	1208	1214	9
0	16	5	291	289	9	10	6	6	62	46	29	15	1	7	0	34	1	8	10	7	103	81	19	0	10	8	1095	1084	9
2	16	5	283	285	9	12	6	6	246	243	8	0	2	7	784	775	7	1	11	7	242	233	9	2	10	8	47	68	47
0	0	6	2727	2717	14	14	6	6	840	843	7	2	2	7	272	280	7	3	11	7	138	154	14	1	1	9	81	56	21
2	0	6	181	182	8	1	7	6	667	671	7	4	2	7	33	3	33	5	11	7	537	513	7	3	1	9	251	251	9
4	0	6	634	649	6	3	7	6	166	162	9	6	2	7	433	435	6	7	11	7	109	114	17	5	1	9	183	194	12
6	0	6	719	711	6	5	7	6	2504	2511	16	8	2	7	327	346	7	0	12	7	142	139	14	0	2	9	27	15	26
8	0	6	517	534	6	7	7	6	81	81	19	10	2	7	201	202	10	2	12	7	154	146	12	2	2	9	30	6	30
10	0	6	958	974	8	9	7	6	465	464	6	12	2	7	516	530	7	4	12	7	256	246	9	4	2	9	201	212	10
12	0	6	725	735	7	11	7	6	493	512	7	14	2	7	90	123	21	0	0	8	2521	2535	17	6	2	9	17	23	16
14	0	6	834	827	7	13	7	6	287	275	8	1	3	7	176	182	9	2	0	8	143	147	11	1	3	9	146	152	11
16	0	6	866	869	8	15	7	6	667	656	7	3	3	7	31	19	31	4	0	8	135	134	7	3	3	9	37	75	37
1	1	6	206	208	7	0	8	6	232	222	8	5	3	7	458	453	6	6	0	8	762	755	7	5	3	9	0	7	1
3	1	6	144	139	9	2	8	6	237	245	8	7	3	7	450	450	6	8	0	8	17	41	16	0	4	9	414	396	7
5	1	6	1752	1755	12	4	8	6	325	320	7	9	3	7	203	213	9	10	0	8	1478	1477	10	2	4	9	0	32	1
7	1	6	56	70	10	6	8	6	255	271	8	11	3	7	763	760	7	1	1	8	118	107	14	4	4	9	90	100	22
9	1	6	406	402	6	8	8	6	443	445	6	13	3	7	26	9	25	3	1	8	54	68	49	1	5	9	0	10	1
11	1	6	185	194	9	10	8	6	9	16	8	0	4	7	942	927	8	5	1	8	426	414	7	3	5	9	160	152	13
13	1	6	28	28	28	12	8	6	251	241	9	2	4	7	155	151	10	7	1	8	207	218	10						

Observed and calculated structure factors for K21

h	k	l	10Fo	10Fc	10s
2	0	0	638	672	4
4	0	0	1208	1226	5
6	0	0	656	672	5
8	0	0	1144	1134	8
10	0	0	1996	1917	9
12	0	0	1461	1469	10
14	0	0	343	326	5
16	0	0	423	423	5
18	0	0	483	482	5
20	0	0	475	469	6
22	0	0	1829	1829	13
1	1	0	701	750	3
3	1	0	278	278	3
5	1	0	640	653	4
7	1	0	451	453	4
9	1	0	1627	1573	9
11	1	0	3108	3002	10
13	1	0	430	431	4
15	1	0	216	231	6
17	1	0	366	361	5
19	1	0	557	551	6
21	1	0	846	860	7
0	2	0	1219	1270	4
2	2	0	284	311	3
4	2	0	598	604	4
6	2	0	156	160	4
8	2	0	265	263	3
10	2	0	583	582	5
12	2	0	414	412	4
14	2	0	869	868	7
16	2	0	796	800	6
18	2	0	174	159	7
20	2	0	59	73	24
22	2	0	240	244	7
1	3	0	298	312	3
3	3	0	400	416	3
7	3	0	527	523	4
9	3	0	872	863	6
11	3	0	519	516	5
13	3	0	343	345	4
15	3	0	984	983	8
17	3	0	1025	1013	8
19	3	0	304	303	6
21	3	0	222	230	8
0	4	0	2260	2303	6
2	4	0	639	633	4
4	4	0	1074	1078	7
6	4	0	4037	3817	8
8	4	0	454	447	4
10	4	0	533	543	5
12	4	0	191	193	5
14	4	0	719	723	6
16	4	0	2114	2119	13
18	4	0	89	84	13
20	4	0	164	155	9
22	4	0	487	489	6
1	5	0	1514	1507	7
3	5	0	143	146	4
5	5	0	3271	3179	8
7	5	0	887	889	6
9	5	0	73	59	10
11	5	0	376	391	4
13	5	0	158	164	7
15	5	0	266	278	5
17	5	0	520	511	5
19	5	0	120	131	11
21	5	0	429	422	6
0	6	0	946	947	6
2	6	0	149	146	4
4	6	0	208	209	4
6	6	0	407	384	4
8	6	0	617	601	5
10	6	0	1546	1550	11
12	6	0	166	171	6
14	6	0	373	361	5
16	6	0	400	403	5
18	6	0	402	390	6
20	6	0	0	20	1
1	7	0	660	652	5
3	7	0	266	256	3
5	7	0	1522	1498	9
7	7	0	470	460	4
9	7	0	1213	1212	8
11	7	0	680	646	6
13	7	0	328	314	5
15	7	0	310	317	5
17	7	0	342	342	6
19	7	0	673	672	6
21	7	0	656	643	6
0	8	0	2824	2766	9
2	8	0	139	119	5
4	8	0	633	620	5
6	8	0	657	655	5
8	8	0	556	571	5
10	8	0	1264	1282	9
12	8	0	121	130	8
14	8	0	65	39	16
16	8	0	291	290	6
18	8	0	24	28	23
20	8	0	324	305	7
1	9	0	204	199	4
3	9	0	324	326	4
5	9	0	1853	1908	10
7	9	0	907	901	7
9	9	0	171	171	6
11	9	0	587	577	5
13	9	0	217	206	6
15	9	0	753	758	6
17	9	0	600	584	6
19	9	0	197	208	8
0	10	0	373	374	4
2	10	0	92	97	9
4	10	0	309	315	4
6	10	0	254	255	5
8	10	0	267	271	5
10	10	0	550	551	5
12	10	0	256	254	6
14	10	0	1057	1064	8
16	10	0	373	367	6
18	10	0	361	370	6
1	11	0	302	284	4
3	11	0	297	297	5
5	11	0	875	895	7
7	11	0	67	88	15
9	11	0	147	146	7
11	11	0	393	408	5
13	11	0	290	301	6
15	11	0	749	756	6
17	11	0	481	472	6
0	12	0	1449	1447	9
2	12	0	161	156	6
4	12	0	438	442	5
6	12	0	615	631	5
8	12	0	212	213	6
10	12	0	694	701	6
12	12	0	566	562	6
14	12	0	204	200	7
16	12	0	34	23	33
1	13	0	618	609	5
3	13	0	193	188	6
5	13	0	332	332	5
7	13	0	473	480	5
9	13	0	276	284	6
11	13	0	962	962	7
13	13	0	234	243	7
15	13	0	252	256	7
0	14	0	1407	1423	10
2	14	0	366	371	5
4	14	0	217	202	6
6	14	0	642	647	6
8	14	0	185	179	7
10	14	0	1260	1274	10
12	14	0	84	91	17
14	14	0	58	14	26
1	15	0	387	378	5
3	15	0	352	344	5
5	15	0	452	452	5
7	15	0	52	72	30
9	15	0	306	296	6
11	15	0	405	408	6
13	15	0	391	396	6
0	16	0	535	524	5
2	16	0	213	226	7
4	16	0	94	82	13
6	16	0	801	811	7
8	16	0	53	15	30
10	16	0	71	64	20
12	16	0	486	490	6
1	17	0	260	253	7
3	17	0	308	294	6
5	17	0	1765	1743	12
7	17	0	79	64	17
9	17	0	50	14	37
0	18	0	318	322	6
2	18	0	254	252	7
4	18	0	118	116	12
6	18	0	322	302	6
8	18	0	260	269	8
1	19	0	196	211	8
3	19	0	129	130	12
1	1	1	109	98	3
3	1	1	377	373	3
5	1	1	775	783	5
7	1	1	28	13	27
9	1	1	209	202	4
11	1	1	771	776	6
13	1	1	240	232	5
15	1	1	212	211	6
17	1	1	674	686	6
19	1	1	489	484	5
21	1	1	644	671	6
0	2	1	170	133	3
2	2	1	552	566	4
4	2	1	240	237	3
6	2	1	271	258	3
8	2	1	608	607	4
10	2	1	86	100	9
12	2	1	891	904	7
14	2	1	50	33	22
16	2	1	637	647	6
18	2	1	48	41	30
20	2	1	337	323	6
22	2	1	259	251	7
1	3	1	306	322	3
3	3	1	226	212	3
5	3	1	255	252	3
7	3	1	415	413	4
9	3	1	315	320	3
11	3	1	361	381	4
13	3	1	267	264	5
15	3	1	76	73	13
17	3	1	321	317	5
19	3	1	207	200	7
21	3	1	397	400	6
0	4	1	1106	1108	6
2	4	1	147	141	4
4	4	1	144	138	4
6	4	1	729	695	5
8	4	1	374	377	4
10	4	1	537	519	5
12	4	1	639	640	5
14	4	1	259	258	5
16	4	1	519	529	5
18	4	1	232	231	6
20	4	1	33	23	33
22	4	1	253	250	7
1	5	1	73	69	7
3	5	1	438	446	4
5	5	1	1395	1348	8
7	5	1	884	866	6
9	5	1	353	340	4
11	5	1	349	375	4
13	5	1	601	606	6
15	5	1	104	112	10
17	5	1	207	197	7
19	5	1	0	17	1
21	5	1	643	639	6
0	6	1	324	301	3
2	6	1	135	121	4
4	6	1	401	384	3
6	6	1	975	977	7
8	6	1	473	458	4
10	6	1	33	14	32
12	6	1	406	397	4
14	6	1	72	73	14
16	6	1	1039	1046	8
18	6	1	236	228	7
20	6	1	478	471	6
1	7	1	87	73	7
3	7	1	455	461	4
5	7	1	805	814	6
7	7	1	182	179	5
9	7	1	400	415	4
11	7	1	46	65	26
13	7	1	108	107	9
15	7	1	133	133	8
17	7	1	213	212	7
19	7	1	180	169	8
0	8	1	558	552	5
2	8	1	128	112	6
4	8	1	70	54	11
6	8	1	133	343	4
8	8	1	59	56	15
10	8	1	89	98	11
12	8	1	458	467	5
14	8	1	493	496	5
16	8	1	509	528	5
18	8	1	258	281	7
20	8	1	334	336	7
1	9	1	876	869	7
3	9	1	81	78	10
5	9	1	516	552	5
7	9	1	342	349	4
9	9	1	89	93	11
11	9	1	1719	1731	12
13	9	1	90	88	12
15	9	1	182	164	7
17	9	1	110	119	12
19	9	1	176	188	9
0	10	1	1452	1496	10
2	10	1	755	742	6
4	10	1	262	270	5
6	10	1	460	461	4
8	10	1	70	75	14
10	10	1	395	402	5
12	10	1	80	25	13
14	10	1	648	653	6
16	10	1	513	499	5
18	10	1	204	224	8
1	11	1	157	162	6
3	11	1	49	51	21
5	11	1	796	808	6
7	11	1	510	499	5
9	11	1	317	319	5
11	11	1	239	246	6
13	11	1	190	198	7
15	11	1	314	297	6
17	11	1	366	382	6
0	12	1	1054	1068	8
2	12	1	561	565	5
4	12	1	134	137	8
6	12	1	753	755	6
8	12	1	99	97	11
10	12	1	64	73	17
12	12	1	236	226	6
14	12	1	68	81	20
16	12	1	806	796	7
1	13	1	416	407	5
3	13	1	266	275	5
5	13	1	1067	1098	8
7	13	1	129	118	8
9	13	1	337	341	5
11	13	1	1249	1228	9
13	13	1	152	144	9
15	13	1	129	134	11
0	14	1	906	914	7
2	14	1	167	169	7
4	14	1	445	459	5
6	14	1	228	223	6
8	14	1	207	198	7
10	14	1	400	407	6
12	14	1	136	111	10
14	14	1	343	338	6
1	15	1	61	60	20
3	15	1	375	387	5
5	15	1	140	153	9
7	15	1	346	342	6
9	15	1	54	49	28
11	15	1	192	186	8
13	15	1	245	231	7
0	16	1	447	441	5
2	16	1	216	200	7
4	16	1	32	37	31
6	16	1	1316	1300	10
8	16	1	345	342	6
10	16	1	63	69	23
12	16	1	66	59	23
1	17	1	75	75	18
3	17	1	198	189	8
5	17	1	856	857	7
7	17	1	236	252	8
9	17	1	328	342	7
0	18	1	294	306	7
2	18	1	97	115	15
4	18	1	370	367	6
6	18	1	328	323	7
1	19	1	456	447	6
3	19	1	428	417	6
0	0	2	3673	3637	6
2	0	2	629	658	4
4	0	2	378	364	3
6	0	2	760	718	5
8	0	2	718	708	5
10	0	2	1606	1566	10
12	0	2	979	979	8
14	0	2	1342	1370	10
16	0	2	927	924	7
18	0	2	576	581	6
20	0	2	191	181	8
22	0	2	379	392	6
1	1	2	555	570	4
3	1	2	678	682	5
5	1	2	1218	1222	7
7	1	2	107	92	6
9	1	2	670	664	5
11	1	2	539	543	5
13	1	2	100	111	9
15	1	2	733	727	6
17	1	2	64	70	17
19	1	2	47	25	46
21	1	2	234	238	7
0	2	2	3901	4154	7
2	2	2	343	345	3
4	2	2	431	435	4
6	2	2	422	422	4
8	2	2	161	153	5
10	2	2	1410	1401	10
12	2	2	593	612	5
14	2	2	18	21	37
16	2	2	270	278	5
18	2	2	31	23	31
20	2	2	136	145	10
22	2	2	574	573	6
1	3	2	444	429	3
3	3	2	175	170	3
5	3	2	1292	1290	8
7	3	2	186	173	4
9	3	2	1434	1429	10
11	3	2	1570	1568	11
13	3	2	335	331	4
15	3	2	261	248	5
17	3	2	374	381	5
19	3	2	788	782	7
21	3	2	722	730	7
0	4	2	2057	2048	7
2	4	2	669	658	4
4	4	2	36	17	21
6	4	2	406	395	4
8	4	2	199	216	4
10	4	2	2126	2161	10
12	4	2	123	129	7
14	4	2	202	200	6
16	4	2	114	121	9
18	4	2	587	570	6
20	4	2	266	267	7
1	5	2	1098	1070	8
3	5	2	63	56	9
5	5	2	1795	1765	9
7	5	2	190	179	4
9	5	2	602	598	5
11	5	2	686	682	5
13	5	2	95	95	10
15	5	2	317	315	5
17	5	2	745	745	6
19	5	2	376	371	6
21	5	2	380	377	6
0	6	2	1168	1171	8
2	6	2	78	84	8
4	6	2	805	818	6
6	6	2	2549	2509	9
8	6	2	309	319	4
10	6	2	152	155	6
12	6	2	348	354	5
14	6	2	779	781	6
16	6	2	1580	1580	11
18	6	2	51	35	33
20	6	2	79	64	17
1	7	2	645	646	5
3	7	2	167	162	5
5	7	2	4665	4592	10
7	7	2	172	177	5
9	7	2	490	502	4
11	7	2	42	11	29
13	7	2	404	404	5
15	7	2	1035	1056	8
17	7	2	1042	1047	8
19	7	2	141	135	10
0	8	2	276	274	4
2	8	2	496	505	5
4	8	2	355	368	4
6	8	2	335	332	4
8	8	2	590	604	5
10	8	2	0	16	1
12	8	2	85	93	12
14	8	2	568	586	5
16	8	2	916	907	7
18	8	2	25	27	24
20	8	2	176	170	9
1	9	2	575	560	5
3	9	2	100	91	8

Observed and calculated structure factors for K21

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	9	2	475	479	5	10	2	3	312	116	4	5	11	3	849	847	7	19	3	4	262	261	7	13	13	4	120	128	12
7	9	2	494	479	5	12	2	3	684	678	5	7	11	3	183	189	7	0	4	4	676	691	5	0	14	4	1379	1381	10
9	9	2	511	513	5	14	2	3	250	254	5	9	11	3	373	370	5	2	4	4	451	445	4	2	14	4	218	212	7
11	9	2	1597	1594	13	16	2	3	1000	1004	8	11	11	3	51	18	27	4	4	4	601	619	5	4	14	4	315	322	6
13	9	2	279	275	5	18	2	3	166	156	8	13	11	3	27	11	26	6	4	4	1987	1969	11	6	14	4	421	428	6
15	9	2	140	134	9	20	2	3	239	231	7	15	11	3	142	136	10	8	4	4	191	193	5	8	14	4	166	153	9
17	9	2	754	752	7	1	3	3	466	446	4	17	11	3	490	490	6	10	4	4	410	420	5	10	14	4	988	990	8
19	9	2	268	267	7	3	3	3	285	273	3	0	12	3	212	205	6	12	4	4	127	127	8	12	14	4	36	49	35
0	10	2	4408	4441	11	5	3	3	1071	1052	7	2	12	3	338	342	5	14	4	4	728	734	6	1	15	4	335	337	6
2	10	2	559	560	5	7	3	3	749	730	5	4	12	3	391	398	5	16	4	4	1562	1553	12	3	15	4	367	356	6
4	10	2	640	646	5	9	3	3	243	252	4	6	12	3	258	246	6	18	4	4	156	153	9	5	15	4	211	204	7
6	10	2	25	30	25	11	3	3	1408	1413	9	8	12	3	0	24	1	1	5	4	1001	981	7	7	15	4	103	77	13
8	10	2	302	308	5	13	3	3	44	30	28	10	12	3	108	98	10	3	5	4	109	92	7	9	15	4	282	269	7
10	10	2	1872	1878	13	15	3	3	138	159	8	12	12	3	231	228	7	5	5	4	1588	1625	11	0	16	4	126	124	11
12	10	2	430	434	5	17	3	3	246	246	6	14	12	3	175	177	9	7	5	4	399	391	4	2	16	4	222	216	7
14	10	2	291	301	6	19	3	3	148	135	9	16	12	3	533	515	6	9	5	4	0	6	1	4	16	4	68	20	22
16	10	2	111	119	12	21	3	3	435	436	6	1	13	3	321	311	5	11	5	4	895	910	7	6	16	4	447	459	6
18	10	2	218	206	8	0	4	3	2186	2141	8	3	13	3	371	392	5	13	5	4	0	13	1	8	16	4	0	25	1
1	11	2	384	379	5	2	4	3	11	3	10	5	13	3	503	506	5	15	5	4	296	298	6	1	17	4	319	306	7
3	11	2	680	693	6	4	4	3	299	288	3	7	13	3	114	104	10	17	5	4	151	133	9	3	17	4	179	195	9
5	11	2	69	74	14	6	4	3	267	266	4	9	13	3	288	283	6	19	5	4	78	79	18	5	17	4	1326	1315	10
7	11	2	19	26	39	8	4	3	162	170	6	11	13	3	527	516	6	0	6	4	2091	2151	10	1	1	5	18	5	18
9	11	2	633	639	6	10	4	3	591	589	5	13	13	3	25	5	25	2	6	4	169	179	5	3	1	5	153	166	6
11	11	2	1811	1827	13	12	4	3	692	707	6	15	13	3	51	42	39	4	6	4	297	285	4	5	1	5	659	658	5
13	11	2	49	27	30	14	4	3	109	95	9	0	14	3	243	249	6	6	6	4	239	235	5	7	1	5	50	42	20
15	11	2	72	89	19	16	4	3	159	148	7	2	14	3	140	132	8	8	6	4	317	311	5	9	1	5	182	187	6
17	11	2	99	85	13	18	4	3	131	130	9	4	14	3	374	373	5	10	6	4	1339	1368	10	11	1	5	203	195	6
0	12	2	1412	1415	10	20	4	3	74	80	19	6	14	3	176	193	7	12	6	4	265	262	5	13	1	5	85	99	13
2	12	2	90	99	11	1	5	3	102	94	7	8	14	3	253	259	7	14	6	4	183	175	7	15	1	5	147	145	8
4	12	2	232	226	5	3	5	3	272	287	4	10	14	3	239	245	7	16	6	4	119	121	10	17	1	5	712	713	6
6	12	2	831	831	7	5	5	3	779	778	6	12	14	3	0	2	1	18	6	4	284	268	7	19	1	5	382	383	6
8	12	2	267	261	6	7	5	3	837	841	6	1	15	3	224	226	7	1	7	4	267	254	4	0	2	5	668	655	5
10	12	2	732	740	6	9	5	3	256	253	5	3	15	3	288	304	6	3	7	4	299	293	4	2	2	5	171	148	5
12	12	2	295	286	6	11	5	3	204	197	6	5	15	3	349	344	6	5	7	4	1329	1342	9	4	2	5	266	278	4
14	12	2	380	377	6	13	5	3	461	465	5	7	15	3	218	214	7	7	7	4	375	358	4	6	2	5	483	482	5
16	12	2	468	470	6	15	5	3	164	169	8	9	15	3	106	103	12	9	7	4	913	945	7	8	2	5	305	304	5
1	13	2	59	64	19	17	5	3	256	256	6	11	15	3	177	370	6	11	7	4	783	783	6	10	2	5	65	66	15
3	13	2	35	16	34	19	5	3	64	72	22	0	16	3	269	269	6	13	7	4	256	254	6	12	2	5	740	739	6
5	13	2	1763	1741	13	0	6	3	657	652	5	2	16	3	60	41	21	15	7	4	272	282	6	14	2	5	42	29	42
7	13	2	17	4	17	2	6	3	167	167	5	4	16	3	229	246	7	17	7	4	416	425	6	16	2	5	230	220	7
9	13	2	0	9	1	4	6	3	605	594	5	6	16	3	1157	1132	9	0	8	4	1982	2000	11	18	2	5	150	129	9
11	13	2	64	79	20	6	6	3	1249	1268	8	8	16	3	295	291	7	2	8	4	33	7	33	1	3	5	95	89	8
13	13	2	135	127	10	8	6	3	324	334	4	10	16	3	219	219	8	4	8	4	338	348	4	3	3	5	210	207	5
15	13	2	551	555	6	10	6	3	97	98	9	1	17	3	156	152	9	6	8	4	597	597	5	5	3	5	474	489	5
0	14	2	387	390	5	12	6	3	346	356	5	3	17	3	220	220	7	8	8	4	431	441	5	7	3	5	93	89	10
2	14	2	293	300	6	14	6	3	41	21	40	5	17	3	563	574	6	10	8	4	1094	1112	8	9	3	5	167	166	6
4	14	2	701	703	6	16	6	3	1088	1099	8	7	17	3	21	7	20	12	8	4	80	76	13	11	3	5	198	196	6
6	14	2	515	511	5	18	6	3	353	361	6	0	18	3	196	191	8	14	8	4	40	29	39	13	3	5	279	276	6
8	14	2	197	188	7	20	6	3	426	423	6	2	18	3	222	222	8	16	8	4	248	242	7	15	3	5	0	17	1
10	14	2	76	77	16	1	7	3	94	108	8	4	18	3	167	179	10	18	8	4	94	80	14	17	3	5	547	533	6
12	14	2	14	19	14	3	7	3	148	155	6	2	0	4	121	318	4	1	9	4	105	98	9	0	4	5	137	139	7
14	14	2	338	335	7	5	7	3	1458	1466	10	4	0	4	598	600	5	3	9	4	205	209	6	2	4	5	96	83	9
1	15	2	672	673	6	7	7	3	207	207	5	6	0	4	101	276	4	5	9	4	1729	1770	12	4	4	5	35	51	35
3	15	2	262	251	6	9	7	3	416	410	4	8	0	4	430	451	4	7	9	4	495	489	5	6	4	5	655	631	5
5	15	2	1505	1502	12	11	7	3	852	853	6	10	0	4	2843	2899	12	9	9	4	90	84	11	8	4	5	285	288	5
7	15	2	472	458	5	13	7	3	112	108	9	12	0	4	1014	1018	8	11	9	4	183	181	7	10	4	5	318	321	5
9	15	2	51	68	10	15	7	3	74	7	16	14	0	4	462	464	5	13	9	4	33	50	13	12	4	5	412	418	5
11	15	2	402	410	6	17	7	3	645	637	6	16	0	4	63	35	19	15	9	4	550	551	6	14	4	5	268	261	6
13	15	2	171	165	9	19	7	3	146	141	10	18	0	4	506	496	5	17	9	4	674	656	6	16	4	5	563	575	6
0	16	2	902	899	7	0	8	3	908	905	7	20	0	4	337	330	6	0	10	4	894	895	7	18	4	5	233	243	7
2	16	2	161	159	8	2	8	3	41	42	30	1	1	4	332	305	3	2	10	4	0	30	1	1	5	5	125	120	7
4	16	2	155	165	9	4	8	3	237	239	5	3	1	4	34	44	33	4	10	4	436	433	5	3	5	5	238	233	5
6	16	2	505	512	6	6	8	3	529	521	5	5	1	4	201	86	4	6	10	4	200	213	6	5	5	5	637	631	5
8	16	2	73	47	18	8	8	3	95	92	9	7	1	4	50	7	17	8	10	4	303	298	5	7	5	5	591	585	5
10	16	2	764	745	7	10	8	3	191	185	6	9	1	4	1164	1188	9	10	10	4	453	455	5	9	5	5	254	261	5
1	17	2	235	221	7	12	8	3	548	547	5	11	1	4	1722	1752	12	12	10	4	260	264	6	11	5	5	315	309	5
3	17	2	370	364	6	14	8	3	283	283	6	13	1	4	229	240	6	14	10	4	788	792	7	13	5	5	408	417	5
5	17	2	73	72	19	16	8	3	85	68	13	15	1	4	127	134	9	16	10	4	473	468	6	15	5	5	119	99	10
7	17	2	124	143	11	18	8	3	106	102	12	17	1	4	52	39	26	1	11	4	195	209	6	17	5	5	138	139	10
9	17	2	315	317	7	1	9	3	541	545	5	19	1	4	512	499	6	3	11	4	354	349	5	0	6	5	257	293	5
0	18	2	715	706	7	3	9	3	154	157	6	0	2	4	320	348	4	5	11	4	1053	1072	8	2	6	5	58	61	16
2	18	2	69	86	22	5	9	3	153	141	6	2	2	4	193	186	4	7	11	4	23	27	23	4	6	5	70	61	13
4	18	2	306	307	7	7	9	3	239	241	5	4	2	4	186	192	4	9	11	4	106	106	10	6	6	5	490	479	5
6	18	2	357	358	7	9	9	3	118	121	8	6	2	4	443	451	4	11	11	4	0	5	1	8	6	5	299	310	5
1	1	3	169	155	4	11	9	3	952	945	7	8	2	4	95	111	9	13	11	4	196	194	8	10	6	5	41	7	41
3	1	3	591	575	4	13	9	3	45	44	44	10	2	4	401	409	4	15	11	4	619	613	6	12	6	5	300	292	6
5	1	3	190	197	4	15	9	3	185	167	8	12	2	4	172	175	5	0	12	4	926	921	7	14	6	5	79	76	15
7	1	3	387	389	4	17	9	3	450	465	6	14	2	4	645	644	5	2	12	4	178	173	7	16	6	5	712	710	6
9	1	3	186	182	5	0	10	3	1041	1075	8	16	2	4	772	780	7	4	12	4	314	315	6	1	7	5	59	50	16
11	1	3	1309	1300	9	2	10	3	731	729	6	18	2	4	158	157	9	6	12	4	313	313	5	3	7	5	392	394	4
13	1	3	341	340	5	4	10	3	354	356	5	20	2	4	48	35	48	8	12	4	240	252	6	5	7	5	275	278	5
15	1	3	271	270	5	6	10	3	258	236	5	1	3	4	178	176	5	10	12	4	505	496	5	7	7	5	298	289	5
17	1	3	309	311	6	8	10	3	124	143	8	3	3	4	362	341	4	12	12	4	392	398	6	9	7	5	287	276	5
19	1	3	466	466	6	10	10	3	200	208	6	5	3	4	3540	3554	10	14	12	4	84	101	17	11	7	5	318	325	6
21	1	3	637	637	6	12	10	3	122	115	9	7	3	4	178	177	5	1	13	4	370	378	5	13	7	5	198	200	7
0	2	3	2351	2320	8	14	10	3	627	634	6	9	3	4	654	661	6	3	13	4	134	134	9	15	7	5	155	169	9
2	2	3	685	639	5	16	10	3	283	285	7	11	3	4	212	218	5	5	13	4	218	225	6	17	7	5	31	57	30
4	2	3	329	285	3	18	10	3	135	150	11	13	3	4	317	319	5	7	13	4	302	286	6	0	8	5	736	740	6
6	2	3	1104	1072	7	1	11	3	272	271	5	15	3	4	854	852	7	9	13	4	298	294	6	2	8	5	201	194	6
8	2	3	717	698	6	3	11	3	44	11	31	17	3	4	785	779	6	11	13	4	778	779	7	4	8	5	104	105	9

Observed and calculated structure factors for K21

h	k	l	10Fo	10Fc	10s
6	8	5	597	588	5
8	8	5	81	73	13
10	8	5	96	80	11
12	8	5	314	315	6
14	8	5	443	446	6
16	8	5	608	610	6
1	9	5	648	647	6
3	9	5	0	27	1
5	9	5	608	602	5
7	9	5	340	338	5
9	9	5	49	71	31
11	9	5	1529	1559	12
13	9	5	128	138	10
15	9	5	164	152	9
0	10	5	1176	1166	9
2	10	5	465	471	5
4	10	5	127	111	9
6	10	5	487	480	5
8	10	5	0	50	1
10	10	5	393	378	5
12	10	5	37	47	37
14	10	5	500	484	6
1	11	5	73	54	14
3	11	5	63	58	19
5	11	5	561	561	6
7	11	5	487	502	5
9	11	5	208	208	7
11	11	5	303	306	6
13	11	5	254	244	7
0	12	5	1045	1064	8
2	12	5	532	529	6
4	12	5	24	28	24
6	12	5	777	777	6
8	12	5	61	58	22
10	12	5	35	10	34
12	12	5	177	176	9
1	13	5	359	349	6
3	13	5	192	196	7
5	13	5	1035	1037	8
7	13	5	229	212	7
9	13	5	314	294	6
11	13	5	1290	1284	10
0	14	5	1061	1048	8
2	14	5	136	137	10
4	14	5	353	353	6
6	14	5	391	396	6
8	14	5	109	118	13
10	14	5	409	419	6
1	15	5	42	44	42
3	15	5	304	312	7
5	15	5	48	8	48
7	15	5	313	315	7
0	16	5	376	357	6
2	16	5	238	239	7
4	16	5	86	89	17
0	0	6	2678	2672	12
2	0	6	112	111	8
4	0	6	529	639	5
6	0	6	671	686	6
8	0	6	429	437	5
10	0	6	948	954	7
12	0	6	726	736	6
14	0	6	791	784	6
16	0	6	916	933	8
1	1	6	184	187	6
3	1	6	76	78	12
5	1	6	1730	1755	12
7	1	6	128	131	8
9	1	6	354	357	5
11	1	6	262	268	6
13	1	6	64	14	18
15	1	6	476	461	6
17	1	6	310	311	7
0	2	6	1724	1738	12
2	2	6	186	186	6
4	2	6	129	130	8
6	2	6	451	460	5
8	2	6	184	177	7
10	2	6	877	881	7
12	2	6	344	346	5
14	2	6	42	49	41
16	2	6	315	329	6
1	3	6	235	225	5
3	3	6	46	10	23
5	3	6	921	941	7
7	3	6	56	67	19
9	3	6	971	958	7
11	3	6	1195	1205	9
13	3	6	138	143	9
15	3	6	140	129	9
17	3	6	384	386	6
0	4	6	2478	2481	12
2	4	6	117	62	8
4	4	6	177	177	5
6	4	6	541	546	5
8	4	6	182	176	7
10	4	6	1416	1408	10
12	4	6	179	146	8
14	4	6	63	12	21
16	4	6	252	266	7
1	5	6	355	356	5
3	5	6	318	324	5
5	5	6	503	487	5
7	5	6	116	113	9
9	5	6	330	335	5
11	5	6	303	302	6
13	5	6	68	62	19
15	5	6	301	288	6
0	6	6	89	76	11
2	6	6	56	52	19
4	6	6	350	341	5
6	6	6	974	966	7
8	6	6	318	321	6
10	6	6	48	52	33
12	6	6	173	178	8
14	6	6	703	703	6
16	6	6	820	819	7
1	7	6	518	520	5
3	7	6	81	67	12
5	7	6	2492	2542	13
7	7	6	109	104	10
9	7	6	374	391	5
11	7	6	353	362	6
13	7	6	250	255	7
15	7	6	713	717	6
0	8	6	188	189	7
2	8	6	228	226	6
4	8	6	392	402	5
6	8	6	246	245	6
8	8	6	356	362	6
10	8	6	145	149	9
12	8	6	128	116	10
14	8	6	410	403	6
1	9	6	416	418	5
3	9	6	81	82	14
5	9	6	26	1	26
7	9	6	537	541	6
9	9	6	344	347	6
11	9	6	731	734	6
13	9	6	79	66	17
0	10	6	2193	2208	14
2	10	6	243	238	6
4	10	6	235	230	6
6	10	6	505	505	5
8	10	6	118	112	11
10	10	6	1332	1314	10
12	10	6	260	265	7
1	11	6	110	121	11
3	11	6	322	317	6
5	11	6	404	414	6
7	11	6	101	107	12
9	11	6	468	469	6
11	11	6	782	779	7
0	12	6	592	586	6
2	12	6	99	107	13
4	12	6	166	176	9
6	12	6	844	863	7
8	12	6	132	108	10
10	12	6	420	405	6
1	13	6	54	53	29
3	13	6	42	22	41
5	13	6	1297	1294	10
7	13	6	137	137	10
0	14	6	52	64	35
2	14	6	351	350	6
4	14	6	116	106	7
6	14	6	171	169	9
1	1	7	63	62	17
3	1	7	189	202	7
5	1	7	50	43	24
7	1	7	292	277	6
9	1	7	128	109	9
11	1	7	711	709	6
13	1	7	240	250	7
15	1	7	206	206	8
0	2	7	729	729	6
2	2	7	342	343	5
4	2	7	78	85	11
6	2	7	483	481	5
8	2	7	278	271	6
10	2	7	76	8	15
12	2	7	451	454	6
14	2	7	122	121	11
1	3	7	212	223	6
3	3	7	30	3	30
5	3	7	461	453	5
7	3	7	373	382	5
9	3	7	175	172	8
11	3	7	849	846	7
13	3	7	0	34	1
0	4	7	1069	1035	8
2	4	7	62	50	18
4	4	7	170	173	7
6	4	7	140	136	8
8	4	7	140	152	9
10	4	7	391	399	6
12	4	7	461	453	6
14	4	7	98	114	14
1	5	7	13	31	12
3	5	7	126	125	9
5	5	7	238	241	6
7	5	7	504	514	5
9	5	7	180	181	8
11	5	7	81	65	16
13	5	7	279	281	7
0	6	7	306	297	6
2	6	7	136	141	8
4	6	7	270	258	6
6	6	7	722	723	6
8	6	7	234	236	7
10	6	7	82	91	15
12	6	7	230	225	7
1	7	7	88	88	13
3	7	7	187	183	7
5	7	7	887	886	7
7	7	7	102	104	13
9	7	7	295	286	6
11	7	7	538	537	6
0	8	7	585	567	5
2	8	7	33	31	33
4	8	7	175	163	7
6	8	7	340	326	6
8	8	7	53	5	30
10	8	7	170	168	9
12	8	7	365	365	6
1	9	7	309	313	6
3	9	7	81	92	15
5	9	7	200	174	7
7	9	7	176	168	8
9	9	7	63	48	23
11	9	7	590	578	6
0	10	7	667	678	6
2	10	7	394	406	6
4	10	7	179	173	8
6	10	7	188	183	8
8	10	7	51	67	45
1	11	7	134	144	10
3	11	7	34	21	33
5	11	7	574	572	6
7	11	7	136	137	10
0	12	7	56	42	31
2	12	7	233	225	7
4	12	7	248	254	7
6	12	7	126	127	12
1	13	7	190	192	8
0	0	8	2575	2601	14
2	0	8	130	129	9
4	0	8	202	208	7
6	0	8	643	656	6
8	0	8	75	76	17
10	0	8	1568	1570	11
12	0	8	511	512	6
1	1	8	132	131	9
3	1	8	90	95	13
5	1	8	381	389	6
7	1	8	216	214	7
9	1	8	650	640	6
11	1	8	558	560	6
0	2	8	244	15	6
2	2	8	96	98	12
4	2	8	234	221	6
6	2	8	517	498	5
8	2	8	55	31	25
10	2	8	210	203	8
1	3	8	105	98	11
3	3	8	247	248	6
5	3	8	1879	1867	12
7	3	8	6	5	6
9	3	8	363	364	6
11	3	8	75	59	18
0	4	8	140	156	9
2	4	8	303	295	6
4	4	8	224	225	7
6	4	8	667	655	6
8	4	8	51	21	31
10	4	8	220	208	8
1	5	8	529	531	6
3	5	8	133	133	9
5	5	8	478	469	6
7	5	8	17	18	17
9	5	8	40	52	39
0	6	8	1867	1853	12
2	6	8	171	168	8
4	6	8	268	260	6
6	6	8	503	501	6
8	6	8	110	116	12
1	7	8	59	59	21
3	7	8	197	195	8
5	7	8	915	917	7
7	7	8	207	202	7
0	8	8	985	988	8
2	8	8	63	53	21
4	8	8	102	102	13
6	8	8	407	411	6
1	9	8	19	10	19
3	9	8	115	93	12
5	9	8	1224	1232	9
0	10	8	1043	1045	8
2	10	8	50	68	42
1	1	9	23	4	23
3	1	9	153	153	9
5	1	9	299	295	7
7	1	9	115	105	12
0	2	9	91	89	14
2	2	9	96	113	14
4	2	9	89	71	14
6	2	9	56	49	26
1	3	9	89	86	15
3	3	9	33	33	33
5	3	9	74	78	19
0	4	9	405	398	6
2	4	9	34	44	34
4	4	9	70	67	19
1	5	9	49	4	38
3	5	9	60	57	26
0	6	9	61	67	25

Observed and calculated structure factors for R22

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	713	722	4	0	8	0	2544	2554	9	1	19	0	124	141	15	3	9	1	35	44	34	1	1	2	544	541	4
4	0	0	1153	1146	6	2	8	0	174	172	5	1	1	1	147	144	3	5	9	1	388	411	5	3	1	2	780	779	6
6	0	0	574	579	5	4	8	0	542	534	5	3	1	1	340	340	3	7	9	1	320	320	5	5	1	2	1040	1032	8
8	0	0	1026	983	7	6	8	0	668	669	6	5	1	1	981	978	7	9	9	1	49	35	35	7	1	2	92	96	8
10	0	0	1771	1741	10	8	8	0	450	464	5	7	1	1	47	15	17	11	9	1	1644	1672	13	9	1	2	614	617	5
12	0	0	1459	1470	11	10	8	0	1198	1180	8	9	1	1	313	303	4	13	9	1	110	120	10	11	1	2	611	627	5
14	0	0	296	286	5	12	8	0	127	126	9	11	1	1	708	717	6	15	9	1	188	179	8	13	1	2	38	21	37
16	0	0	323	318	5	14	8	0	112	94	11	13	1	1	282	284	5	17	9	1	107	115	14	15	1	2	678	674	6
18	0	0	435	436	6	16	8	0	140	147	6	15	1	1	236	226	6	19	9	1	196	215	9	17	1	2	54	68	30
20	0	0	422	421	6	18	8	0	47	40	47	17	1	1	680	694	6	0	10	1	1332	1372	9	19	1	2	18	19	17
22	0	0	1840	1819	12	20	8	0	314	292	7	19	1	1	497	501	6	2	10	1	737	738	6	21	1	2	328	315	7
1	1	0	895	839	3	1	9	0	88	75	11	21	1	1	640	641	6	4	10	1	204	203	6	0	2	2	4071	4076	8
3	1	0	254	250	3	3	9	0	349	356	4	0	2	1	158	178	3	6	10	1	483	487	5	2	2	2	382	370	3
5	1	0	516	517	4	5	9	0	1850	1872	11	2	2	1	534	556	4	8	10	1	121	125	10	4	2	2	482	472	4
7	1	0	397	395	4	7	9	0	878	861	7	4	2	1	388	384	3	10	10	1	328	337	5	6	2	2	490	477	4
9	1	0	1512	1492	9	9	9	0	61	75	23	6	2	1	295	282	3	12	10	1	52	19	35	8	2	2	226	210	4
11	1	0	2978	2966	11	11	9	0	677	649	6	8	2	1	533	531	4	14	10	1	619	612	6	10	2	2	1348	1354	10
13	1	0	427	420	5	13	9	0	214	197	7	10	2	1	46	4	27	16	10	1	453	457	6	12	2	2	577	578	5
15	1	0	247	252	6	15	9	0	719	731	6	12	2	1	882	881	7	18	10	1	188	197	9	14	2	2	61	14	41
17	1	0	375	383	6	17	9	0	545	541	6	14	2	1	128	112	9	1	11	1	98	119	12	16	2	2	316	327	6
19	1	0	528	526	6	19	9	0	180	178	10	16	2	1	564	574	5	3	11	1	73	76	17	18	2	2	64	40	23
21	1	0	834	817	7	0	10	0	274	286	5	18	2	1	56	9	31	5	11	1	806	817	6	20	2	2	108	106	14
0	2	0	1241	1273	4	2	10	0	106	110	10	20	2	1	319	309	7	7	11	1	506	505	5	1	3	2	496	485	4
2	2	0	316	337	3	4	10	0	290	295	5	22	2	1	261	262	8	9	11	1	266	274	6	3	3	2	201	198	4
4	2	0	566	576	4	6	10	0	287	289	5	1	3	1	366	373	4	11	11	1	217	220	7	5	3	2	1096	1102	8
6	2	0	136	138	5	8	10	0	283	291	5	3	3	1	260	251	4	13	11	1	180	177	8	7	3	2	239	226	4
8	2	0	260	248	4	10	10	0	493	507	5	5	3	1	377	375	4	15	11	1	298	282	7	9	3	2	1344	1360	10
10	2	0	574	577	5	12	10	0	270	277	6	7	3	1	402	398	4	17	11	1	419	433	6	11	3	2	1467	1504	11
12	2	0	428	437	5	14	10	0	1029	1056	8	9	3	1	236	238	4	0	12	1	964	988	8	13	3	2	328	332	5
14	2	0	854	852	7	16	10	0	333	299	6	11	3	1	338	347	4	2	12	1	547	555	5	15	3	2	228	217	6
16	2	0	793	788	6	18	10	0	396	395	6	13	3	1	212	219	6	4	12	1	144	150	9	17	3	2	417	413	5
18	2	0	120	117	11	1	11	0	279	274	5	15	3	1	105	94	11	6	12	1	716	707	6	19	3	2	765	776	7
20	2	0	61	74	32	3	11	0	242	243	6	17	3	1	294	296	6	8	12	1	84	83	17	21	3	2	663	672	7
22	2	0	242	240	8	5	11	0	728	742	6	19	3	1	180	177	9	10	12	1	39	46	39	0	4	2	1768	1750	7
1	3	0	310	312	3	7	11	0	74	89	18	21	3	1	364	359	7	12	12	1	232	225	7	2	4	2	620	619	5
3	3	0	533	544	4	9	11	0	60	85	24	0	4	1	1203	1210	6	14	12	1	75	70	21	4	4	2	76	65	10
5	3	0	4878	4782	8	11	11	0	466	481	5	2	4	1	138	134	5	16	12	1	740	731	7	6	4	2	345	337	4
7	3	0	548	519	4	13	11	0	214	227	8	4	4	1	152	145	5	1	13	1	449	436	5	8	4	2	86	95	11
9	3	0	866	848	6	15	11	0	740	736	6	6	4	1	695	657	5	3	13	1	306	307	5	10	4	2	1990	2023	11
11	3	0	400	398	4	17	11	0	467	464	6	8	4	1	375	364	4	5	13	1	987	1008	8	12	4	2	152	158	8
13	3	0	262	267	6	0	12	0	1475	1502	10	10	4	1	539	522	5	7	13	1	91	87	15	14	4	2	167	164	8
15	3	0	916	901	7	2	12	0	197	195	7	12	4	1	670	664	5	9	13	1	293	291	6	16	4	2	0	11	-1
17	3	0	1015	1007	8	4	12	0	333	329	5	14	4	1	269	267	6	11	13	1	1175	1188	9	18	4	2	531	515	5
19	3	0	298	295	7	6	12	0	551	558	6	16	4	1	493	499	5	13	13	1	180	166	9	20	4	2	260	264	8
21	3	0	317	317	7	8	12	0	195	197	7	18	4	1	243	244	7	15	13	1	160	167	11	1	5	2	978	973	6
0	4	0	2024	2057	6	10	12	0	721	715	6	20	4	1	71	20	23	0	14	1	839	862	7	3	5	2	57	48	14
2	4	0	655	656	5	12	12	0	507	509	6	1	5	1	100	115	7	2	14	1	173	175	8	5	5	2	1852	1828	9
4	4	0	947	936	7	14	12	0	129	128	12	3	5	1	408	412	4	4	14	1	398	398	5	7	5	2	242	229	5
6	4	0	3922	3808	9	16	12	0	19	35	18	5	5	1	1211	1179	8	6	14	1	264	263	6	9	5	2	487	491	5
8	4	0	427	415	4	1	13	0	547	556	6	7	5	1	852	840	6	8	14	1	239	232	7	11	5	2	670	657	5
10	4	0	468	461	5	3	13	0	213	222	7	9	5	1	460	440	4	10	14	1	354	369	6	13	5	2	84	75	15
12	4	0	249	257	5	5	13	0	328	312	6	11	5	1	270	295	5	12	14	1	156	147	10	15	5	2	307	302	6
14	4	0	672	668	6	7	13	0	485	487	5	13	5	1	572	564	5	14	14	1	296	303	7	17	5	2	708	710	6
16	4	0	2070	2066	14	9	13	0	328	323	6	15	5	1	121	127	10	1	15	1	29	23	28	19	5	2	362	358	6
18	4	0	163	82	9	11	13	0	896	909	8	17	5	1	213	202	7	3	15	1	376	381	6	21	5	2	396	373	7
20	4	0	159	168	11	13	13	0	279	287	7	19	5	1	48	11	47	5	15	1	137	135	11	0	6	2	1077	1078	7
22	4	0	523	511	6	15	13	0	256	260	8	21	5	1	602	603	6	7	15	1	351	346	6	2	6	2	50	55	18
1	5	0	1490	1481	7	0	14	0	1275	1299	9	0	6	1	523	509	4	9	15	1	38	34	38	4	6	2	826	826	6
3	5	0	59	70	12	2	14	0	379	372	5	2	6	1	112	109	6	11	15	1	144	130	11	6	6	2	2484	2464	10
5	5	0	3128	3058	9	4	14	0	203	212	7	4	6	1	277	270	4	13	15	1	219	210	9	8	6	2	289	290	5
7	5	0	915	890	6	6	14	0	701	717	7	6	6	1	962	960	6	0	16	1	356	361	6	10	6	2	143	123	8
9	5	0	55	15	21	8	14	0	138	139	11	8	6	1	540	526	5	2	16	1	202	190	8	12	6	2	365	373	5
11	5	0	398	416	5	10	14	0	1202	1222	9	10	6	1	133	111	9	4	16	1	45	46	44	14	6	2	807	803	7
13	5	0	235	242	6	12	14	0	68	73	27	12	6	1	358	360	5	6	16	1	1305	1277	9	16	6	2	1537	1543	12
15	5	0	215	237	7	14	14	0	0	33	1	14	6	1	27	10	27	8	16	1	350	350	7	18	6	2	53	8	47
17	5	0	490	492	6	1	15	0	313	312	6	16	6	1	975	985	8	10	16	1	18	30	17	20	6	2	72	67	24
19	5	0	159	164	10	3	15	0	359	364	6	18	6	1	263	265	7	12	16	1	58	39	44	1	7	2	671	661	5
21	5	0	446	446	6	5	15	0	514	520	5	20	6	1	482	471	6	1	17	1	104	109	15	3	7	2	103	89	9
0	6	0	763	781	5	7	15	0	91	104	16	1	7	1	133	134	6	3	17	1	212	203	8	5	7	2	4448	4396	11
2	6	0	186	188	4	9	15	0	201	196	8	3	7	1	483	473	4	5	17	1	793	802	7	7	7	2	179	182	6
4	6	0	274	274	4	11	15	0	429	414	6	5	7	1	730	745	6	7	17	1	234	223	8	9	7	2	446	460	5
6	6	0	477	471	4	13	15	0	376	384	7	7	7	1	209	207	6	9	17	1	299	309	8	11	7	2	108	102	11
8	6	0	684	676	6	0	16	0	546	559	6	9	7	1	359	374	5	0	18	1	318	314	7	13	7	2	333	337	5
10	6	0	1430	1455	11	2	16	0	250	250	7	11	7	1	72	91	16	2	18	1	108	111	15	15	7	2	993	1001	7
12	6	0	165	168	8	4	16	0	148	151	10	13	7	1	67	76	19	4	18	1	329	321	7	17	7	2	1026	1029	8
14	6	0	411	407	5	6	16	0	771	775	7	15	7	1	118	110	11	6	18	1	295	295	8	19	7	2	100	104	16
16	6	0	490	491	5	8	16	0	72	80	25	17	7	1	241	252	7	1	19	1	419	409	7	0	8	2	416	429	4
18	6	0	365	366	6	10	16	0	91	97	18	19	7	1	165	155	10	3	19	1	409	411	7	2	8	2	520	521	5
20	6	0	45	1	45	12	16	0	468	470	6	0	8	1	463	446	4	0	0	2	3273	3336	7	4	8	2	229	233	5
1	7	0	606	585	4	1	17	0	313	315	7	2	8	1	112	102	8	2	0	2	651	659	5	6	8	2	362	357	5
3	7	0	236	237	4	3	17	0	275	279	7	4	8	1	28	19	28	4	0	2	231	225	3	8	8	2	568	587	5
5	7	0	1369	1362	9	5	17	0	1678	1692	13	6	8	1	272	288	5	6	0	2	737	717	6	10	8	2	76	71	16
7	7	0	530	521	5	7	17	0	42	29	42	8	8	1	53	53	26	8	0	2	638	632	5	12	8	2	65	53	20
9	7	0	1132	1121	9	9	17	0	43	39	43	10	8	1	132	137	9	10	0	2	1477	1445	10	14	8	2	504	505	5
11	7	0	616	596	6	0	18	0	388	384	6	12	8	1	473	475	5	12	0	2	1055	1054	8	16	8	2	866	874	7
13	7	0	293	304	6	2	18	0	271	277	7	14	8	1	506	499	5	14	0	2	1298	1307	10	18	8	2	0	9	1
15	7	0	284	301	6	4	18	0	55	61	55	16	8	1	498	499	6	16	0	2	826	847	7	20	8	2	199	193	10
17	7	0	373	373	6	6	18	0	285	287	8	18	8	1	299	296	7	18	0	2	602	595	6	1	9	2	509	507	5
19	7	0	658	652	6	8	18	0	311	293	7	20	8	1	332	336	7	20	0	2	185	186	9	3	9	2	142	114	8
21	7	0	592	588	7	1	19	0	202	182	9	1	9	1	908	901	7	22	0	2	402	403	7	5	9	2	537	523	5

Observed and calculated structure factors for K22

h	k	l	10Fo	10Fc	10s
7	9	2	496	487	5
9	9	2	574	580	5
11	9	2	1573	1583	11
13	9	2	206	212	7
15	9	2	143	132	10
17	9	2	750	739	7
19	9	2	298	286	7
0	10	2	4330	4312	12
2	10	2	600	597	5
4	10	2	668	664	6
6	10	2	111	113	11
8	10	2	262	267	6
10	10	2	1772	1802	13
12	10	2	410	404	5
14	10	2	301	317	6
16	10	2	206	196	9
18	10	2	190	185	9
1	11	2	428	427	5
3	11	2	686	699	6
5	11	2	43	19	42
7	11	2	35	11	34
9	11	2	544	558	6
11	11	2	1775	1790	14
13	11	2	34	28	34
15	11	2	96	94	15
17	11	2	55	66	47
0	12	2	1290	1299	10
2	12	2	92	99	14
4	12	2	167	164	8
6	12	2	812	820	7
8	12	2	195	201	8
10	12	2	674	685	6
12	12	2	283	285	7
14	12	2	446	434	6
16	12	2	482	487	6
1	13	2	132	139	10
3	13	2	55	63	29
5	13	2	1680	1700	14
7	13	2	0	19	1
9	13	2	74	64	20
11	13	2	136	139	11
13	13	2	110	118	14
15	13	2	523	528	6
0	14	2	329	333	6
2	14	2	329	328	6
4	14	2	681	682	6
6	14	2	493	487	6
8	14	2	201	191	8
10	14	2	81	71	20
12	14	2	7	8	6
14	14	2	306	313	7
1	15	2	639	636	6
3	15	2	229	225	7
5	15	2	1437	1418	10
7	15	2	456	455	6
9	15	2	0	7	1
11	15	2	432	427	6
13	15	2	135	120	13
0	16	2	898	899	7
2	16	2	152	157	10
4	16	2	81	81	20
6	16	2	560	561	6
8	16	2	27	45	26
10	16	2	750	747	7
1	17	2	255	248	8
3	17	2	370	373	7
5	17	2	75	58	24
7	17	2	127	136	14
9	17	2	325	322	7
0	18	2	664	640	6
2	18	2	104	88	16
4	18	2	267	270	8
6	18	2	372	372	7
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7	1	3	358	354	4
9	1	3	260	260	5
11	1	3	1242	1250	9
13	1	3	389	378	5
15	1	3	283	284	6
17	1	3	323	323	6
19	1	3	485	486	6
21	1	3	624	613	6
0	2	3	2119	2069	8
2	2	3	663	638	5
4	2	3	170	167	5
6	2	3	1076	1040	8
8	2	3	644	630	5
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12	2	3	649	663	6
14	2	3	304	314	5
16	2	3	938	949	7
18	2	3	186	196	9
20	2	3	228	228	9
1	3	3	515	508	4
3	3	3	235	234	4
5	3	3	987	969	7
7	3	3	701	700	6
9	3	3	198	193	6
11	3	3	1375	1384	10
13	3	3	40	4	40
15	3	3	168	179	8
17	3	3	249	256	7
19	3	3	107	107	15
21	3	3	406	404	7
0	4	3	2250	2196	9
2	4	3	44	24	23
4	4	3	318	308	4
6	4	3	293	280	4
8	4	3	168	169	6
10	4	3	595	593	5
12	4	3	707	718	6
14	4	3	125	111	10
16	4	3	114	116	12
18	4	3	143	142	11
20	4	3	67	68	28
1	5	3	65	64	13
3	5	3	236	245	4
5	5	3	653	631	5
7	5	3	841	824	7
9	5	3	325	334	5
11	5	3	121	125	9
13	5	3	432	426	5
15	5	3	183	183	8
17	5	3	251	258	7
19	5	3	57	49	38
0	6	3	497	497	4
2	6	3	162	157	6
4	6	3	500	481	5
6	6	3	1268	1265	9
8	6	3	382	384	5
10	6	3	158	167	8
12	6	3	304	314	6
14	6	3	76	75	17
16	6	3	1055	1053	8
18	6	3	374	389	7
20	6	3	428	427	7
1	7	3	170	154	6
3	7	3	177	196	6
5	7	3	1404	1405	11
7	7	3	191	186	6
9	7	3	386	393	5
11	7	3	864	870	7
13	7	3	131	131	10
15	7	3	54	22	31
17	7	3	672	663	6
19	7	3	148	125	12
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2	8	3	36	42	36
4	8	3	262	260	5
6	8	3	561	570	5
8	8	3	107	98	11
10	8	3	230	234	6
12	8	3	557	554	6
14	8	3	290	293	6
16	8	3	38	26	38
18	8	3	125	120	12
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3	9	3	157	168	8
5	9	3	263	256	6
7	9	3	200	205	7
9	9	3	61	56	22
11	9	3	894	898	7
13	9	3	85	73	16
15	9	3	175	174	9
17	9	3	431	449	6
0	10	3	967	966	7
2	10	3	713	730	6
4	10	3	290	296	5
6	10	3	251	259	6
8	10	3	187	192	7
10	10	3	143	148	9
12	10	3	68	73	22
14	10	3	587	597	6
16	10	3	248	244	8
1	11	3	226	224	6
3	11	3	43	38	43
5	11	3	866	863	7
7	11	3	211	204	7
9	11	3	340	335	6
11	11	3	56	46	32
13	11	3	0	2	1
15	11	3	125	122	13
17	11	3	545	540	6
0	12	3	122	130	10
2	12	3	126	129	6
4	12	3	397	407	5
6	12	3	204	202	7
8	12	3	23	17	22
10	12	3	51	65	46
12	12	3	234	224	7
14	12	3	145	158	11
16	12	3	467	443	6
1	13	3	339	334	6
3	13	3	410	411	5
5	13	3	412	418	6
7	13	3	135	129	10
9	13	3	230	225	7
11	13	3	489	474	6
13	13	3	24	23	24
15	13	3	73	70	25
0	14	3	210	199	7
2	14	3	131	133	11
4	14	3	321	319	6
6	14	3	155	156	10
8	14	3	287	289	7
10	14	3	199	207	9
12	14	3	72	41	25
1	15	3	187	186	9
3	15	3	290	297	7
5	15	3	316	325	7
7	15	3	225	220	8
9	15	3	96	86	18
11	15	3	331	315	7
0	16	3	203	190	9
2	16	3	60	34	32
4	16	3	238	253	8
6	16	3	1121	1106	8
8	16	3	293	297	7
10	16	3	168	176	11
1	17	3	169	176	11
3	17	3	216	224	9
5	17	3	515	512	6
7	17	3	40	29	40
0	18	3	189	188	10
2	18	3	209	217	10
4	18	3	141	136	13
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2	0	4	361	370	4
4	0	4	563	579	5
6	0	4	353	349	4
8	0	4	343	343	4
10	0	4	2680	2747	12
12	0	4	1012	1016	8
14	0	4	418	419	5
16	0	4	83	67	16
18	0	4	459	451	6
20	0	4	314	300	7
1	1	4	368	371	4
3	1	4	42	19	28
5	1	4	180	168	6
7	1	4	50	50	25
9	1	4	1097	1111	8
11	1	4	1687	1734	12
13	1	4	233	233	6
15	1	4	142	150	10
17	1	4	65	63	24
19	1	4	477	477	6
0	2	4	319	339	4
2	2	4	222	221	5
4	2	4	367	356	4
6	2	4	457	475	5
8	2	4	78	89	14
10	2	4	386	396	5
12	2	4	390	400	5
14	2	4	636	633	6
16	2	4	769	774	7
18	2	4	135	119	11
20	2	4	71	38	25
1	3	4	185	198	5
3	3	4	435	427	4
5	3	4	1345	1365	11
7	3	4	174	188	6
9	3	4	636	652	6
11	3	4	128	124	9
13	3	4	246	253	6
15	3	4	789	785	7
17	3	4	764	776	7
19	3	4	245	253	8
0	4	4	515	537	5
2	4	4	471	469	5
4	4	4	509	521	5
6	4	4	1953	1977	11
8	4	4	178	184	7
10	4	4	348	350	5
12	4	4	181	179	7
14	4	4	676	677	6
16	4	4	1494	1504	10
18	4	4	146	147	11
1	5	4	982	977	7
3	5	4	127	131	8
5	5	4	1503	1531	11
7	5	4	413	410	5
9	5	4	35	36	34
11	5	4	912	931	7
13	5	4	80	85	16
15	5	4	257	263	7
17	5	4	122	121	12
19	5	4	99	106	17
0	6	4	1994	2034	11
2	6	4	192	210	6
4	6	4	337	327	5
6	6	4	170	166	7
8	6	4	372	374	5
10	6	4	1304	1302	9
12	6	4	263	259	6
14	6	4	216	219	8
16	6	4	202	193	8
18	6	4	259	252	8
1	7	4	222	207	6
3	7	4	267	277	5
5	7	4	1235	1240	8
7	7	4	407	406	5
9	7	4	859	878	7
11	7	4	726	743	6
13	7	4	254	247	7
15	7	4	261	270	7
17	7	4	453	452	6
0	8	4	1768	1856	12
2	8	4	47	43	37
4	8	4	275	284	5
6	8	4	608	604	6
8	8	4	361	362	5
10	8	4	1026	1030	8
12	8	4	85	73	15
14	8	4	70	79	22
16	8	4	304	293	7
18	8	4	20	19	20
1	9	4	34	21	33
3	9	4	229	235	6
5	9	4	1751	1753	13
7	9	4	480	474	5
9	9	4	43	11	43
11	9	4	247	239	7
13	9	4	81	53	18
15	9	4	528	534	6
17	9	4	618	618	6
0	10	4	811	813	7
2	10	4	45	36	45
4	10	4	397	402	5
6	10	4	177	179	8
8	10	4	309	303	6
10	10	4	425	422	6
12	10	4	289	283	6
14	10	4	789	795	7
16	10	4	410	414	7
1	11	4	190	185	7
3	11	4	305	306	6
5	11	4	948	964	8
7	11	4	31	14	30
9	11	4	56	52	30
11	11	4	36	55	35
13	11	4	141	140	11
15	11	4	607	601	6
0	12	4	987	972	8
2	12	4	204	193	7
4	12	4	218	234	7
6	12	4	253	261	7
8	12	4	237	228	7
10	12	4	514	513	6
12	12	4	348	359	7
14	12	4	21	50	21
1	13	4	335	336	6
3	13	4	153	156	9
5	13	4	210	200	8
7	13	4	305	296	6
9	13	4	322	327	7
11	13	4	731	729	7
13	13	4	159	168	11
0	14	4	1294	1279	9
2	14	4	238	220	7
4	14	4	310	317	7
6	14	4	489	483	6
8	14	4	132	120	12
10	14	4	951	956	8
12	14	4	47	41	46
1	15	4	285	275	7
3	15	4	358	363	6
5	15	4	248	260	8
7	15	4	70	42	25
9	15	4	190	188	10
0	16	4	148	151	11
2	16	4	241	240	8
4	16	4	91	78	19
6	16	4	441	430	6
8	16	4	54	19	54
1	17	4	170	158	7
3	17	4	185	186	10
1	1	5	45	39	32
3	1	5	140	149	8
5	1	5	768	762	6
7	1	5	29	18	29
9	1	5	246	258	6
11	1	5	158	152	8
13	1	5	128	139	10
15	1	5	154	151	9
17	1	5	712	715	6
19	1	5	380	393	7
0	2	5	829	819	6
2	2	5	148	138	7
4	2	5	364	373	4
6	2	5	485	488	5
8	2	5	253	257	6
10	2	5	108	126	11
12	2	5	696	706	6
14	2	5	0	33	1
16	2	5	156	160	10
18	2	5	101	98	16
1	3	5	136	131	8
3	3	5	230	228	6
5	3	5	556	562	5
7	3	5	66	73	19
9	3	5	110	106	11
11	3	5	229	224	7
13	3	5	240	240	7
15	3	5	0	27	1
17	3	5	511	513	6
0	4	5	184	183	6
2	4	5	77	73	15
4	4	5	75	60	15
6	4	5	616	610	5
8	4	5	273	288	6
10	4	5	336	322	5
12	4	5	431	441	5
14	4	5	262	270	7
16	4	5	564	553	6
18	4	5	244	255	8
1	5	5	136	141	8
3	5	5	231	214	6
5	5	5	527	522	5
7	5	5	577	568	5
9	5	5	318	328	6
11	5	5	259	250	6
13	5	5	383	388	6
15	5	5	92	107	17
17	5	5	186	142	9
0	6	5	381	413	5
2	6	5	52	68	29
4	6	5	43	24	42
6	6	5	489	474	5
8	6	5	339	347	5
10	6	5	45	62	44
12	6	5	246	255	7
14	6	5	45	21	44
16	6	5	664	656	6
1	7	5	87	79	14
3	7	5	398	412	5
5	7	5	224	218	6
7	7	5	301	306	6
9	7	5	255	251	6
11	7	5	323	319	6
13	7	5	161	169	10
15	7	5	150	154	11
17	7	5	69	28	27
0	8	5	662	671	6
2	8	5	195	190	7
4	8	5	91	94	13
6	8	5	549	543	5
8	8	5	80	70	16

Observed and calculated structure factors for K22

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
10	8	5	112	111	12	1	1	6	182	175	7	2	8	6	245	240	7	11	3	7	821	825	7	5	1	8	443	450	6
12	8	5	331	328	6	3	1	6	143	144	8	4	8	6	313	313	6	13	3	7	66	55	26	7	1	8	250	235	7
14	8	5	437	444	6	5	1	6	1612	1654	13	6	8	6	269	262	6	0	4	7	1084	1067	8	9	1	8	600	595	6
16	8	5	608	588	6	7	1	6	120	127	10	8	8	6	361	351	6	2	4	7	49	53	41	11	1	8	542	540	6
1	9	5	677	670	6	9	1	6	329	138	6	10	8	6	180	185	9	4	4	7	200	187	7	0	2	8	32	7	32
3	9	5	57	15	24	11	1	6	209	208	7	12	8	6	109	84	14	6	4	7	146	146	9	2	2	8	117	107	13
5	9	5	518	511	5	13	1	6	76	86	19	14	8	6	355	349	7	8	4	7	140	138	10	4	2	8	211	213	8
7	9	5	315	315	6	15	1	6	434	424	6	1	9	6	384	380	6	10	4	7	391	399	6	6	2	8	507	500	6
9	9	5	0	23	1	17	1	6	297	307	7	3	9	6	62	54	26	12	4	7	457	454	6	8	2	8	53	24	40
11	9	5	1508	1515	11	0	2	6	1688	1698	12	5	9	6	17	20	17	14	4	7	122	114	14	10	2	8	215	206	8
13	9	5	158	155	10	2	2	6	197	204	7	7	9	6	545	541	6	1	5	7	50	5	36	1	3	8	97	102	14
15	9	5	176	163	10	4	2	6	158	153	8	9	9	6	385	383	6	3	5	7	99	110	14	3	3	8	287	281	7
0	10	5	1083	1070	8	6	2	6	496	495	5	11	9	6	743	727	7	5	5	7	163	173	9	5	3	8	1762	1770	12
2	10	5	467	466	5	8	2	6	208	210	7	13	9	6	29	28	28	7	5	7	490	497	6	7	3	8	26	7	25
4	10	5	88	67	15	10	2	6	831	848	7	0	10	6	2107	2120	15	9	5	7	238	234	8	9	3	8	350	344	7
6	10	5	511	488	5	12	2	6	335	326	6	2	10	6	278	262	7	11	5	7	33	27	33	11	3	8	126	116	12
8	10	5	84	83	16	14	2	6	63	47	26	4	10	6	242	244	7	13	5	7	269	256	8	0	4	8	230	248	8
10	10	5	330	325	6	16	2	6	376	370	7	6	10	6	550	561	6	0	6	7	212	224	7	2	4	8	307	313	7
12	10	5	87	77	19	1	3	6	263	262	6	8	10	6	84	88	19	2	6	7	134	135	10	4	4	8	172	167	9
14	10	5	464	451	6	3	3	6	12	39	12	10	10	6	1259	1250	10	4	6	7	201	205	8	6	4	8	664	660	6
1	11	5	0	29	1	5	3	6	846	838	7	12	10	6	248	246	8	6	6	7	725	724	7	8	4	8	0	17	1
3	11	5	65	77	23	7	3	6	106	107	12	1	11	6	150	160	10	8	6	7	254	259	7	10	4	8	171	162	10
5	11	5	559	558	6	9	3	6	928	916	7	3	11	6	147	137	6	10	6	7	131	116	12	1	5	8	538	526	6
7	11	5	501	502	6	11	3	6	1167	1165	9	5	11	6	472	481	6	12	6	7	210	198	9	3	5	8	139	154	11
9	11	5	172	173	9	13	3	6	152	150	9	7	11	6	142	138	11	1	7	7	74	98	20	5	5	8	415	418	6
11	11	5	301	296	7	15	3	6	96	109	16	9	11	6	402	396	6	3	7	7	182	196	9	7	5	8	35	24	35
13	11	5	223	226	9	17	3	6	393	408	7	11	11	6	765	755	7	5	7	7	855	848	7	9	5	8	75	85	23
0	12	5	1004	1009	8	0	4	6	2302	2320	13	0	12	6	508	504	6	7	7	7	124	108	11	0	6	8	1768	1788	13
2	12	5	522	526	6	2	4	6	43	41	42	2	12	6	117	108	14	9	7	7	285	280	7	2	6	8	195	189	9
4	12	5	0	22	1	4	4	6	312	328	5	4	12	6	161	135	10	11	7	7	546	549	6	4	6	8	300	286	7
6	12	5	744	741	7	6	4	6	498	511	5	6	12	6	861	860	7	0	8	7	631	625	6	6	6	8	461	456	6
8	12	5	0	47	1	8	4	6	91	102	14	8	12	6	55	64	44	2	8	7	39	33	38	8	6	8	149	151	11
10	12	5	29	12	28	10	4	6	1312	1333	10	10	12	6	369	363	7	4	8	7	197	185	8	1	7	8	39	31	38
12	12	5	178	180	10	12	4	6	179	167	9	1	13	6	59	6	33	6	8	7	168	355	6	3	7	8	199	194	9
1	13	5	387	370	6	14	4	6	39	9	18	3	13	6	49	41	49	8	8	7	0	18	1	5	7	8	870	856	7
3	13	5	209	212	8	16	4	6	190	192	9	5	13	6	1266	1259	9	10	8	7	189	191	10	7	7	8	222	236	9
5	13	5	967	975	8	1	5	6	310	295	5	7	13	6	114	113	15	1	9	7	143	347	6	0	8	8	911	903	8
7	13	5	191	183	9	3	5	6	314	316	5	0	14	6	96	107	18	3	9	7	94	101	16	2	8	8	0	30	1
9	13	5	253	255	8	5	5	6	527	519	5	2	14	6	375	372	7	5	9	7	241	237	8	4	8	8	86	65	20
11	13	5	1260	1256	9	7	5	6	92	77	14	4	14	6	289	291	8	7	9	7	127	132	13	6	8	8	423	421	7
0	14	5	1013	1000	8	9	5	6	283	284	6	6	14	6	153	154	12	9	9	7	0	2	1	1	9	8	0	34	1
2	14	5	145	148	12	11	5	6	312	315	6	1	1	7	93	77	13	0	10	7	618	615	6	3	9	8	121	110	13
4	14	5	327	317	7	13	5	6	78	70	20	3	1	7	192	194	7	2	10	7	403	412	6	5	9	8	1242	1228	10
6	14	5	414	415	7	15	5	6	277	284	7	5	1	7	109	111	11	4	10	7	139	139	12	0	10	8	1017	992	8
8	14	5	143	147	12	0	6	6	211	132	7	7	1	7	272	266	6	6	10	7	211	199	9	2	10	8	66	63	30
10	14	5	383	383	7	2	6	6	97	72	12	9	1	7	150	153	9	8	10	7	112	102	15	1	1	9	0	17	1
1	15	5	69	70	26	4	6	6	346	347	5	11	1	7	671	679	7	1	11	7	129	124	12	3	1	9	131	133	12
3	15	5	106	114	7	6	6	6	949	943	7	13	1	7	266	278	7	3	11	7	35	16	35	5	1	9	347	348	7
5	15	5	30	7	29	8	6	6	295	297	6	15	1	7	217	219	8	5	11	7	587	586	6	0	2	9	165	166	10
7	15	5	318	319	7	10	6	6	58	17	27	0	2	7	633	632	6	7	11	7	129	136	13	2	2	9	97	96	17
0	16	5	122	103	7	12	6	6	189	193	9	2	2	7	136	130	5	0	12	7	24	21	21	4	2	9	145	139	12
2	16	5	230	225	9	14	6	6	710	708	6	4	2	7	52	25	29	2	12	7	204	209	9	6	2	9	64	46	27
4	16	5	70	76	28	16	6	6	782	781	7	6	2	7	476	477	5	4	12	7	273	273	8	1	1	9	99	109	16
0	0	6	2492	2519	12	1	7	6	518	524	5	8	2	7	258	256	7	0	0	8	2448	2476	15	3	3	9	35	0	34
2	0	6	117	121	10	3	7	6	109	101	12	10	2	7	63	48	25	2	0	8	140	136	10	5	3	9	155	122	10
4	0	6	551	558	5	5	7	6	2398	2424	14	12	2	7	444	443	6	4	0	8	188	175	8	0	4	9	427	425	6
6	0	6	688	686	6	7	7	6	87	115	16	14	2	7	186	177	9	6	0	8	666	685	6	2	4	9	69	44	25
8	0	6	396	400	5	9	7	6	357	350	6	1	3	7	242	233	6	8	0	8	0	29	1	4	4	9	71	66	25
10	0	6	887	891	7	11	7	6	422	435	6	3	3	7	0	13	1	10	0	8	1476	1491	10	1	5	9	4	24	3
12	0	6	771	789	6	13	7	6	213	213	8	5	3	7	410	399	5	12	0	8	528	530	6	3	5	9	47	58	47
14	0	6	751	748	7	15	7	6	681	685	7	7	3	7	186	186	6	1	1	8	157	158	10						
16	0	6	871	888	7	0	8	6	316	285	6	9	3	7	125	143	11	3	1	8	87	88	16						

Observed and calculated structure factors for K23

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	782	792	3	4	8	0	464	452	4	3	1	1	403	394	3	7	9	1	302	306	4	7	1	2	115	109	4
4	0	0	1267	1280	5	6	8	0	625	626	5	5	1	1	936	944	6	9	9	1	50	37	15	9	1	2	678	685	5
6	0	0	485	507	4	8	8	0	184	185	4	7	1	1	128	113	4	11	9	1	1633	1661	11	11	1	2	706	704	5
8	0	0	794	763	6	10	8	0	1259	1259	8	9	1	1	457	448	3	13	9	1	90	92	9	13	1	2	30	12	30
10	0	0	3592	3604	10	12	8	0	204	211	5	11	1	1	774	794	5	15	9	1	100	96	9	15	1	2	645	641	5
12	0	0	1359	1372	9	14	8	0	139	136	6	13	1	1	392	387	4	17	9	1	155	150	7	17	1	2	112	105	8
14	0	0	262	251	4	16	8	0	314	324	5	15	1	1	80	77	9	19	9	1	177	187	7	19	1	2	29	1	28
16	0	0	174	171	5	18	8	0	77	73	13	17	1	1	703	721	6	0	10	1	1234	1254	9	21	1	2	366	355	5
18	0	0	522	520	5	20	8	0	323	315	5	19	1	1	460	476	5	2	10	1	791	784	6	0	2	2	4056	4003	7
20	0	0	266	267	5	1	9	0	8	6	8	21	1	1	835	812	7	4	10	1	256	262	4	2	2	2	420	411	3
22	0	0	1643	1653	11	3	9	0	458	463	4	0	2	1	154	175	3	6	10	1	441	447	4	4	2	2	571	559	4
1	1	0	824	848	3	5	9	0	1777	1815	9	2	2	1	502	529	3	8	10	1	184	178	5	6	2	2	513	501	4
3	1	0	248	238	2	7	9	0	834	828	6	4	2	1	517	515	3	10	10	1	253	253	4	8	2	2	335	331	3
5	1	0	461	476	3	9	9	0	0	22	1	6	2	1	298	279	3	12	10	1	10	18	9	10	2	2	1263	1257	9
7	1	0	401	393	3	11	9	0	692	687	6	8	2	1	554	556	4	14	10	1	634	629	5	12	2	2	504	507	4
9	1	0	1595	1593	8	13	9	0	227	229	5	10	2	1	208	224	4	16	10	1	282	291	5	14	2	2	72	71	10
11	1	0	2850	2881	10	15	9	0	551	558	5	12	2	1	923	932	7	18	10	1	269	260	6	16	2	2	175	372	4
13	1	0	321	326	4	17	9	0	456	450	5	14	2	1	132	136	6	1	11	1	188	193	4	18	2	2	48	5	21
15	1	0	252	261	4	19	9	0	232	227	6	16	2	1	622	636	5	3	11	1	207	205	4	20	2	2	62	16	16
17	1	0	347	350	4	0	10	0	278	289	3	18	2	1	32	40	32	5	11	1	702	724	6	1	3	2	469	468	3
19	1	0	589	594	5	2	10	0	42	38	18	20	2	1	184	182	6	7	11	1	537	529	5	3	3	2	251	247	3
21	1	0	758	752	6	4	10	0	165	177	4	22	2	1	219	227	6	9	11	1	325	321	4	5	3	2	1036	1022	7
0	2	0	1248	1263	4	6	10	0	281	275	4	1	3	1	359	358	3	11	11	1	319	326	4	7	3	2	224	215	3
2	2	0	325	342	3	8	10	0	330	333	4	3	3	1	277	269	3	13	11	1	142	144	7	9	3	2	1516	1537	9
4	2	0	611	616	4	10	10	0	538	538	5	5	3	1	368	351	3	15	11	1	130	125	7	11	3	2	1349	1377	10
6	2	0	94	96	4	12	10	0	189	192	5	7	3	1	482	472	3	17	11	1	439	450	5	13	3	2	457	456	4
8	2	0	243	241	3	14	10	0	1169	1169	8	9	3	1	230	241	3	0	12	1	1074	1080	7	15	3	2	188	180	5
10	2	0	618	628	5	16	10	0	211	211	6	11	3	1	238	250	4	2	12	1	514	515	5	17	3	2	354	356	5
12	2	0	166	369	4	18	10	0	537	532	5	13	3	1	246	252	4	4	12	1	117	118	6	19	3	2	828	836	7
14	2	0	838	845	6	1	11	0	328	330	4	15	3	1	63	45	11	6	12	1	641	642	5	21	3	2	524	534	5
16	2	0	759	733	6	3	11	0	212	214	4	17	3	1	315	308	4	8	12	1	118	119	7	0	4	2	1767	1724	7
18	2	0	61	34	14	5	11	0	788	795	6	19	3	1	210	207	6	10	12	1	159	157	6	2	4	2	583	571	4
20	2	0	159	152	7	7	11	0	104	108	7	21	3	1	310	318	6	12	12	1	254	259	5	4	4	2	66	10	7
22	2	0	299	304	6	9	11	0	94	98	8	0	4	1	1121	1121	6	14	12	1	41	65	40	6	4	2	217	205	3
1	3	0	401	392	3	11	11	0	512	524	5	2	4	1	97	100	4	16	12	1	671	692	6	8	4	2	26	22	26
3	3	0	693	690	4	13	11	0	105	120	9	4	4	1	252	247	3	1	13	1	400	394	4	10	4	2	1925	1978	10
5	3	0	4665	4648	8	15	11	0	848	854	7	6	4	1	751	726	6	3	13	1	379	382	4	12	4	2	227	232	4
7	3	0	555	539	4	17	11	0	455	470	5	8	4	1	450	452	4	5	13	1	935	953	7	14	4	2	259	258	4
9	3	0	1021	1027	8	0	12	0	1448	1491	10	10	4	1	308	292	3	7	13	1	54	62	16	16	4	2	62	72	13
11	3	0	265	258	3	2	12	0	269	271	4	12	4	1	712	722	5	9	13	1	308	317	5	18	4	2	464	454	5
13	3	0	264	267	4	4	12	0	213	201	4	14	4	1	268	261	4	11	13	1	1106	1108	8	20	4	2	109	308	5
15	3	0	821	823	6	6	12	0	576	568	5	16	4	1	599	600	5	13	13	1	173	162	6	1	5	2	913	894	5
17	3	0	950	929	7	8	12	0	194	200	5	18	4	1	270	263	5	15	13	1	257	256	6	3	5	2	39	34	12
19	3	0	270	271	5	10	12	0	641	632	5	20	4	1	90	82	11	0	14	1	706	712	6	5	5	2	1818	1773	8
21	3	0	455	441	5	12	12	0	482	479	5	1	5	1	142	142	3	2	14	1	260	256	5	7	5	2	269	255	3
0	4	0	2071	2088	6	14	12	0	64	72	15	3	5	1	482	485	3	4	14	1	413	421	4	9	5	2	160	361	4
2	4	0	636	636	4	16	12	0	138	119	8	5	5	1	1401	1404	7	6	14	1	262	269	5	11	5	2	626	619	5
4	4	0	984	995	6	1	13	0	471	481	4	7	5	1	872	862	6	8	14	1	301	298	5	13	5	2	77	73	10
6	4	0	3767	3682	8	3	13	0	208	216	5	9	5	1	580	561	4	10	14	1	207	217	6	15	5	2	242	243	5
8	4	0	479	470	4	5	13	0	375	379	4	11	5	1	245	270	4	12	14	1	179	180	7	17	5	2	709	708	6
10	4	0	450	454	4	7	13	0	516	517	4	13	5	1	570	571	5	14	14	1	377	364	5	19	5	2	199	394	5
12	4	0	317	318	4	9	13	0	467	462	5	15	5	1	95	89	8	1	15	1	29	15	29	21	5	2	470	457	5
14	4	0	835	831	6	11	13	0	885	884	7	17	5	1	236	219	5	3	15	1	331	336	5	0	6	2	1110	1094	7
16	4	0	1964	1976	12	13	13	0	307	323	5	19	5	1	53	50	21	5	15	1	213	213	5	2	6	2	78	84	6
18	4	0	92	93	10	15	13	0	259	260	6	21	5	1	721	701	6	7	15	1	341	343	5	4	6	2	989	978	6
20	4	0	252	244	6	0	14	0	1350	1379	9	0	6	1	567	545	4	9	15	1	64	45	16	6	6	2	2199	2355	9
1	5	0	1484	1471	6	2	14	0	369	372	4	2	6	1	155	149	3	11	15	1	123	117	9	8	6	2	247	245	4
3	5	0	0	11	1	4	14	0	221	226	5	4	6	1	209	206	3	13	15	1	168	170	7	10	6	2	0	22	1
5	5	0	3172	3067	8	6	14	0	778	786	6	6	6	1	897	878	6	0	16	1	270	273	5	12	6	2	418	413	4
7	5	0	883	879	6	8	14	0	82	87	10	8	6	1	582	569	4	2	16	1	246	244	5	14	6	2	940	951	7
9	5	0	110	124	6	10	14	0	1291	1301	9	10	6	1	142	137	5	4	16	1	0	2	1	16	6	2	1438	1443	10
11	5	0	369	390	4	12	14	0	52	61	23	12	6	1	330	320	4	6	16	1	1270	1278	9	18	6	2	42	46	41
13	5	0	353	371	4	14	14	0	0	18	1	14	6	1	44	13	19	8	16	1	345	345	5	20	6	2	89	77	11
15	5	0	249	249	5	1	15	0	227	224	5	16	6	1	994	1003	7	10	16	1	61	58	19	1	7	2	774	761	5
17	5	0	476	470	5	3	15	0	411	416	4	18	6	1	297	294	5	12	16	1	81	60	14	3	7	2	52	62	11
19	5	0	204	207	6	5	15	0	516	523	5	20	6	1	441	437	5	1	17	1	92	81	10	5	7	2	4511	4368	11
21	5	0	348	348	5	7	15	0	5	44	4	1	7	1	140	141	4	3	17	1	298	294	5	7	7	2	158	161	4
0	6	0	773	784	5	9	15	0	94	100	11	3	7	1	589	572	4	5	17	1	729	734	6	9	7	2	505	508	4
2	6	0	239	237	3	11	15	0	386	391	5	5	7	1	487	488	4	7	17	1	227	232	6	11	7	2	189	193	5
4	6	0	442	451	3	13	15	0	430	426	5	7	7	1	214	213	4	9	17	1	376	382	5	13	7	2	292	291	4
6	6	0	617	606	5	0	16	0	606	613	5	9	7	1	445	451	4	0	18	1	310	312	5	15	7	2	900	922	7
8	6	0	749	739	6	2	16	0	217	221	5	11	7	1	14	30	13	2	18	1	87	88	12	17	7	2	918	929	7
10	6	0	1315	1327	9	4	16	0	220	216	6	13	7	1	74	63	10	4	18	1	333	333	5	19	7	2	82	90	13
12	6	0	224	228	4	6	16	0	807	811	6	15	7	1	23	22	23	6	18	1	330	332	6	0	8	2	492	491	4
14	6	0	493	495	5	8	16	0	87	98	11	17	7	1	221	227	5	1	19	1	347	344	5	2	8	2	511	502	4
16	6	0	597	590	5	10	16	0	70	67	15	19	7	1	137	133	8	3	19	1	434	431	5	4	8	2	119	132	5
18	6	0	352	349	5	12	16	0	440	446	5	0	8	1	596	563	4	0	0	2	3242	3305	7	6	8	2	428	420	4
20	6	0	53	35	22	1	17	0	317	317	5	2	8	1	26	8	25	2	0	2	639	651	4	8	8	2	603	606	5
1	7	0	643	637	4	3	17	0	281	278	5	4	8	1	98	109	6	4	0	2	279	279	3	10	8	2	7	21	7
3	7	0	163	160	3	5	17	0	1787	1798	14	6	8	1	283	291	3	6	0	2	742	711	5	12	8	2	136	126	6
5	7	0	1384	1383	8	7	17	0	35	49	34	8	8	1	112	88	6	8	0	2	577	569	4	14	8	2	527	525	5
7	7	0	508	501	4	9	17	0	68	58	15	10	8	1	26	17	25	10	0	2	1395	1370	9	16	8	2	874	880	7
9	7	0	1160	1175	9	0	18	0	348	345	5	12	8	1	487	489	4	12	0	2	974	996	8	18	8	2	63	63	17
11	7	0	569	525	5	2	18	0	323	333	5	14	8	1	560	550	5	14	0	2	1317	1325	9	1	9	2	466	465	4
13	7	0	373	371	4	4	18	0	0	20	1	16	8	1	672	662	5	16	0	2	682	694	6	3	9	2	88	82	7
15	7	0	260	259	5	6	18	0	266	269	6	18	8	1	352	347	5	18	0	2	801	791	6	5	9	2	512	503	4
17	7	0	287	287	5	8	18	0	357	338	5	20	8	1	255	259	6	20	0	2	94	94	11	7	9	2	469	447	4
19	7	0	711	710	6	1	19	0	220	209	6	1	9	1	968	951	7	1	1	2	563	572	4	9	9	2	688	694	5
0	8	0	2508	2476	8	3	19	0	121	118	10	3	9	1	87	84	7	3	1	2	886	876	6	11	9	2	1547	1573	11
2	8	0	228	223	3	1	1	1	177	173	2	5	9	1	351	373	4	5	1	2	956	958	7	13	9	2	84	89	10

Observed and calculated structure factors for K23

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	268	279	5	20	2	3	114	112	9	17	11	3	555	558	5	10	4	4	307	316	4	10	14	4	1031	1027	8
17	9	2	652	664	6	1	3	3	559	542	4	0	12	3	189	190	5	12	4	4	212	212	5	12	14	4	48	10	26
19	9	2	305	306	6	3	3	3	234	224	3	2	12	3	297	296	4	14	4	4	805	823	6	1	15	4	191	188	6
0	10	2	4290	4307	12	5	3	3	1037	1015	8	4	12	3	167	171	4	16	4	4	1380	1413	10	3	15	4	416	412	5
2	10	2	693	693	5	7	3	3	743	730	5	6	12	3	134	132	7	18	4	4	158	153	7	5	15	4	242	245	6
4	10	2	768	770	5	9	3	3	195	185	4	8	12	3	54	48	15	1	5	4	1019	1018	7	7	15	4	86	85	13
6	10	2	123	134	6	11	3	3	1291	1323	10	10	12	3	154	149	6	3	5	4	198	200	4	9	15	4	101	101	10
8	10	2	222	221	4	13	3	3	47	43	16	12	12	3	266	258	5	5	5	4	1457	1495	10	0	16	4	167	173	7
10	10	2	1782	1814	11	15	3	3	120	124	7	14	12	3	144	154	8	7	5	4	436	436	4	2	16	4	193	201	6
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16	10	2	266	268	5	21	3	3	385	380	5	3	13	3	484	488	5	13	5	4	208	207	5	8	16	4	47	23	28
18	10	2	215	231	6	0	4	3	2199	2143	8	5	13	3	343	341	4	15	5	4	249	254	5	1	17	4	386	381	5
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9	11	2	602	591	5	10	4	3	428	413	4	15	13	3	166	164	7	4	6	4	438	437	4	7	1	5	45	30	17
11	11	2	1739	1768	12	12	4	3	783	785	6	0	14	3	59	50	14	6	6	4	106	95	7	9	1	5	364	368	4
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2	12	2	57	47	13	1	5	3	49	44	10	10	14	3	72	51	14	16	6	4	260	253	5	19	1	5	364	377	5
4	12	2	74	58	10	3	5	3	300	309	3	12	14	3	43	56	16	18	6	4	259	249	6	0	2	5	792	787	6
6	12	2	869	866	7	5	5	3	824	810	6	1	15	3	175	170	6	1	7	4	222	216	4	2	2	5	110	91	6
8	12	2	115	125	7	7	5	3	847	850	6	3	15	3	259	246	5	3	7	4	235	237	4	4	2	5	470	483	4
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13	13	2	74	73	14	8	6	3	420	421	4	1	17	3	148	149	8	6	8	4	584	576	5	7	3	5	89	99	8
15	13	2	514	512	5	10	6	3	165	178	5	3	17	3	310	305	5	8	8	4	302	305	4	9	3	5	107	95	7
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4	14	2	682	688	5	16	6	3	1074	1083	8	0	18	3	203	208	7	14	8	4	123	118	8	15	3	5	51	17	20
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14	14	2	365	364	5	5	7	3	1230	1219	9	6	0	4	455	452	4	5	9	4	1700	1721	11	6	4	5	646	635	5
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5	15	2	1428	1432	10	11	7	3	835	836	6	12	0	4	930	930	7	11	9	4	257	259	5	12	4	5	491	498	5
7	15	2	532	524	5	13	7	3	131	136	6	14	0	4	195	404	4	13	9	4	75	77	12	14	4	5	253	260	5
9	15	2	103	99	10	15	7	3	131	114	7	16	0	4	217	214	5	15	9	4	379	391	5	16	4	5	637	627	5
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13	15	2	105	94	10	19	7	3	108	101	10	20	0	4	162	157	7	0	10	4	840	846	7	1	5	5	170	164	5
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2	16	2	117	106	8	2	8	3	109	105	6	3	1	4	72	56	8	4	10	4	446	449	4	5	5	5	641	648	5
4	16	2	29	7	28	4	8	3	336	343	4	5	1	4	260	241	3	6	10	4	211	212	5	7	5	5	585	586	5
6	16	2	563	562	5	6	8	3	601	593	5	7	1	4	0	14	1	8	10	4	145	142	4	9	5	5	404	416	4
8	16	2	84	92	12	8	8	3	76	75	9	9	1	4	1186	1212	8	10	10	4	462	470	5	11	5	5	244	230	5
10	16	2	712	710	6	10	8	3	111	122	7	11	1	4	1630	1644	11	12	10	4	230	230	5	13	5	5	199	187	4
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9	17	2	367	358	5	1	9	3	605	597	5	0	2	4	292	318	3	5	11	4	1028	1036	7	4	6	5	63	64	11
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4	18	2	242	247	6	7	9	3	226	216	4	6	2	4	484	506	4	11	11	4	74	67	12	10	6	5	87	82	9
6	18	2	419	414	5	9	9	3	71	67	10	8	2	4	62	69	10	13	11	4	89	65	10	12	6	5	225	226	5
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3	1	1	610	589	4	13	9	3	67	57	13	12	2	4	365	364	4	0	12	4	941	941	7	16	6	5	683	669	6
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9	1	1	389	391	4	0	10	3	832	851	6	18	2	4	32	13	32	6	12	4	248	250	5	5	7	5	61	58	13
11	1	1	1321	1327	10	2	10	3	781	788	6	20	2	4	99	103	11	8	12	4	250	248	5	7	7	5	328	319	4
13	1	1	462	464	4	4	10	3	369	369	4	1	3	4	278	279	3	10	12	4	431	420	5	9	7	5	309	306	4
15	1	1	150	143	6	6	10	3	212	213	5	3	3	4	556	545	4	12	12	4	319	316	5	11	7	5	363	363	4
17	1	1	345	342	5	8	10	3	242	249	4	5	3	4	3230	3256	10	14	12	4	41	10	40	13	7	5	169	170	6
19	1	1	445	465	5	10	10	3	69	60	11	7	3	4	204	207	4	1	13	4	260	262	5	15	7	5	60	57	18
21	1	1	812	781	6	12	10	3	87	86	9	9	3	4	782	798	6	3	13	4	133	135	7	17	7	5	44	43	32
0	2	3	2154	2127	7	14	10	3	616	619	5	11	3	4	21	9	20	5	13	4	251	247	5	0	8	5	727	738	6
2	2	3	595	577	4	16	10	3	86	88	11	13	3	4	243	252	5	7	13	4	303	306	5	2	8	5	145	137	6
4	2	3	11	12	22	1	11	3	289	288	4	15	3	4	716	712	6	9	13	4	459	457	5	4	8	5	29	16	29
6	2	3	1088	1069	8	3	11	3	158	158	5	17	3	4	711	712	6	11	13	4	710	703	6	6	8	5	538	530	5
8	2	3	678	661	5	5	11	3	775	791	6	19	3	4	216	234	6	13	13	4	200	185	6	8	8	5	82	88	10
10	2	3	270	273	4	7	11	3	224	221	5	0	4	4	487	516	4	0	14	4	1342	1353	9	10	8	5	22	5	21
12	2	3	684	701	5	9	11	3	381	384	4	2	4	4	441	430	4	2	14	4	213	216	6	12	8	5	349	354	5
14	2	3	338	340	4	11	11	3	48	40	19	4	4	4	563	590	5	4	14	4	331	330	5	14	8	5	486	480	5
16	2	3	1031	1030	7	13	11	3	31	34	31	6	4	4	1878	1877	10	6	14	4	535	539	5	16	8	5	730	712	6
18	2	3	235	224	5	15	11	3	46	21	28	8	4	4	206	216	4	8	14	4	68	71	14	1	9	5	685	693	5

Observed and calculated structure factors for K23

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	9	5	34	34	34	9	1	6	373	379	4	10	8	6	127	121	8	2	4	7	94	88	9	9	1	8	666	651	6
5	9	5	485	478	5	11	1	6	170	179	6	12	8	6	145	144	8	4	4	7	265	260	5	11	1	8	506	492	5
7	9	5	319	313	4	13	1	6	100	100	9	14	8	6	163	367	5	6	4	7	112	106	8	0	2	8	45	18	25
9	9	5	17	32	36	15	1	6	410	410	5	1	9	6	345	341	5	8	4	7	191	190	6	2	2	8	116	108	8
11	9	5	1511	1503	10	17	1	6	302	294	6	3	9	6	79	79	11	10	4	7	260	266	5	4	2	8	236	231	6
13	9	5	138	140	7	0	2	6	1609	1650	11	5	9	6	36	10	35	12	4	7	490	482	5	6	2	8	520	514	5
15	9	5	108	109	10	2	2	6	240	240	4	7	9	6	509	517	5	14	4	7	113	122	9	8	2	8	0	20	1
0	10	5	983	976	7	4	2	6	229	226	5	9	9	6	471	466	5	1	5	7	14	19	13	10	2	8	223	225	6
2	10	5	498	510	5	6	2	6	527	527	5	11	9	6	717	708	6	3	5	7	165	162	6	1	3	8	150	149	7
4	10	5	119	120	7	8	2	6	286	289	4	13	9	6	89	55	11	5	5	7	277	271	5	3	3	8	357	355	5
6	10	5	465	456	4	10	2	6	767	770	6	0	10	6	2079	2093	13	7	5	7	492	508	5	5	3	8	1726	1712	11
8	10	5	131	129	7	12	2	6	284	280	5	2	10	6	337	340	5	9	5	7	308	311	5	7	3	8	0	4	1
10	10	5	265	252	5	14	2	6	19	13	19	4	10	6	337	339	5	11	5	7	67	23	16	9	3	8	440	437	5
12	10	5	76	73	13	16	2	6	413	412	5	6	10	6	599	596	5	13	5	7	264	258	6	11	3	8	188	181	7
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3	11	5	160	172	6	5	3	6	786	796	6	12	10	6	165	167	7	4	6	7	179	184	6	4	4	8	204	205	6
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7	11	5	523	530	5	9	3	6	1030	1041	7	3	11	6	356	356	5	8	6	7	268	280	5	8	4	8	30	42	29
9	11	5	223	212	6	11	3	6	1072	1090	8	5	11	6	453	460	5	10	6	7	158	154	7	10	4	8	151	140	8
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13	11	5	203	205	6	15	3	6	90	78	11	9	11	6	431	429	5	1	7	7	80	78	11	3	5	8	174	176	6
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2	12	5	502	501	5	2	4	6	0	12	1	0	12	6	480	483	5	5	7	7	741	723	6	7	5	8	37	36	36
4	12	5	41	49	34	4	4	6	162	161	4	2	12	6	84	87	12	7	7	7	128	118	8	9	5	8	151	141	8
6	12	5	687	694	6	6	4	6	452	458	4	4	12	6	75	85	14	9	7	7	347	344	5	0	6	8	1784	1799	14
8	12	5	71	71	14	8	4	6	40	53	27	6	12	6	911	916	7	11	7	7	516	513	5	2	6	8	216	221	6
10	12	5	68	68	15	10	4	6	1325	1323	10	8	12	6	30	3	29	0	8	7	570	565	5	4	6	8	158	357	5
12	12	5	208	212	6	12	4	6	226	225	6	10	12	6	403	391	5	2	8	7	96	92	10	6	6	8	422	420	5
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7	13	5	178	171	6	3	5	6	332	338	4	7	13	6	135	137	8	10	8	7	109	95	9	5	7	8	874	883	7
9	13	5	278	283	6	5	5	6	460	454	4	0	14	6	57	46	20	1	9	7	388	387	5	7	7	8	242	245	6
11	13	5	1227	1200	9	7	5	6	54	44	16	2	14	6	392	393	5	3	9	7	80	70	12	0	8	8	871	870	7
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4	14	5	339	342	5	13	5	6	63	64	16	3	1	7	225	220	5	9	9	7	39	13	38	6	8	8	410	408	5
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8	14	5	197	200	7	0	6	6	156	152	6	7	1	7	262	255	5	2	10	7	431	435	5	3	9	8	183	176	7
1	15	5	96	99	11	2	6	6	55	22	14	9	1	7	229	223	5	4	10	7	174	171	7	5	9	8	1212	1218	9
3	15	5	285	280	5	4	6	6	466	476	5	11	1	7	711	707	6	6	10	7	201	194	6	0	10	8	1029	1019	7
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2	16	5	270	272	6	12	6	6	201	203	6	2	2	7	125	121	4	5	11	7	559	556	5	5	1	9	108	104	6
4	16	5	123	110	9	14	6	6	825	822	7	4	2	7	41	26	26	7	11	7	147	156	8	0	2	9	132	129	8
0	0	6	2489	2528	11	1	7	6	601	608	5	6	2	7	466	455	5	0	12	7	17	20	17	2	2	9	56	54	21
2	0	6	114	121	7	3	7	6	204	205	5	8	2	7	257	261	5	2	12	7	195	188	7	4	2	9	228	228	6
4	0	6	570	585	5	5	7	6	2355	2395	12	10	2	7	60	53	17	4	12	7	262	262	6	6	2	9	73	15	16
6	0	6	676	698	6	7	7	6	90	87	10	12	2	7	507	503	5	0	0	8	2379	2419	13	1	1	9	149	152	8
8	0	6	377	375	4	9	7	6	393	400	5	14	2	7	189	183	7	2	0	8	188	178	6	3	1	9	0	8	1
10	0	6	860	870	7	11	7	6	501	505	5	1	3	7	204	207	5	4	0	8	266	263	5	5	1	9	161	88	7
12	0	6	779	780	6	13	7	6	172	169	7	3	3	7	35	36	35	6	0	8	730	735	6	0	4	9	439	438	5
14	0	6	767	762	6	15	7	6	617	614	6	5	3	7	169	376	4	8	0	8	56	58	21	2	4	9	25	54	25
16	0	6	810	811	6	0	8	6	325	312	4	7	3	7	433	438	5	10	0	8	1419	1407	10	4	4	9	62	73	18
1	1	6	175	179	5	2	8	6	230	227	5	9	3	7	174	164	6	1	1	8	143	134	7	1	5	9	0	22	1
3	1	6	207	210	5	4	8	6	257	256	5	11	3	7	776	766	6	3	1	8	94	101	10	3	5	9	88	80	12
5	1	6	1624	1632	11	6	8	6	298	297	5	13	3	7	41	53	40	5	1	8	484	484	5						
7	1	6	110	103	7	8	8	6	365	363	5	0	4	7	1023	1013	7	7	1	8	221	219	6						

Observed and calculated structure factors for K24

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	662	668	4	6	8	0	619	633	5	5	1	1	739	747	6	9	9	1	89	65	12	11	1	2	687	696	6
4	0	0	1355	1330	6	8	8	0	467	473	5	7	1	1	219	203	4	11	9	1	1673	1671	13	13	1	2	68	63	15
6	0	0	545	553	4	10	8	0	1419	1401	10	9	1	1	477	471	4	13	9	1	34	17	34	15	1	2	707	723	6
8	0	0	970	950	7	12	8	0	243	252	6	11	1	1	802	823	6	15	9	1	27	4	26	17	1	2	112	120	10
10	0	0	1974	1757	10	14	8	0	97	106	12	13	1	1	336	331	5	17	9	1	153	158	10	19	1	2	69	40	21
12	0	0	1385	1402	9	16	8	0	277	271	6	15	1	1	48	52	28	19	9	1	151	180	11	21	1	2	334	323	7
14	0	0	282	280	5	18	8	0	35	12	35	17	1	1	729	730	6	0	10	1	1298	1307	9	0	2	2	4009	4062	7
16	0	0	231	225	6	20	8	0	362	363	7	19	1	1	466	477	6	2	10	1	797	796	6	2	2	2	358	352	3
18	0	0	694	688	6	1	9	0	147	128	6	21	1	1	935	908	8	4	10	1	348	366	4	4	2	2	529	518	4
20	0	0	318	321	7	3	9	0	429	432	4	0	2	1	166	119	3	6	10	1	397	403	4	6	2	2	444	431	4
22	0	0	1564	1583	12	5	9	0	1814	1814	11	2	2	1	376	395	3	8	10	1	120	122	9	8	2	2	315	311	4
1	1	0	752	790	3	7	9	0	907	911	7	4	2	1	509	510	4	10	10	1	288	274	5	10	2	2	1312	1295	9
3	1	0	119	310	3	9	9	0	94	91	11	6	2	1	278	270	3	12	10	1	45	33	45	12	2	2	523	529	5
5	1	0	575	592	4	11	9	0	624	616	6	8	2	1	747	753	5	14	10	1	714	702	6	14	2	2	125	130	8
7	1	0	378	379	3	13	9	0	260	260	6	10	2	1	434	457	4	16	10	1	267	280	7	16	2	2	357	351	5
9	1	0	1704	1655	9	15	9	0	547	554	6	12	2	1	936	939	7	18	10	1	346	344	7	18	2	2	54	60	28
11	1	0	2950	2847	11	17	9	0	474	482	6	14	2	1	93	96	11	1	11	1	319	328	5	20	2	2	29	17	29
13	1	0	260	263	5	19	9	0	332	329	7	16	2	1	713	729	6	3	11	1	266	264	5	1	3	2	422	417	4
15	1	0	188	203	7	0	10	0	312	324	4	18	2	1	63	68	21	5	11	1	617	643	5	3	3	2	170	168	4
17	1	0	318	323	6	2	10	0	74	74	13	20	2	1	94	94	14	7	11	1	441	442	5	5	3	2	1126	1120	8
19	1	0	621	623	6	4	10	0	146	156	4	22	2	1	250	248	8	9	11	1	425	424	5	7	3	2	244	241	4
21	1	0	758	762	7	6	10	0	314	282	5	1	3	1	297	301	3	11	11	1	410	407	5	9	3	2	1606	1629	10
0	2	0	1190	1208	4	8	10	0	411	417	5	3	3	1	238	224	3	13	11	1	113	120	11	11	3	2	1340	1348	9
2	2	0	344	361	3	10	10	0	590	597	5	5	3	1	252	242	3	15	11	1	41	34	41	13	3	2	576	575	6
4	2	0	611	614	4	12	10	0	173	173	7	7	3	1	513	509	4	17	11	1	360	373	7	15	3	2	236	231	6
6	2	0	47	53	15	14	10	0	1199	1196	9	9	3	1	317	324	4	0	12	1	1168	1165	8	17	3	2	327	328	6
8	2	0	220	228	4	16	10	0	251	245	7	11	3	1	238	241	5	2	12	1	507	511	5	19	3	2	877	879	7
10	2	0	604	620	5	18	10	0	617	610	6	13	3	1	328	329	5	4	12	1	102	103	10	21	3	2	556	563	6
12	2	0	131	140	4	1	11	0	400	399	5	15	3	1	0	1	1	6	12	1	639	645	5	0	4	2	1988	1955	7
14	2	0	831	847	7	3	11	0	272	271	5	17	3	1	365	364	6	8	12	1	161	142	8	2	4	2	717	710	5
16	2	0	752	740	6	5	11	0	873	907	7	19	3	1	229	226	7	10	12	1	213	226	7	4	4	2	8	36	7
18	2	0	88	96	14	7	11	0	111	135	10	21	3	1	337	346	7	12	12	1	254	253	7	6	4	2	193	168	4
20	2	0	180	180	9	9	11	0	133	139	9	0	4	1	1013	1021	7	14	12	1	79	98	18	8	4	2	134	148	6
22	2	0	145	329	7	11	11	0	542	551	6	2	4	1	0	24	1	16	12	1	710	699	7	10	4	2	2126	2158	11
1	3	0	421	409	3	13	11	0	138	140	9	4	4	1	327	318	3	1	13	1	367	364	5	12	4	2	269	274	5
3	3	0	586	596	5	15	11	0	971	961	8	6	4	1	820	780	6	3	13	1	360	362	5	14	4	2	264	270	6
7	3	0	485	467	4	17	11	0	493	503	6	8	4	1	507	507	4	5	13	1	977	1003	8	16	4	2	78	48	15
9	3	0	1078	1083	8	0	12	0	1370	1393	10	10	4	1	189	167	5	7	13	1	69	48	18	18	4	2	529	521	6
11	3	0	271	274	5	2	12	0	252	259	6	12	4	1	708	715	6	9	13	1	375	372	6	20	4	2	386	378	6
13	3	0	181	379	4	4	12	0	294	291	5	14	4	1	295	299	5	11	13	1	1097	1111	9	1	5	2	1008	990	6
15	3	0	911	913	7	6	12	0	645	648	6	16	4	1	631	643	6	13	13	1	113	105	12	3	5	2	0	8	1
17	3	0	940	938	7	8	12	0	235	242	6	18	4	1	225	234	7	15	13	1	241	243	8	5	5	2	1759	1723	9
19	3	0	269	271	7	10	12	0	578	570	5	20	4	1	158	145	9	0	14	1	652	680	6	7	5	2	208	192	5
21	3	0	415	400	6	12	12	0	545	540	6	1	5	1	143	155	4	2	14	1	307	299	6	9	5	2	434	437	4
0	4	0	2330	2332	6	14	12	0	150	159	10	3	5	1	641	647	5	4	14	1	517	520	5	11	5	2	665	654	5
2	4	0	752	728	5	16	12	0	148	139	11	5	5	1	1604	1623	8	6	14	1	178	182	7	13	5	2	126	120	8
4	4	0	1059	1067	7	1	13	0	535	541	5	7	5	1	842	824	6	8	14	1	302	295	6	15	5	2	226	227	6
6	4	0	3852	3625	9	3	13	0	250	261	6	9	5	1	554	548	5	10	14	1	164	175	9	17	5	2	776	789	7
8	4	0	577	577	5	5	13	0	358	368	5	11	5	1	294	314	5	12	14	1	128	123	11	19	5	2	453	450	6
10	4	0	586	596	5	7	13	0	581	577	6	13	5	1	701	714	6	14	14	1	445	435	6	21	5	2	518	509	6
12	4	0	149	341	5	9	13	0	376	384	6	15	5	1	243	233	6	1	15	1	60	71	21	0	6	2	1164	1145	9
14	4	0	896	902	7	11	13	0	885	889	7	17	5	1	253	243	6	3	15	1	302	312	6	2	6	2	26	10	26
16	4	0	1937	1964	14	13	13	0	344	343	6	19	5	1	96	99	14	5	15	1	265	277	7	4	6	2	945	948	6
18	4	0	165	171	9	15	13	0	297	300	7	21	5	1	826	821	7	7	15	1	266	273	7	6	6	2	2436	2368	10
20	4	0	113	312	7	0	14	0	1422	1414	11	0	6	1	379	356	4	9	15	1	94	92	15	8	6	2	209	212	5
1	5	0	1577	1546	7	2	14	0	425	425	5	2	6	1	249	244	3	11	15	1	202	178	8	10	6	2	65	46	15
3	5	0	43	36	17	4	14	0	227	210	6	4	6	1	243	244	4	13	15	1	127	122	12	12	6	2	470	475	5
5	5	0	3277	3131	8	6	14	0	807	823	7	6	6	1	864	862	7	0	16	1	275	270	6	14	6	2	950	950	7
7	5	0	918	906	6	8	14	0	105	125	13	8	6	1	507	493	5	2	16	1	265	267	7	16	6	2	1409	1431	10
9	5	0	95	100	9	10	14	0	1389	1388	11	10	6	1	0	13	1	4	16	1	60	51	24	18	6	2	98	96	13
11	5	0	380	396	5	12	14	0	46	49	45	12	6	1	320	309	5	6	16	1	1256	1249	10	20	6	2	0	18	1
13	5	0	137	349	5	14	14	0	46	48	45	14	6	1	59	7	20	8	16	1	370	374	6	1	7	2	831	810	6
15	5	0	295	303	6	1	15	0	304	293	6	16	6	1	1055	1043	8	10	16	1	67	59	25	3	7	2	24	21	23
17	5	0	417	433	6	3	15	0	448	443	5	18	6	1	223	225	7	12	16	1	77	69	21	5	7	2	4552	4477	11
19	5	0	182	182	8	5	15	0	454	474	5	20	6	1	0	404	-1	1	17	1	5	35	5	7	7	2	182	187	6
21	5	0	296	295	7	7	15	0	39	16	38	1	7	1	34	20	34	3	17	1	291	276	7	9	7	2	522	526	5
0	6	0	895	905	6	9	15	0	175	172	9	3	7	1	644	629	5	5	17	1	746	752	7	11	7	2	194	206	6
2	6	0	132	134	5	11	15	0	422	422	6	5	7	1	436	433	4	7	17	1	258	259	8	13	7	2	394	387	5
4	6	0	177	388	4	13	15	0	490	492	6	7	7	1	153	153	6	9	17	1	438	429	7	15	7	2	990	1001	8
6	6	0	565	553	5	0	16	0	545	539	6	9	7	1	582	578	5	0	18	1	270	269	7	17	7	2	900	886	7
8	6	0	700	690	5	2	16	0	228	220	7	11	7	1	52	31	22	2	18	1	46	43	46	19	7	2	80	99	19
10	6	0	1421	1408	9	4	16	0	124	128	11	13	7	1	47	75	14	4	18	1	423	422	6	0	8	2	405	408	4
12	6	0	122	319	5	6	16	0	842	852	7	15	7	1	97	88	12	6	18	1	426	419	7	2	8	2	563	548	5
14	6	0	450	453	5	8	16	0	79	74	18	17	7	1	161	177	9	1	19	1	368	356	7	4	8	2	177	196	6
16	6	0	555	555	6	10	16	0	47	24	47	19	7	1	175	173	9	0	0	2	3326	3527	7	6	8	2	369	359	4
18	6	0	194	391	6	12	16	0	474	467	7	0	8	1	672	657	5	2	0	2	721	734	5	8	8	2	699	705	6
20	6	0	49	5	48	1	17	0	268	268	7	2	8	1	46	60	21	4	0	2	362	356	3	10	8	2	119	124	9
1	7	0	733	714	5	3	17	0	322	322	6	4	8	1	157	175	6	6	0	2	767	729	5	12	8	2	208	206	6
3	7	0	206	206	4	5	17	0	1813	1812	13	6	8	1	311	326	4	8	0	2	765	746	5	14	8	2	562	581	6
5	7	0	1512	1506	9	7	17	0	10	28	10	8	8	1	138	135	7	10	0	2	1525	1489	10	16	8	2	896	902	7
7	7	0	487	480	4	9	17	0	33	17	32	10	8	1	125	113	8	12	0	2	953	957	7	18	8	2	154	133	10
9	7	0	1252	1254	9	0	18	0	326	341	7	12	8	1	432	436	5	14	0	2	1415	1415	10	1	9	2	570	565	5
11	7	0	538	494	5	2	18	0	339	335	7	14	8	1	560	561	5	16	0	2	729	742	6	3	9	2	80	68	12
13	7	0	461	474	5	4	18	0	70	61	22	16	8	1	747	735	6	18	0	2	960	955	7	5	9	2	479	481	5
15	7	0	307	308	6	6	18	0	194	207	9	18	8	1	323	316	7	20	0	2	115	110	12	7	9	2	488	478	5
17	7	0	206	217	7	8	18	0	363	351	7	20	8	1	167	185	10	1	1	2	583	587	4	9	9	2	628	628	6
19	7	0	764	772	7	1	19	0	278	275	8	1	9	1	956	952	7	3	1	2	805	797	6	11	9	2	1632	1617	11
0	8	0	2683	2619	9	3	19	0	118	96	13	3	9	1	159	151	6	5	1	2	1116	1121	8	13	9	2	79	79	14
2	8	0	159	161	5	1	1	1	186	171	3	5	9	1	488	522	5	7	1	2	175	170	4	15	9	2	304	309	6
4	8	0	504	501	4	3	1	1	530	516	4	7	9	1	254	253	5	9	1	2	715	714	6	17	9	2	700	690	6

Observed and calculated structure factors for K24

h	k	l	10Fo	10Fc	10s
19	9	2	274	272	8
0	10	2	4457	4347	12
2	10	2	648	643	6
4	10	2	728	728	6
6	10	2	123	103	8
8	10	2	290	285	5
10	10	2	1866	1882	14
12	10	2	340	339	6
14	10	2	381	366	6
16	10	2	228	228	8
18	10	2	312	300	7
1	11	2	324	313	5
3	11	2	767	766	6
5	11	2	108	108	10
7	11	2	23	16	23
9	11	2	651	648	6
11	11	2	1730	1698	12
13	11	2	0	17	1
15	11	2	313	305	7
17	11	2	119	106	13
0	12	2	1382	1367	10
2	12	2	52	18	23
4	12	2	135	114	8
6	12	2	917	927	8
8	12	2	188	182	7
10	12	2	828	819	7
12	12	2	282	283	7
14	12	2	503	494	6
16	12	2	378	391	7
1	13	2	158	154	8
3	13	2	93	79	12
5	13	2	1766	1796	14
7	13	2	76	79	16
9	13	2	105	96	12
11	13	2	112	112	12
13	13	2	85	77	16
15	13	2	578	566	6
0	14	2	476	469	5
2	14	2	146	349	6
4	14	2	678	701	6
6	14	2	417	412	6
8	14	2	213	218	7
10	14	2	231	222	7
12	14	2	70	55	21
14	14	2	172	182	7
1	15	2	617	623	6
3	15	2	255	264	7
5	15	2	1476	1486	10
7	15	2	548	556	6
9	15	2	50	50	37
11	15	2	395	408	7
13	15	2	143	137	11
0	16	2	900	898	7
2	16	2	125	136	11
4	16	2	111	110	13
6	16	2	495	491	6
8	16	2	110	97	14
10	16	2	691	696	7
1	17	2	203	196	8
3	17	2	433	426	6
5	17	2	184	180	9
7	17	2	43	49	42
9	17	2	123	115	7
0	18	2	759	737	7
2	18	2	63	48	26
4	18	2	273	275	7
6	18	2	414	427	7
1	1	3	274	267	3
3	1	3	701	694	5
5	1	3	279	289	3
7	1	3	195	201	5
9	1	3	417	422	4
11	1	3	1392	1358	10
13	1	3	411	419	5
15	1	3	45	20	37
17	1	3	333	340	6
19	1	3	439	461	6
21	1	3	885	868	7
0	2	3	2395	2358	8
2	2	3	500	471	4
4	2	3	0	6	1
6	2	3	1120	1090	8
8	2	3	832	812	6
10	2	3	453	465	5
12	2	3	689	693	6
14	2	3	314	308	5
16	2	3	1103	1104	8
18	2	3	145	126	9
20	2	3	62	18	24
1	3	3	523	508	4
3	3	3	276	272	3
5	3	3	1111	1104	7
7	3	3	757	747	6
9	3	3	240	231	5
11	3	3	1295	1320	10
13	3	3	91	104	12
15	3	3	58	71	21
17	3	3	216	223	7
19	3	3	156	154	10
21	3	3	410	405	7
0	4	3	2125	2056	9
2	4	3	82	90	8
4	4	3	421	414	4
6	4	3	213	214	5
8	4	3	274	279	5
10	4	3	319	299	5
12	4	3	783	787	6
14	4	3	126	130	9
16	4	3	239	237	6
18	4	3	155	143	9
20	4	3	22	70	21
1	5	3	39	32	25
3	5	3	420	425	4
5	5	3	991	995	7
7	5	3	828	823	6
9	5	3	412	420	5
11	5	3	159	148	7
13	5	3	537	545	5
15	5	3	145	132	9
17	5	3	286	300	7
19	5	3	133	136	11
0	6	3	637	642	5
2	6	3	73	66	11
4	6	3	476	463	4
6	6	3	1186	1197	9
8	6	3	372	369	4
10	6	3	58	72	19
12	6	3	275	267	6
14	6	3	80	71	14
16	6	3	1107	1114	9
18	6	3	363	359	6
20	6	3	361	366	7
1	7	3	114	90	7
3	7	3	326	328	4
5	7	3	1173	1173	9
7	7	3	218	214	5
9	7	3	561	559	5
11	7	3	795	792	6
13	7	3	134	135	9
15	7	3	187	186	8
17	7	3	630	619	6
19	7	3	144	148	11
0	8	3	851	847	7
2	8	3	164	167	6
4	8	3	388	399	4
6	8	3	564	564	5
8	8	3	44	26	31
10	8	3	56	31	22
12	8	3	554	546	5
14	8	3	353	343	6
16	8	3	243	231	7
18	8	3	149	146	10
1	9	3	593	588	5
3	9	3	118	100	8
5	9	3	176	175	6
7	9	3	169	177	7
9	9	3	129	111	8
11	9	3	885	881	7
13	9	3	44	18	44
15	9	3	40	37	40
17	9	3	507	508	6
0	10	3	886	907	7
2	10	3	790	809	6
4	10	3	453	465	5
6	10	3	182	184	7
8	10	3	197	209	7
10	10	3	92	77	12
12	10	3	124	134	10
14	10	3	699	695	6
16	10	3	81	86	18
1	11	3	405	406	5
3	11	3	212	224	6
5	11	3	727	724	6
7	11	3	144	137	8
9	11	3	477	483	5
11	11	3	107	109	12
13	11	3	52	70	37
15	11	3	122	107	11
17	11	3	493	495	6
0	12	3	270	266	6
2	12	3	275	282	6
4	12	3	367	359	5
6	12	3	133	125	9
8	12	3	75	85	16
10	12	3	215	217	7
12	12	3	258	259	7
14	12	3	175	178	9
16	12	3	409	398	7
1	13	3	254	249	6
3	13	3	468	465	5
5	13	3	380	390	6
7	13	3	140	151	9
9	13	3	316	313	6
11	13	3	405	389	6
13	13	3	24	37	24
0	14	3	49	30	34
2	14	3	267	264	6
4	14	3	431	455	6
6	14	3	237	245	7
8	14	3	368	355	6
10	14	3	0	16	1
12	14	3	45	2	44
1	15	3	240	242	7
3	15	3	231	215	7
5	15	3	442	456	6
7	15	3	130	131	11
9	15	3	149	160	10
11	15	3	370	355	7
0	16	3	124	94	11
2	16	3	88	79	16
4	16	3	176	181	8
6	16	3	1106	1079	8
8	16	3	282	295	7
10	16	3	88	96	18
1	17	3	86	101	17
3	17	3	280	276	7
5	17	3	462	456	6
7	17	3	96	6	16
0	18	3	237	246	8
2	18	3	163	158	10
0	0	4	6226	6609	11
2	0	4	374	381	4
4	0	4	771	771	6
6	0	4	459	448	4
8	0	4	290	298	5
10	0	4	2694	2701	12
12	0	4	927	934	7
14	0	4	428	437	5
16	0	4	172	171	8
18	0	4	666	646	6
20	0	4	186	186	9
1	1	4	263	259	4
3	1	4	38	26	30
5	1	4	197	177	5
7	1	4	51	14	19
9	1	4	1246	1273	10
11	1	4	1605	1610	13
13	1	4	123	116	9
15	1	4	135	145	9
17	1	4	0	12	1
19	1	4	559	561	6
0	2	4	264	293	4
2	2	4	230	239	4
4	2	4	378	370	4
6	2	4	506	533	5
8	2	4	54	57	19
10	2	4	408	422	5
12	2	4	344	347	5
14	2	4	617	626	6
16	2	4	718	743	6
18	2	4	85	69	16
20	2	4	116	121	13
1	3	4	285	291	4
3	3	4	488	480	4
5	3	4	3351	3358	11
7	3	4	138	149	7
9	3	4	835	837	6
11	3	4	38	18	38
13	3	4	339	343	5
15	3	4	787	780	6
17	3	4	715	714	7
19	3	4	234	229	8
0	4	4	623	646	5
2	4	4	490	484	5
4	4	4	632	651	5
6	4	4	1810	1816	11
8	4	4	281	294	5
10	4	4	400	415	5
12	4	4	209	214	7
14	4	4	861	873	7
16	4	4	1384	1403	10
18	4	4	230	216	7
1	5	4	1074	1076	8
3	5	4	175	167	6
5	5	4	1492	1544	11
7	5	4	449	453	5
9	5	4	102	96	10
11	5	4	953	946	7
13	5	4	170	180	8
15	5	4	291	291	6
17	5	4	34	44	34
19	5	4	116	121	12
0	6	4	2081	2136	11
2	6	4	148	163	6
4	6	4	380	383	4
6	6	4	159	146	6
8	6	4	378	381	5
10	6	4	1277	1288	9
12	6	4	417	411	5
14	6	4	246	242	7
16	6	4	212	224	8
18	6	4	286	289	7
1	7	4	278	267	5
3	7	4	266	276	5
5	7	4	1314	1357	10
7	7	4	409	400	5
9	7	4	958	966	7
11	7	4	686	678	6
13	7	4	414	401	5
15	7	4	285	289	7
17	7	4	338	337	7
0	8	4	1881	1909	12
2	8	4	13	12	13
4	8	4	237	246	5
6	8	4	593	586	5
8	8	4	370	384	5
10	8	4	1208	1215	9
12	8	4	170	166	8
14	8	4	102	103	13
16	8	4	231	225	8
18	8	4	62	55	29
1	9	4	74	65	13
3	9	4	314	312	5
5	9	4	1727	1719	13
7	9	4	523	516	5
9	9	4	41	16	41
11	9	4	195	201	7
13	9	4	92	96	15
15	9	4	185	188	6
17	9	4	588	581	6
0	10	4	875	869	7
2	10	4	20	17	20
4	10	4	418	430	5
6	10	4	204	212	7
8	10	4	405	403	5
10	10	4	515	513	6
12	10	4	197	220	8
14	10	4	921	906	7
16	10	4	378	389	7
1	11	4	258	249	6
3	11	4	343	346	5
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7	11	4	44	47	44
9	11	4	87	70	14
11	11	4	91	89	15
13	11	4	86	79	17
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0	12	4	849	864	7
2	12	4	275	277	6
4	12	4	170	165	8
6	12	4	303	306	6
8	12	4	296	291	6
10	12	4	356	364	6
12	12	4	380	360	6
14	12	4	71	55	20
1	13	4	320	308	6
3	13	4	155	164	9
5	13	4	239	235	7
7	13	4	345	348	6
9	13	4	399	400	6
11	13	4	715	711	7
13	13	4	181	197	10
0	14	4	1355	1384	10
2	14	4	262	252	7
4	14	4	313	322	6
6	14	4	559	567	6
8	14	4	102	95	14
10	14	4	1113	1097	9
12	14	4	32	20	31
1	15	4	243	243	7
3	15	4	440	431	6
5	15	4	312	205	6
7	15	4	156	138	10
9	15	4	162	160	10
0	16	4	107	107	14
2	16	4	196	198	8
4	16	4	92	83	16
6	16	4	488	471	6
8	16	4	0	6	1
1	17	4	347	342	7
3	17	4	217	208	8
1	1	5	74	78	12
3	1	5	275	279	5
5	1	5	592	584	5
7	1	5	74	82	13
9	1	5	385	384	5
11	1	5	240	232	6
13	1	5	162	161	8
15	1	5	70	63	18
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19	1	5	368	384	7
0	2	5	633	627	5
2	2	5	33	15	12
4	2	5	473	478	5
6	2	5	481	480	5
8	2	5	392	403	5
10	2	5	194	195	7
12	2	5	754	756	6
14	2	5	0	27	1
16	2	5	285	284	7
18	2	5	159	158	10
1	3	5	115	115	8
3	3	5	203	195	5
5	3	5	456	471	5
7	3	5	106	107	9
9	3	5	142	141	7
11	3	5	277	275	6
13	3	5	350	336	6
15	3	5	30	53	29
17	3	5	558	557	6
0	4	5	80	79	11
2	4	5	60	6	16
4	4	5	166	170	6
6	4	5	662	662	6
8	4	5	355	374	5
10	4	5	100	84	11
12	4	5	479	486	5
14	4	5	298	293	6
16	4	5	643	653	6
18	4	5	264	256	7
1	5	5	182	170	6
3	5	5	363	366	5
5	5	5	794	779	6
7	5	5	558	558	5
9	5	5	409	411	5
11	5	5	259	255	6
13	5	5	495	489	5
15	5	5	166	157	9
17	5	5	182	182	9
0	6	5	309	337	5
2	6	5	142	143	7
4	6	5	25	35	25
6	6	5	414	405	5
8	6	5	307	319	5
10	6	5	0	7	1
12	6	5	236	227	7
14	6	5	40	18	40
16	6	5	710	699	6
1	7	5	43	16	33
3	7	5	492	502	5
5	7	5	61	34	18
7	7	5	289	290	6
9	7	5	391	387	5
11	7	5	392	395	6
13	7	5	210	190	7
15	7	5	0	11	1
17	7	5	93	82	17
0	8	5	788	801	6
2	8	5	108	87	10
4	8	5	30	33	30
6	8	5	553	559	6
8	8	5	119	125	10
10	8	5	58	65	23
12	8	5	314	310	6
14	8	5	493	489	6
16	8	5	774	764	7
1	9	5	670	684	6
3	9	5	88	75	13
5	9	5	557	564	6
7	9	5	281	282	6

Observed and calculated structure factors for K24

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
9	9	5	61	54	21	15	1	6	474	475	6	14	8	6	411	408	7	4	4	7	299	295	6	9	1	8	695	686	7
11	9	5	1493	1500	11	17	1	6	304	298	7	1	9	6	396	397	6	6	4	7	85	80	14	11	1	8	474	478	6
13	9	5	77	83	18	0	2	6	1679	1677	12	3	9	6	55	87	26	8	4	7	232	224	7	0	2	8	0	20	1
15	9	5	60	41	29	2	2	6	223	219	5	5	9	6	114	33	11	10	4	7	170	183	9	2	2	8	114	104	10
0	10	5	1011	1005	8	4	2	6	207	210	6	7	9	6	526	531	6	12	4	7	474	472	6	4	2	8	229	227	7
2	10	5	510	513	5	6	2	6	504	496	5	9	9	6	432	426	6	14	4	7	156	148	10	6	2	8	534	525	6
4	10	5	192	191	7	8	2	6	281	278	6	11	9	6	736	732	6	1	5	7	14	31	14	8	2	8	5	11	5
6	10	5	423	417	5	10	2	6	779	792	6	13	9	6	47	75	46	1	5	7	230	227	6	10	2	8	243	228	7
8	10	5	97	84	12	12	2	6	284	289	6	0	10	6	2085	2117	15	5	5	7	373	376	6	1	3	8	156	159	9
10	10	5	266	264	7	14	2	6	47	22	47	2	10	6	299	301	6	7	5	7	487	488	6	3	3	8	327	318	6
12	10	5	26	36	26	16	2	6	396	397	7	4	10	6	103	115	6	9	5	7	306	303	6	5	3	8	1775	1758	13
14	10	5	532	523	6	1	3	6	216	213	6	6	10	6	581	582	6	11	5	7	70	56	19	7	3	8	35	28	35
1	11	5	165	168	8	3	3	6	52	54	24	8	10	6	114	102	12	13	5	7	342	338	7	9	3	8	462	458	6
3	11	5	197	204	7	5	3	6	846	839	7	10	10	6	1291	1277	9	0	6	7	290	285	6	11	3	8	183	177	9
5	11	5	426	427	6	7	3	6	115	110	9	12	10	6	170	178	10	2	6	7	88	99	14	0	4	8	178	197	8
7	11	5	466	469	6	9	3	6	1097	1097	8	1	11	6	58	52	24	4	6	7	211	213	7	2	4	8	325	319	6
9	11	5	267	279	7	11	3	6	1069	1073	8	3	11	6	176	176	6	6	6	7	673	671	6	4	4	8	244	244	7
11	11	5	440	441	6	13	3	6	311	309	6	5	11	6	414	419	6	8	6	7	235	252	7	6	4	8	570	578	6
13	11	5	192	194	9	15	3	6	113	106	13	7	11	6	105	112	13	10	6	7	88	94	16	8	4	8	101	90	14
0	12	5	1137	1140	9	0	4	6	2417	2432	13	9	11	6	492	481	6	12	6	7	192	183	9	10	4	8	186	190	9
2	12	5	505	499	5	2	4	6	82	78	12	11	11	6	664	670	6	1	7	7	61	39	20	1	5	8	580	573	6
4	12	5	57	58	26	4	4	6	377	380	5	0	12	6	546	544	6	3	7	7	275	281	6	3	5	8	147	148	10
6	12	5	708	704	6	6	4	6	435	438	5	2	12	6	76	66	17	5	7	7	699	694	6	5	5	8	429	417	6
8	12	5	96	88	14	8	4	6	115	117	10	4	12	6	128	122	11	7	7	7	140	137	10	7	5	8	54	41	34
10	12	5	124	121	12	10	4	6	1419	1427	10	6	12	6	955	947	7	9	7	7	398	399	6	9	5	8	127	128	12
12	12	5	201	201	9	12	4	6	249	258	7	8	12	6	61	44	28	11	7	7	489	492	6	0	6	8	1831	1830	13
1	13	5	310	308	6	14	4	6	74	79	20	10	12	6	457	445	6	0	8	7	510	499	5	2	6	8	167	178	9
3	13	5	262	266	7	16	4	6	167	168	10	1	13	6	0	3	1	2	8	7	137	140	10	4	6	8	337	328	6
5	13	5	942	963	8	1	5	6	265	265	5	3	13	6	47	33	46	4	8	7	314	311	6	6	6	8	439	444	6
7	13	5	156	164	10	3	5	6	360	360	5	5	13	6	1341	1326	9	6	8	7	313	311	6	8	6	8	180	171	9
9	13	5	327	327	7	5	5	6	428	426	5	7	13	6	199	203	9	8	8	7	20	53	19	1	7	8	64	70	24
11	13	5	1219	1194	9	7	5	6	71	78	16	0	14	6	29	27	28	10	8	7	17	26	17	3	7	8	192	187	8
0	14	5	860	854	7	9	5	6	237	223	6	2	14	6	411	403	6	1	9	7	373	380	6	5	7	8	915	904	7
2	14	5	244	243	7	11	5	6	362	348	6	4	14	6	299	301	7	1	9	7	20	42	19	7	7	8	217	227	8
4	14	5	418	410	6	13	5	6	42	34	42	1	1	7	88	83	12	5	9	7	161	152	9	0	8	8	937	928	7
6	14	5	353	355	7	15	5	6	199	203	8	3	1	7	278	276	6	7	9	7	76	91	20	2	8	8	70	58	21
8	14	5	194	196	9	0	6	6	138	135	8	5	1	7	45	8	39	9	9	7	0	16	1	4	8	8	52	41	41
1	15	5	18	30	17	2	6	6	50	44	24	7	1	7	233	219	6	0	10	7	612	607	6	6	8	8	419	420	6
3	15	5	268	264	7	4	6	6	465	471	5	9	1	7	234	237	7	2	10	7	442	441	6	1	9	8	38	9	37
5	15	5	106	111	13	6	6	6	865	862	7	11	1	7	724	724	7	4	10	7	231	220	7	3	9	8	188	175	9
7	15	5	250	265	8	8	6	6	257	260	6	13	1	7	109	115	7	6	10	7	186	186	9	5	9	8	1198	1213	9
0	16	5	246	256	8	10	6	6	101	75	13	15	1	7	72	70	22	8	10	7	100	96	15	0	10	8	1027	1023	8
2	16	5	290	289	7	12	6	6	215	231	7	0	2	7	721	714	6	1	11	7	215	219	8	2	10	8	82	85	19
0	0	6	2648	2614	12	14	6	6	835	826	7	2	2	7	285	279	6	3	11	7	138	139	11	1	1	9	44	60	43
2	0	6	158	154	7	1	7	6	634	641	6	4	2	7	25	15	24	5	11	7	512	519	6	3	1	9	218	215	8
4	0	6	612	620	5	3	7	6	169	168	7	6	2	7	443	444	5	7	11	7	96	110	16	5	1	9	219	234	8
6	0	6	684	694	6	5	7	6	2423	2453	14	8	2	7	127	130	6	0	12	7	111	83	11	0	2	9	59	49	26
8	0	6	454	465	5	7	7	6	92	93	12	10	2	7	158	148	9	2	12	7	156	171	10	2	2	9	27	19	26
10	0	6	926	923	7	9	7	6	418	425	6	12	2	7	518	513	6	4	12	7	255	252	7	4	2	9	237	222	8
12	0	6	755	760	7	11	7	6	507	515	6	14	2	7	164	151	9	0	0	8	2441	2482	15	6	2	9	18	16	17
14	0	6	814	818	7	13	7	6	235	233	8	1	3	7	179	184	7	2	0	8	136	145	10	1	1	9	162	153	9
16	0	6	836	839	7	15	7	6	660	654	7	3	3	7	29	14	29	4	0	8	298	289	6	3	1	9	35	39	35
1	1	6	185	187	6	0	8	6	260	257	6	5	3	7	422	422	5	6	0	8	734	735	7	5	1	9	13	28	12
3	1	6	167	164	7	2	8	6	250	245	6	7	3	7	441	440	6	8	0	8	89	14	15	0	4	9	411	403	6
5	1	6	1701	1716	13	4	8	6	102	298	6	9	3	7	191	189	8	10	0	8	1455	1454	10	2	4	9	0	29	1
7	1	6	59	62	19	6	8	6	253	260	6	11	3	7	767	755	7	1	1	8	109	107	11	4	4	9	82	92	18
9	1	6	373	381	5	8	8	6	423	420	6	13	3	7	23	11	23	3	1	8	92	83	13	1	5	9	0	16	1
11	1	6	180	185	8	10	8	6	64	55	22	0	4	7	980	945	7	5	1	8	455	447	6	3	5	9	132	129	11
13	1	6	49	55	18	12	8	6	194	197	8	2	4	7	129	128	9	7	1	8	221	217	7						

Observed and calculated structure factors for K25

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	592	610	4	2	8	0	145	143	5	1	1	1	196	183	3	5	9	1	497	523	5	5	1	2	1195	1211	7
4	0	0	1284	1292	6	4	8	0	429	420	4	3	1	1	537	531	4	7	9	1	338	336	4	7	1	2	201	191	3
6	0	0	693	695	5	6	8	0	553	557	5	5	1	1	655	653	4	9	9	1	89	85	9	9	1	2	687	692	5
8	0	0	931	916	6	8	8	0	494	495	4	7	1	1	147	130	4	11	9	1	1710	1748	12	11	1	2	592	600	5
10	0	0	3828	3826	11	10	8	0	1439	1432	11	9	1	1	446	443	4	13	9	1	27	12	27	13	1	2	113	100	7
12	0	0	1335	1383	10	12	8	0	197	213	5	11	1	1	924	951	7	15	9	1	27	5	26	15	1	2	683	694	6
14	0	0	193	186	5	14	8	0	129	135	8	13	1	1	340	339	4	17	9	1	187	194	7	17	1	2	92	75	10
16	0	0	305	300	5	16	8	0	233	239	6	15	1	1	56	54	16	19	9	1	140	150	9	19	1	2	22	32	21
18	0	0	652	652	6	18	8	0	0	5	1	17	1	1	715	724	6	0	10	1	1237	1268	8	21	1	2	299	273	6
20	0	0	257	257	6	20	8	0	350	342	6	19	1	1	426	439	5	2	10	1	794	781	6	0	2	2	4266	4169	8
22	0	0	1590	1605	11	1	9	0	185	171	4	21	1	1	1033	989	8	4	10	1	324	321	4	2	2	2	306	310	3
1	1	0	678	715	3	3	9	0	398	398	4	0	2	1	299	242	3	6	10	1	435	432	5	4	2	2	476	483	4
3	1	0	232	221	3	5	9	0	1885	1910	10	2	2	1	421	438	3	8	10	1	152	149	6	6	2	2	194	380	3
5	1	0	593	593	4	7	9	0	924	906	7	4	2	1	510	506	4	10	10	1	257	250	5	8	2	2	280	266	3
7	1	0	487	489	4	9	9	0	76	71	11	6	2	1	168	154	3	12	10	1	24	24	23	10	2	2	1330	1312	10
9	1	0	1740	1755	9	11	9	0	530	522	5	8	2	1	724	722	5	14	10	1	626	629	6	12	2	2	526	542	5
11	1	0	2866	2867	11	13	9	0	303	302	5	10	2	1	485	516	4	16	10	1	262	269	6	14	2	2	152	158	6
13	1	0	270	270	4	15	9	0	513	518	5	12	2	1	978	983	7	18	10	1	308	306	6	16	2	2	311	310	5
15	1	0	245	248	5	17	9	0	486	490	5	14	2	1	113	116	7	1	11	1	292	297	4	18	2	2	97	70	10
17	1	0	294	294	5	19	9	0	329	317	6	16	2	1	813	823	6	3	11	1	321	319	4	20	2	2	47	45	40
19	1	0	644	639	6	0	10	0	433	450	4	18	2	1	0	13	1	5	11	1	552	563	5	1	3	2	377	379	3
21	1	0	784	784	7	2	10	0	39	50	30	20	2	1	97	103	12	7	11	1	492	490	5	3	3	2	271	262	3
0	2	0	1288	1295	4	4	10	0	473	485	4	22	2	1	184	189	8	9	11	1	380	382	5	5	3	2	1190	1186	8
2	2	0	258	270	3	6	10	0	221	217	5	1	3	1	312	312	3	11	11	1	452	456	5	7	3	2	138	124	5
4	2	0	708	711	5	8	10	0	323	339	4	3	3	1	221	216	3	13	11	1	82	93	13	9	3	2	1666	1718	10
6	2	0	114	119	5	10	10	0	595	610	5	5	3	1	234	225	3	15	11	1	21	10	21	11	3	2	1385	1405	10
8	2	0	279	276	3	12	10	0	124	118	8	7	3	1	538	527	4	17	11	1	388	397	6	13	3	2	537	536	5
10	2	0	668	677	5	14	10	0	1240	1240	9	9	3	1	268	280	4	0	12	1	1226	1250	9	15	3	2	204	198	5
12	2	0	283	282	4	16	10	0	267	269	6	11	3	1	252	253	4	2	12	1	470	468	5	17	3	2	100	298	5
14	2	0	869	863	6	18	10	0	599	591	6	13	3	1	302	312	4	4	12	1	84	75	11	19	3	2	857	854	7
16	2	0	720	713	6	1	11	0	327	325	4	15	3	1	44	5	22	6	12	1	656	647	5	21	3	2	565	557	6
18	2	0	115	84	8	3	11	0	303	306	4	17	3	1	338	335	5	8	12	1	183	180	6	0	4	2	2175	2162	8
20	2	0	213	202	7	5	11	0	1034	1055	8	19	3	1	218	215	6	10	12	1	297	296	5	2	4	2	703	705	5
22	2	0	351	336	6	7	11	0	170	174	6	21	3	1	358	359	6	12	12	1	294	296	5	4	4	2	0	18	1
1	3	0	331	322	3	9	11	0	126	125	8	0	4	1	881	879	6	14	12	1	50	61	27	6	4	2	335	312	3
3	3	0	532	532	4	11	11	0	443	446	5	2	4	1	29	42	29	16	12	1	765	768	7	8	4	2	191	188	4
5	3	0	5084	4965	9	13	11	0	165	173	7	4	4	1	313	305	3	1	13	1	339	341	5	10	4	2	2115	2169	11
7	3	0	517	468	4	15	11	0	956	955	7	6	4	1	881	850	6	3	13	1	372	372	5	12	4	2	315	320	4
9	3	0	1063	1070	7	17	11	0	420	422	6	8	4	1	546	546	5	5	13	1	993	999	8	14	4	2	282	280	5
11	3	0	382	383	4	0	12	0	1472	1515	11	10	4	1	126	103	6	7	13	1	87	91	11	16	4	2	71	56	14
13	3	0	405	414	4	2	12	0	263	254	5	12	4	1	718	725	5	9	13	1	360	362	5	18	4	2	508	505	5
15	3	0	891	898	7	4	12	0	278	279	5	14	4	1	254	257	5	11	13	1	1080	1094	8	20	4	2	171	160	6
17	3	0	928	931	7	6	12	0	683	688	6	16	4	1	713	729	6	13	13	1	92	105	12	1	5	2	1019	1007	8
19	3	0	212	215	6	8	12	0	164	175	6	18	4	1	244	237	6	15	13	1	269	269	6	3	5	2	109	111	5
21	3	0	369	360	6	10	12	0	616	599	5	20	4	1	138	138	9	0	14	1	598	608	5	5	5	2	1756	1768	9
0	4	0	2394	2372	7	12	12	0	538	532	5	1	5	1	131	133	4	2	14	1	318	316	5	7	5	2	183	168	4
2	4	0	613	615	4	14	12	0	139	130	8	3	5	1	607	612	4	4	14	1	453	462	5	9	5	2	440	445	4
4	4	0	1156	1173	7	16	12	0	91	109	15	5	5	1	1779	1786	8	6	14	1	242	242	6	11	5	2	643	652	5
6	4	0	3732	3627	9	1	13	0	492	491	5	7	5	1	922	890	7	8	14	1	313	311	5	13	5	2	41	38	27
8	4	0	571	551	4	3	13	0	172	173	6	9	5	1	556	549	4	10	14	1	118	120	9	15	5	2	245	247	5
10	4	0	572	562	5	5	13	0	498	503	5	11	5	1	368	402	4	12	14	1	136	145	9	17	5	2	769	758	6
12	4	0	281	285	4	7	13	0	504	506	5	13	5	1	627	641	6	14	14	1	425	418	6	19	5	2	454	444	5
14	4	0	963	962	7	9	13	0	510	515	5	15	5	1	272	259	5	1	15	1	14	19	14	21	5	2	491	477	6
16	4	0	1995	2016	13	11	13	0	956	975	8	17	5	1	247	233	6	3	15	1	238	244	6	0	6	2	1211	1215	8
18	4	0	151	132	7	13	13	0	315	317	6	19	5	1	60	62	19	5	15	1	364	371	5	2	6	2	117	143	5
20	4	0	299	287	6	15	13	0	248	264	7	21	5	1	903	857	7	7	15	1	312	312	5	4	6	2	1087	1092	7
22	4	0	399	411	6	0	14	0	1583	1598	10	0	6	1	302	278	3	9	15	1	79	82	14	6	6	2	2343	2340	10
1	5	0	1450	1454	7	2	14	0	394	394	5	2	6	1	226	218	3	11	15	1	208	191	7	8	6	2	247	236	4
3	5	0	54	43	9	4	14	0	210	225	6	4	6	1	220	219	3	13	15	1	97	98	12	10	6	2	0	21	1
5	5	0	3220	3195	9	6	14	0	671	683	6	6	6	1	913	895	6	0	16	1	303	296	5	12	6	2	387	395	4
7	5	0	844	831	6	8	14	0	96	115	11	8	6	1	472	449	4	2	16	1	280	279	6	14	6	2	1011	1014	8
9	5	0	174	175	4	10	14	0	1386	1418	10	10	6	1	28	19	27	4	16	1	62	52	18	16	6	2	1474	1467	11
11	5	0	327	341	4	12	14	0	78	78	16	12	6	1	345	337	4	6	16	1	1248	1257	9	18	6	2	84	69	13
13	5	0	351	361	4	14	14	0	0	4	1	14	6	1	18	4	18	8	16	1	288	300	6	20	6	2	79	71	15
15	5	0	292	300	5	1	15	0	276	267	5	16	6	1	1104	1118	8	10	16	1	50	56	14	1	7	2	724	714	5
17	5	0	471	468	5	3	15	0	418	419	5	18	6	1	253	243	6	12	16	1	125	118	10	3	7	2	0	15	1
19	5	0	223	220	6	5	15	0	460	456	5	20	6	1	406	398	6	1	17	1	0	51	1	5	7	2	4668	4642	12
21	5	0	256	267	7	7	15	0	68	35	16	1	7	1	104	83	6	3	17	1	327	326	6	7	7	2	223	205	4
0	6	0	1070	1066	7	9	15	0	146	157	8	3	7	1	639	633	5	5	17	1	698	692	6	9	7	2	524	525	5
2	6	0	112	121	5	11	15	0	377	376	6	5	7	1	315	315	3	7	17	1	257	250	7	11	7	2	37	43	37
4	6	0	399	415	3	13	15	0	442	443	6	7	7	1	155	158	5	9	17	1	439	431	6	13	7	2	365	373	5
6	6	0	503	492	4	0	16	0	609	607	5	9	7	1	511	525	5	0	18	1	214	218	7	15	7	2	967	969	7
8	6	0	632	623	5	2	16	0	160	159	8	11	7	1	53	34	17	2	18	1	69	44	18	17	7	2	912	915	7
10	6	0	1385	1408	10	4	16	0	195	199	7	13	7	1	41	62	30	4	18	1	356	373	6	19	7	2	41	52	41
12	6	0	317	328	4	6	16	0	909	908	7	15	7	1	102	96	10	6	18	1	392	383	6	0	8	2	360	362	4
14	6	0	442	459	5	8	16	0	54	55	25	17	7	1	158	157	7	1	19	1	330	332	6	2	8	2	443	432	4
16	6	0	483	488	5	10	16	0	0	21	1	19	7	1	139	140	9	3	19	1	408	395	6	4	8	2	229	236	4
18	6	0	395	394	5	12	16	0	423	432	6	0	8	1	873	853	6	0	0	2	3628	3606	8	6	8	2	420	405	4
20	6	0	14	18	34	1	17	0	233	221	6	2	8	1	45	57	16	2	0	2	599	628	4	8	8	2	619	620	5
1	7	0	763	728	5	3	17	0	298	302	6	4	8	1	138	150	5	4	0	2	471	459	4	10	8	2	114	120	8
3	7	0	132	132	5	5	17	0	1953	1948	12	6	8	1	154	167	4	6	0	2	707	672	5	12	8	2	210	218	5
5	7	0	1523	1537	9	7	17	0	51	52	31	8	8	1	181	182	5	8	0	2	622	610	5	14	8	2	609	615	6
7	7	0	441	427	4	9	17	0	39	46	18	10	8	1	230	218	5	10	0	2	1460	1468	10	16	8	2	896	913	7
9	7	0	1312	1310	10	0	18	0	216	220	7	12	8	1	491	491	5	12	0	2	891	897	7	18	8	2	118	106	10
11	7	0	622	573	5	2	18	0	274	285	6	14	8	1	541	553	5	14	0	2	1355	1370	9	1	9	2	495	495	4
13	7	0	410	423	4	4	18	0	112	112	11	16	8	1	849	840	7	16	0	2	736	743	6	3	9	2	55	41	15
15	7	0	292	265	5	6	18	0	198	203	7	18	8	1	325	323	6	18	0	2	906	896	7	5	9	2	468	458	4
17	7	0	205	206	6	8	18	0	337	317	6	20	8	1	164	180	8	20	0	2	65	61	18	7	9	2	426	409	4
19	7	0	720	727	6	1	19	0	247	246	7	1	9	1	975	959	7	1	1	2	491	498	4	9	9	2	712	707	6
0	8	0	2760	2694	9	3	19	0	62	47	22	3	9	1	183	179	5	3	1	2	739	735	5	11	9	2	1612	1610	12

Observed and calculated structure factors for K25

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
13	9	2	31	53	31	18	2	1	169	171	7	15	11	3	146	146	9	6	4	4	1837	1829	11	6	14	4	449	467	5
15	9	2	339	348	5	20	2	1	29	37	28	17	11	3	487	492	6	8	4	4	261	259	4	8	14	4	92	90	13
17	9	2	611	624	6	1	3	1	556	533	4	0	12	3	364	358	5	10	4	4	367	380	4	10	14	4	1140	1122	8
19	9	2	280	273	7	3	3	1	275	270	3	2	12	3	262	257	5	12	4	4	177	175	6	12	14	4	61	39	23
0	10	2	4576	4530	13	5	3	1	1144	1139	9	4	12	3	338	327	5	14	4	4	921	919	7	1	15	4	225	222	7
2	10	2	655	664	6	7	3	1	763	755	6	6	12	3	158	150	7	16	4	4	1430	1442	10	3	15	4	410	410	6
4	10	2	756	762	6	9	3	3	209	209	5	8	12	3	114	103	9	18	4	4	178	178	8	5	15	4	193	191	7
6	10	2	24	9	23	11	3	3	1323	1339	9	10	12	3	267	276	6	1	5	4	1025	1013	7	7	15	4	159	150	9
8	10	2	290	292	5	13	3	1	97	102	9	12	12	3	293	287	6	3	5	4	162	153	5	9	15	4	157	150	9
10	10	2	1888	1940	13	15	3	1	91	73	10	14	12	3	143	149	9	5	5	4	1531	1582	11	0	16	4	160	163	8
12	10	2	311	313	5	17	3	1	231	233	6	16	12	3	471	469	6	7	5	4	404	403	4	2	16	4	147	149	9
14	10	2	364	368	5	19	3	3	139	138	9	1	13	3	229	231	6	9	5	4	144	159	6	4	16	4	135	137	10
16	10	2	161	167	8	21	3	3	432	432	6	3	13	3	467	472	5	11	5	4	893	904	7	6	16	4	517	521	6
18	10	2	312	304	6	0	4	3	2029	1976	9	5	13	3	388	388	5	13	5	4	197	205	6	8	16	4	37	11	36
1	11	2	298	300	4	2	4	3	70	81	8	7	13	3	94	111	11	15	5	4	299	290	5	1	17	4	111	105	6
3	11	2	719	712	6	4	4	3	415	401	4	9	13	3	284	295	6	17	5	4	74	82	15	3	17	4	197	192	8
5	11	2	201	200	5	6	4	3	170	167	5	11	13	3	387	376	5	19	5	4	151	145	8	1	1	5	84	88	9
7	11	2	31	26	11	8	4	3	306	312	4	13	13	3	37	26	16	0	6	4	2232	2277	11	3	1	5	276	279	4
9	11	2	705	714	6	10	4	3	270	261	4	15	13	3	197	180	8	2	6	4	143	149	6	5	1	5	520	523	5
11	11	2	1719	1760	13	12	4	3	771	792	6	0	14	3	61	62	19	4	6	4	397	392	4	7	1	5	40	37	27
13	11	2	149	43	7	14	4	3	86	100	11	2	14	3	273	271	6	6	6	4	202	205	5	9	1	5	362	372	4
15	11	2	298	287	6	16	4	3	303	299	5	4	14	3	392	398	5	8	6	4	334	328	4	11	1	5	314	318	5
17	11	2	83	76	15	18	4	3	149	148	8	6	14	3	200	200	7	10	6	4	1284	1301	10	13	1	5	170	176	7
0	12	2	1391	1381	10	20	4	3	75	74	16	8	14	3	166	163	5	12	6	4	411	420	5	15	1	5	68	64	15
2	12	2	0	17	1	1	5	3	62	57	10	10	14	3	60	46	22	14	6	4	255	253	6	17	1	5	738	711	6
4	12	2	54	46	17	3	5	3	401	414	4	12	14	3	0	23	1	16	6	4	154	154	8	19	1	5	341	348	6
6	12	2	892	881	7	5	5	3	1093	1102	8	1	15	3	200	201	7	18	6	4	309	295	6	0	2	5	560	548	5
8	12	2	156	149	7	7	5	3	869	875	7	3	15	3	170	168	7	1	7	4	275	273	4	2	2	5	49	38	18
10	12	2	824	840	7	9	5	3	421	430	4	5	15	3	560	566	6	3	7	4	210	206	5	4	2	5	484	483	5
12	12	2	242	238	6	11	5	3	199	204	5	7	15	3	173	177	8	5	7	4	1366	1402	9	6	2	5	408	403	4
14	12	2	550	535	6	13	5	3	482	487	5	9	15	3	140	135	9	7	7	4	166	357	4	8	2	5	391	386	4
16	12	2	362	357	6	15	5	3	156	158	7	11	15	3	423	399	6	9	7	4	1014	1020	7	10	2	5	229	236	5
1	13	2	149	148	7	17	5	3	301	300	6	0	16	3	171	164	7	11	7	4	758	757	6	12	2	5	783	777	6
3	13	2	67	65	15	19	5	3	102	97	12	2	16	3	129	113	9	13	7	4	362	358	5	14	2	5	50	43	25
5	13	2	1932	1931	13	0	6	3	666	667	5	4	16	3	166	172	8	15	7	4	253	255	6	16	2	5	163	155	5
7	13	2	88	89	11	2	6	3	75	68	9	6	16	3	1106	1116	8	17	7	4	334	334	6	18	2	5	122	115	10
9	13	2	153	139	7	4	6	3	448	433	4	8	16	3	242	246	7	0	8	4	1942	1997	11	1	3	5	117	124	7
11	13	2	46	45	33	6	6	3	1206	1202	8	10	16	3	103	109	13	2	8	4	0	2	1	3	3	5	193	189	5
13	13	2	108	118	11	8	6	3	324	319	4	1	17	3	108	126	12	4	8	4	195	188	5	5	3	5	463	477	4
15	13	2	544	547	6	10	6	3	64	75	13	3	17	3	328	332	6	6	8	4	511	504	5	7	3	5	112	119	8
0	14	2	514	519	5	12	6	3	299	301	5	5	17	3	424	420	6	8	8	4	387	393	5	9	3	5	120	112	8
2	14	2	304	295	5	14	6	3	76	77	13	7	17	3	43	7	42	10	8	4	1207	1246	9	11	3	5	265	267	5
4	14	2	757	764	6	16	6	3	1169	1180	9	0	18	3	281	279	6	12	8	4	118	128	9	13	3	5	329	318	5
6	14	2	463	449	5	18	6	3	369	370	6	2	18	3	138	154	10	14	8	4	119	121	9	15	3	5	70	49	15
8	14	2	196	195	6	20	6	3	365	364	6	4	18	3	183	191	8	16	8	4	181	187	7	17	3	5	521	528	6
10	14	2	206	216	7	1	7	3	142	137	6	0	0	4	7054	6762	13	18	8	4	74	58	17	0	4	5	41	15	27
12	14	2	82	82	13	3	7	3	314	332	4	2	0	4	363	367	4	1	9	4	88	94	10	2	4	5	32	26	32
14	14	2	435	440	6	5	7	3	1079	1073	8	4	0	4	744	758	6	1	9	4	280	283	5	4	4	5	151	153	6
1	15	2	552	556	5	7	7	3	198	204	5	6	0	4	362	350	4	5	9	4	1764	1784	12	6	4	5	739	705	6
3	15	2	303	307	5	9	7	3	514	516	5	8	0	4	281	276	4	7	9	4	527	523	5	8	4	5	380	388	4
5	15	2	1514	1529	11	11	7	3	782	772	6	10	0	4	2650	2732	12	9	9	4	0	3	1	10	4	5	47	35	22
7	15	2	533	525	5	13	7	3	120	128	8	12	0	4	931	927	7	11	9	4	137	136	8	12	4	5	487	501	5
9	15	2	122	116	9	15	7	3	192	194	6	14	0	4	357	359	5	13	9	4	153	141	7	14	4	5	249	254	6
11	15	2	361	363	6	17	7	3	591	579	5	16	0	4	123	124	9	15	9	4	349	357	6	16	4	5	717	725	6
13	15	2	152	142	9	19	7	3	103	105	12	18	0	4	613	608	6	17	9	4	570	575	6	18	4	5	270	264	6
0	16	2	1022	1013	7	0	8	3	711	691	5	20	0	4	143	142	9	0	10	4	967	965	7	1	5	5	179	166	5
2	16	2	139	130	8	2	8	3	153	161	6	1	1	4	210	208	4	2	10	4	79	76	11	3	5	5	349	347	4
4	16	2	105	104	11	4	8	3	375	377	4	3	1	4	105	88	6	4	10	4	514	527	5	5	5	5	891	886	6
6	16	2	190	189	6	6	8	3	542	532	5	5	1	4	228	197	4	6	10	4	267	261	5	7	5	5	615	606	5
8	16	2	74	77	16	8	8	3	34	16	33	7	1	4	84	72	9	8	10	4	349	343	5	9	5	5	399	407	5
10	16	2	715	712	6	10	8	3	50	51	22	9	1	4	1314	1338	9	10	10	4	533	532	5	11	5	5	330	329	5
1	17	2	209	198	7	12	8	3	575	587	5	11	1	4	1571	1621	12	12	10	4	158	170	8	13	5	5	426	428	5
3	17	2	398	388	6	14	8	3	351	345	5	13	1	4	137	136	7	14	10	4	945	948	8	15	5	5	179	179	7
5	17	2	250	241	7	16	8	3	148	310	5	15	1	4	180	180	6	16	10	4	413	415	6	17	5	5	174	170	8
7	17	2	41	9	41	18	8	3	161	157	8	17	1	4	49	30	27	1	11	4	180	183	6	0	6	5	254	286	5
9	17	2	396	392	6	1	9	3	587	585	5	19	1	4	578	583	6	3	11	4	164	366	5	2	6	5	110	123	8
0	18	2	849	836	7	3	9	3	70	61	12	0	2	4	308	325	3	5	11	4	1225	1257	9	4	6	5	46	51	23
2	18	2	0	23	1	5	9	3	221	205	5	2	2	4	177	181	4	7	11	4	79	81	12	6	6	5	440	435	4
4	18	2	260	258	7	7	9	3	246	244	5	4	2	4	443	439	4	9	11	4	72	67	14	8	6	5	294	300	5
6	18	2	435	439	6	9	9	3	118	115	8	6	2	4	481	495	4	11	11	4	0	11	1	10	6	5	33	11	33
1	1	3	295	285	3	11	9	3	915	933	7	8	2	4	94	92	9	13	11	4	109	110	11	12	6	5	245	243	6
3	1	3	695	699	5	13	9	3	46	20	25	10	2	4	441	456	4	15	11	4	809	811	7	14	6	5	54	18	22
5	1	3	379	380	3	15	9	3	35	34	35	12	2	4	295	302	5	0	12	4	938	932	7	16	6	5	767	763	7
7	1	3	260	254	4	17	9	3	539	540	6	14	2	4	643	642	6	2	12	4	264	267	5	1	7	5	55	52	17
9	1	3	383	395	4	0	10	3	823	831	6	16	2	4	724	730	6	4	12	4	156	157	7	3	7	5	504	509	5
11	1	3	1444	1466	11	2	10	3	775	780	6	18	2	4	71	60	17	6	12	4	323	326	5	5	7	5	53	45	18
13	1	3	411	417	4	4	10	3	416	417	4	20	2	4	144	144	9	8	12	4	221	232	6	7	7	5	282	291	5
15	1	3	41	18	40	6	10	3	184	179	6	1	3	4	236	230	4	10	12	4	382	377	5	9	7	5	350	352	5
17	1	3	342	346	5	8	10	3	223	218	5	3	3	4	452	444	4	12	12	4	360	352	6	11	7	5	398	394	5
19	1	3	422	431	5	10	10	3	48	48	21	5	3	4	3430	3475	11	14	12	4	0	36	1	13	7	5	165	174	7
21	1	3	982	952	7	12	10	3	130	130	8	7	3	4	152	151	6	1	13	4	262	264	6	15	7	5	53	2	24
0	2	3	2482	2474	8	14	10	3	615	616	6	9	3	4	818	826	6	3	13	4	91	95	11	17	7	5	107	87	12
2	2	3	522	500	4	16	10	3	57	55	25	11	3	4	102	109	8	5	13	4	337	328	5	0	8	5	911	923	7
4	2	3	38	2	18	1	11	3	397	389	4	13	3	4	347	363	5	7	13	4	293	294	6	2	8	5	98	94	9
6	2	3	1201	1176	9	3	11	3	261	259	5	15	3	4	758	768	6	9	13	4	492	502	5	4	8	5	0	13	1
8	2	3	798	795	6	5	11	3	632	620	6	17	3	4	717	717	7	11	13	4	752	762	6	6	8	5	596	580	5
10	2	3	523	538	5	7	11	3	197	191	6	19	3	4	187	188	7	13	13	4	163	182	9	8	8	5	147	152	7
12	2	3	729	742	6	9	11	3	437	441	5	0	4	4	660	679	5	0	14	4	1514	1515	10	10	8	5	149	145	7
14	2	3	325	319	5	11	11	3	184	183	7	2	4	4	398	387	4	2	14	4	235	233	6	12	8	5	354	359	5
16	2	3	1198	1204	9	13	11	3	88	75	12	4	4	4	707	731	6	4	14	4	322	331	6	14	8	5	484	477	5

Observed and calculated structure factors for K25

h	k	l	10Fo	10Fc	10s
16	8	5	862	851	7
1	9	5	672	688	6
3	9	5	100	85	9
5	9	5	589	580	5
7	9	5	359	347	5
9	9	5	65	71	16
11	9	5	1533	1563	12
13	9	5	81	86	14
15	9	5	0	19	1
0	10	5	1002	990	7
2	10	5	509	513	5
4	10	5	178	167	6
6	10	5	463	451	5
8	10	5	99	113	11
10	10	5	262	250	6
12	10	5	17	41	17
14	10	5	491	478	6
1	11	5	147	146	7
3	11	5	256	257	6
5	11	5	386	381	5
7	11	5	501	495	5
9	11	5	261	257	6
11	11	5	474	465	5
13	11	5	159	163	8
0	12	5	1168	1186	9
2	12	5	474	467	5
4	12	5	84	78	12
6	12	5	692	689	6
8	12	5	120	115	10
10	12	5	168	176	8
12	12	5	238	244	7
1	13	5	298	292	6
3	13	5	283	273	6
5	13	5	949	962	8
7	13	5	187	195	8
9	13	5	326	323	6
11	13	5	1190	1183	9
0	14	5	825	815	7
2	14	5	287	268	6
4	14	5	372	373	6
6	14	5	403	402	6
8	14	5	211	216	7
1	15	5	80	73	15
3	15	5	193	205	8
5	15	5	176	173	8
7	15	5	297	289	6
0	16	5	258	253	7
2	16	5	283	290	7
4	16	5	138	149	10
0	0	6	2646	2669	12
2	0	6	105	96	8
4	0	6	663	672	5
6	0	6	722	724	6
8	0	6	397	393	5
10	0	6	923	932	7
12	0	6	706	721	6
14	0	6	786	797	7
16	0	6	830	861	7
1	1	6	130	130	7
3	1	6	148	142	6
5	1	6	1752	1782	12
7	1	6	53	40	18
9	1	6	369	379	5
11	1	6	257	254	6
13	1	6	54	22	21
15	1	6	457	457	5
17	1	6	338	323	6
0	2	6	1694	1717	12
2	2	6	198	188	5
4	2	6	196	194	6
6	2	6	465	473	5
8	2	6	253	251	5
10	2	6	794	792	6
12	2	6	296	300	5
14	2	6	21	42	21
16	2	6	373	376	6
1	3	6	187	191	6
3	3	6	103	109	9
5	3	6	862	866	7
7	3	6	23	46	22
9	3	6	1153	1150	8
11	3	6	1079	1103	8
13	3	6	296	291	6
15	3	6	84	87	14
17	3	6	332	327	6
0	4	6	2514	2540	13
2	4	6	71	83	13
4	4	6	361	360	5
6	4	6	518	517	5
8	4	6	143	142	7
10	4	6	1440	1445	11
12	4	6	284	286	6
14	4	6	88	95	13
16	4	6	258	252	6
1	5	6	263	269	5
3	5	6	297	297	5
5	5	6	441	434	5
7	5	6	98	86	10
9	5	6	247	238	6
11	5	6	349	353	5
13	5	6	72	76	17
15	5	6	220	215	7
0	6	6	111	117	8
2	6	6	29	25	29
4	6	6	554	553	5
6	6	6	863	841	7
8	6	6	277	279	5
10	6	6	110	108	9
12	6	6	187	181	7
14	6	6	866	861	7
1	7	6	578	593	5
3	7	6	157	166	7
5	7	6	2491	2535	14
7	7	6	103	109	10
9	7	6	421	419	5
11	7	6	419	421	5
13	7	6	232	219	6
15	7	6	638	636	6
0	8	6	268	258	5
2	8	6	201	184	6
4	8	6	321	320	5
6	8	6	269	272	6
8	8	6	166	370	5
10	8	6	62	59	19
12	8	6	224	212	7
14	8	6	436	433	6
1	9	6	359	356	5
3	9	6	97	112	11
5	9	6	82	40	13
7	9	6	484	480	5
9	9	6	480	478	6
11	9	6	745	745	6
13	9	6	60	75	24
0	10	6	2223	2240	14
2	10	6	333	321	5
4	10	6	342	338	5
6	10	6	501	504	5
8	10	6	110	95	10
10	10	6	1292	1311	9
12	10	6	172	169	8
1	11	6	46	44	38
3	11	6	343	340	5
5	11	6	371	368	6
7	11	6	74	81	17
9	11	6	533	518	6
11	11	6	712	710	6
0	12	6	534	530	5
2	12	6	46	36	46
4	12	6	78	75	15
6	12	6	939	938	7
8	12	6	34	26	33
10	12	6	461	451	6
1	13	6	38	11	38
3	13	6	35	40	35
5	13	6	1451	1445	11
7	13	6	201	201	7
0	14	6	33	50	33
2	14	6	356	351	6
4	14	6	342	347	6
6	14	6	149	144	10
1	1	7	96	85	10
3	1	7	270	271	5
5	1	7	53	43	19
7	1	7	264	257	6
9	1	7	221	224	6
11	1	7	777	784	7
13	1	7	323	327	6
15	1	7	73	68	18
0	2	7	781	773	6
2	2	7	101	299	5
4	2	7	18	19	18
6	2	7	493	487	5
8	2	7	115	317	5
10	2	7	191	193	7
12	2	7	545	547	6
14	2	7	169	157	8
1	3	7	183	183	6
3	3	7	0	19	1
5	3	7	421	419	5
7	3	7	447	461	5
9	3	7	189	183	7
11	3	7	771	762	7
13	3	7	23	27	22
0	4	7	920	901	7
2	4	7	120	125	9
4	4	7	299	289	5
6	4	7	57	50	19
8	4	7	231	241	6
10	4	7	143	157	8
12	4	7	465	472	5
14	4	7	118	122	11
1	5	7	40	26	40
3	5	7	230	226	6
5	5	7	434	444	5
7	5	7	509	516	5
9	5	7	312	312	6
11	5	7	99	95	12
13	5	7	299	298	6
0	6	7	304	295	5
2	6	7	96	100	11
4	6	7	201	197	6
6	6	7	678	676	6
8	6	7	211	225	7
10	6	7	114	96	10
12	6	7	205	203	7
1	7	7	60	54	17
3	7	7	278	286	6
5	7	7	650	634	6
7	7	7	127	144	9
9	7	7	371	371	6
11	7	7	467	470	6
0	8	7	413	406	5
2	8	7	141	134	8
4	8	7	294	302	6
6	8	7	291	294	6
8	8	7	63	69	20
10	8	7	48	33	35
1	9	7	397	389	5
3	9	7	34	16	33
5	9	7	164	161	8
7	9	7	113	125	11
9	9	7	40	18	39
0	10	7	564	569	6
2	10	7	423	424	6
4	10	7	193	190	7
6	10	7	192	187	8
8	10	7	100	100	11
1	11	7	215	210	7
3	11	7	154	152	9
5	11	7	459	453	6
7	11	7	155	147	9
0	12	7	128	137	10
2	12	7	162	159	9
4	12	7	219	230	7
0	0	8	2540	2557	15
2	0	8	143	137	8
4	0	8	287	285	6
6	0	8	689	681	6
8	0	8	38	7	37
10	0	8	1466	1468	11
1	1	8	81	84	14
3	1	8	120	115	10
5	1	8	450	464	5
7	1	8	172	172	8
9	1	8	709	717	6
11	1	8	493	486	6
0	2	8	46	10	31
2	2	8	71	74	15
4	2	8	264	264	6
6	2	8	538	512	5
8	2	8	37	34	37
10	2	8	249	242	7
1	3	8	113	125	10
3	3	8	302	310	6
5	3	8	1791	1824	12
7	3	8	32	25	32
9	3	8	459	456	6
11	3	8	100	116	13
0	4	8	159	171	8
2	4	8	263	262	6
4	4	8	281	282	6
6	4	8	598	598	6
8	4	8	65	64	19
10	4	8	166	171	9
1	5	8	533	545	5
3	5	8	135	139	9
5	5	8	460	453	5
7	5	8	0	14	1
9	5	8	171	164	8
0	6	8	1899	1915	12
2	6	8	181	179	8
4	6	8	337	334	6
6	6	8	494	483	6
8	6	8	158	150	9
1	7	8	75	64	16
3	7	8	120	134	10
5	7	8	960	955	7
7	7	8	190	201	8
0	8	8	1004	995	7
2	8	8	66	51	19
4	8	8	26	19	25
6	8	8	167	357	6
1	9	8	39	4	38
3	9	8	162	157	9
5	9	8	1239	1238	9
0	10	8	1089	1084	8
2	10	8	152	139	9
1	1	9	58	70	24
3	1	9	216	207	7
5	1	9	197	193	8
0	2	9	53	16	28
2	2	9	12	26	12
4	2	9	247	234	7
6	2	9	40	33	19
1	3	9	177	167	8
3	3	9	13	36	13
5	3	9	0	20	1
0	4	9	381	374	6
2	4	9	38	46	38
4	4	9	71	77	18
1	5	9	0	12	1
3	5	9	106	114	12

Observed and calculated structure factors for K26

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	555	583	4	4	8	0	499	486	5	3	1	1	429	420	4	7	9	1	390	373	6	3	1	2	645	644	5
4	0	0	1138	1167	6	6	8	0	560	565	6	5	1	1	749	742	5	9	9	1	87	104	24	5	1	2	1248	1259	9
6	0	0	728	761	6	8	8	0	570	556	6	7	1	1	29	12	28	11	9	1	1746	1747	12	7	1	2	164	157	7
8	0	0	1089	1083	7	10	8	0	1332	1336	11	9	1	1	270	271	5	13	9	1	71	63	34	9	1	2	633	626	6
10	0	0	3944	3938	10	12	8	0	124	119	15	11	1	1	840	872	7	15	9	1	126	132	17	11	1	2	501	511	6
12	0	0	1376	1435	10	14	8	0	85	96	26	13	1	1	266	263	7	17	9	1	151	162	16	13	1	2	141	119	12
14	0	0	248	233	7	16	8	0	256	254	9	15	1	1	146	151	12	19	9	1	172	173	14	15	1	2	721	726	7
16	0	0	443	429	6	18	8	0	27	13	26	17	1	1	703	706	7	0	10	1	1378	1406	10	17	1	2	0	27	1
18	0	0	525	523	6	20	8	0	324	311	9	19	1	1	474	470	7	2	10	1	755	754	7	19	1	2	49	11	49
20	0	0	379	382	8	1	9	0	203	202	9	21	1	1	784	774	7	4	10	1	213	236	10	21	1	2	238	233	11
22	0	0	1762	1788	11	3	9	0	286	285	7	0	2	1	234	193	4	6	10	1	487	479	6	0	2	2	4358	4243	7
1	1	0	655	696	4	5	9	0	1967	1968	12	2	2	1	530	541	4	8	10	1	104	107	19	2	2	2	278	277	5
3	1	0	196	192	4	7	9	0	928	909	7	4	2	1	342	344	4	10	10	1	335	344	7	4	2	2	407	405	4
5	1	0	575	600	5	9	9	0	143	146	13	6	2	1	179	162	6	12	10	1	14	23	14	6	2	2	382	372	4
7	1	0	497	507	5	11	9	0	530	526	6	8	2	1	609	631	5	14	10	1	602	605	7	8	2	2	147	134	9
9	1	0	1645	1665	10	13	9	0	276	273	8	10	2	1	213	217	7	16	10	1	454	440	7	10	2	2	1380	1408	9
11	1	0	2991	2958	11	15	9	0	689	703	7	12	2	1	921	943	7	18	10	1	236	232	11	12	2	2	589	611	6
13	1	0	395	407	6	17	9	0	563	574	7	14	2	1	79	85	23	1	11	1	168	183	12	14	2	2	65	71	34
15	1	0	258	268	8	19	9	0	229	219	11	16	2	1	711	721	7	3	11	1	154	164	13	16	2	2	259	263	8
17	1	0	314	325	7	0	10	0	393	418	6	18	2	1	17	16	16	5	11	1	701	695	6	18	2	2	0	15	1
19	1	0	561	570	7	2	10	0	43	14	42	20	2	1	279	277	9	7	11	1	509	502	6	20	2	2	74	94	38
21	1	0	843	849	8	4	10	0	422	424	6	22	2	1	237	232	11	9	11	1	299	307	8	1	3	2	386	379	4
0	2	0	1274	1338	5	6	10	0	226	228	9	1	3	1	335	334	4	11	11	1	307	311	8	3	3	2	260	258	5
2	2	0	235	251	4	8	10	0	238	257	9	3	3	1	237	224	5	13	11	1	93	126	24	5	3	2	1257	1240	9
4	2	0	666	685	5	10	10	0	555	566	6	5	3	1	269	261	5	15	11	1	186	203	13	7	3	2	108	98	12
6	2	0	200	194	5	12	10	0	186	187	11	7	3	1	451	456	5	17	11	1	415	408	8	9	3	2	1473	1541	11
8	2	0	303	303	5	14	10	0	1125	1108	9	9	3	1	273	280	6	0	12	1	1108	1126	8	11	3	2	1508	1532	12
10	2	0	620	644	6	16	10	0	328	342	9	11	3	1	338	350	6	2	12	1	525	534	6	13	3	2	355	347	6
12	2	0	337	351	6	18	10	0	409	419	8	13	3	1	257	262	7	4	12	1	69	87	39	15	3	2	224	213	9
14	2	0	858	874	7	1	11	0	220	249	10	15	3	1	80	66	24	6	12	1	701	695	7	17	3	2	342	346	7
16	2	0	749	766	7	3	11	0	313	322	7	17	3	1	303	306	8	8	12	1	159	133	13	19	3	2	789	786	7
18	2	0	103	102	20	5	11	0	964	978	8	19	3	1	183	198	12	10	12	1	109	138	20	21	3	2	672	680	7
20	2	0	101	115	25	7	11	0	123	141	16	21	3	1	391	394	8	12	12	1	286	281	9	0	4	2	2217	2171	8
22	2	0	291	271	10	9	11	0	110	116	18	0	4	1	999	996	6	14	12	1	65	79	64	2	4	2	728	704	6
1	3	0	249	248	4	11	11	0	377	371	7	2	4	1	103	124	11	16	12	1	819	788	8	4	4	2	73	58	17
3	3	0	408	404	4	13	11	0	260	267	9	4	4	1	190	176	6	1	13	1	385	379	7	6	4	2	476	463	5
7	3	0	499	488	5	15	11	0	823	818	7	6	4	1	797	751	6	3	13	1	278	302	9	8	4	2	227	240	7
9	3	0	884	894	7	17	11	0	414	411	8	8	4	1	455	452	5	5	13	1	1064	1061	8	10	4	2	2142	2180	12
11	3	0	506	525	6	0	12	0	1494	1518	11	10	4	1	407	389	5	7	13	1	111	120	20	12	4	2	225	231	8
13	3	0	380	385	6	2	12	0	145	162	14	12	4	1	648	667	6	9	13	1	342	339	8	14	4	2	193	201	10
15	3	0	967	965	8	4	12	0	384	373	7	14	4	1	250	239	8	11	13	1	1231	1175	10	16	4	2	135	142	14
17	3	0	1009	994	8	6	12	0	654	649	6	16	4	1	599	608	6	13	13	1	129	135	19	18	4	2	536	541	7
19	3	0	248	249	9	8	12	0	166	153	12	18	4	1	240	231	9	15	13	1	188	174	14	20	4	2	310	308	9
21	3	0	247	251	11	10	12	0	702	703	7	20	4	1	31	12	31	0	14	1	760	791	7	1	5	2	1076	1064	8
0	4	0	2226	2292	7	12	12	0	545	544	7	1	5	1	72	94	17	2	14	1	213	214	11	3	5	2	148	150	8
2	4	0	590	577	5	14	12	0	158	152	15	3	5	1	462	479	5	4	14	1	411	418	7	5	5	2	1888	1828	10
4	4	0	1113	1124	8	16	12	0	0	31	1	5	5	1	1548	1513	9	6	14	1	241	263	10	7	5	2	146	145	10
6	4	0	3792	3746	9	1	13	0	535	535	6	7	5	1	920	898	7	8	14	1	256	249	10	9	5	2	540	541	6
8	4	0	454	444	5	3	13	0	176	167	12	9	5	1	402	407	6	10	14	1	293	315	10	11	5	2	675	676	6
10	4	0	523	521	6	5	13	0	443	431	7	11	5	1	388	407	6	12	14	1	128	130	20	13	5	2	75	19	27
12	4	0	196	195	9	7	13	0	453	452	7	13	5	1	599	601	6	14	14	1	350	339	9	15	5	2	333	321	7
14	4	0	805	801	7	9	13	0	419	398	7	15	5	1	50	21	49	1	15	1	30	12	30	17	5	2	727	733	7
16	4	0	2079	2113	15	11	13	0	1018	987	8	17	5	1	233	225	9	3	15	1	265	302	10	19	5	2	401	387	8
18	4	0	92	63	23	13	13	0	251	257	11	19	5	1	30	18	30	5	15	1	233	252	11	21	5	2	416	389	8
20	4	0	181	170	13	15	13	0	256	255	11	21	5	1	696	701	8	7	15	1	329	334	9	0	6	2	1207	1196	8
22	4	0	464	469	8	0	14	0	1499	1545	11	0	6	1	309	287	4	9	15	1	53	39	52	2	6	2	136	150	10
1	5	0	1421	1416	8	2	14	0	393	372	7	2	6	1	159	150	8	11	15	1	191	173	14	4	6	2	964	964	8
3	5	0	112	112	10	4	14	0	187	203	12	4	6	1	318	314	5	13	15	1	149	162	19	6	6	2	2508	2419	11
5	5	0	3290	3214	9	6	14	0	587	600	7	6	6	1	973	977	7	0	16	1	403	387	8	8	6	2	301	305	6
7	5	0	846	836	6	8	14	0	150	169	15	8	6	1	458	446	5	2	16	1	204	228	13	10	6	2	102	106	18
9	5	0	45	53	44	10	14	0	1318	1320	11	10	6	1	52	33	52	4	16	1	71	20	47	12	6	2	313	320	7
11	5	0	322	342	6	12	14	0	59	107	58	12	6	1	380	379	6	6	16	1	1295	1246	10	14	6	2	874	878	7
13	5	0	202	211	9	14	14	0	38	5	37	14	6	1	43	43	43	8	16	1	299	307	10	16	6	2	1541	1566	11
15	5	0	288	278	7	1	15	0	317	325	9	16	6	1	1067	1087	9	10	16	1	22	32	22	18	6	2	51	19	51
17	5	0	520	508	6	3	15	0	346	336	8	18	6	1	247	246	10	12	16	1	120	105	23	20	6	2	107	85	24
19	5	0	166	178	14	5	15	0	478	465	7	20	6	1	458	445	8	1	17	1	49	98	49	1	7	2	611	603	5
21	5	0	385	371	8	7	15	0	30	26	30	1	7	1	97	111	14	3	17	1	237	236	12	3	7	2	123	135	12
0	6	0	1040	1057	7	9	15	0	237	231	11	3	7	1	530	526	5	5	17	1	781	791	8	5	7	2	4753	4676	11
2	6	0	90	103	13	11	15	0	381	379	9	5	7	1	610	615	5	7	17	1	246	250	12	7	7	2	196	197	9
4	6	0	246	249	5	13	15	0	358	374	9	7	7	1	165	162	10	9	17	1	331	336	10	9	7	2	489	481	6
6	6	0	384	381	5	0	16	0	583	577	7	9	7	1	397	410	6	0	18	1	217	258	14	11	7	2	43	59	42
8	6	0	562	546	5	2	16	0	166	174	15	11	7	1	71	44	30	2	18	1	94	83	32	13	7	2	197	397	7
10	6	0	1498	1531	12	4	16	0	178	155	14	13	7	1	54	69	53	4	18	1	314	330	10	15	7	2	1016	1027	8
12	6	0	232	236	8	6	16	0	836	824	8	15	7	1	46	64	45	6	18	1	313	309	11	17	7	2	1024	1024	8
14	6	0	381	384	6	8	16	0	18	38	17	17	7	1	200	196	11	8	18	1	40	66	40	19	7	2	91	90	28
16	6	0	389	398	7	10	16	0	76	62	47	19	7	1	133	147	19	1	19	1	355	379	11	0	8	2	320	313	6
18	6	0	401	405	7	12	16	0	457	442	8	0	8	1	700	697	6	3	19	1	353	378	10	2	8	2	442	428	5
20	6	0	65	28	64	1	17	0	202	214	14	2	8	1	59	58	35	0	0	2	3463	3597	7	4	8	2	325	331	6
1	7	0	683	689	5	3	17	0	275	291	11	4	8	1	0	25	1	2	0	2	584	587	5	6	8	2	394	380	6
3	7	0	155	167	8	5	17	0	1878	1846	13	6	8	1	337	351	6	4	0	2	430	419	4	8	8	2	550	548	6
5	7	0	1493	1485	10	7	17	0	75	21	47	8	8	1	95	116	20	6	0	2	715	683	6	10	8	2	38	7	37
7	7	0	437	414	5	9	17	0	0	43	1	10	8	1	45	19	44	8	0	2	585	590	5	12	8	2	131	125	15
9	7	0	1246	1244	10	0	18	0	220	262	14	12	8	1	500	505	6	10	0	2	1528	1505	11	14	8	2	590	585	6
11	7	0	675	638	7	2	18	0	214	226	14	14	8	1	508	502	6	12	0	2	910	930	7	16	8	2	904	912	8
13	7	0	306	305	7	4	18	0	145	148	19	16	8	1	632	631	7	14	0	2	1303	1335	10	18	8	2	55	15	54
15	7	0	261	277	8	6	18	0	254	275	12	18	8	1	291	281	9	16	0	2	862	872	7	20	8	2	196	180	14
17	7	0	301	296	8	8	18	0	245	245	13	20	8	1	310	307	9	18	0	2	639	638	7	1	9	2	501	481	6
19	7	0	656	665	7	1	19	0	174	191	18	1	9	1	908	892	7	20	0	2	144	128	16	3	9	2	55	64	54
21	7	0	664	648	7	3	19	0	93	79	36	3	9	1	113	111	16	22	0	2	361	359	9	5	9	2	498	469	6
0	8	0	2740	2755	10	1	1	1	155	140	4	5	9	1	493	525	6	1	1	2	466	469	5	7	9	2	431	425	6

Observed and calculated structure factors for K26

h	k	l	10Fo	10Fc	10s
9	9	2	616	617	6
11	9	2	1600	1574	12
13	9	2	194	193	11
15	9	2	226	206	10
17	9	2	700	680	7
19	9	2	288	278	10
0	10	2	4549	4533	13
2	10	2	592	576	6
4	10	2	675	672	6
6	10	2	67	23	16
8	10	2	320	323	7
10	10	2	1950	1937	15
12	10	2	376	383	7
14	10	2	312	315	8
16	10	2	120	100	20
18	10	2	243	241	11
1	11	2	330	342	7
3	11	2	655	647	7
5	11	2	119	119	17
7	11	2	55	47	54
9	11	2	688	694	7
11	11	2	1844	1822	13
13	11	2	52	59	52
15	11	2	133	126	19
17	11	2	76	78	44
0	12	2	1391	1430	10
2	12	2	71	54	35
4	12	2	146	115	14
6	12	2	808	788	7
8	12	2	215	218	10
10	12	2	784	771	7
12	12	2	246	244	10
14	12	2	465	450	7
16	12	2	417	423	8
1	13	2	77	78	33
3	13	2	0	8	1
5	13	2	1903	1858	12
7	13	2	0	44	1
9	13	2	59	45	58
11	13	2	62	40	61
13	13	2	159	165	16
15	13	2	565	569	8
0	14	2	446	431	7
2	14	2	232	258	11
4	14	2	772	754	7
6	14	2	480	479	7
8	14	2	159	160	15
10	14	2	102	107	25
12	14	2	72	54	52
14	14	2	381	397	9
1	15	2	583	577	7
3	15	2	261	266	10
5	15	2	1508	1524	12
7	15	2	469	458	8
9	15	2	0	22	1
11	15	2	385	363	8
13	15	2	148	163	19
0	16	2	984	985	8
2	16	2	144	169	18
4	16	2	111	155	24
6	16	2	453	447	8
8	16	2	58	9	58
10	16	2	774	757	8
1	17	2	227	226	13
3	17	2	347	345	10
5	17	2	128	126	22
7	17	2	66	81	65
9	17	2	369	366	10
0	18	2	773	766	8
2	18	2	63	54	62
4	18	2	264	277	12
6	18	2	348	365	10
1	1	3	220	208	5
3	1	3	617	614	5
5	1	3	264	260	5
7	1	3	361	362	5
9	1	3	237	236	7
11	1	3	1167	1384	11
13	1	3	351	354	6
15	1	3	216	217	9
17	1	3	336	342	8
19	1	3	439	460	7
21	1	3	751	742	8
0	2	3	2461	2376	9
2	2	3	633	611	5
4	2	3	219	190	6
6	2	3	1156	1136	9
8	2	3	730	725	6
10	2	3	245	238	7
12	2	3	711	728	7
14	2	3	297	289	7
16	2	3	1073	1089	9
18	2	3	157	173	15
20	2	3	204	208	12
1	3	3	508	495	5
3	3	3	269	268	5
5	3	3	1120	1080	9
7	3	3	759	739	6
9	3	3	237	226	7
11	3	3	1377	1397	11
13	3	3	0	53	1
15	3	3	139	152	14
17	3	3	243	239	9
19	3	3	147	123	15
21	3	3	444	444	8
0	4	3	2175	2058	10
2	4	3	25	28	25
4	4	3	327	326	5
6	4	3	224	219	7
8	4	3	238	237	7
10	4	3	490	488	6
12	4	3	719	727	7
14	4	3	94	89	21
16	4	3	213	206	10
18	4	3	134	133	17
20	4	3	0	35	1
1	5	3	109	96	13
3	5	3	306	305	6
5	5	3	894	879	7
7	5	3	887	880	7
9	5	3	101	305	7
11	5	3	233	209	8
13	5	3	453	459	6
15	5	3	101	92	20
17	5	3	281	290	9
19	5	3	68	54	50
0	6	3	664	655	6
2	6	3	153	122	10
4	6	3	545	518	5
6	6	3	1259	1261	10
8	6	3	314	309	7
10	6	3	85	101	23
12	6	3	345	345	7
14	6	3	0	47	1
16	6	3	1149	1144	9
18	6	3	177	171	8
20	6	3	420	408	8
1	7	3	133	128	13
3	7	3	231	233	8
5	7	3	1331	1294	10
7	7	3	206	219	9
9	7	3	425	428	6
11	7	3	831	821	7
13	7	3	150	128	13
15	7	3	57	61	57
17	7	3	608	600	7
19	7	3	126	113	20
0	8	3	836	807	7
2	8	3	81	71	25
4	8	3	242	245	8
6	8	3	528	523	6
8	8	3	50	51	49
10	8	3	109	108	18
12	8	3	566	581	6
14	8	3	106	297	8
16	8	3	146	143	16
18	8	3	108	113	24
1	9	3	556	560	6
3	9	3	103	110	20
5	9	3	187	179	11
7	9	3	251	261	8
9	9	3	115	114	17
11	9	3	962	953	8
13	9	3	36	23	36
15	9	3	151	135	15
17	9	3	493	498	8
0	10	3	938	956	8
2	10	3	725	742	7
4	10	3	325	334	7
6	10	3	242	225	9
8	10	3	178	172	11
10	10	3	161	142	13
12	10	3	108	122	21
14	10	3	603	590	7
16	10	3	192	219	14
1	11	3	276	291	8
3	11	3	115	110	17
5	11	3	746	736	7
7	11	3	215	203	10
9	11	3	362	362	8
11	11	3	60	60	60
13	11	3	57	37	56
15	11	3	65	49	64
17	11	3	492	497	8
0	12	3	266	273	9
2	12	3	334	319	7
4	12	3	339	352	8
6	12	3	220	211	10
8	12	3	59	57	59
10	12	3	146	150	16
12	12	3	272	269	10
14	12	3	170	164	15
16	12	3	521	505	8
1	13	3	263	280	9
3	13	3	413	403	7
5	13	3	467	464	7
7	13	3	68	98	44
9	13	3	271	269	10
11	13	3	513	472	7
13	13	3	28	4	28
15	13	3	101	77	28
0	14	3	135	122	17
2	14	3	169	169	14
4	14	3	326	339	9
6	14	3	153	166	16
8	14	3	281	298	10
10	14	3	147	151	17
12	14	3	0	19	1
1	15	3	189	188	13
3	15	3	223	237	12
5	15	3	457	453	8
7	15	3	203	214	13
9	15	3	106	88	25
11	15	3	394	377	9
0	16	3	236	249	12
2	16	3	43	74	42
4	16	3	195	191	14
6	16	3	1153	1108	9
8	16	3	263	264	11
10	16	3	134	185	22
1	17	3	155	176	18
3	17	3	242	256	13
5	17	3	533	525	8
7	17	3	82	4	40
0	18	3	201	230	15
2	18	3	211	197	14
4	18	3	174	148	17
2	0	4	303	318	5
4	0	4	604	614	6
6	0	4	258	244	7
8	0	4	409	402	6
10	0	4	2881	2890	13
12	0	4	990	991	8
14	0	4	381	390	7
16	0	4	64	24	41
18	0	4	536	518	7
20	0	4	269	264	10
1	1	4	271	263	6
3	1	4	94	88	16
5	1	4	169	138	9
7	1	4	56	46	46
9	1	4	1264	1254	9
11	1	4	1688	1725	14
13	1	4	234	236	9
15	1	4	170	169	12
17	1	4	0	15	1
19	1	4	534	525	7
0	2	4	361	364	5
2	2	4	168	164	9
4	2	4	445	436	5
6	2	4	421	441	6
8	2	4	133	128	13
10	2	4	437	444	6
12	2	4	346	340	7
14	2	4	633	655	7
16	2	4	742	765	7
18	2	4	101	105	24
20	2	4	62	74	62
1	3	4	160	158	9
3	3	4	370	354	6
5	3	4	3593	3588	12
7	3	4	170	168	10
9	3	4	660	695	7
11	3	4	225	223	9
13	3	4	343	341	7
15	3	4	836	837	8
17	3	4	755	771	7
19	3	4	218	223	11
0	4	4	675	685	6
2	4	4	412	393	6
4	4	4	653	666	6
6	4	4	1967	1942	12
8	4	4	181	185	10
10	4	4	390	391	6
12	4	4	124	130	15
14	4	4	779	795	8
16	4	4	1531	1551	12
18	4	4	110	129	24
1	5	4	979	943	8
3	5	4	108	108	16
5	5	4	1594	1641	13
7	5	4	384	377	6
9	5	4	69	82	33
11	5	4	875	883	7
13	5	4	100	71	20
15	5	4	283	294	9
17	5	4	142	135	17
19	5	4	114	113	23
0	6	4	2230	2258	12
2	6	4	139	148	13
4	6	4	311	306	7
6	6	4	252	247	8
8	6	4	283	276	8
10	6	4	1367	1376	10
12	6	4	126	319	7
14	6	4	212	204	10
16	6	4	96	108	25
18	6	4	303	289	10
1	7	4	272	274	8
3	7	4	215	218	9
5	7	4	1328	1352	9
7	7	4	339	329	7
9	7	4	965	984	8
11	7	4	795	794	7
13	7	4	249	248	9
15	7	4	252	253	10
17	7	4	177	196	8
0	8	4	2021	2044	13
2	8	4	0	10	1
4	8	4	239	243	9
6	8	4	518	511	6
8	8	4	442	432	6
10	8	4	1166	1171	9
12	8	4	61	58	60
14	8	4	115	78	19
16	8	4	210	207	12
18	8	4	50	67	49
1	9	4	117	108	17
3	9	4	176	179	11
5	9	4	1854	1829	14
7	9	4	523	514	6
9	9	4	0	63	1
11	9	4	154	150	14
13	9	4	121	119	18
15	9	4	502	510	7
17	9	4	635	642	8
0	10	4	923	916	7
2	10	4	26	42	25
4	10	4	497	508	6
6	10	4	216	226	10
8	10	4	268	275	9
10	10	4	473	472	7
12	10	4	195	207	12
14	10	4	850	847	8
16	10	4	479	456	8
1	11	4	190	156	11
3	11	4	384	369	7
5	11	4	1150	1174	9
7	11	4	58	33	57
9	11	4	73	80	37
11	11	4	61	44	60
13	11	4	188	178	14
15	11	4	683	678	7
0	12	4	965	968	8
2	12	4	171	171	13
4	12	4	253	262	10
6	12	4	301	319	9
8	12	4	194	195	12
10	12	4	505	492	7
12	12	4	401	381	8
14	12	4	29	70	29
1	13	4	309	306	9
3	13	4	95	107	26
5	13	4	280	280	9
7	13	4	249	260	11
9	13	4	404	397	8
11	13	4	814	784	8
13	13	4	122	140	23
0	14	4	1457	1477	11
2	14	4	231	218	11
4	14	4	299	319	10
6	14	4	404	403	8
8	14	4	151	144	17
10	14	4	1050	1040	9
12	14	4	41	61	41
1	15	4	283	289	10
3	15	4	317	340	10
5	15	4	199	216	14
7	15	4	147	109	18
9	15	4	203	222	14
0	16	4	140	162	20
2	16	4	175	175	16
4	16	4	73	86	57
6	16	4	474	470	8
8	16	4	62	17	61
1	17	4	281	284	11
3	17	4	196	196	15
5	17	4	1434	1392	11
1	1	5	68	41	29
3	1	5	201	194	9
5	1	5	633	618	6
7	1	5	45	33	45
9	1	5	231	242	9
11	1	5	260	263	8
13	1	5	120	131	16
15	1	5	84	97	28
17	1	5	696	722	7
19	1	5	365	367	9
0	2	5	624	615	6
2	2	5	153	133	12
4	2	5	350	357	6
6	2	5	411	416	6
8	2	5	309	315	7
10	2	5	65	18	37
12	2	5	756	758	7
14	2	5	47	13	46
16	2	5	288	279	9
18	2	5	133	114	18
1	3	5	110	116	16
3	3	5	231	212	8
5	3	5	506	504	6
7	3	5	119	105	15
9	3	5	159	130	12
11	3	5	208	213	10
13	3	5	275	271	8
15	3	5	0	5	1
17	3	5	512	514	7
0	4	5	53	60	53
2	4	5	74	70	28
4	4	5	74	71	28
6	4	5	669	666	7
8	4	5	329	338	7
10	4	5	253	232	8
12	4	5	459	454	7
14	4	5	247	241	9
16	4	5	626	641	7
18	4	5	260	252	10
1	5	5	149	137	12
3	5	5	251	251	8
5	5	5	736	728	7
7	5	5	604	621	7
9	5	5	313	305	7
11	5	5	356	341	7
13	5	5	402	407	7
15	5	5	37	34	36
17	5	5	151	163	16
0	6	5	242	278	8
2	6	5	71	80	31
4	6	5	10	13	9
6	6	5	499	493	6
8	6	5	307	304	7
10	6	5	0	12	1
12	6	5	274	271	9
14	6	5	73	53	36
16	6	5	747	748	8
1	7	5	81	68	27
3	7	5	434	448	6
5	7	5	148	145	13
7	7	5	268	278	8
9	7	5	289	274	8
11	7	5	324	341	8
13	7	5	179	165	13
15	7	5	91	120	30
17	7	5	83	58	36
0	8	5	828	830	7
2	8	5	181	172	11
4	8	5	80	101	28
6	8	5	572	580	7
8	8	5	113	107	18
10	8	5	81	6	29

Observed and calculated structure factors for K26

h	k	l	10Fo	10Fc	10s
12	8	5	377	366	8
14	8	5	451	443	8
16	8	5	712	695	7
1	9	5	666	661	6
3	9	5	0	50	1
5	9	5	598	596	7
7	9	5	361	362	8
9	9	5	67	85	45
11	9	5	1620	1585	12
13	9	5	151	120	16
15	9	5	147	132	17
0	10	5	1108	1111	9
2	10	5	499	495	6
4	10	5	124	99	17
6	10	5	499	497	7
8	10	5	91	81	26
10	10	5	346	332	8
12	10	5	74	42	42
14	10	5	468	457	8
1	11	5	82	68	30
3	11	5	137	140	16
5	11	5	508	487	7
7	11	5	498	506	7
9	11	5	197	202	13
11	11	5	340	350	9
13	11	5	194	184	13
0	12	5	1077	1096	9
2	12	5	516	515	7
4	12	5	51	71	50
6	12	5	728	726	7
8	12	5	87	82	32
10	12	5	58	56	58
12	12	5	241	233	12
1	13	5	322	330	9
3	13	5	219	218	12
5	13	5	1031	1023	8
7	13	5	207	214	13
9	13	5	294	298	10
11	13	5	1273	1254	10
0	14	5	956	960	8
2	14	5	187	186	14
4	14	5	343	342	9
6	14	5	438	422	8
8	14	5	169	169	16
10	14	5	337	344	10
1	15	5	24	86	23
3	15	5	230	254	13
5	15	5	129	69	21
7	15	5	121	310	10
0	16	5	304	317	11
2	16	5	252	254	12
4	16	5	126	122	23
0	0	6	2656	2674	14
2	0	6	105	79	17
4	0	6	663	676	6
6	0	6	677	706	6
8	0	6	386	383	7
10	0	6	938	941	8
12	0	6	716	716	7
14	0	6	759	779	8
16	0	6	921	929	8
1	1	6	139	138	13
3	1	6	104	78	17
5	1	6	1794	1810	12
7	1	6	78	89	26
9	1	6	145	151	7
11	1	6	293	286	8
13	1	6	58	18	58
15	1	6	478	464	7
17	1	6	351	337	9
0	2	6	1787	1791	14
2	2	6	182	163	10
4	2	6	142	128	13
6	2	6	446	453	6
8	2	6	170	172	12
10	2	6	858	883	8
12	2	6	344	348	8
14	2	6	53	14	53
16	2	6	326	336	9
1	3	6	202	190	10
3	3	6	86	88	23
5	3	6	902	905	7
7	3	6	27	25	26
9	3	6	1032	1048	8
11	3	6	1182	1188	9
13	3	6	159	159	14
15	3	6	116	102	21
17	3	6	369	357	9
0	4	6	2542	2570	14
2	4	6	110	87	17
4	4	6	342	339	7
6	4	6	571	582	7
8	4	6	203	190	10
10	4	6	1443	1450	11
12	4	6	213	211	11
14	4	6	85	42	31
16	4	6	105	291	10
1	5	6	349	346	7
3	5	6	268	270	8
5	5	6	518	516	6
7	5	6	137	123	14
9	5	6	323	318	8
11	5	6	322	311	8
13	5	6	99	101	24
15	5	6	299	297	10
0	6	6	114	95	17
2	6	6	0	3	1
4	6	6	434	451	7
6	6	6	920	911	8
8	6	6	330	325	8
10	6	6	0	12	1
12	6	6	140	152	17
14	6	6	780	776	8
16	6	6	791	798	8
1	7	6	508	513	6
3	7	6	73	85	33
5	7	6	2570	2603	16
7	7	6	123	115	18
9	7	6	385	380	7
11	7	6	352	345	8
13	7	6	254	247	11
15	7	6	713	701	8
0	8	6	243	235	9
2	8	6	172	185	12
4	8	6	196	186	7
6	8	6	262	261	9
8	8	6	331	331	8
10	8	6	162	144	15
12	8	6	149	146	17
14	8	6	406	412	8
1	9	6	380	369	7
3	9	6	112	97	19
5	9	6	20	8	19
7	9	6	498	505	7
9	9	6	417	416	8
11	9	6	759	740	8
13	9	6	78	24	38
0	10	6	2254	2285	16
2	10	6	251	265	10
4	10	6	268	261	10
6	10	6	467	473	7
8	10	6	105	111	24
10	10	6	1348	1351	10
12	10	6	240	231	12
1	11	6	73	94	43
3	11	6	293	302	10
5	11	6	397	396	8
7	11	6	14	90	14
9	11	6	499	502	8
11	11	6	770	782	8
0	12	6	583	580	7
2	12	6	64	78	63
4	12	6	75	109	45
6	12	6	871	863	8
8	12	6	80	79	40
10	12	6	418	420	9
1	13	6	39	49	39
3	13	6	0	15	1
5	13	6	1409	1403	11
7	13	6	152	158	18
0	14	6	30	19	30
2	14	6	320	320	10
4	14	6	363	348	9
6	14	6	213	169	14
1	1	7	91	70	22
3	1	7	223	221	10
5	1	7	25	16	24
7	1	7	301	289	8
9	1	7	122	136	18
11	1	7	731	758	8
13	1	7	282	275	10
15	1	7	181	183	14
0	2	7	757	762	7
2	2	7	136	139	7
4	2	7	0	46	1
6	2	7	515	515	6
8	2	7	297	292	8
10	2	7	51	55	51
12	2	7	514	509	7
14	2	7	141	149	18
1	3	7	225	215	9
3	3	7	52	12	52
5	3	7	448	441	7
7	3	7	422	426	7
9	3	7	171	174	13
11	3	7	850	831	8
13	3	7	71	35	46
0	4	7	1022	995	8
2	4	7	74	62	31
4	4	7	234	206	9
6	4	7	103	107	21
8	4	7	186	182	12
10	4	7	333	333	8
12	4	7	451	462	8
14	4	7	95	103	29
1	5	7	0	10	1
3	5	7	150	146	14
5	5	7	313	307	8
7	5	7	527	535	7
9	5	7	240	223	10
11	5	7	91	90	29
13	5	7	295	278	10
0	6	7	306	302	8
2	6	7	139	128	16
4	6	7	242	231	10
6	6	7	704	722	7
8	6	7	228	225	11
10	6	7	64	97	63
12	6	7	222	227	12
1	7	7	103	81	21
3	7	7	232	225	10
5	7	7	786	789	7
7	7	7	139	128	17
9	7	7	333	308	9
11	7	7	522	519	8
0	8	7	506	513	7
2	8	7	82	53	30
4	8	7	197	184	12
6	8	7	335	322	8
8	8	7	41	14	41
10	8	7	124	110	21
12	8	7	380	377	9
1	9	7	361	348	8
3	9	7	87	65	31
5	9	7	168	178	15
7	9	7	176	165	14
9	9	7	34	16	34
11	9	7	603	605	8
0	10	7	622	619	7
2	10	7	422	419	8
4	10	7	167	159	15
6	10	7	182	189	14
8	10	7	113	89	24
1	11	7	160	153	16
3	11	7	40	72	40
5	11	7	538	521	7
7	11	7	132	152	21
0	12	7	48	80	48
2	12	7	227	214	12
4	12	7	206	216	14
6	12	7	131	111	20
1	13	7	171	188	16
0	0	8	2590	2678	17
2	0	8	133	125	17
4	0	8	217	206	11
6	0	8	633	635	7
8	0	8	54	46	53
10	0	8	1566	1594	12
12	0	8	508	525	8
1	1	8	100	101	23
3	1	8	114	135	20
5	1	8	429	439	7
7	1	8	189	182	13
9	1	8	683	692	7
11	1	8	534	546	8
0	2	8	44	6	43
2	2	8	68	75	44
4	2	8	272	265	9
6	2	8	498	489	7
8	2	8	112	50	21
10	2	8	260	236	10
1	3	8	95	87	24
3	3	8	277	264	9
5	3	8	1908	1920	14
7	3	8	0	9	1
9	3	8	374	388	9
11	3	8	0	54	1
0	4	8	173	164	13
2	4	8	262	265	10
4	4	8	269	256	10
6	4	8	634	659	7
8	4	8	0	9	1
10	4	8	212	192	12
1	5	8	490	516	7
3	5	8	153	145	16
5	5	8	494	489	7
7	5	8	0	9	1
9	5	8	121	112	21
0	6	8	1929	1940	14
2	6	8	183	170	13
4	6	8	290	290	9
6	6	8	495	503	8
8	6	8	108	107	25
1	7	8	35	68	34
3	7	8	153	152	16
5	7	8	967	945	9
7	7	8	213	190	12
0	8	8	1037	1043	9
2	8	8	72	51	52
4	8	8	86	51	33
6	8	8	369	364	9
1	9	8	0	7	1
3	9	8	81	85	39
5	9	8	1261	1281	10
0	10	8	1056	1062	9
2	10	8	128	114	21
1	1	9	0	19	1
3	1	9	169	161	15
5	1	9	289	270	10
0	2	9	0	58	1
2	2	9	109	95	23
4	2	9	126	136	20
6	2	9	65	8	64
1	3	9	125	114	20
3	3	9	46	18	45
5	3	9	81	78	36
0	4	9	176	389	9
2	4	9	73	57	43
4	4	9	68	60	67
1	5	9	0	15	-1
3	5	9	64	69	64
0	6	9	105	66	25

Observed and calculated structure factors for K27

h	k	l	10Fo	10Fc	10s
2	0	0	652	649	4
4	0	0	1268	1276	8
6	0	0	627	644	5
8	0	0	917	906	7
10	0	0	3779	3749	14
12	0	0	1357	1384	10
14	0	0	206	196	10
16	0	0	275	273	9
18	0	0	605	585	7
20	0	0	271	254	11
22	0	0	1612	1668	12
1	1	0	678	697	4
3	1	0	191	183	5
5	1	0	519	514	5
7	1	0	509	508	5
9	1	0	1720	1728	12
11	1	0	2883	2885	14
13	1	0	315	319	7
15	1	0	276	275	9
17	1	0	275	292	9
19	1	0	616	617	8
21	1	0	776	788	8
0	2	0	1301	1350	6
2	2	0	227	244	4
4	2	0	709	729	5
6	2	0	155	161	8
8	2	0	311	301	5
10	2	0	673	682	6
12	2	0	286	285	7
14	2	0	845	869	8
16	2	0	719	709	7
18	2	0	42	20	41
20	2	0	179	178	15
22	2	0	327	330	11
1	3	0	326	325	4
3	3	0	516	520	5
5	3	0	4970	4889	11
7	3	0	512	491	5
9	3	0	1021	1013	8
11	3	0	378	377	6
13	3	0	378	386	7
15	3	0	872	870	8
17	3	0	937	947	9
19	3	0	213	222	12
21	3	0	171	364	10
0	4	0	2172	2217	9
2	4	0	579	563	5
4	4	0	1193	1181	8
6	4	0	3698	3644	12
8	4	0	490	486	5
10	4	0	470	468	6
12	4	0	234	233	9
14	4	0	920	925	8
16	4	0	2011	2020	15
18	4	0	109	96	21
20	4	0	246	237	12
22	4	0	193	401	10
1	5	0	1428	1425	9
3	5	0	68	61	18
5	5	0	3215	3187	11
7	5	0	829	811	6
9	5	0	154	161	10
11	5	0	309	330	7
13	5	0	300	311	8
15	5	0	287	281	8
17	5	0	591	513	7
19	5	0	215	220	13
21	5	0	293	300	11
0	6	0	983	973	7
2	6	0	152	159	8
4	6	0	407	417	5
6	6	0	532	518	5
8	6	0	641	623	6
10	6	0	1381	1387	10
12	6	0	267	273	8
14	6	0	446	452	7
16	6	0	506	504	7
18	6	0	380	378	9
20	6	0	71	16	52
1	7	0	743	718	6
3	7	0	125	139	11
5	7	0	1449	1460	10
7	7	0	433	421	6
9	7	0	1275	1281	10
11	7	0	615	571	7
13	7	0	371	371	7
15	7	0	236	238	10
17	7	0	230	226	11
19	7	0	686	707	8
0	8	0	2599	2646	13
2	8	0	155	159	10
4	8	0	435	436	5
6	8	0	568	564	6
8	8	0	486	491	6
10	8	0	1358	1349	12
12	8	0	164	182	13
14	8	0	127	135	17
16	8	0	263	270	10
18	8	0	81	4	35
20	8	0	337	308	10
1	9	0	115	105	14
3	9	0	403	405	6
5	9	0	1869	1896	14
7	9	0	894	877	7
9	9	0	50	48	49
11	9	0	617	587	6
13	9	0	276	274	9
15	9	0	531	558	7
17	9	0	497	490	8
19	9	0	279	271	11
0	10	0	378	386	6
2	10	0	73	53	28
4	10	0	460	476	6
6	10	0	256	251	8
8	10	0	303	300	8
10	10	0	549	557	6
12	10	0	125	121	17
14	10	0	1197	1207	10
16	10	0	267	254	11
18	10	0	516	526	9
1	11	0	288	292	8
3	11	0	318	310	7
5	11	0	965	975	8
7	11	0	153	156	13
9	11	0	103	106	20
11	11	0	423	428	8
13	11	0	184	199	13
15	11	0	896	891	9
17	11	0	403	429	9
0	12	0	1521	1535	11
2	12	0	242	239	9
4	12	0	295	283	8
6	12	0	641	652	7
8	12	0	161	171	13
10	12	0	637	649	7
12	12	0	533	527	7
14	12	0	136	121	18
16	12	0	114	93	24
1	13	0	483	466	7
3	13	0	126	140	16
5	13	0	456	443	7
7	13	0	452	464	7
9	13	0	522	519	7
11	13	0	938	947	9
13	13	0	268	285	11
15	13	0	235	240	12
0	14	0	1540	1549	11
2	14	0	392	397	8
4	14	0	216	223	11
6	14	0	686	680	7
8	14	0	140	130	17
10	14	0	1362	1377	10
12	14	0	64	82	64
14	14	0	0	5	1
1	15	0	268	266	10
3	15	0	398	404	8
5	15	0	497	494	8
7	15	0	66	15	60
9	15	0	150	153	17
11	15	0	375	380	9
13	15	0	439	427	9
0	16	0	597	609	7
2	16	0	170	162	14
4	16	0	212	223	13
6	16	0	876	864	8
8	16	0	41	43	40
10	16	0	0	38	1
12	16	0	437	433	9
1	17	0	237	246	12
3	17	0	274	288	11
5	17	0	1920	1910	15
7	17	0	39	44	38
9	17	0	71	60	60
0	18	0	286	275	11
2	18	0	267	283	12
4	18	0	57	87	57
6	18	0	236	243	13
8	18	0	308	315	11
1	19	0	222	226	14
3	19	0	0	60	1
1	1	1	154	145	5
3	1	1	475	472	5
5	1	1	782	782	6
7	1	1	93	84	13
9	1	1	392	394	5
11	1	1	867	896	7
13	1	1	347	346	7
15	1	1	38	45	38
17	1	1	712	725	8
19	1	1	463	458	8
21	1	1	914	883	9
0	2	1	132	70	7
2	2	1	488	501	4
4	2	1	446	447	5
6	2	1	215	216	6
8	2	1	629	639	5
10	2	1	324	338	6
12	2	1	969	979	8
14	2	1	101	114	20
16	2	1	723	734	7
18	2	1	58	24	58
20	2	1	172	188	16
22	2	1	202	207	15
1	3	1	316	317	5
3	3	1	243	229	5
5	3	1	279	274	5
7	3	1	503	500	5
9	3	1	248	259	7
11	3	1	246	261	8
13	3	1	291	290	8
15	3	1	52	37	52
17	3	1	324	316	8
19	3	1	204	205	11
21	3	1	340	348	10
0	4	1	985	996	7
2	4	1	92	92	13
4	4	1	253	244	5
6	4	1	839	795	6
8	4	1	492	497	6
10	4	1	246	224	8
12	4	1	709	724	7
14	4	1	231	248	9
16	4	1	669	672	7
18	4	1	252	244	11
20	4	1	93	83	30
1	5	1	95	105	12
3	5	1	539	544	5
5	5	1	1648	1612	11
7	5	1	901	897	7
9	5	1	510	529	6
11	5	1	328	350	7
13	5	1	596	598	7
15	5	1	129	125	17
17	5	1	235	221	11
19	5	1	63	39	63
21	5	1	784	764	8
0	6	1	408	386	5
2	6	1	168	168	8
4	6	1	276	259	6
6	6	1	897	878	7
8	6	1	484	485	6
10	6	1	78	78	25
12	6	1	356	355	7
14	6	1	0	8	1
16	6	1	1063	1070	9
18	6	1	275	271	11
20	6	1	439	430	9
1	7	1	127	128	11
3	7	1	589	571	5
5	7	1	446	435	5
7	7	1	205	200	9
9	7	1	454	469	6
11	7	1	0	8	1
13	7	1	52	74	51
15	7	1	55	28	54
17	7	1	215	189	12
19	7	1	143	128	18
0	8	1	755	737	6
2	8	1	56	12	37
4	8	1	91	100	18
6	8	1	314	329	7
8	8	1	146	148	12
10	8	1	122	106	15
12	8	1	499	499	7
14	8	1	542	550	7
16	8	1	758	749	8
18	8	1	319	336	10
20	8	1	231	243	13
1	9	1	958	934	8
3	9	1	155	149	11
5	9	1	442	454	6
7	9	1	330	347	7
9	9	1	44	85	43
11	9	1	1714	1726	12
13	9	1	31	46	31
15	9	1	80	67	33
17	9	1	188	191	14
19	9	1	130	172	22
0	10	1	1256	1286	10
2	10	1	786	778	7
4	10	1	296	297	7
6	10	1	447	436	6
8	10	1	159	153	12
10	10	1	271	265	8
12	10	1	0	8	1
14	10	1	614	620	8
16	10	1	289	301	10
18	10	1	281	275	11
1	11	1	209	218	10
3	11	1	265	249	8
5	11	1	665	679	7
7	11	1	541	537	6
9	11	1	332	333	8
11	11	1	387	383	8
13	11	1	134	128	17
15	11	1	61	92	60
17	11	1	423	437	9
0	12	1	1152	1179	9
2	12	1	487	477	6
4	12	1	106	91	18
6	12	1	668	653	7
8	12	1	183	169	12
10	12	1	221	223	11
12	12	1	289	287	9
14	12	1	0	44	1
16	12	1	736	746	8
1	13	1	343	350	8
3	13	1	363	364	8
5	13	1	966	1000	9
7	13	1	88	85	27
9	13	1	340	347	9
11	13	1	1108	1102	9
13	13	1	132	131	20
15	13	1	270	260	11
0	14	1	685	696	7
2	14	1	290	282	9
4	14	1	445	438	7
6	14	1	263	267	10
8	14	1	306	298	9
10	14	1	187	198	14
12	14	1	183	169	15
14	14	1	398	391	9
1	15	1	51	27	50
3	15	1	285	288	10
5	15	1	272	285	10
7	15	1	355	349	9
9	15	1	70	63	49
11	15	1	158	132	17
13	15	1	128	146	22
0	16	1	316	312	9
2	16	1	257	241	11
4	16	1	0	19	1
6	16	1	1279	1290	10
8	16	1	277	290	11
10	16	1	55	41	54
12	16	1	115	92	25
1	17	1	83	66	36
3	17	1	309	313	10
5	17	1	732	732	8
7	17	1	256	244	12
9	17	1	425	413	9
0	18	1	254	281	12
2	18	1	83	79	38
4	18	1	335	349	10
6	18	1	350	338	10
1	19	1	327	316	11
3	19	1	402	403	10
0	0	2	3513	3467	9
2	0	2	563	580	5
4	0	2	468	457	5
6	0	2	767	724	6
8	0	2	562	553	6
10	0	2	1447	1393	11
12	0	2	876	879	8
14	0	2	1357	1358	10
16	0	2	730	728	8
18	0	2	797	783	8
20	0	2	88	56	32
1	1	2	499	511	5
3	1	2	735	738	6
5	1	2	1161	1149	8
7	1	2	153	158	9
9	1	2	680	668	6
11	1	2	603	603	7
13	1	2	92	95	22
15	1	2	667	675	7
17	1	2	78	72	33
19	1	2	0	22	1
21	1	2	291	286	11
0	2	2	4162	4135	10
2	2	2	325	329	5
4	2	2	482	486	5
6	2	2	423	417	5
8	2	2	256	246	7
10	2	2	1297	1316	10
12	2	2	530	550	6
14	2	2	104	131	19
16	2	2	320	324	9
18	2	2	64	50	63
20	2	2	55	17	55
1	3	2	366	369	5
3	3	2	286	281	5
5	3	2	1144	1114	9
7	3	2	121	105	11
9	3	2	1623	1662	11
11	3	2	1410	1411	10
13	3	2	461	460	6
15	3	2	177	171	12
17	3	2	298	291	10
19	3	2	842	833	8
21	3	2	556	569	9
0	4	2	2067	2029	10
2	4	2	663	652	5
4	4	2	59	21	24
6	4	2	335	310	5
8	4	2	155	164	10
10	4	2	2013	2092	15
12	4	2	265	262	8
14	4	2	257	264	9
16	4	2	16	41	15
18	4	2	500	497	8
20	4	2	316	320	11
1	5	2	1017	990	7
3	5	2	99	109	13
5	5	2	1813	1785	12
7	5	2	196	180	9
9	5	2	445	447	6
11	5	2	633	638	7
13	5	2	52	12	52
15	5	2	263	267	9
17	5	2	763	745	8
19	5	2	423	420	9
21	5	2	470	455	9
0	6	2	1149	1136	8
2	6	2	157	166	8
4	6	2	1088	1088	8
6	6	2	2337	2331	13
8	6	2	264	271	8
10	6	2	0	7	1
12	6	2	352	351	7
14	6	2	994	994	9
16	6	2	1471	1478	12
18	6	2	14	29	14
20	6	2	16	79	15
1	7	2	719	701	6
3	7	2	25	22	25
5	7	2	4529	4582	15
7	7	2	210	196	9
9	7	2	501	510	6
11	7	2	40	54	40
13	7	2	369	368	8
15	7	2	935	949	9
17	7	2	947	950	8
19	7	2	53	55	52
0	8	2	422	415	6
2	8	2	424	416	5
4	8	2	250	246	8
6	8	2	406	401	6
8	8	2	580	579	6
10	8	2	70	47	29
12	8	2	202	200	10
14	8	2	587	603	7
16	8	2	894	906	8
18	8	2	69	70	62
1	9	2	457	445	6
3	9	2	0	32	1
5	9	2	478	444	6
7	9	2	401	396	7
9	9	2	726	719	7
11	9	2	1577	1573	12

Observed and calculated structure factors for K27

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
13	9	2	106	111	21	18	2	3	203	201	14	15	11	3	60	55	60	6	4	4	1817	1846	15	6	14	4	466	457	8
15	9	2	321	318	9	20	2	3	119	117	23	17	11	3	554	538	9	8	4	4	202	213	10	8	14	4	124	106	21
17	9	2	630	625	8	1	3	3	551	531	5	0	12	3	296	288	8	10	4	4	111	325	8	10	14	4	1083	1085	9
19	9	2	297	294	11	3	3	3	270	265	6	2	12	3	263	273	9	12	4	4	156	143	13	12	14	4	34	46	34
0	10	2	4363	4489	16	5	3	3	1116	1098	9	4	12	3	341	342	8	14	4	4	877	888	8	1	15	4	221	220	13
2	10	2	667	667	7	7	3	3	747	737	7	6	12	3	155	147	14	16	4	4	1452	1449	11	3	15	4	397	401	9
4	10	2	748	753	7	9	3	3	200	194	10	8	12	3	61	86	60	18	4	4	156	150	17	5	15	4	203	218	14
6	10	2	29	35	28	11	3	3	1316	1342	10	10	12	3	221	210	11	1	5	4	993	978	8	7	15	4	151	134	18
8	10	2	285	284	8	13	3	3	0	84	1	12	12	3	290	287	10	3	5	4	139	141	13	9	15	4	174	146	16
10	10	2	1874	1897	14	15	3	3	90	108	25	14	12	3	149	137	18	5	5	4	1542	1578	12	0	16	4	158	168	17
12	10	2	330	332	8	17	3	3	254	253	11	16	12	3	465	446	9	7	5	4	395	384	7	2	16	4	174	157	16
14	10	2	355	354	9	19	3	3	116	128	24	1	13	3	241	239	10	9	5	4	144	151	13	4	16	4	153	152	19
16	10	2	167	188	17	21	3	3	413	420	10	3	13	3	449	462	7	11	5	4	879	898	8	6	16	4	502	487	9
18	10	2	290	279	11	0	4	3	2133	2053	11	5	13	3	170	389	8	13	5	4	169	163	13	8	16	4	48	17	47
1	11	2	329	343	7	2	4	3	24	50	23	7	13	3	98	118	25	15	5	4	275	277	10	1	17	4	318	325	11
3	11	2	688	696	7	4	4	3	369	363	5	9	13	3	265	278	11	17	5	4	114	117	23	3	17	4	205	185	15
5	11	2	119	127	17	6	4	3	214	200	8	11	13	3	389	380	9	19	5	4	154	143	18	1	1	5	59	61	50
7	11	2	0	10	1	8	4	3	277	275	7	13	13	3	74	3	44	0	6	4	2171	2216	14	3	1	5	231	237	9
9	11	2	702	697	7	10	4	3	373	362	7	15	13	3	173	168	16	2	6	4	179	173	10	5	1	5	606	607	6
11	11	2	1800	1802	13	12	4	3	777	788	7	0	14	3	49	20	48	4	6	4	191	398	6	7	1	5	43	10	43
13	11	2	83	43	29	14	4	3	112	95	19	2	14	3	249	239	10	6	6	4	191	182	10	9	1	5	332	331	8
15	11	2	224	221	12	16	4	3	238	246	11	4	14	3	362	374	9	8	6	4	335	328	7	11	1	5	290	279	9
17	11	2	94	89	31	18	4	3	169	154	15	6	14	3	160	175	15	10	6	4	1254	1283	11	13	1	5	176	190	13
0	12	2	1344	1376	10	20	4	3	13	25	13	8	14	3	351	348	9	12	6	4	164	171	8	15	1	5	43	12	42
2	12	2	65	1	40	1	5	3	91	85	15	10	14	3	0	22	1	14	6	4	251	250	10	17	1	5	747	735	8
4	12	2	63	47	48	3	5	3	361	360	5	12	14	3	46	46	45	16	6	4	154	167	17	19	1	5	338	358	11
6	12	2	884	856	7	5	5	3	959	957	8	1	15	3	151	160	17	18	6	4	277	278	12	0	2	5	647	644	6
8	12	2	162	164	13	7	5	3	881	883	8	3	15	3	225	221	12	1	7	4	276	272	8	2	2	5	83	89	24
10	12	2	813	810	8	9	5	3	408	413	6	5	15	3	491	486	8	3	7	4	209	199	9	4	2	5	426	437	6
12	12	2	253	229	10	11	5	3	184	159	11	7	15	3	200	215	14	5	7	4	1356	1341	10	6	2	5	438	438	7
14	12	2	532	522	8	13	5	3	445	448	7	9	15	3	118	112	23	7	7	4	347	345	7	8	2	5	331	328	8
16	12	2	369	374	10	15	5	3	0	37	1	11	15	3	358	341	10	9	7	4	976	1000	8	10	2	5	109	112	19
1	13	2	189	175	11	17	5	3	286	285	10	0	16	3	164	168	16	11	7	4	737	752	7	12	2	5	766	775	7
3	13	2	45	73	44	19	5	3	65	77	64	2	16	3	76	82	42	13	7	4	315	313	9	14	2	5	33	41	33
5	13	2	1844	1882	15	0	6	3	585	591	6	4	16	3	182	199	15	15	7	4	224	232	12	16	2	5	279	287	11
7	13	2	46	49	45	2	6	3	117	100	13	6	16	3	1147	1136	10	17	7	4	344	348	10	18	2	5	99	82	29
9	13	2	134	142	18	4	6	3	475	463	6	8	16	3	261	246	11	0	8	4	1895	1957	12	1	3	5	129	119	14
11	13	2	74	83	40	6	6	3	1187	1196	9	10	16	3	124	125	23	2	8	4	49	18	48	3	3	5	202	200	10
13	13	2	129	115	20	8	6	3	340	342	7	1	17	3	113	138	25	4	8	4	196	197	10	5	3	5	495	500	6
15	13	2	519	525	9	10	6	3	144	131	13	3	17	3	321	326	11	6	8	4	533	512	6	7	3	5	115	117	17
0	14	2	469	468	7	12	6	3	313	310	8	5	17	3	460	453	9	8	8	4	390	385	7	9	3	5	105	106	19
2	14	2	299	300	9	14	6	3	43	78	43	7	17	3	0	9	1	10	8	4	1171	1181	9	11	3	5	258	267	10
4	14	2	748	762	8	16	6	3	1140	1135	10	0	18	3	205	227	15	12	8	4	135	107	16	13	3	5	297	293	9
6	14	2	483	473	8	18	6	3	394	392	9	2	18	3	194	186	15	14	8	4	100	115	25	15	3	5	13	20	13
8	14	2	201	192	12	20	6	3	376	390	10	4	18	3	187	171	16	16	8	4	202	215	14	17	3	5	527	517	8
10	14	2	150	163	17	1	7	3	180	168	9	0	0	4	6895	6677	15	18	8	4	79	55	46	0	4	5	27	56	26
12	14	2	77	72	41	3	7	3	265	277	7	2	0	4	188	390	5	1	9	4	72	51	31	2	4	5	54	51	54
14	14	2	432	421	9	5	7	3	1180	1168	9	4	0	4	700	727	7	3	9	4	260	272	9	4	4	5	114	118	17
1	15	2	554	552	7	7	7	3	171	170	11	6	0	4	171	370	6	5	9	4	1775	1783	14	6	4	5	681	670	7
3	15	2	308	301	9	9	7	3	469	470	6	8	0	4	270	274	8	7	9	4	497	502	7	8	4	5	347	355	7
5	15	2	1515	1514	11	11	7	3	810	811	8	10	0	4	2655	2691	16	9	9	4	56	14	56	10	4	5	120	117	18
7	15	2	504	500	8	13	7	3	112	118	20	12	0	4	913	933	9	11	9	4	175	180	13	12	4	5	493	497	7
9	15	2	85	111	35	15	7	3	123	136	19	14	0	4	350	362	8	13	9	4	126	122	19	14	4	5	238	243	11
11	15	2	366	369	9	17	7	3	622	614	8	16	0	4	150	138	15	15	9	4	187	192	9	16	4	5	675	679	8
13	15	2	164	154	18	19	7	3	73	93	72	18	0	4	567	559	8	17	9	4	584	583	9	18	4	5	268	266	12
0	16	2	1002	1019	9	0	8	3	818	792	7	20	0	4	133	144	22	0	10	4	918	919	8	1	5	5	147	147	13
2	16	2	137	135	19	2	8	3	113	122	16	1	1	4	225	223	7	2	10	4	51	82	51	3	5	5	300	296	8
4	16	2	66	77	66	4	8	3	339	335	7	3	1	4	102	97	16	4	10	4	524	524	7	5	5	5	776	777	7
6	16	2	454	449	9	6	8	3	574	564	6	5	1	4	262	229	7	6	10	4	218	235	11	7	5	5	613	614	7
8	16	2	46	66	46	8	8	3	0	23	1	7	1	4	53	68	51	8	10	4	316	312	8	9	5	5	389	392	7
10	16	2	720	728	8	10	8	3	69	50	34	9	1	4	1293	1309	11	10	10	4	480	485	7	11	5	5	290	291	9
1	17	2	240	224	12	12	8	3	575	594	7	11	1	4	1614	1637	12	12	10	4	181	171	14	13	5	5	389	398	8
3	17	2	372	377	9	14	8	3	350	339	9	13	1	4	167	172	13	14	10	4	932	918	9	15	5	5	96	77	28
5	17	2	201	182	14	16	8	3	233	224	12	15	1	4	192	193	13	16	10	4	411	403	9	17	5	5	165	161	18
7	17	2	33	12	33	18	8	3	180	172	16	17	1	4	19	31	19	1	11	4	157	162	13	0	6	5	301	342	8
9	17	2	413	394	9	1	9	3	567	569	6	19	1	4	574	565	8	3	11	4	361	366	8	2	6	5	89	96	21
0	18	2	799	797	8	3	9	3	77	79	27	0	2	4	333	349	6	5	11	4	1193	1191	9	4	6	5	54	25	54
2	18	2	33	21	33	5	9	3	261	261	8	2	2	4	162	168	10	7	11	4	70	64	18	6	6	5	433	425	7
4	18	2	231	240	13	7	9	3	256	252	8	4	2	4	454	447	6	9	11	4	80	57	32	8	6	5	323	326	8
6	18	2	409	406	10	9	9	3	116	107	17	6	2	4	448	468	6	11	11	4	36	24	35	10	6	5	39	39	39
1	1	3	249	250	5	11	9	3	914	915	8	8	2	4	109	111	18	13	11	4	142	130	18	12	6	5	258	255	10
3	1	3	654	654	6	13	9	3	0	18	1	10	2	4	445	458	7	15	11	4	773	754	8	14	6	5	67	25	51
5	1	3	274	266	6	15	9	3	86	89	32	12	2	4	304	302	8	0	12	4	961	959	8	16	6	5	738	726	8
7	1	3	293	289	6	17	9	3	527	535	8	14	2	4	645	646	7	2	12	4	241	246	10	1	7	5	67	77	37
9	1	3	344	350	6	0	10	3	835	857	7	16	2	4	729	726	8	4	12	4	149	168	15	3	7	5	456	474	7
11	1	3	1410	1418	11	2	10	3	754	769	7	18	2	4	0	5	1	6	12	4	294	305	9	5	7	5	26	31	25
13	1	3	420	425	7	4	10	3	397	393	7	20	2	4	121	123	24	8	12	4	220	219	11	7	7	5	297	308	8
15	1	3	91	109	25	6	10	3	189	190	11	1	3	4	231	228	7	10	12	4	433	423	8	9	7	5	315	314	9
17	1	3	362	345	8	8	10	3	212	215	10	3	3	4	458	442	6	12	12	4	356	355	10	11	7	5	360	363	9
19	1	3	450	449	9	10	10	3	68	60	41	5	3	4	3380	3423	15	14	12	4	77	35	43	13	7	5	177	175	15
21	1	3	889	852	9	12	10	3	101	108	23	7	3	4	167	170	11	1	13	4	243	250	11	15	7	5	55	50	55
0	2	3	2358	2321	11	14	10	3	611	602	8	9	3	4	770	784	7	3	13	4	77	82	17	17	7	5	75	67	51
2	2	3	576	561	5	16	10	3	100	80	28	11	3	4	108	104	18	5	13	4	296	287	9	0	8	5	833	837	7
4	2	3	77	66	17	1	11	3	332	318	8	13	3	4	335	341	8	7	13	4	259	266	11	2	8	5	137	125	15
6	2	3	1154	1119	9	3	11	3	181	188	11	15	3	4	762	749	8	9	13	4	526	497	8	4	8	5	0	18	1
8	2	3	729	726	7	5	11	3	733	726	7	17	3	4	725	727	8	11	13	4	746	747	8	6	8	5	555	551	7
10	2	3	360	374	7	7	11	3	234	233	10	19	3	4	194	194	15	13	13	4	167	158	17	8	8	5	143	123	15
12	2	3	706	717	7	9	11	3	387	390	8	0	4	4	564	589	6	0	14	4	1473	1480	11	10	8	5	55	61	54
14	2	3	313	317	8	11	11	3	119	111	19	2	4	4	168	166	6	2	14	4	236	236	11	12	8	5	371	362	9
16	2	3	1114	1122	9	13	11	3	45	41	45	4	4	4	696	721	7	4	14	4	333	331	9	14	8	5	484	471	9

Observed and calculated structure factors for K27

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
16	8	5	795	779	8	7	1	6	70	64	35	8	8	6	334	348	9	0	4	7	964	948	8	9	1	8	707	705	8
1	9	5	673	675	7	9	1	6	377	370	8	10	8	6	96	108	28	2	4	7	71	91	42	11	1	8	476	496	9
3	9	5	81	66	28	11	1	6	239	246	11	12	8	6	187	192	15	4	4	7	253	249	10	0	2	8	50	4	49
5	9	5	547	534	7	13	1	6	59	28	58	14	8	6	436	419	9	6	4	7	83	80	31	2	2	8	95	73	27
7	9	5	352	345	8	15	1	6	443	441	9	1	9	6	336	332	8	8	4	7	207	207	12	4	2	8	263	262	11
9	9	5	65	73	52	17	1	6	317	323	11	3	9	6	87	116	28	10	4	7	235	230	12	6	2	8	499	494	8
11	9	5	1530	1548	12	0	2	6	1682	1709	13	5	9	6	67	37	49	12	4	7	470	480	9	8	2	8	60	40	59
13	9	5	117	111	22	2	2	6	196	195	11	7	9	6	463	476	8	14	4	7	116	110	25	10	2	8	249	236	12
15	9	5	83	83	41	4	2	6	192	189	11	9	9	6	492	483	8	1	5	7	36	7	35	1	3	8	147	117	16
0	10	5	1021	1008	9	6	2	6	476	488	7	11	9	6	713	718	8	3	5	7	177	185	13	3	3	8	291	306	10
2	10	5	517	509	7	8	2	6	229	236	11	13	9	6	82	38	42	5	5	7	358	358	9	5	3	8	1820	1798	14
4	10	5	132	143	17	10	2	6	798	798	8	0	10	6	2193	2213	16	7	5	7	512	526	8	7	3	8	37	14	36
6	10	5	468	453	7	12	2	6	295	305	10	2	10	6	325	325	9	9	5	7	303	298	10	9	3	8	434	428	9
8	10	5	120	115	20	14	2	6	67	24	56	4	10	6	327	324	9	11	5	7	0	61	1	11	3	8	137	114	22
10	10	5	277	267	11	16	2	6	388	386	10	6	10	6	524	521	8	13	5	7	256	270	13	0	4	8	191	199	14
12	10	5	43	53	42	1	3	6	249	193	9	8	10	6	100	87	28	0	6	7	248	251	11	2	4	8	258	258	11
14	10	5	482	470	9	3	3	6	109	109	18	10	10	6	1301	1284	10	2	6	7	116	114	20	4	4	8	276	273	11
1	11	5	111	94	19	5	3	6	832	833	8	12	10	6	163	181	18	4	6	7	200	210	12	6	4	8	620	616	8
3	11	5	208	208	11	7	3	6	75	39	32	1	11	6	69	76	49	6	6	7	669	669	8	8	4	8	41	38	41
5	11	5	471	466	8	9	3	6	1103	1107	9	3	11	6	332	334	10	8	6	7	219	244	12	10	4	8	156	150	19
7	11	5	512	527	8	11	3	6	1079	1112	10	5	11	6	396	411	9	10	6	7	110	125	25	1	5	8	516	536	8
9	11	5	210	222	13	13	3	6	245	241	12	7	11	6	105	86	25	12	6	7	220	206	13	3	5	8	151	147	17
11	11	5	410	409	9	15	3	6	91	73	32	9	11	6	516	502	8	1	7	7	72	78	42	5	5	8	459	444	9
13	11	5	189	189	15	17	3	6	323	327	11	11	11	6	745	742	8	3	7	7	252	257	10	7	5	8	70	21	61
0	12	5	1118	1128	9	0	4	6	2465	2475	17	0	12	6	505	522	8	5	7	7	699	683	8	9	5	8	151	150	19
2	12	5	488	477	8	2	4	6	74	65	31	2	12	6	0	50	1	7	7	7	120	115	21	0	6	8	1875	1873	14
4	12	5	44	68	43	4	4	6	161	357	8	4	12	6	92	77	10	9	7	7	348	341	10	2	6	8	182	183	15
6	12	5	692	689	7	6	4	6	516	523	7	6	12	6	914	915	8	11	7	7	487	491	9	4	6	8	339	331	10
8	12	5	112	103	22	8	4	6	131	136	17	8	12	6	0	35	1	0	8	7	486	474	8	6	6	8	466	467	9
10	12	5	115	116	24	10	4	6	1398	1398	11	10	12	6	445	422	9	2	8	7	126	96	19	8	6	8	124	148	24
12	12	5	240	235	13	12	4	6	265	253	10	1	13	6	35	7	35	4	8	7	276	259	10	1	7	8	41	52	40
1	13	5	296	306	10	14	4	6	75	79	48	3	13	6	14	53	14	6	8	7	358	320	9	3	7	8	172	136	15
3	13	5	264	265	11	16	4	6	232	243	13	5	13	6	1412	1407	11	8	8	7	57	36	57	5	7	8	947	928	9
5	13	5	982	968	9	1	5	6	274	268	8	7	13	6	173	172	17	10	8	7	24	46	24	7	7	8	177	204	16
7	13	5	164	183	17	3	5	6	288	291	8	0	14	6	19	13	18	1	9	7	385	372	9	0	8	8	988	971	9
9	13	5	295	306	11	5	5	6	465	455	7	2	14	6	351	351	10	3	9	7	0	33	1	2	8	8	29	37	28
11	13	5	1190	1191	10	7	5	6	83	86	29	4	14	6	340	347	11	5	9	7	190	198	15	4	8	8	68	24	67
0	14	5	894	877	8	9	5	6	229	246	11	6	14	6	161	154	18	7	9	7	132	136	20	6	8	8	164	365	10
2	14	5	230	239	12	11	5	6	346	354	9	1	1	7	59	71	59	9	9	7	83	18	37	1	9	8	0	15	1
4	14	5	344	353	10	13	5	6	105	83	26	3	1	7	244	240	10	0	10	7	587	576	8	3	9	8	162	142	17
6	14	5	431	420	9	15	5	6	244	237	12	5	1	7	66	25	47	2	10	7	419	425	9	5	9	8	1250	1240	10
8	14	5	191	207	15	0	6	6	155	145	14	7	1	7	276	266	10	4	10	7	183	181	15	0	10	8	1050	1055	9
1	15	5	110	111	25	2	6	6	0	26	1	9	1	7	209	194	12	6	10	7	187	183	15	2	10	8	140	137	20
3	15	5	238	240	13	4	6	6	540	541	7	11	1	7	755	750	8	8	10	7	92	106	33	1	1	9	55	46	55
5	15	5	79	100	46	6	6	6	845	843	8	13	1	7	330	332	10	1	11	7	162	166	17	3	1	9	190	179	16
7	15	5	324	321	11	8	6	6	298	301	9	15	1	7	116	123	26	3	11	7	118	113	24	5	1	9	239	246	13
0	16	5	245	262	13	10	6	6	135	106	17	0	2	7	700	699	8	5	11	7	515	516	9	0	2	9	47	48	47
2	16	5	267	261	12	12	6	6	169	157	15	2	2	7	330	320	8	7	11	7	161	173	18	2	2	9	63	59	62
4	16	5	117	125	26	14	6	6	855	845	8	4	2	7	46	3	46	0	12	7	84	96	37	4	2	9	220	205	14
0	0	6	2577	2608	16	1	7	6	563	572	7	6	2	7	461	466	8	2	12	7	169	178	17	6	2	9	16	12	15
2	0	6	77	79	30	3	7	6	157	153	14	8	2	7	283	281	10	4	12	7	240	236	13	1	3	9	138	146	21
4	0	6	645	658	7	5	7	6	2515	2505	18	10	2	7	110	107	25	0	0	8	2497	2531	20	3	3	9	57	23	57
6	0	6	690	706	7	7	7	6	109	107	21	12	2	7	538	529	8	2	0	8	163	150	15	5	3	9	34	40	34
8	0	6	371	371	8	9	7	6	394	397	8	14	2	7	137	158	22	4	0	8	261	257	11	0	4	9	417	404	9
10	0	6	885	893	8	11	7	6	397	420	9	1	3	7	188	189	12	6	0	8	676	675	8	2	4	9	0	58	1
12	0	6	701	714	8	13	7	6	219	220	13	3	3	7	0	25	1	8	0	8	0	3	1	4	4	9	78	60	45
14	0	6	781	777	8	15	7	6	630	628	9	5	3	7	413	402	8	10	0	8	1463	1450	11	1	5	9	76	7	44
16	0	6	847	853	8	0	8	6	285	280	9	7	3	7	437	442	8	1	1	8	62	87	61	3	5	9	73	85	72
1	1	6	139	140	15	2	8	6	181	178	13	9	3	7	176	173	14	3	1	8	110	122	24						
3	1	6	151	140	14	4	8	6	313	324	9	11	3	7	767	755	8	5	1	8	469	472	8						
5	1	6	1697	1742	14	6	8	6	297	276	9	13	3	7	36	32	35	7	1	8	158	168	17						

Observed and calculated structure factors for K28

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	634	642	4	4	8	0	377	375	4	1	1	1	463	453	4	7	9	1	332	336	5	7	1	2	180	172	4
4	0	0	1229	1221	6	6	8	0	560	557	5	5	1	1	863	874	6	9	9	1	24	50	23	9	1	2	627	632	5
6	0	0	611	618	5	8	8	0	471	472	5	7	1	1	98	90	7	11	9	1	1667	1702	11	11	1	2	628	630	5
8	0	0	895	873	7	10	8	0	1334	1325	10	9	1	1	446	438	4	13	9	1	71	63	19	13	1	2	76	73	15
10	0	0	1707	3697	10	12	8	0	164	168	8	11	1	1	836	860	7	15	9	1	70	85	22	15	1	2	647	655	6
12	0	0	1384	1403	11	14	8	0	169	168	8	13	1	1	372	364	5	17	9	1	199	176	8	17	1	2	72	60	19
14	0	0	182	176	7	16	8	0	317	295	6	15	1	1	70	66	17	19	9	1	180	185	10	19	1	2	35	20	34
16	0	0	241	247	6	18	8	0	52	22	43	17	1	1	715	727	7	0	10	1	1240	1246	9	21	1	2	327	324	7
18	0	0	600	566	6	20	8	0	323	318	7	19	1	1	458	473	6	2	10	1	778	772	6	0	2	2	4241	4122	7
20	0	0	235	238	8	1	9	0	97	84	10	21	1	1	880	870	7	4	10	1	262	260	5	2	2	2	329	319	3
22	0	0	1676	1682	12	3	9	0	387	386	4	0	2	1	48	74	11	6	10	1	434	444	5	4	2	2	487	480	4
1	1	0	681	715	3	5	9	0	1893	1895	11	2	2	1	478	500	4	8	10	1	164	172	8	6	2	2	435	425	4
3	1	0	172	160	3	7	9	0	892	873	7	4	2	1	501	502	4	10	10	1	246	250	6	8	2	2	246	243	4
5	1	0	441	445	4	9	9	0	59	27	23	6	2	1	243	228	3	12	10	1	28	16	27	10	2	2	1277	1304	9
7	1	0	502	499	4	11	9	0	615	599	6	8	2	1	601	613	5	14	10	1	621	613	6	12	2	2	530	549	5
9	1	0	1718	1711	9	13	9	0	286	287	6	10	2	1	283	284	4	16	10	1	270	288	7	14	2	2	117	124	10
11	1	0	2923	2863	11	15	9	0	543	547	6	12	2	1	940	956	7	18	10	1	269	266	8	16	2	2	338	332	6
13	1	0	332	334	5	17	9	0	490	486	6	14	2	1	152	156	8	1	11	1	193	206	7	18	2	2	63	46	24
15	1	0	294	300	5	19	9	0	256	257	8	16	2	1	697	702	6	3	11	1	261	262	6	20	2	2	38	30	38
17	1	0	293	299	6	0	10	0	298	313	5	18	2	1	17	39	16	5	11	1	668	693	6	1	3	2	174	168	3
19	1	0	622	612	6	2	10	0	70	55	16	20	2	1	173	171	9	7	11	1	548	540	5	3	3	2	311	309	3
21	1	0	760	767	7	4	10	0	461	476	5	22	2	1	206	203	9	9	11	1	329	331	5	5	3	2	1034	1016	7
0	2	0	1366	1376	4	6	10	0	274	272	5	1	3	1	339	337	3	11	11	1	376	375	6	7	3	2	119	112	7
2	2	0	226	239	3	8	10	0	278	286	6	3	3	1	246	240	4	13	11	1	114	117	12	9	3	2	1630	1641	10
4	2	0	714	730	5	10	10	0	515	511	5	5	3	1	332	330	4	15	11	1	84	97	19	11	3	2	1345	1377	11
6	2	0	168	169	4	12	10	0	133	138	10	7	3	1	489	489	4	17	11	1	433	451	6	13	3	2	432	440	5
8	2	0	314	309	4	14	10	0	1179	1203	9	9	3	1	241	238	4	0	12	1	1087	1109	9	15	3	2	158	145	8
10	2	0	674	701	6	16	10	0	217	210	8	11	3	1	239	243	5	2	12	1	481	483	5	17	3	2	311	309	6
12	2	0	294	296	5	18	10	0	532	525	6	13	3	1	256	268	6	4	12	1	109	102	11	19	3	2	831	831	7
14	2	0	866	876	7	1	11	0	284	267	5	15	3	1	53	43	27	6	12	1	635	629	6	21	3	2	515	530	6
16	2	0	708	704	6	3	11	0	297	298	5	17	3	1	314	312	6	8	12	1	161	153	8	0	4	2	1942	1927	7
18	2	0	44	18	43	5	11	0	917	920	7	19	3	1	201	206	8	10	12	1	179	180	8	2	4	2	673	664	5
20	2	0	187	178	9	7	11	0	174	175	7	21	3	1	329	325	7	12	12	1	284	284	7	4	4	2	68	40	11
22	2	0	359	336	7	9	11	0	72	56	18	0	4	1	1026	1040	7	14	12	1	64	35	27	6	4	2	329	314	4
1	3	0	314	311	3	11	11	0	437	462	6	2	4	1	81	88	8	16	12	1	717	723	7	8	4	2	128	138	8
3	3	0	548	547	4	13	11	0	180	184	9	4	4	1	251	251	3	1	13	1	378	367	5	10	4	2	2017	2041	11
5	3	0	4883	4797	8	15	11	0	874	885	8	6	4	1	818	780	6	3	13	1	375	375	5	12	4	2	285	295	5
7	3	0	497	482	4	17	11	0	394	411	7	8	4	1	497	500	5	5	13	1	956	957	8	14	4	2	237	231	6
9	3	0	999	988	8	0	12	0	1546	1578	12	10	4	1	268	249	5	7	13	1	89	78	15	16	4	2	56	9	28
11	3	0	343	342	4	2	12	0	240	244	6	12	4	1	742	732	6	9	13	1	322	319	6	18	4	2	504	495	6
13	3	0	358	366	5	4	12	0	241	238	6	14	4	1	260	255	6	11	13	1	1096	1086	8	20	4	2	319	315	7
15	3	0	851	838	7	6	12	0	622	626	6	16	4	1	648	659	6	13	13	1	150	142	11	1	5	2	1000	971	6
17	3	0	962	956	8	8	12	0	140	147	9	18	4	1	245	256	7	15	13	1	273	268	8	3	5	2	135	129	6
19	3	0	209	218	8	10	12	0	677	663	6	20	4	1	86	86	19	0	14	1	661	678	6	5	5	2	1902	1836	9
21	3	0	416	411	6	12	12	0	519	503	6	1	5	1	109	113	6	2	14	1	289	277	6	7	5	2	203	191	5
0	4	0	2112	2088	6	14	12	0	77	91	22	3	5	1	522	523	4	4	14	1	407	415	5	9	5	2	425	419	5
2	4	0	569	566	4	16	12	0	102	94	17	5	5	1	1541	1517	8	6	14	1	265	280	7	11	5	2	641	647	6
4	4	0	1134	1131	7	1	13	0	427	418	5	7	5	1	911	885	6	8	14	1	321	315	6	13	5	2	41	7	41
6	4	0	1749	1625	9	3	13	0	155	156	8	9	5	1	581	565	5	10	14	1	197	196	8	15	5	2	273	264	6
8	4	0	466	459	5	5	13	0	424	419	5	11	5	1	316	317	5	12	14	1	172	182	10	17	5	2	749	735	6
10	4	0	420	424	5	7	13	0	465	469	5	13	5	1	578	574	6	14	14	1	388	384	7	19	5	2	411	416	6
12	4	0	257	253	5	9	13	0	539	537	6	15	5	1	133	116	10	1	15	1	52	30	35	21	5	2	461	447	6
14	4	0	886	897	7	11	13	0	931	924	8	17	5	1	216	221	8	3	15	1	282	284	6	0	6	2	1069	1071	7
16	4	0	2029	1997	14	13	13	0	297	297	7	19	5	1	0	18	1	5	15	1	242	252	7	2	6	2	153	168	6
18	4	0	98	83	14	15	13	0	210	226	9	21	5	1	746	742	7	7	15	1	353	352	6	4	6	2	1094	1105	8
20	4	0	234	227	8	0	14	0	1479	1493	11	0	6	1	486	471	4	9	15	1	76	71	21	6	6	2	2363	2299	10
1	5	0	1403	1392	7	2	14	0	393	400	5	2	6	1	170	172	5	11	15	1	117	121	14	8	6	2	280	277	5
3	5	0	65	53	11	4	14	0	201	205	7	4	6	1	217	207	4	13	15	1	156	145	11	10	6	2	40	29	19
5	5	0	3285	3160	8	6	14	0	697	696	6	6	6	1	894	880	7	0	16	1	245	255	7	12	6	2	338	343	5
7	5	0	812	799	6	8	14	0	116	122	12	8	6	1	522	508	5	2	16	1	244	244	7	14	6	2	992	1004	8
9	5	0	178	185	6	10	14	0	1324	1338	9	10	6	1	116	115	10	4	16	1	18	10	18	16	6	2	1457	1460	10
11	5	0	310	335	5	12	14	0	93	98	18	12	6	1	336	335	5	6	16	1	1267	1269	10	18	6	2	40	28	19
13	5	0	320	327	5	14	14	0	0	24	1	14	6	1	51	24	30	8	16	1	296	306	7	20	6	2	90	106	19
15	5	0	270	273	6	1	15	0	241	230	7	16	6	1	1052	1046	8	10	16	1	133	70	13	1	7	2	692	684	5
17	5	0	503	504	6	3	15	0	396	399	6	18	6	1	280	277	7	12	16	1	99	90	18	3	7	2	97	17	9
19	5	0	221	233	8	5	15	0	535	534	6	20	6	1	424	431	6	1	17	1	68	82	26	5	7	2	4758	4504	11
21	5	0	297	308	7	7	15	0	33	12	33	1	7	1	150	146	5	3	17	1	322	316	7	7	7	2	219	218	5
0	6	0	913	921	6	9	15	0	107	109	14	3	7	1	589	586	5	5	17	1	719	703	7	9	7	2	470	477	5
2	6	0	154	156	5	11	15	0	188	181	6	5	7	1	413	418	4	7	17	1	206	225	9	11	7	2	64	85	20
4	6	0	409	415	4	13	15	0	418	412	7	7	7	1	196	204	6	9	17	1	411	394	7	13	7	2	148	151	5
6	6	0	539	531	5	0	16	0	605	606	6	9	7	1	439	458	5	0	18	1	279	295	8	15	7	2	912	925	8
8	6	0	636	635	5	2	16	0	182	168	9	11	7	1	0	9	1	2	18	1	83	73	21	17	7	2	968	962	7
10	6	0	1340	1351	9	4	16	0	268	263	7	13	7	1	42	58	41	4	18	1	334	334	7	19	7	2	47	38	47
12	6	0	277	280	5	6	16	0	834	841	7	15	7	1	37	32	37	6	18	1	336	334	7	0	8	2	485	490	5
14	6	0	453	457	5	8	16	0	57	69	38	17	7	1	199	202	8	1	19	1	344	330	7	2	8	2	425	416	4
16	6	0	551	548	6	10	16	0	66	34	27	19	7	1	129	137	12	3	19	1	396	400	7	4	8	2	195	205	6
18	6	0	390	385	6	12	16	0	408	416	7	0	8	1	681	668	5	0	0	2	3096	3324	7	6	8	2	410	403	5
20	6	0	34	36	34	1	17	0	257	261	7	2	8	1	46	9	24	2	0	2	550	571	4	8	8	2	556	559	5
1	7	0	718	710	5	3	17	0	293	293	7	4	8	1	88	107	11	4	0	2	418	414	3	10	8	2	26	13	26
3	7	0	105	113	8	5	17	0	1897	1883	13	6	8	1	309	311	4	6	0	2	770	733	6	12	8	2	176	177	8
5	7	0	1381	1358	9	7	17	0	51	41	50	8	8	1	124	138	9	8	0	2	526	509	4	14	8	2	573	574	6
7	7	0	463	441	4	9	17	0	75	56	25	10	8	1	84	72	14	10	0	2	1346	1329	10	16	8	2	881	883	7
9	7	0	1252	1249	9	0	18	0	310	313	7	12	8	1	516	513	5	12	0	2	918	925	7	18	8	2	67	58	28
11	7	0	571	540	5	2	18	0	291	295	7	14	8	1	565	569	6	14	0	2	1307	1334	10	1	9	2	425	412	5
13	7	0	329	345	6	4	18	0	102	66	17	16	8	1	740	726	7	16	0	2	700	688	6	3	9	2	57	38	22
15	7	0	215	219	7	6	18	0	226	240	9	18	8	1	363	347	6	18	0	2	780	776	7	5	9	2	456	441	5
17	7	0	255	248	7	8	18	0	332	311	7	20	8	1	239	252	8	20	0	2	84	64	18	7	9	2	390	386	5
19	7	0	678	693	7	1	19	0	194	185	10	1	9	1	962	947	7	1	1	2	471	480	4	9	9	2	744	754	6
0	8	0	2659	2582	9	3	19	0	66	65	32	3	9	1	131	133	8	3	1	2	757	747	6	11	9	2	1566	1569	11
2	8	0	147	153	6	1	1	1	170	162	3	5	9	1	367	380	5	5	1	2	1092	1079	8	13	9	2	83	96	16

Observed and calculated structure factors for K28

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	330	329	6	20	2	3	109	106	15	17	11	3	566	547	6	8	4	4	186	196	7	8	14	4	92	100	18
17	9	2	609	618	7	1	3	3	549	538	4	0	12	3	245	237	6	10	4	4	279	287	5	10	14	4	1048	1050	8
19	9	2	295	304	8	3	3	3	243	246	4	2	12	3	276	271	6	12	4	4	158	162	8	12	14	4	24	55	24
0	10	2	4666	4436	12	5	3	3	1088	1059	7	4	12	3	357	358	5	14	4	4	864	864	7	1	15	4	193	198	9
2	10	2	669	661	6	7	3	3	744	736	6	6	12	3	135	132	10	16	4	4	1431	1428	11	3	15	4	405	393	6
4	10	2	747	746	6	9	3	3	188	186	6	8	12	3	89	75	15	18	4	4	145	142	11	5	15	4	263	257	8
6	10	2	55	61	24	11	3	3	1320	1328	10	10	12	3	161	176	9	1	5	4	962	957	7	7	15	4	133	116	13
8	10	2	277	282	6	13	3	3	77	65	15	12	12	3	266	272	7	3	5	4	154	144	7	9	15	4	121	113	14
10	10	2	1838	1867	13	15	3	3	132	117	9	14	12	3	113	125	15	5	5	4	1540	1558	11	0	16	4	180	163	10
12	10	2	319	326	6	17	3	3	260	251	7	16	12	3	411	418	7	7	5	4	374	374	5	2	16	4	168	163	10
14	10	2	342	349	6	19	3	3	116	127	13	1	13	3	252	256	7	9	5	4	188	172	6	4	16	4	193	185	10
16	10	2	218	223	8	21	3	3	399	402	7	3	13	3	474	473	5	11	5	4	879	901	7	6	16	4	458	467	6
18	10	2	278	268	8	0	4	3	2187	2094	9	5	13	3	338	342	6	13	5	4	180	173	8	8	16	4	0	5	1
1	11	2	358	355	5	2	4	3	42	49	24	7	13	3	119	126	12	15	5	4	266	271	7	1	17	4	345	337	7
3	11	2	684	688	6	4	4	3	379	368	4	9	13	3	255	251	7	17	5	4	116	113	13	3	17	4	181	191	11
5	11	2	73	72	17	6	4	3	219	215	5	11	13	3	376	364	6	19	5	4	172	156	10	1	1	5	75	73	14
7	11	2	14	11	34	8	4	3	275	275	5	13	13	3	0	10	1	0	6	4	2131	2176	11	3	1	5	224	228	5
9	11	2	649	662	6	10	4	3	394	387	5	15	13	3	181	173	11	2	6	4	168	175	7	5	1	5	671	664	6
11	11	2	1760	1778	14	12	4	3	787	789	7	0	14	3	0	7	1	4	6	4	390	399	5	7	1	5	19	16	18
13	11	2	41	50	41	14	4	3	108	106	11	2	14	3	223	233	7	6	6	4	176	169	7	9	1	5	359	364	5
15	11	2	216	210	8	16	4	3	222	227	7	4	14	3	338	351	6	8	6	4	344	340	5	11	1	5	257	255	6
17	11	2	89	75	19	18	4	3	157	160	10	6	14	3	156	165	9	10	6	4	1258	1255	9	13	1	5	181	201	8
0	12	2	1339	1344	10	20	4	3	68	33	27	8	14	3	376	365	6	12	6	4	363	371	5	15	1	5	0	25	1
2	12	2	19	8	18	1	5	3	78	77	11	10	14	3	27	23	27	14	6	4	258	256	7	17	1	5	739	735	7
4	12	2	0	1	1	3	5	3	336	345	4	12	14	3	82	63	20	16	6	4	206	201	8	19	1	5	369	371	7
6	12	2	824	834	7	5	5	3	894	877	7	1	15	3	167	160	9	18	6	4	279	280	7	0	2	5	710	714	6
8	12	2	139	150	10	7	5	3	868	871	7	3	15	3	211	212	8	1	7	4	275	264	5	2	2	5	86	80	12
10	12	2	802	798	7	9	5	3	431	446	5	5	15	3	457	465	6	3	7	4	196	187	6	4	2	5	471	475	5
12	12	2	216	218	8	11	5	3	140	129	8	7	15	3	212	214	9	5	7	4	1262	1277	10	6	2	5	434	441	5
14	12	2	557	555	6	13	5	3	429	428	5	9	15	3	129	121	12	7	7	4	375	364	5	8	2	5	315	316	5
16	12	2	374	379	7	15	5	3	5	30	5	11	15	3	353	334	7	9	7	4	982	976	7	10	2	5	71	80	17
1	13	2	203	197	7	17	5	3	282	286	7	0	16	3	121	115	13	11	7	4	719	730	6	12	2	5	748	750	6
3	13	2	42	66	42	19	5	3	64	58	28	2	16	3	85	83	19	13	7	4	305	294	6	14	2	5	78	76	18
5	13	2	1870	1869	14	0	6	3	517	518	5	4	16	3	210	209	8	15	7	4	212	217	8	16	2	5	258	255	7
7	13	2	5	45	5	2	6	3	107	98	8	6	16	3	1144	1125	8	17	7	4	356	369	7	18	2	5	71	79	24
9	13	2	159	156	9	4	6	3	439	421	4	8	16	3	271	258	8	0	8	4	1874	1916	12	1	3	5	127	130	9
11	13	2	110	108	13	6	6	3	1186	1191	9	10	16	3	95	94	20	2	8	4	19	15	18	3	3	5	215	210	6
13	13	2	120	122	13	8	6	3	366	362	5	1	17	3	154	155	11	4	8	4	150	154	8	5	3	5	544	540	5
15	13	2	505	511	6	10	6	3	141	159	8	3	17	3	319	327	7	6	8	4	505	503	5	7	3	5	92	108	12
0	14	2	400	409	5	12	6	3	298	300	5	5	17	3	435	431	6	8	8	4	366	372	5	9	3	5	87	88	14
2	14	2	301	305	6	14	6	3	99	106	13	7	17	3	0	31	1	10	8	4	1155	1161	8	11	3	5	284	285	6
4	14	2	733	751	7	16	6	3	1123	1116	8	0	18	3	217	217	9	12	8	4	91	94	15	13	3	5	279	277	6
6	14	2	450	454	6	18	6	3	411	403	6	2	18	3	173	181	11	14	8	4	152	143	10	15	3	5	22	20	21
8	14	2	178	186	8	20	6	3	400	394	7	4	18	3	157	154	12	16	8	4	237	235	8	17	3	5	515	513	6
10	14	2	117	131	13	1	7	3	179	178	6	0	0	4	6050	6591	11	18	8	4	52	42	51	0	4	5	88	80	13
12	14	2	53	61	52	3	7	3	282	295	5	2	0	4	171	379	4	1	9	4	18	27	37	2	4	5	71	49	15
14	14	2	397	406	7	5	7	3	1179	1152	9	4	0	4	676	694	5	3	9	4	258	265	6	4	4	5	126	121	9
1	15	2	510	518	6	7	7	3	177	173	7	6	0	4	390	383	4	5	9	4	1756	1774	13	6	4	5	672	663	6
3	15	2	297	296	6	9	7	3	470	470	5	8	0	4	257	258	5	7	9	4	492	492	5	8	4	5	352	362	5
5	15	2	1477	1486	10	11	7	3	803	813	7	10	0	4	2608	2650	12	9	9	4	0	34	1	10	4	5	154	134	8
7	15	2	496	485	6	13	7	3	137	135	10	12	0	4	933	952	7	11	9	4	206	197	7	12	4	5	503	506	5
9	15	2	156	153	11	15	7	3	147	145	10	14	0	4	353	345	5	13	9	4	131	130	11	14	4	5	249	250	7
11	15	2	377	372	7	17	7	3	635	619	6	16	0	4	160	166	9	15	9	4	368	380	7	16	4	5	674	677	6
13	15	2	150	144	12	19	7	3	88	101	19	18	0	4	560	547	6	17	9	4	571	573	6	18	4	5	277	276	8
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4	16	2	20	46	20	4	8	3	345	342	5	3	1	4	118	110	7	4	10	4	524	528	5	5	5	5	720	727	6
6	16	2	464	469	6	6	8	3	584	575	5	5	1	4	291	282	4	6	10	4	211	211	7	7	5	5	615	603	5
8	16	2	67	52	27	8	8	3	0	32	1	7	1	4	78	64	13	8	10	4	297	300	6	9	5	5	422	416	5
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1	17	2	236	238	8	12	8	3	607	599	6	11	1	4	1603	1620	12	12	10	4	172	181	9	13	5	5	376	386	6
3	17	2	388	378	6	14	8	3	366	359	6	13	1	4	183	182	7	14	10	4	919	918	8	15	5	5	58	73	14
5	17	2	165	151	10	16	8	3	213	196	8	15	1	4	215	214	7	16	10	4	359	363	7	17	5	5	157	159	10
7	17	2	0	22	1	18	8	3	181	175	10	17	1	4	0	23	1	1	11	4	148	141	9	0	6	5	370	399	5
9	17	2	404	394	7	1	9	3	587	584	5	19	1	4	560	560	6	3	11	4	350	356	6	2	6	5	101	101	11
0	18	2	786	769	7	3	9	3	87	90	13	0	2	4	343	367	4	5	11	4	1113	1149	9	4	6	5	33	61	32
2	18	2	44	20	43	5	9	3	326	323	5	2	2	4	166	162	6	7	11	4	71	78	20	6	6	5	433	431	5
4	18	2	205	215	9	7	9	3	240	237	6	4	2	4	450	451	4	9	11	4	29	17	28	8	6	5	331	340	5
6	18	2	422	412	7	9	9	3	89	69	14	6	2	4	425	459	5	11	11	4	21	2	21	10	6	5	80	68	15
1	1	3	262	260	3	11	9	3	886	889	7	8	2	4	116	117	9	13	11	4	107	116	15	12	6	5	246	237	7
3	1	3	641	634	5	13	9	3	44	32	44	10	2	4	467	471	5	15	11	4	762	747	7	14	6	5	61	2	27
5	1	3	198	196	4	15	9	3	105	101	14	12	2	4	300	309	6	0	12	4	974	989	8	16	6	5	719	705	7
7	1	3	285	288	4	17	9	3	515	519	6	14	2	4	652	654	6	2	12	4	244	249	7	1	7	5	86	83	13
9	1	3	179	383	4	0	10	3	801	809	6	16	2	4	723	722	6	4	12	4	139	134	10	3	7	5	485	488	5
11	1	3	1154	1389	10	2	10	3	757	769	6	18	2	4	0	2	1	6	12	4	281	282	6	5	7	5	20	14	20
13	1	3	433	440	5	4	10	3	353	364	5	20	2	4	115	124	15	8	12	4	207	199	8	7	7	5	312	312	6
15	1	3	129	129	9	6	10	3	191	192	7	1	3	4	214	218	5	10	12	4	430	434	6	9	7	5	298	307	6
17	1	3	346	350	6	8	10	3	222	235	7	3	3	4	473	451	4	12	12	4	337	335	7	11	7	5	362	373	6
19	1	3	456	465	6	10	10	3	56	41	26	5	3	4	3312	3364	11	14	12	4	62	11	32	13	7	5	177	159	9
21	1	3	881	842	7	12	10	3	94	91	15	7	3	4	166	162	7	1	13	4	232	220	7	15	7	5	38	49	38
0	2	3	2281	2219	8	14	10	3	594	598	6	9	3	4	761	765	6	3	13	4	91	89	15	17	7	5	29	57	29
2	2	3	580	554	4	16	10	3	67	66	27	11	3	4	96	79	12	5	13	4	253	257	7	0	8	5	799	802	6
4	2	3	61	19	12	1	11	3	311	311	5	13	3	4	326	327	6	7	13	4	256	266	7	2	8	5	132	124	9
6	2	3	1109	1107	8	3	11	3	193	201	7	15	3	4	729	724	6	9	13	4	512	515	6	4	8	5	38	16	38
8	2	3	728	710	6	5	11	3	742	741	6	17	3	4	736	737	7	11	13	4	712	718	7	6	8	5	542	541	5
10	2	3	332	337	5	7	11	3	227	233	7	19	3	4	189	190	9	13	13	4	151	164	12	8	8	5	134	122	10
12	2	3	716	726	6	9	11	3	392	390	5	0	4	4	485	508	5	0	14	4	1421	1428	10	10	8	5	67	42	21
14	2	3	349	353	5	11	11	3	123	109	11	2	4	4	374	370	4	2	14	4	248	239	7	12	8	5	384	376	6
16	2	3	1085	1104	9	13	11	3	78	52	19	4	4	4	666	689	6	4	14	4	311	315	7	14	8	5	487	489	6
18	2	3	218	221	8	15	11	3	53	50	52	6	4	4	1836	1840	11	6	14	4	465	476	6	16	8	5	789	768	7

Observed and calculated structure factors for K28

h	k	l	10Fo	10Fc	10s
1	9	5	680	687	6
3	9	5	70	62	19
5	9	5	508	484	5
7	9	5	337	337	6
9	9	5	71	48	20
11	9	5	1528	1537	11
13	9	5	106	120	15
15	9	5	108	101	15
0	10	5	952	983	8
2	10	5	500	506	5
4	10	5	128	123	10
6	10	5	466	452	5
8	10	5	138	127	10
10	10	5	269	256	7
12	10	5	45	69	45
14	10	5	472	466	6
1	11	5	83	88	17
3	11	5	224	218	7
5	11	5	463	468	6
7	11	5	530	527	6
9	11	5	220	224	8
11	11	5	405	409	6
13	11	5	177	179	10
0	12	5	1073	1083	8
2	12	5	481	476	5
4	12	5	47	59	47
6	12	5	670	675	6
8	12	5	96	99	16
10	12	5	112	87	14
12	12	5	246	234	8
1	13	5	326	315	6
3	13	5	270	270	7
5	13	5	947	942	8
7	13	5	184	181	9
9	13	5	282	287	7
11	13	5	1194	1180	9
0	14	5	873	861	7
2	14	5	231	235	8
4	14	5	326	341	7
6	14	5	431	430	6
8	14	5	208	217	9
1	15	5	96	109	18
3	15	5	222	235	9
5	15	5	75	74	22
7	15	5	298	321	8
0	16	5	238	222	8
2	16	5	267	262	8
4	16	5	121	116	14
0	0	6	2456	2540	12
2	0	6	81	71	14
4	0	6	647	650	6
6	0	6	673	687	6
8	0	6	357	346	5
10	0	6	857	857	7
12	0	6	721	732	7
14	0	6	765	770	7
16	0	6	825	825	7
1	1	6	128	122	9
3	1	6	146	143	8
5	1	6	1665	1711	13
7	1	6	69	58	17
9	1	6	347	349	6
11	1	6	238	236	7
13	1	6	48	40	48
15	1	6	428	424	6
17	1	6	338	329	7
0	2	6	1667	1703	12
2	2	6	193	190	7
4	2	6	194	183	7
6	2	6	491	492	5
8	2	6	232	231	7
10	2	6	790	790	7
12	2	6	300	306	6
14	2	6	31	21	31
16	2	6	390	395	7
1	3	6	174	184	7
3	3	6	132	123	9
5	3	6	772	778	6
7	3	6	39	40	38
9	3	6	1104	1100	8
11	3	6	1072	1085	8
13	3	6	227	226	8
15	3	6	52	54	52
17	3	6	337	336	7
0	4	6	2409	2418	13
2	4	6	74	70	16
4	4	6	320	327	5
6	4	6	509	521	5
8	4	6	107	121	12
10	4	6	1327	1365	10
12	4	6	278	265	6
14	4	6	62	58	29
16	4	6	203	212	9
1	5	6	257	261	6
3	5	6	267	279	6
5	5	6	477	477	5
7	5	6	71	83	18
9	5	6	230	233	7
11	5	6	340	351	6
13	5	6	104	100	15
15	5	6	228	236	8
0	6	6	227	188	6
2	6	6	65	27	19
4	6	6	546	551	6
6	6	6	824	822	7
8	6	6	314	305	6
10	6	6	143	132	10
12	6	6	160	156	10
14	6	6	862	851	7
1	7	6	566	567	6
3	7	6	155	153	8
5	7	6	2468	2455	14
7	7	6	130	121	10
9	7	6	383	376	5
11	7	6	426	450	6
13	7	6	208	211	9
15	7	6	619	612	6
0	8	6	342	330	6
2	8	6	176	177	8
4	8	6	292	302	6
6	8	6	281	270	6
8	8	6	342	335	6
10	8	6	148	133	10
12	8	6	185	181	9
14	8	6	413	400	7
1	9	6	329	311	6
3	9	6	123	112	11
5	9	6	62	41	24
7	9	6	484	472	6
9	9	6	524	505	6
11	9	6	711	714	7
13	9	6	50	48	49
0	10	6	2182	2181	15
2	10	6	317	318	6
4	10	6	339	320	6
6	10	6	520	539	6
8	10	6	126	87	12
10	10	6	1257	1263	9
12	10	6	190	184	10
1	11	6	92	86	16
3	11	6	345	331	6
5	11	6	440	454	6
7	11	6	106	102	15
9	11	6	482	473	6
11	11	6	726	721	7
0	12	6	502	497	6
2	12	6	0	43	1
4	12	6	62	45	30
6	12	6	893	903	7
8	12	6	30	26	29
10	12	6	412	413	7
1	13	6	38	20	38
3	13	6	50	48	49
5	13	6	1394	1399	10
7	13	6	163	170	10
0	14	6	0	35	1
2	14	6	351	358	7
4	14	6	348	336	7
6	14	6	160	147	11
1	1	7	76	80	16
3	1	7	241	239	6
5	1	7	61	55	25
7	1	7	273	263	6
9	1	7	213	215	7
11	1	7	739	742	7
13	1	7	324	335	7
15	1	7	153	139	11
0	2	7	668	664	6
2	2	7	306	310	6
4	2	7	27	22	27
6	2	7	470	465	5
8	2	7	301	285	6
10	2	7	93	90	16
12	2	7	534	522	6
14	2	7	193	185	9
1	3	7	196	191	7
3	3	7	0	27	1
5	3	7	381	389	6
7	3	7	432	443	6
9	3	7	160	169	9
11	3	7	752	751	7
13	3	7	61	37	30
0	4	7	1002	963	8
2	4	7	108	94	12
4	4	7	277	260	6
6	4	7	112	81	12
8	4	7	213	209	8
10	4	7	230	240	8
12	4	7	476	475	6
14	4	7	135	121	12
1	5	7	47	13	46
3	5	7	172	184	8
5	5	7	324	324	6
7	5	7	509	515	6
9	5	7	326	318	6
11	5	7	89	45	17
13	5	7	240	262	8
0	6	7	218	224	7
2	6	7	98	108	14
4	6	7	189	183	8
6	6	7	678	676	6
8	6	7	237	247	7
10	6	7	124	138	13
12	6	7	200	197	9
1	7	7	61	79	27
3	7	7	270	265	7
5	7	7	699	676	6
7	7	7	129	120	12
9	7	7	338	346	7
11	7	7	503	498	6
0	8	7	519	514	6
2	8	7	81	98	19
4	8	7	271	269	7
6	8	7	315	323	7
8	8	7	52	29	51
10	8	7	94	68	17
1	9	7	380	385	6
3	9	7	5	38	5
5	9	7	239	233	8
7	9	7	110	124	14
9	9	7	31	11	30
0	10	7	550	555	6
2	10	7	412	422	6
4	10	7	163	163	10
6	10	7	187	188	9
8	10	7	123	116	14
1	11	7	165	165	11
3	11	7	121	123	14
5	11	7	543	534	6
7	11	7	168	169	10
0	12	7	65	58	28
2	12	7	177	177	10
4	12	7	247	245	8
0	0	8	2463	2485	15
2	0	8	146	143	10
4	0	8	247	241	7
6	0	8	689	692	7
8	0	8	0	11	1
10	0	8	1428	1426	10
1	1	8	86	89	16
3	1	8	131	130	11
5	1	8	504	509	6
7	1	8	165	174	10
9	1	8	678	693	7
11	1	8	485	478	6
0	2	8	13	5	12
2	2	8	71	67	21
4	2	8	268	270	7
6	2	8	498	486	6
8	2	8	47	44	46
10	2	8	239	246	8
1	3	8	113	114	13
3	3	8	307	308	6
5	3	8	1765	1767	13
7	3	8	44	21	43
9	3	8	409	417	6
11	3	8	144	134	12
0	4	8	241	255	7
2	4	8	270	258	7
4	4	8	259	259	7
6	4	8	607	606	6
8	4	8	0	23	1
10	4	8	120	119	14
1	5	8	517	518	6
3	5	8	151	145	10
5	5	8	442	433	6
7	5	8	0	6	1
9	5	8	184	170	9
0	6	8	1890	1856	13
2	6	8	174	184	10
4	6	8	334	334	7
6	6	8	476	463	6
8	6	8	157	151	11
1	7	8	59	58	33
3	7	8	238	129	12
5	7	8	903	892	8
7	7	8	211	210	9
0	8	8	944	949	8
2	8	8	56	40	38
4	8	8	19	3	19
6	8	8	366	360	7
1	9	8	0	29	1
3	9	8	145	138	12
5	9	8	1226	1238	10
0	10	8	1070	1027	8
2	10	8	150	138	11
1	1	9	43	57	43
3	1	9	185	178	9
5	1	9	269	275	8
0	2	9	78	74	21
2	2	9	68	48	25
4	2	9	228	228	8
6	2	9	26	12	25
1	3	9	151	152	11
3	3	9	47	17	46
5	3	9	57	60	42
0	4	9	424	418	6
2	4	9	73	54	24
4	4	9	74	65	23
1	5	9	36	7	36
3	5	9	86	90	20

Observed and calculated structure factors for K29

h	k	l	10Fo	10Fc	10s
2	0	0	544	569	1
4	0	0	1224	1244	5
6	0	0	630	657	4
8	0	0	1146	1139	7
10	0	0	1680	1852	9
12	0	0	1328	1354	10
14	0	0	257	245	4
16	0	0	391	383	4
18	0	0	643	627	5
20	0	0	334	339	5
22	0	0	1657	1633	12
1	1	0	663	690	3
3	1	0	269	261	2
5	1	0	591	598	4
7	1	0	481	484	3
9	1	0	1642	1673	8
11	1	0	2907	2894	9
13	1	0	333	338	4
15	1	0	230	235	5
17	1	0	266	272	5
19	1	0	555	564	5
21	1	0	809	805	7
0	2	0	1285	1317	4
2	2	0	273	284	2
4	2	0	677	692	4
6	2	0	146	152	3
8	2	0	283	281	1
10	2	0	634	643	5
12	2	0	307	311	4
14	2	0	837	853	6
16	2	0	741	744	6
18	2	0	74	23	11
20	2	0	152	148	7
22	2	0	319	316	6
1	3	0	321	317	3
3	3	0	370	375	3
7	3	0	494	480	4
9	3	0	968	967	7
11	3	0	431	428	4
13	3	0	454	456	4
15	3	0	931	944	7
17	3	0	934	922	7
19	3	0	251	250	6
21	3	0	294	283	6
0	4	0	2299	2301	5
2	4	0	649	642	5
4	4	0	1153	1153	6
6	4	0	3791	3641	7
8	4	0	534	527	4
10	4	0	553	553	4
12	4	0	203	204	4
14	4	0	821	837	6
16	4	0	2036	2036	12
18	4	0	124	99	7
20	4	0	220	226	6
22	4	0	410	407	5
1	5	0	1463	1453	6
3	5	0	124	112	3
5	5	0	3397	3209	7
7	5	0	888	859	6
9	5	0	71	90	8
11	5	0	326	343	4
13	5	0	222	228	4
15	5	0	273	275	5
17	5	0	483	470	5
19	5	0	175	176	6
21	5	0	306	308	6
0	6	0	1032	1034	7
2	6	0	72	82	6
4	6	0	308	312	3
6	6	0	488	473	4
8	6	0	558	534	4
10	6	0	1494	1485	10
12	6	0	259	263	4
14	6	0	411	409	4
16	6	0	466	463	5
18	6	0	412	422	5
20	6	0	50	24	24
1	7	0	754	741	5
3	7	0	228	238	3
5	7	0	1558	1505	8
7	7	0	438	430	4
9	7	0	1274	1258	10
11	7	0	619	577	5
13	7	0	404	410	4
15	7	0	279	284	5
17	7	0	223	217	5
19	7	0	688	682	6
0	8	0	2743	2690	8
2	8	0	129	125	4
4	8	0	520	501	4
6	8	0	581	580	4
8	8	0	566	562	4
10	8	0	1367	1353	10
12	8	0	200	209	5
14	8	0	104	101	8
16	8	0	237	243	5
18	8	0	40	43	40
20	8	0	322	306	6
1	9	0	157	150	4
3	9	0	323	321	3
5	9	0	1888	1916	9
7	9	0	913	901	7
9	9	0	112	121	6
11	9	0	587	578	5
13	9	0	304	298	4
15	9	0	623	633	5
17	9	0	532	520	5
19	9	0	261	246	6
0	10	0	373	394	4
2	10	0	72	71	9
4	10	0	424	424	4
6	10	0	250	244	4
8	10	0	359	375	4
10	10	0	587	593	5
12	10	0	144	148	6
14	10	0	1144	1131	8
16	10	0	310	311	5
18	10	0	524	517	5
1	11	0	317	316	4
3	11	0	333	341	4
5	11	0	950	963	7
7	11	0	125	131	6
9	11	0	127	126	6
11	11	0	421	432	4
13	11	0	264	260	5
15	11	0	858	868	6
17	11	0	462	463	5
0	12	0	1454	1468	10
2	12	0	189	184	5
4	12	0	356	349	4
6	12	0	649	657	5
8	12	0	168	171	5
10	12	0	656	663	6
12	12	0	543	538	5
14	12	0	166	161	7
16	12	0	101	81	11
1	13	0	497	503	5
3	13	0	229	234	5
5	13	0	519	419	4
7	13	0	494	498	5
9	13	0	415	411	4
11	13	0	938	930	7
13	13	0	290	303	5
15	13	0	283	285	6
0	14	0	1529	1554	12
2	14	0	428	429	4
4	14	0	205	201	5
6	14	0	694	693	6
8	14	0	228	225	5
10	14	0	1370	1364	9
12	14	0	67	87	15
14	14	0	65	32	16
1	15	0	324	327	5
3	15	0	381	377	5
5	15	0	477	475	5
7	15	0	6	22	6
9	15	0	218	226	6
11	15	0	388	383	5
13	15	0	426	427	5
0	16	0	561	577	5
2	16	0	204	205	6
4	16	0	156	160	7
6	16	0	792	799	6
8	16	0	75	74	13
10	16	0	45	55	31
12	16	0	438	447	5
1	17	0	246	248	5
3	17	0	366	361	5
5	17	0	1844	1854	14
7	17	0	44	1	43
9	17	0	51	21	22
0	18	0	278	280	6
2	18	0	291	287	5
4	18	0	131	120	8
6	18	0	259	264	6
8	18	0	321	320	6
1	19	0	236	235	6
3	19	0	128	105	8
1	1	1	138	126	3
3	1	1	503	502	4
5	1	1	719	729	5
7	1	1	135	115	4
9	1	1	377	365	3
11	1	1	837	844	6
13	1	1	262	272	4
15	1	1	76	68	10
17	1	1	707	708	6
19	1	1	497	507	5
21	1	1	838	810	6
0	2	1	237	188	3
2	2	1	436	460	3
4	2	1	375	374	3
6	2	1	254	239	3
8	2	1	717	737	5
10	2	1	295	315	3
12	2	1	940	945	7
14	2	1	108	99	7
16	2	1	723	717	6
18	2	1	40	53	39
20	2	1	200	199	6
22	2	1	229	236	7
1	3	1	299	298	3
3	3	1	210	204	3
5	3	1	238	232	3
7	3	1	500	494	4
9	3	1	312	313	3
11	3	1	293	299	4
13	3	1	308	311	4
15	3	1	42	37	23
17	3	1	338	337	5
19	3	1	205	207	6
21	3	1	362	367	6
0	4	1	1021	1010	6
2	4	1	68	75	6
4	4	1	231	227	3
6	4	1	798	747	6
8	4	1	512	511	4
10	4	1	323	297	4
12	4	1	682	691	5
14	4	1	274	275	4
16	4	1	628	610	5
18	4	1	207	218	6
20	4	1	83	64	12
1	5	1	103	104	4
3	5	1	632	634	4
5	5	1	1603	1588	7
7	5	1	876	856	6
9	5	1	473	469	4
11	5	1	347	372	4
13	5	1	694	697	6
15	5	1	99	87	8
17	5	1	232	237	5
19	5	1	0	17	1
21	5	1	758	752	6
0	6	1	342	313	3
2	6	1	203	193	3
4	6	1	345	329	3
6	6	1	900	896	7
8	6	1	476	459	4
10	6	1	16	23	16
12	6	1	378	370	4
14	6	1	41	17	23
16	6	1	1048	1052	8
18	6	1	240	217	6
20	6	1	429	431	5
1	7	1	74	76	6
3	7	1	581	572	4
5	7	1	567	567	4
7	7	1	161	162	4
9	7	1	483	489	4
11	7	1	27	17	26
13	7	1	66	63	11
15	7	1	37	12	37
17	7	1	198	191	6
19	7	1	175	171	7
0	8	1	698	678	5
2	8	1	7	31	6
4	8	1	63	59	9
6	8	1	318	312	3
8	8	1	154	163	5
10	8	1	60	54	12
12	8	1	465	479	4
14	8	1	550	558	5
16	8	1	678	671	6
18	8	1	286	283	5
20	8	1	250	257	6
1	9	1	906	897	6
3	9	1	188	178	4
5	9	1	538	549	4
7	9	1	311	316	4
9	9	1	80	84	9
11	9	1	1687	1703	11
13	9	1	32	18	31
15	9	1	78	69	11
17	9	1	159	161	7
19	9	1	199	207	7
0	10	1	1390	1392	9
2	10	1	800	794	6
4	10	1	338	334	4
6	10	1	405	417	4
8	10	1	106	106	7
10	10	1	323	323	4
12	10	1	37	56	17
14	10	1	677	671	6
16	10	1	353	365	5
18	10	1	274	271	6
1	11	1	217	228	4
3	11	1	216	216	4
5	11	1	698	707	5
7	11	1	484	488	4
9	11	1	359	363	4
11	11	1	327	329	5
13	11	1	116	110	8
15	11	1	136	148	8
17	11	1	191	197	5
0	12	1	1157	1168	9
2	12	1	500	489	4
4	12	1	84	88	8
6	12	1	657	664	5
8	12	1	195	192	5
10	12	1	195	185	6
12	12	1	370	271	5
14	12	1	54	67	20
16	12	1	748	756	6
1	13	1	346	344	4
3	13	1	320	314	4
5	13	1	1039	1060	8
7	13	1	115	104	7
9	13	1	367	368	5
11	13	1	1149	1143	8
13	13	1	121	110	9
15	13	1	193	197	7
0	14	1	739	769	6
2	14	1	265	264	5
4	14	1	485	486	5
6	14	1	233	220	5
8	14	1	281	284	5
10	14	1	269	269	5
12	14	1	114	120	8
14	14	1	407	404	5
1	15	1	47	17	19
3	15	1	288	292	5
5	15	1	236	236	5
7	15	1	312	314	5
9	15	1	68	60	14
11	15	1	194	167	6
13	15	1	142	141	8
0	16	1	367	368	5
2	16	1	229	231	5
4	16	1	40	33	40
6	16	1	1244	1249	9
8	16	1	282	301	6
10	16	1	47	13	28
12	16	1	89	96	13
1	17	1	31	18	31
3	17	1	261	256	5
5	17	1	804	803	6
7	17	1	277	268	6
9	17	1	411	413	5
0	18	1	287	290	5
2	18	1	94	63	10
4	18	1	382	383	5
6	18	1	370	357	5
1	19	1	356	353	5
3	19	1	384	391	5
0	0	2	3352	3562	6
2	0	2	646	661	5
4	0	2	441	442	3
6	0	2	756	724	5
8	0	2	729	709	5
10	0	2	1496	1474	9
12	0	2	870	872	6
14	0	2	1355	1350	9
16	0	2	807	828	6
18	0	2	795	776	6
20	0	2	112	113	9
22	0	2	212	226	7
1	1	2	515	517	4
3	1	2	632	636	4
5	1	2	1205	1218	7
7	1	2	163	163	3
9	1	2	652	648	5
11	1	2	563	575	5
13	1	2	142	146	6
15	1	2	734	718	6
17	1	2	89	83	9
19	1	2	35	13	14
21	1	2	253	254	6
2	2	2	288	291	3
4	2	2	454	448	3
6	2	2	398	391	3
8	2	2	179	168	4
10	2	2	1367	1358	9
12	2	2	540	555	5
14	2	2	86	98	9
16	2	2	294	284	5
18	2	2	75	58	12
20	2	2	0	37	1
1	3	2	357	358	3
3	3	2	169	164	3
5	3	2	1223	1195	7
7	3	2	136	132	4
9	3	2	1556	1589	9
11	3	2	1432	1448	10
13	3	2	468	464	4
15	3	2	239	227	5
17	3	2	281	282	5
19	3	2	792	795	7
21	3	2	629	632	6
0	4	2	2168	2114	7
2	4	2	757	735	5
4	4	2	26	12	26
6	4	2	316	325	3
8	4	2	266	274	3
10	4	2	2133	2165	10
12	4	2	220	227	4
14	4	2	233	223	5
16	4	2	77	74	11
18	4	2	565	552	5
20	4	2	330	332	5
1	5	2	1074	1039	7
3	5	2	86	91	5
5	5	2	1830	1779	8
7	5	2	173	154	4
9	5	2	495	495	4
11	5	2	664	652	5
13	5	2	57	55	14
15	5	2	290	289	5
17	5	2	759	757	6
19	5	2	402	398	5
21	5	2	444	437	5
0	6	2	1190	1188	8
2	6	2	92	95	5
4	6	2	995	990	6
6	6	2	2425	2352	9
8	6	2	245	241	4
10	6	2	86	92	8
12	6	2	347	347	4
14	6	2	895	903	7
16	6	2	1479	1490	10
18	6	2	19	20	18
20	6	2	55	59	22
1	7	2	714	703	5
3	7	2	162	165	4
5	7	2	4847	4625	10
7	7	2	189	189	4
9	7	2	487	496	4
11	7	2	34	37	34
13	7	2	457	462	5
15	7	2	997	1002	7
17	7	2	910	925	7
19	7	2	66	86	17
0	8	2	166	166	4
2	8	2	463	460	4
4	8	2	300	309	3
6	8	2	388	377	4
8	8	2	614	614	5
10	8	2	43	44	20
12	8	2	201	207	5
14	8	2	572	576	5
16	8	2	913	911	7
18	8	2	64	71	16
1	9	2	484	475	4
3	9	2	67	63	9
5	9	2	475	462	4
7	9	2	430	429	4
9	9	2	633	637	5
11	9	2	1573	1553	11
13	9	2	144	144	6

Observed and calculated structure factors for K29

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	251	247	5	1	3	3	499	482	4	0	12	3	291	295	4	12	4	4	118	125	8	12	14	4	27	43	27
17	9	2	649	646	6	1	3	3	304	300	3	2	12	3	276	278	4	14	4	4	801	822	6	1	15	4	279	282	5
19	9	2	279	272	6	5	3	3	1121	1106	8	4	12	3	334	341	4	16	4	4	1476	1473	11	3	15	4	390	383	5
0	10	2	4597	4477	11	7	3	3	751	748	5	6	12	3	171	167	6	18	4	4	161	157	7	5	15	4	216	218	6
2	10	2	554	560	5	9	3	3	225	233	4	8	12	3	112	111	8	1	5	4	983	981	7	7	15	4	152	144	7
4	10	2	701	702	5	11	3	3	1294	1348	10	10	12	3	174	184	7	3	5	4	122	126	5	9	15	4	203	206	6
6	10	2	64	25	11	13	3	3	93	95	8	12	12	3	278	264	6	5	5	4	1582	1607	10	0	16	4	151	151	7
8	10	2	384	387	4	15	3	3	120	110	7	14	12	3	155	156	7	7	5	4	410	410	4	2	16	4	183	187	7
10	10	2	1902	1926	12	17	3	3	210	213	6	16	12	3	467	465	5	9	5	4	89	88	9	4	16	4	86	99	13
12	10	2	340	333	5	19	3	3	132	128	9	1	13	3	250	244	5	11	5	4	872	887	6	6	16	4	442	442	5
14	10	2	324	329	5	21	3	3	407	424	5	3	13	3	410	422	4	13	5	4	80	89	12	8	16	4	22	4	21
16	10	2	133	131	8	0	4	3	2132	2057	8	5	13	3	437	454	5	15	5	4	264	275	5	1	17	4	320	322	6
18	10	2	322	305	6	2	4	3	56	57	9	7	13	3	104	106	9	17	5	4	115	94	9	3	17	4	245	240	6
1	11	2	321	308	4	4	4	3	348	349	3	9	13	3	295	305	6	19	5	4	105	105	10	1	1	5	34	40	34
3	11	2	716	715	5	6	4	3	232	228	3	11	13	3	438	436	5	0	6	4	2182	2224	10	3	1	5	240	256	4
5	11	2	119	123	6	8	4	3	259	275	4	13	13	3	9	26	9	2	6	4	119	123	6	5	1	5	586	599	5
7	11	2	54	40	14	10	4	3	429	416	4	15	13	3	142	109	8	4	6	4	336	337	4	7	1	5	28	20	28
9	11	2	681	686	5	12	4	3	739	748	6	0	14	3	107	103	8	6	6	4	185	185	5	9	1	5	296	302	4
11	11	2	1779	1769	12	14	4	3	118	112	7	2	14	3	226	227	5	8	6	4	258	255	4	11	1	5	249	243	5
13	11	2	33	35	32	16	4	3	197	206	6	4	14	3	396	413	5	10	6	4	1321	1337	9	13	1	5	121	128	8
15	11	2	207	200	6	18	4	3	127	124	8	6	14	3	212	207	6	12	6	4	351	344	4	15	1	5	15	35	14
17	11	2	125	126	9	20	4	3	39	2	39	8	14	3	343	343	5	14	6	4	203	209	6	17	1	5	728	720	6
0	12	2	1419	1426	11	1	5	3	90	91	6	10	14	3	97	101	10	16	6	4	165	157	7	19	1	5	402	395	6
2	12	2	47	49	17	3	5	3	406	416	4	12	14	3	0	9	1	18	6	4	316	305	6	0	2	5	610	597	5
4	12	2	107	108	7	5	5	3	952	943	7	1	15	3	188	191	6	1	7	4	314	296	4	2	2	5	79	67	8
6	12	2	850	843	6	7	5	3	847	844	6	3	15	3	199	210	6	3	7	4	294	288	4	4	2	5	166	176	4
8	12	2	197	213	5	9	5	3	340	352	4	5	15	3	440	433	5	5	7	4	1352	1354	10	6	2	5	455	462	4
10	12	2	769	780	6	11	5	3	187	179	5	7	15	3	190	186	6	7	7	4	355	346	4	8	2	5	384	387	4
12	12	2	259	257	5	13	5	3	525	536	5	9	15	3	119	118	9	9	7	4	976	975	7	10	2	5	91	87	9
14	12	2	465	459	5	15	5	3	38	3	38	11	15	3	376	362	5	11	7	4	726	743	6	12	2	5	753	749	6
16	12	2	391	384	5	17	5	3	293	297	5	0	16	3	230	219	6	13	7	4	343	346	5	14	2	5	36	29	35
1	13	2	142	133	6	19	5	3	60	57	18	2	16	3	68	62	14	15	7	4	251	265	6	16	2	5	283	269	5
3	13	2	24	6	24	0	6	3	645	642	5	4	16	3	176	187	6	17	7	4	326	326	6	18	2	5	144	143	8
5	13	2	1841	1839	12	2	6	3	101	91	5	6	16	3	1089	1100	8	0	8	4	1930	1976	10	1	3	5	98	95	7
7	13	2	71	64	12	4	6	3	546	526	4	8	16	3	246	242	6	2	8	4	20	5	19	3	3	5	193	187	4
9	13	2	84	75	10	6	6	3	1210	1200	9	10	16	3	142	165	9	4	8	4	244	249	4	5	3	5	464	475	4
11	13	2	77	90	12	8	6	3	331	323	4	1	17	3	112	114	9	6	8	4	541	529	5	7	3	5	109	111	7
13	13	2	166	167	7	10	6	3	79	87	9	3	17	3	279	270	6	8	8	4	432	442	4	9	3	5	153	144	6
15	13	2	566	568	5	12	6	3	337	333	4	5	17	3	534	526	5	10	8	4	1176	1175	8	11	3	5	228	241	5
0	14	2	479	479	5	14	6	3	66	67	12	7	17	3	37	13	37	12	8	4	141	133	7	13	3	5	305	305	5
2	14	2	324	325	5	16	6	3	1112	1110	8	0	18	3	198	206	7	14	8	4	84	90	12	15	3	5	28	17	27
4	14	2	742	739	6	18	6	3	373	363	5	2	18	3	172	174	7	16	8	4	199	197	6	17	3	5	519	527	5
6	14	2	417	434	5	20	6	3	390	391	5	4	18	3	193	198	7	18	8	4	101	94	11	0	4	5	73	72	10
8	14	2	239	235	6	1	7	3	120	113	5	2	0	4	319	331	3	1	9	4	85	76	8	2	4	5	84	34	8
10	14	2	170	168	7	3	7	3	259	268	4	4	0	4	673	696	5	3	9	4	207	207	5	4	4	5	108	105	7
12	14	2	47	60	40	5	7	3	1262	1262	10	6	0	4	340	338	4	5	9	4	1795	1780	11	6	4	5	652	643	5
14	14	2	360	374	6	7	7	3	213	212	4	8	0	4	423	426	4	7	9	4	498	506	5	8	4	5	351	366	4
1	15	2	608	604	5	9	7	3	476	484	4	10	0	4	2705	2785	11	9	9	4	52	45	16	10	4	5	181	170	5
3	15	2	274	276	5	11	7	3	809	802	6	12	0	4	884	911	7	11	9	4	180	182	7	12	4	5	461	469	5
5	15	2	1506	1501	10	13	7	3	131	132	7	14	0	4	409	413	5	13	9	4	143	137	7	14	4	5	263	268	5
7	15	2	513	524	5	15	7	3	108	99	8	16	0	4	55	33	18	15	9	4	457	453	5	16	4	5	640	631	6
9	15	2	17	22	16	17	7	3	613	599	6	18	0	4	612	601	6	17	9	4	608	596	6	18	4	5	250	245	6
11	15	2	173	183	8	19	7	3	134	135	9	20	0	4	213	210	7	0	10	4	906	903	7	1	5	5	126	124	6
0	16	2	975	971	7	0	8	3	851	825	7	1	1	4	216	234	3	2	10	4	40	13	23	3	5	5	346	342	4
2	16	2	171	168	6	2	8	3	133	133	5	3	1	4	83	62	7	4	10	4	482	495	4	5	5	5	757	762	6
4	16	2	113	133	9	4	8	3	106	102	4	5	1	4	177	158	4	6	10	4	206	217	5	7	5	5	587	586	5
6	16	2	486	490	5	6	8	3	546	543	5	7	1	4	49	44	14	8	10	4	370	374	4	9	5	5	337	343	4
8	16	2	34	13	33	8	8	3	34	17	33	9	1	4	1252	1274	8	10	10	4	497	498	5	11	5	5	306	295	5
10	16	2	735	734	6	10	8	3	90	86	8	11	1	4	1617	1661	11	12	10	4	178	180	6	13	5	5	455	470	5
1	17	2	234	231	6	12	8	3	545	564	5	13	1	4	191	183	5	14	10	4	855	850	7	15	5	5	54	46	19
3	17	2	426	421	5	14	8	3	330	337	5	15	1	4	151	160	7	16	10	4	433	431	5	17	5	5	176	175	7
5	17	2	147	156	8	16	8	3	179	175	7	17	1	4	56	37	18	1	11	4	201	196	5	0	6	5	264	296	4
7	17	2	49	74	24	18	8	3	127	114	8	19	1	4	531	518	5	3	11	4	392	402	4	2	6	5	106	108	7
9	17	2	363	354	6	1	9	3	553	548	5	0	2	4	332	354	3	5	11	4	1141	1160	8	4	6	5	40	19	22
0	18	2	777	759	6	3	9	3	73	74	9	2	2	4	192	193	4	7	11	4	48	16	22	6	6	5	431	440	4
2	18	2	61	34	16	5	9	3	191	161	5	4	2	4	425	424	4	9	11	4	22	67	22	8	6	5	294	297	5
4	18	2	265	275	6	7	9	3	229	220	4	6	2	4	440	470	4	11	11	4	0	4	1	10	6	5	56	10	15
6	18	2	367	379	6	9	9	3	115	116	7	8	2	4	89	98	8	13	11	4	182	179	7	12	6	5	277	267	5
1	1	3	211	213	3	11	9	3	905	909	7	10	2	4	417	438	4	15	11	4	738	727	6	14	6	5	19	29	18
3	1	3	699	689	5	13	9	3	45	19	21	12	2	4	311	311	4	0	12	4	918	922	7	16	6	5	698	710	6
5	1	3	270	279	3	15	9	3	102	91	12	14	2	4	636	630	5	2	12	4	208	205	5	1	7	5	51	43	14
7	1	3	272	278	3	17	9	3	481	495	5	16	2	4	737	745	6	4	12	4	218	224	5	3	7	5	452	469	4
9	1	3	315	324	4	0	10	3	965	954	7	18	2	4	13	34	12	6	12	4	298	318	5	5	7	5	134	118	6
11	1	3	1336	1357	10	2	10	3	785	788	6	20	2	4	92	96	12	8	12	4	211	228	6	7	7	5	281	278	4
13	1	3	153	160	4	4	10	3	415	428	4	1	3	4	218	224	3	10	12	4	457	447	5	9	7	5	331	326	5
15	1	3	129	133	7	6	10	3	187	178	5	3	3	4	353	341	3	12	12	4	402	371	5	11	7	5	349	356	5
17	1	3	337	342	5	8	10	3	186	184	5	5	3	4	3460	3494	10	14	12	4	65	64	17	13	7	5	167	166	7
19	1	3	474	492	5	10	10	3	130	120	6	7	3	4	148	164	5	1	13	4	276	274	5	15	7	5	79	79	14
21	1	3	810	775	7	12	10	3	206	148	5	9	3	4	736	750	6	3	13	4	166	149	6	17	7	5	69	59	15
0	2	3	2419	2378	7	14	10	3	633	658	6	11	3	4	139	139	6	5	13	4	247	268	5	0	8	5	803	798	6
2	2	3	542	522	4	16	10	3	154	152	7	13	3	4	191	196	4	7	13	4	275	289	6	2	8	5	124	120	6
4	2	3	145	137	4	1	11	3	321	327	4	15	3	4	803	805	7	9	13	4	407	414	5	4	8	5	62	49	13
6	2	3	1104	1076	8	3	11	3	166	167	5	17	3	4	718	703	6	11	13	4	759	732	6	6	8	5	558	550	5
8	2	3	825	813	6	5	11	3	751	752	6	19	3	4	212	217	7	13	13	4	160	170	7	8	8	5	136	138	7
10	2	3	326	337	4	7	11	3	183	185	5	0	4	4	644	662	5	0	14	4	1467	1474	10	10	8	5	97	22	9
12	2	3	708	720	6	9	11	3	411	418	4	2	4	4	431	424	4	2	14	4	261	259	5	12	8	5	477	353	5
14	2	3	310	309	4	11	11	3	60	67	15	4	4	4	667	696	5	4	14	4	306	315	5	14	8	5	476	474	5
16	2	3	1062	1084	8	13	11	3	70	61	15	6	4	4	1823	1848	10	6	14	4	463	472	5	16	8	5	721	710	6
18	2	3	143	139	7	15	11	3	23	2	23	8	4	4	236	243	4	8	14	4	194	188	6	1	9	5	660	648	5
20	2	3	115	123	10	17	11	3	492	494	5	10	4	4	400	396	4	10	14	4	1078	1067	8	3	9	5	104	91	8

Observed and calculated structure factors for K29

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	9	5	604	596	5	13	1	6	0	9	1	1	9	6	348	359	5	6	4	7	117	107	8	11	1	8	498	511	6
7	9	5	300	322	6	15	1	6	471	461	5	3	9	6	87	95	10	8	4	7	244	210	5	0	2	8	44	17	11
9	9	5	75	71	12	17	1	6	287	293	6	5	9	6	33	26	33	10	4	7	266	275	6	2	2	8	86	85	11
11	9	5	1520	1525	11	0	2	6	1707	1721	11	7	9	6	499	496	5	12	4	7	449	458	5	4	2	8	258	250	6
13	9	5	94	81	10	2	2	6	183	181	5	9	9	6	438	430	5	14	4	7	134	131	8	6	2	8	666	498	6
15	9	5	85	87	12	4	2	6	167	162	5	11	9	6	716	716	6	1	5	7	27	17	27	8	2	8	42	31	41
0	10	5	1103	1086	8	6	2	6	454	460	5	13	9	6	0	17	1	3	5	7	211	211	5	10	2	8	231	232	6
2	10	5	504	513	5	8	2	6	193	194	5	0	10	6	2214	2211	13	5	5	7	341	342	5	1	3	8	131	128	8
4	10	5	170	172	6	12	2	6	279	303	6	2	10	6	256	259	5	7	5	7	524	500	5	3	3	8	246	251	6
6	10	5	434	436	5	14	2	6	0	4	1	4	10	6	290	297	5	9	5	7	257	249	6	5	3	8	1786	1828	14
8	10	5	35	77	34	16	2	6	338	348	6	6	10	6	518	515	5	11	5	7	65	59	16	7	3	8	0	12	-1
10	10	5	311	311	5	1	3	6	194	174	5	8	10	6	150	151	7	13	5	7	316	327	6	9	3	8	408	410	5
12	10	5	12	17	12	3	3	6	53	46	15	10	10	6	1318	1309	10	0	6	7	272	278	5	11	3	8	98	106	12
14	10	5	499	501	5	5	3	6	872	870	6	12	10	6	185	185	7	2	6	7	106	115	9	0	4	8	164	172	7
1	11	5	99	94	9	7	3	6	50	46	18	1	11	6	38	62	37	4	6	7	228	239	6	2	4	8	283	282	5
3	11	5	176	170	6	9	3	6	1054	1062	8	3	11	6	338	337	5	6	6	7	670	673	6	4	4	8	279	267	5
5	11	5	496	487	5	13	3	6	239	237	5	5	11	6	403	400	5	8	6	7	227	227	6	6	4	8	590	603	6
7	11	5	493	493	5	15	3	6	119	105	9	7	11	6	90	85	11	10	6	7	99	97	10	8	4	8	56	53	20
9	11	5	244	237	6	17	3	6	307	308	6	9	11	6	496	499	5	12	6	7	225	224	6	10	4	8	197	179	7
11	11	5	160	160	5	0	4	6	2444	2499	11	11	11	6	737	732	6	1	7	7	62	62	15	1	5	8	521	526	5
13	11	5	168	177	8	2	4	6	109	102	7	0	12	6	573	568	5	3	7	7	257	255	5	3	5	8	146	139	7
0	12	5	1129	1117	8	4	4	6	353	357	4	2	12	6	75	88	13	5	7	7	766	753	6	5	5	8	460	460	5
2	12	5	479	479	5	6	4	6	498	502	5	4	12	6	104	115	10	7	7	7	133	130	8	7	5	8	49	34	25
4	12	5	83	74	11	8	4	6	198	207	6	6	12	6	886	891	7	9	7	7	347	350	5	9	5	8	102	111	12
6	12	5	692	692	6	10	4	6	1398	1422	10	8	12	6	86	67	12	11	7	7	499	494	5	0	6	8	1847	1365	14
8	12	5	116	122	8	12	4	6	206	211	6	10	12	6	412	412	5	0	8	7	504	507	5	2	6	8	161	158	7
10	12	5	97	89	11	14	4	6	58	46	17	1	13	6	25	9	25	2	8	7	112	101	9	4	6	8	298	300	6
12	12	5	208	222	7	16	4	6	243	242	6	3	13	6	40	8	19	4	8	7	231	229	6	6	6	8	458	450	5
1	13	5	301	297	5	1	5	6	309	308	4	5	13	6	1342	1367	10	6	8	7	321	320	5	8	6	8	89	99	12
3	13	5	225	227	6	3	5	6	309	312	4	7	13	6	168	176	8	8	8	7	47	58	29	1	7	8	89	75	12
5	13	5	996	1004	8	5	5	6	490	479	4	0	14	6	13	16	13	10	8	7	87	85	12	3	7	8	204	194	7
7	13	5	196	204	6	7	5	6	105	112	9	2	14	6	375	369	5	1	9	7	345	337	5	5	7	8	919	910	7
9	13	5	332	321	5	9	5	6	283	268	5	4	14	6	326	331	6	3	9	7	28	27	28	7	7	8	184	192	7
11	13	5	1220	1212	9	11	5	6	314	328	5	6	14	6	146	128	8	5	9	7	179	158	7	0	8	8	994	974	7
0	14	5	931	932	7	13	5	6	63	68	17	1	1	7	74	62	12	7	9	7	103	126	10	2	8	8	71	55	15
2	14	5	233	218	6	15	5	6	253	253	6	3	1	7	246	250	5	9	9	7	44	25	40	4	8	8	69	54	16
4	14	5	378	384	5	0	6	6	125	107	6	5	1	7	39	19	31	0	10	7	622	623	6	6	8	8	376	375	5
6	14	5	370	384	5	2	6	6	72	10	11	7	1	7	264	258	5	2	10	7	427	425	5	1	9	8	0	3	1
8	14	5	183	188	7	4	6	6	476	481	5	9	1	7	164	171	8	4	10	7	205	205	6	1	9	8	118	109	9
1	15	5	91	78	11	6	6	6	860	858	7	11	1	7	715	720	6	6	10	7	168	163	7	5	9	8	1212	1223	9
3	15	5	242	245	6	8	6	6	292	289	5	13	1	7	264	274	6	8	10	7	67	83	16	0	10	8	1034	1026	8
5	15	5	63	61	18	10	6	6	106	38	10	15	1	7	132	138	9	1	11	7	181	167	7	2	10	8	94	80	12
7	15	5	286	293	6	12	6	6	166	160	7	0	2	7	745	739	6	3	11	7	116	107	9	1	1	9	20	26	19
0	16	5	123	103	6	14	6	6	789	792	6	2	2	7	310	300	5	5	11	7	543	526	5	3	1	9	199	199	7
2	16	5	247	256	6	1	7	6	552	570	5	4	2	7	0	41	1	7	11	7	142	140	8	5	1	9	243	260	6
4	16	5	137	137	9	3	7	6	92	79	9	6	2	7	450	447	5	0	12	7	100	96	10	0	2	9	42	42	42
0	0	6	2546	2612	11	5	7	6	2511	2526	12	8	2	7	344	324	5	2	12	7	182	176	7	2	2	9	51	42	25
2	0	6	121	121	7	7	7	6	90	95	10	10	2	7	98	98	11	4	12	7	221	222	7	4	2	9	160	153	8
4	0	6	664	663	5	9	7	6	405	399	5	12	2	7	506	508	5	0	0	8	2512	2557	13	6	2	9	26	28	26
6	0	6	654	681	6	11	7	6	393	402	5	14	2	7	142	145	8	2	0	8	117	129	9	1	3	9	112	111	10
8	0	6	455	459	5	13	7	6	293	288	6	1	3	7	175	179	6	4	0	8	261	251	5	3	3	9	50	46	27
10	0	6	894	917	7	15	7	6	658	662	6	3	3	7	31	17	31	6	0	8	667	663	6	5	3	9	57	52	22
12	0	6	678	675	6	0	8	6	250	258	5	5	3	7	444	433	5	8	0	8	74	77	15	0	4	9	407	392	5
14	0	6	759	770	6	2	8	6	187	200	6	7	3	7	427	430	5	10	0	8	1486	1493	12	2	4	9	48	45	27
16	0	6	880	889	7	4	8	6	360	365	5	9	3	7	185	196	7	12	0	8	460	466	5	4	4	9	54	57	24
1	1	6	168	159	5	6	8	6	252	261	5	11	3	7	769	772	6	1	1	8	86	88	11	1	5	9	0	13	1
3	1	6	92	72	8	8	8	6	379	365	5	13	3	7	0	21	1	3	1	8	112	108	9	3	5	9	122	112	9
5	1	6	1713	1755	11	10	8	6	131	115	8	0	4	7	981	966	8	5	1	8	447	443	5						
7	1	6	65	78	13	12	8	6	198	200	6	2	4	7	100	98	9	7	1	8	172	177	9						
9	1	6	346	349	5	14	8	6	406	401	5	4	4	7	244	230	5	9	1	8	675	687	6						

Observed and calculated structure factors for K30

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	690	717	4	2	8	0	168	161	5	1	1	1	134	126	3	1	9	1	883	869	7	22	0	2	577	582	6
4	0	0	1017	1025	5	4	8	0	623	611	5	3	1	1	257	258	3	3	9	1	72	3	12	1	1	2	548	546	4
6	0	0	604	604	4	6	8	0	708	720	6	5	1	1	1069	1057	6	5	9	1	418	430	4	3	1	2	755	736	5
8	0	0	1152	1140	8	8	8	0	493	506	5	7	1	1	41	51	14	7	9	1	321	330	4	5	1	2	1027	1020	7
10	0	0	3930	3864	9	10	8	0	1080	1079	8	9	1	1	170	167	4	9	9	1	25	24	25	7	1	2	61	55	9
12	0	0	1450	1488	10	12	8	0	90	79	10	11	1	1	612	633	5	11	9	1	1677	1704	12	9	1	2	578	576	5
14	0	0	156	341	4	14	8	0	87	60	11	13	1	1	216	217	5	13	9	1	173	169	7	11	1	2	564	569	5
16	0	0	466	455	5	16	8	0	382	368	6	15	1	1	366	365	5	15	9	1	274	272	6	13	1	2	10	12	9
18	0	0	313	313	5	18	8	0	0	31	1	17	1	1	667	676	6	17	9	1	65	73	19	15	1	2	690	692	6
20	0	0	534	532	5	20	8	0	272	270	7	19	1	1	568	555	5	19	9	1	246	242	7	17	1	2	28	30	28
22	0	0	1981	1997	13	1	9	0	114	101	7	21	1	1	432	443	6	0	10	1	1491	1493	10	19	1	2	40	74	40
1	1	0	847	885	3	3	9	0	266	266	4	0	2	1	206	221	3	2	10	1	725	722	6	21	1	2	269	272	7
3	1	0	293	282	3	5	9	0	1891	1936	10	2	2	1	604	609	4	4	10	1	118	120	8	0	2	2	4079	4109	7
5	1	0	571	574	4	7	9	0	866	860	7	4	2	1	279	277	3	6	10	1	538	552	5	2	2	2	388	378	3
7	1	0	156	160	3	9	9	0	143	133	7	6	2	1	286	269	3	8	10	1	105	105	8	4	2	2	451	434	3
9	1	0	1358	1352	9	11	9	0	671	656	6	8	2	1	475	478	4	10	10	1	414	421	5	6	2	2	509	504	4
11	1	0	3101	3080	10	13	9	0	171	178	7	10	2	1	257	253	4	12	10	1	4	18	3	8	2	2	120	110	6
13	1	0	542	537	5	15	9	0	874	888	7	12	2	1	798	818	6	14	10	1	605	599	6	10	2	2	1414	1417	10
15	1	0	223	231	5	17	9	0	641	632	6	14	2	1	117	109	7	16	10	1	630	625	6	12	2	2	622	618	5
17	1	0	443	440	5	19	9	0	78	69	17	16	2	1	465	481	5	18	10	1	143	133	10	14	2	2	128	87	7
19	1	0	450	446	5	0	10	0	290	300	4	18	2	1	10	30	10	1	11	1	20	38	20	16	2	2	286	276	5
21	1	0	915	900	7	2	10	0	217	218	5	20	2	1	422	423	6	3	11	1	73	32	12	18	2	2	107	99	11
0	2	0	1210	1244	4	4	10	0	221	221	5	22	2	1	302	299	7	5	11	1	921	912	7	20	2	2	206	211	7
2	2	0	173	182	3	6	10	0	290	282	4	1	3	1	397	405	3	7	11	1	482	494	5	22	2	2	631	632	6
4	2	0	481	495	4	8	10	0	232	254	5	3	3	1	275	261	3	9	11	1	230	239	6	1	3	2	569	556	4
6	2	0	145	157	4	10	10	0	500	502	5	5	3	1	433	427	3	11	11	1	112	109	9	3	3	2	141	133	4
8	2	0	226	220	4	12	10	0	389	391	5	7	3	1	338	337	3	13	11	1	179	179	7	5	3	2	1215	1201	8
10	2	0	520	515	4	14	10	0	938	947	7	9	3	1	217	221	4	15	11	1	459	447	6	7	3	2	279	272	3
12	2	0	550	558	5	16	10	0	377	375	6	11	3	1	412	436	4	17	11	1	441	442	6	9	3	2	1134	1140	8
14	2	0	855	843	6	18	10	0	290	282	7	13	3	1	189	183	5	0	12	1	915	909	7	11	3	2	1614	1658	11
16	2	0	862	865	7	1	11	0	242	246	5	15	3	1	159	161	7	2	12	1	601	600	5	13	3	2	189	186	6
18	2	0	273	267	6	3	11	0	222	229	5	17	3	1	271	260	6	4	12	1	172	173	6	15	3	2	280	281	5
20	2	0	0	0	1	5	11	0	643	650	6	19	3	1	182	175	7	6	12	1	777	782	6	17	3	2	496	499	5
22	2	0	156	153	10	7	11	0	35	42	34	21	3	1	411	410	6	8	12	1	72	63	14	19	3	2	709	716	6
1	3	0	262	264	3	9	11	0	76	96	13	0	4	1	1312	1313	6	10	12	1	70	66	15	21	3	2	818	797	7
3	3	0	443	456	4	11	11	0	440	458	5	2	4	1	181	178	3	12	12	1	211	206	7	0	4	2	1742	1713	7
7	3	0	540	556	5	13	11	0	294	294	6	4	4	1	60	48	9	14	12	1	78	81	16	2	4	2	621	611	4
9	3	0	703	699	5	15	11	0	626	624	6	6	4	1	603	565	4	16	12	1	818	788	7	4	4	2	120	123	5
11	3	0	520	522	5	17	11	0	491	485	6	8	4	1	309	298	3	1	13	1	511	506	5	6	4	2	471	450	4
13	3	0	222	221	5	0	12	0	1509	1527	11	10	4	1	776	776	6	3	13	1	255	246	5	8	4	2	99	106	7
15	3	0	976	976	7	2	12	0	169	137	6	12	4	1	607	614	5	5	13	1	1076	1086	8	10	4	2	1971	2023	11
17	3	0	1054	1054	8	4	12	0	406	406	4	14	4	1	280	273	5	7	13	1	127	119	8	12	4	2	77	84	11
19	3	0	151	147	6	6	12	0	525	520	5	16	4	1	401	395	5	9	13	1	260	266	6	14	4	2	146	104	7
21	3	0	212	208	7	8	12	0	192	196	6	18	4	1	225	224	6	11	13	1	1299	1314	10	16	4	2	86	77	12
0	4	0	2028	2036	6	10	12	0	808	802	7	20	4	1	121	113	10	13	13	1	190	195	7	18	4	2	553	551	5
2	4	0	721	711	5	12	12	0	516	511	5	22	4	1	365	363	6	15	13	1	80	79	18	20	4	2	240	231	7
4	4	0	813	804	5	14	12	0	122	137	11	1	5	1	93	103	6	0	14	1	994	1028	7	1	5	2	1022	991	8
6	4	0	3947	3954	8	16	12	0	68	51	20	3	5	1	326	326	3	2	14	1	133	114	8	3	5	2	54	55	11
8	4	0	167	157	3	1	13	0	635	635	6	5	5	1	974	945	6	4	14	1	373	374	5	5	5	2	1889	1878	9
10	4	0	499	499	4	3	13	0	278	274	5	7	5	1	841	834	6	6	14	1	267	266	6	7	5	2	244	243	4
12	4	0	218	219	5	5	13	0	294	293	5	9	5	1	347	342	4	8	14	1	208	208	7	9	5	2	542	552	5
14	4	0	483	483	5	7	13	0	490	495	5	11	5	1	287	298	4	10	14	1	523	530	6	11	5	2	684	689	6
16	4	0	2204	2186	13	9	13	0	201	198	7	13	5	1	566	571	5	12	14	1	133	128	10	13	5	2	101	81	9
18	4	0	0	11	1	11	13	0	946	952	8	15	5	1	348	350	5	14	14	1	256	257	7	15	5	2	364	360	5
20	4	0	114	105	11	13	13	0	258	264	7	17	5	1	192	191	7	1	15	1	61	45	18	17	5	2	666	664	6
22	4	0	605	596	6	15	13	0	304	303	6	19	5	1	46	28	38	3	15	1	409	418	5	19	5	2	307	299	6
1	5	0	1537	1500	7	0	14	0	1243	1249	9	21	5	1	481	488	6	5	15	1	90	67	13	21	5	2	295	295	7
3	5	0	87	91	6	2	14	0	354	341	5	0	6	1	550	521	4	7	15	1	356	362	6	0	6	2	1115	1122	8
5	5	0	3035	3036	8	4	14	0	229	231	6	2	6	1	61	57	10	9	15	1	14	4	14	2	6	2	88	5	6
7	5	0	959	967	7	6	14	0	685	699	6	4	6	1	323	320	3	11	15	1	166	151	9	4	6	2	651	645	5
9	5	0	153	154	5	8	14	0	203	182	7	6	6	1	1063	1053	7	13	15	1	251	240	7	6	6	2	2571	2593	10
11	5	0	456	467	5	10	14	0	1142	1148	9	8	6	1	516	520	5	0	16	1	470	470	5	8	6	2	315	314	4
13	5	0	132	130	7	12	14	0	69	84	23	10	6	1	133	113	6	2	16	1	162	155	7	10	6	2	271	267	5
15	5	0	187	197	6	14	14	0	0	20	1	12	6	1	379	372	4	4	16	1	107	97	11	12	6	2	350	348	5
17	5	0	483	490	5	1	15	0	361	375	5	14	6	1	58	35	16	6	16	1	1319	1320	10	14	6	2	642	651	6
19	5	0	118	122	10	3	15	0	313	317	5	16	6	1	964	973	8	8	16	1	369	372	6	16	6	2	1646	1670	11
21	5	0	539	537	6	5	15	0	563	538	5	18	6	1	275	269	6	10	16	1	109	110	12	18	6	2	86	82	14
0	6	0	752	762	5	7	15	0	175	183	7	20	6	1	493	492	6	12	16	1	49	19	42	20	6	2	42	54	41
2	6	0	193	187	3	9	15	0	263	261	7	1	7	1	160	154	4	1	17	1	160	151	8	1	7	2	632	599	5
4	6	0	132	138	5	11	15	0	440	438	6	3	7	1	410	411	4	3	17	1	139	141	9	3	7	2	190	187	4
6	6	0	383	376	4	13	15	0	341	345	7	5	7	1	986	996	7	5	17	1	898	913	7	5	7	2	4308	4424	10
8	6	0	644	642	5	0	16	0	559	568	5	7	7	1	205	201	5	7	17	1	244	238	7	7	7	2	157	150	6
10	6	0	1557	1568	11	2	16	0	312	311	6	9	7	1	279	281	4	9	17	1	224	217	8	9	7	2	420	436	4
12	6	0	103	92	9	4	16	0	87	100	13	11	7	1	150	162	6	0	18	1	322	313	6	11	7	2	106	46	8
14	6	0	368	361	5	6	16	0	727	743	6	13	7	1	80	50	12	2	18	1	138	132	9	13	7	2	160	355	5
16	6	0	414	417	5	8	16	0	108	104	12	15	7	1	244	247	6	4	18	1	311	319	6	15	7	2	1043	1061	8
18	6	0	394	393	6	10	16	0	178	164	8	17	7	1	297	294	6	6	18	1	264	262	7	17	7	2	1119	1128	8
20	6	0	51	35	31	12	16	0	500	503	6	19	7	1	175	181	8	1	19	1	487	484	6	19	7	2	161	162	8
1	7	0	519	511	4	1	17	0	359	353	6	21	7	1	102	88	13	3	19	1	402	409	6	0	8	2	361	371	4
3	7	0	126	127	3	3	17	0	307	303	6	0	8	1	336	326	4	0	0	2	3484	3383	6	2	8	2	562	567	5
5	7	0	1382	1365	9	5	17	0	1678	1666	12	2	8	1	204	187	4	2	0	2	715	707	5	4	8	2	262	277	4
7	7	0	569	567	5	7	17	0	113	94	12	4	8	1	165	150	5	4	0	2	106	99	5	6	8	2	360	355	4
9	7	0	1037	1033	7	9	17	0	70	37	19	6	8	1	274	281	4	6	0	2	691	661	5	8	8	2	543	560	5
11	7	0	698	669	6	0	18	0	411	429	6	8	8	1	31	26	31	8	0	2	690	682	5	10	8	2	154	166	7
13	7	0	240	233	5	2	18	0	262	254	7	10	8	1	261	284	5	10	0	2	1556	1538	10	12	8	2	135	61	8
15	7	0	142	147	5	4	18	0	118	96	11	12	8	1	502	485	5	12	0	2	1159	1166	9	14	8	2	470	450	5
17	7	0	501	504	6	6	18	0	357	344	6	14	8	1	471	473	5	14	0	2	1242	1251	8	16	8	2	878	882	7
19	7	0	599	603	6	8	18	0	260	261	7	16	8	1	330	321	6	16	0	2	979	986	7	18	8	2	73	60	17
21	7	0	620	611	6	1	19	0	163	149	9	18	8	1	234	242	7	18	0	2	397	407	5	20	8	2	153	149	10
0	8	0	2604	2590	9	3	19	0	193	199	9	20	8	1	418	408	6	20	0	2	265	260	6	1	9	2	562	555	5

Observed and calculated structure factors for K30

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	9	2	204	200	5	8	2	3	586	596	5	1	11	3	65	69	14	17	3	4	812	823	6	9	13	4	220	212	7
5	9	2	622	603	5	10	2	3	184	191	5	5	11	3	948	959	8	19	3	4	302	301	6	11	13	4	798	788	7
7	9	2	551	552	5	12	2	3	637	647	5	7	11	3	192	195	6	0	4	4	555	583	5	13	13	4	162	161	9
9	9	2	461	464	5	14	2	3	308	316	5	9	11	3	293	298	5	2	4	4	545	540	5	0	14	4	1232	1255	10
11	9	2	1602	1613	10	16	2	3	851	860	7	11	11	3	148	153	8	4	4	4	396	393	4	2	14	4	239	205	7
13	9	2	301	305	6	18	2	3	175	180	8	13	11	3	0	7	1	6	4	4	2127	2124	10	4	14	4	333	331	6
15	9	2	58	16	22	20	2	3	335	339	6	15	11	3	296	275	6	8	4	4	150	151	6	6	14	4	461	464	5
17	9	2	856	837	7	1	3	3	500	485	4	17	11	3	536	544	6	10	4	4	185	408	4	8	14	4	186	172	8
19	9	2	293	283	7	3	3	3	238	231	3	0	12	3	62	66	16	12	4	4	188	187	6	10	14	4	909	904	7
0	10	2	4365	4355	11	5	3	3	943	915	7	2	12	3	176	369	5	14	4	4	513	525	5	12	14	4	51	49	38
2	10	2	609	532	5	7	3	3	689	690	5	4	12	3	435	439	5	16	4	4	1606	1621	12	1	15	4	349	340	6
4	10	2	601	609	5	9	3	3	195	192	5	6	12	3	287	283	5	18	4	4	104	108	12	3	15	4	338	332	6
6	10	2	124	124	7	11	3	3	1453	1444	9	8	12	3	0	10	1	20	4	4	56	69	30	5	15	4	276	278	6
8	10	2	288	301	5	13	3	3	40	32	39	10	12	3	31	34	30	1	5	4	970	960	7	7	15	4	0	15	1
10	10	2	1800	1825	13	15	3	3	239	252	6	12	12	3	200	187	7	3	5	4	122	123	6	9	15	4	258	245	7
12	10	2	443	443	5	17	3	3	263	260	6	14	12	3	167	174	9	5	5	4	1524	1542	11	0	16	4	175	173	8
14	10	2	282	279	6	19	3	3	99	98	12	16	12	3	512	494	6	7	5	4	429	434	4	2	16	4	312	298	6
16	10	2	161	132	8	21	3	3	451	444	6	1	13	3	425	410	5	9	5	4	54	57	18	4	16	4	65	21	22
18	10	2	143	136	10	0	4	3	2338	2263	8	3	13	3	159	365	5	11	5	4	943	952	7	6	16	4	421	418	6
1	11	2	487	482	5	2	4	3	0	1	1	5	13	3	484	493	5	13	5	4	47	17	25	8	16	4	59	38	26
3	11	2	691	692	6	4	4	3	257	249	4	7	13	3	116	115	9	15	5	4	239	250	6	1	17	4	374	375	6
5	11	2	80	76	12	6	4	3	327	319	4	9	13	3	202	202	7	17	5	4	149	147	9	3	17	4	227	215	7
7	11	2	19	24	18	8	4	3	105	118	8	11	13	3	592	593	6	19	5	4	59	69	25	5	17	4	1292	1270	10
9	11	2	511	513	5	10	4	3	794	800	6	13	13	3	48	48	41	0	6	4	1968	2004	10	1	1	5	27	16	27
11	11	2	1825	1869	14	12	4	3	640	644	5	15	13	3	0	20	1	2	6	4	200	216	5	3	1	5	81	95	10
13	11	2	51	40	27	14	4	3	119	119	8	0	14	3	370	355	5	4	6	4	247	253	5	5	1	5	831	847	7
15	11	2	62	12	20	16	4	3	25	31	24	2	14	3	79	72	13	6	6	4	199	198	5	7	1	5	41	50	28
17	11	2	84	65	15	18	4	3	100	104	12	4	14	3	279	282	6	8	6	4	340	346	5	9	1	5	168	164	6
0	12	2	1330	1318	10	20	4	3	159	146	9	6	14	3	125	140	9	10	6	4	1368	1379	10	11	1	5	91	98	11
2	12	2	193	196	6	1	5	3	73	70	9	8	14	3	272	269	6	12	6	4	161	169	8	13	1	5	82	89	12
4	12	2	248	254	5	3	5	3	170	178	4	10	14	3	361	365	6	14	6	4	182	186	7	15	1	5	250	259	6
6	12	2	769	785	7	5	5	3	470	454	4	12	14	3	58	40	25	16	6	4	137	144	9	17	1	5	698	699	6
8	12	2	253	249	6	7	5	3	811	811	6	1	15	3	203	202	7	18	6	4	251	256	7	19	1	5	424	436	6
10	12	2	611	618	6	9	5	3	251	250	5	3	15	3	327	332	6	1	7	4	186	169	5	0	2	5	882	877	6
12	12	2	323	331	6	11	5	3	154	135	6	5	15	3	247	257	7	3	7	4	145	343	4	2	2	5	205	192	5
14	12	2	376	165	6	13	5	3	435	444	5	7	15	3	236	242	7	5	7	4	1216	1237	9	4	2	5	282	284	4
16	12	2	583	589	6	15	5	3	374	378	5	9	15	3	62	58	21	7	7	4	422	431	4	6	2	5	477	485	5
1	13	2	73	86	13	17	5	3	240	241	6	11	15	3	344	330	6	9	7	4	801	811	6	8	2	5	220	218	5
3	13	2	21	11	20	19	5	3	30	9	29	0	16	3	293	282	6	11	7	4	809	789	6	10	2	5	289	314	5
5	13	2	1687	1680	11	0	6	3	509	493	4	2	16	3	40	7	39	13	7	4	184	184	7	12	2	5	655	659	6
7	13	2	64	67	17	2	6	3	197	191	4	4	16	3	301	296	6	15	7	4	302	303	6	14	2	5	19	25	18
9	13	2	10	15	9	4	6	3	530	520	5	6	16	3	1140	1142	9	17	7	4	558	548	6	16	2	5	81	81	14
11	13	2	131	142	10	6	6	3	1339	1340	10	8	16	3	333	327	6	0	8	4	1814	1870	11	18	2	5	145	136	9
13	13	2	183	171	8	8	6	3	367	368	4	10	16	3	248	244	7	2	8	4	41	50	36	1	3	5	136	135	6
15	13	2	580	577	6	10	6	3	173	166	6	1	17	3	223	219	7	4	8	4	352	353	4	3	3	5	244	241	5
0	14	2	271	272	6	12	6	3	334	337	5	3	17	3	181	179	8	6	8	4	646	650	5	5	3	5	576	592	5
2	14	2	327	141	5	14	6	3	74	61	13	5	17	3	609	608	6	8	8	4	382	389	5	7	3	5	46	47	22
4	14	2	682	683	6	16	6	3	1047	1051	8	7	17	3	40	22	40	10	8	4	943	945	7	9	3	5	109	107	9
6	14	2	519	519	5	18	6	3	412	399	6	0	18	3	214	199	8	12	8	4	50	36	22	11	3	5	170	172	7
8	14	2	216	202	7	20	6	3	444	446	6	2	18	3	227	235	8	14	8	4	33	43	33	13	3	5	205	211	6
10	14	2	0	2	1	1	7	3	156	152	5	4	18	3	140	132	10	16	8	4	327	323	7	15	3	5	71	80	17
12	14	2	42	29	41	3	7	3	116	134	7	2	0	4	317	329	4	18	8	4	0	25	1	17	3	5	474	482	6
14	14	2	256	264	7	5	7	3	1608	1610	10	4	0	4	432	446	4	1	9	4	67	33	13	0	4	5	249	241	5
1	15	2	714	706	6	7	7	3	214	213	5	6	0	4	266	261	4	3	9	4	153	153	6	2	4	5	110	92	8
3	15	2	193	189	7	9	7	3	318	317	5	8	0	4	457	457	4	5	9	4	1756	1813	12	4	4	5	0	4	1
5	15	2	1445	1434	10	11	7	3	912	927	7	10	0	4	2886	2892	12	7	9	4	467	464	5	6	4	5	575	574	5
7	15	2	434	438	5	13	7	3	156	157	7	12	0	4	1074	1074	8	9	9	4	64	58	16	8	4	5	265	263	5
9	15	2	106	95	11	15	7	3	103	95	12	14	0	4	448	458	5	11	9	4	255	244	6	10	4	5	482	485	5
11	15	2	470	467	6	17	7	3	702	680	6	16	0	4	91	69	12	13	9	4	29	39	28	12	4	5	395	399	5
13	15	2	147	144	10	19	7	3	152	140	10	18	0	4	378	378	6	15	9	4	650	665	6	14	4	5	290	284	6
0	16	2	888	893	8	0	8	3	1090	1089	8	20	0	4	419	414	6	17	9	4	694	691	6	16	4	5	498	487	6
2	16	2	184	181	7	2	8	3	34	25	33	1	1	4	486	473	4	0	10	4	814	821	6	18	4	5	230	236	7
4	16	2	103	115	12	4	8	3	166	164	5	3	1	4	17	30	16	2	10	4	147	120	7	1	5	5	143	132	6
6	16	2	624	633	6	6	8	3	558	549	5	5	1	4	91	75	8	4	10	4	359	353	5	3	5	5	184	162	5
8	16	2	64	5	21	8	8	3	127	129	7	7	1	4	112	122	7	6	10	4	173	171	6	5	5	5	401	391	4
10	16	2	811	807	7	10	8	3	361	356	5	9	1	4	960	978	7	8	10	4	283	286	5	7	5	5	552	562	5
1	17	2	276	287	6	12	8	3	533	529	5	11	1	4	1823	1861	12	10	10	4	399	414	5	9	5	5	263	263	5
3	17	2	389	393	6	14	8	3	260	266	6	13	1	4	309	311	5	12	10	4	357	357	6	11	5	5	259	258	6
5	17	2	0	9	1	16	8	3	119	131	12	15	1	4	115	107	9	14	10	4	683	700	6	13	5	5	401	405	5
7	17	2	240	248	7	18	8	3	104	47	12	17	1	4	129	139	9	16	10	4	481	475	6	15	5	5	278	270	6
9	17	2	313	306	7	1	9	3	573	589	5	19	1	4	404	407	6	1	11	4	198	191	6	17	5	5	131	128	10
0	18	2	600	594	6	3	9	3	210	203	5	0	2	4	304	326	4	3	11	4	298	296	5	0	6	5	377	407	4
2	18	2	140	142	10	5	9	3	237	222	5	2	2	4	259	254	4	5	11	4	852	873	7	2	6	5	43	41	25
4	18	2	320	316	6	7	9	3	188	190	6	4	2	4	312	302	4	7	11	4	87	69	11	4	6	5	38	4	38
6	18	2	160	159	6	9	9	3	49	35	21	6	2	4	433	464	4	9	11	4	50	72	28	6	6	5	545	546	5
1	1	3	170	158	4	11	9	3	930	946	7	8	2	4	78	78	11	11	11	4	60	55	20	8	6	5	342	346	5
3	1	3	485	479	4	13	9	3	108	107	10	10	2	4	350	351	4	13	11	4	186	190	8	10	6	5	59	65	19
5	1	3	47	41	13	15	9	3	260	246	6	12	2	4	467	478	5	15	11	4	504	495	6	12	6	5	265	255	6
7	1	3	425	423	4	17	9	3	370	392	6	14	2	4	629	625	6	0	12	4	1012	1022	8	14	6	5	43	40	43
9	1	3	132	138	6	0	10	3	1091	1088	8	16	2	4	821	833	7	2	12	4	129	133	9	16	6	5	667	649	6
11	1	3	1180	1172	8	2	10	3	697	706	6	18	2	4	244	255	7	4	12	4	313	315	5	1	7	5	107	94	9
13	1	3	321	318	5	4	10	3	218	214	5	20	2	4	42	23	42	6	12	4	246	253	6	3	7	5	361	377	5
15	1	3	419	418	5	6	10	3	332	325	5	1	3	4	129	144	6	8	12	4	221	219	6	5	7	5	389	373	5
17	1	3	319	324	6	8	10	3	161	167	7	3	3	4	356	358	4	10	12	4	607	608	6	7	7	5	289	294	5
19	1	3	554	543	5	10	10	3	232	239	6	5	3	4	3522	3449	10	12	12	4	386	381	6	9	7	5	190	189	6
21	1	3	425	428	6	12	10	3	62	66	19	7	3	4	204	210	5	14	12	4	69	63	21	11	7	5	273	270	6
0	2	3	2057	1985	8	14	10	3	578	583	6	9	3	4	521	536	5	1	13	4	421	416	5	13	7	5	136	140	9
2	2	3	743	700	5	16	10	3	434	411	6	11	3	4	222	228	5	3	13	4	213	215	7	15	7	5	239	252	7
4	2	3	293	289	3	18	10	3	76	76	18	13	3	4	222	220	6	5	13	4	201	208	7	17	7	5	0	9	1
6	2	3	1041	1009	7	1	11	3	148	152	7	15	3	4	860	860	7	7	13	4	310	314	6	0	8	5	584	607	5

Observed and calculated structure factors for K30

h	k	l	10Fo	10Fc	10s
2	8	5	242	237	5
4	8	5	169	168	6
6	8	5	563	557	5
8	8	5	64	65	16
10	8	5	200	207	7
12	8	5	371	332	6
14	8	5	446	440	6
16	8	5	474	467	6
1	9	5	677	675	6
3	9	5	46	2	24
5	9	5	554	545	5
7	9	5	313	311	5
9	9	5	0	4	1
11	9	5	1543	1562	12
13	9	5	186	184	8
15	9	5	217	222	7
0	10	5	1187	1181	9
2	10	5	458	450	5
4	10	5	0	0	1
6	10	5	551	549	5
8	10	5	61	64	19
10	10	5	404	401	6
12	10	5	89	83	14
14	10	5	444	437	6
1	11	5	18	25	17
3	11	5	31	0	31
5	11	5	643	633	6
7	11	5	472	495	5
9	11	5	159	148	8
11	11	5	214	213	7
13	11	5	205	223	8
0	12	5	959	972	8
2	12	5	554	550	5
4	12	5	40	5	39
6	12	5	797	806	7
8	12	5	51	44	30
10	12	5	105	84	12
12	12	5	169	164	9
1	13	5	437	435	5
3	13	5	149	158	9
5	13	5	1038	1052	8
7	13	5	203	204	7
9	13	5	231	227	8
11	13	5	1381	1370	10
0	14	5	1169	1143	8
2	14	5	156	96	9
4	14	5	289	292	6
6	14	5	428	430	6
8	14	5	114	123	12
10	14	5	517	520	6
1	15	5	46	55	46
3	15	5	341	345	6
5	15	5	80	63	17
7	15	5	317	332	7
0	16	5	374	384	6
2	16	5	204	198	8
4	16	5	40	15	39
0	0	6	2586	2567	12
2	0	6	173	164	6
4	0	6	484	485	5
6	0	6	714	709	6
8	0	6	418	438	5
10	0	6	950	958	7
12	0	6	829	827	7
14	0	6	723	706	6
16	0	6	992	981	8
1	1	6	202	190	5
3	1	6	100	100	9
5	1	6	1629	1658	12
7	1	6	166	168	7
9	1	6	308	320	5
11	1	6	219	234	6
13	1	6	85	92	14
15	1	6	433	433	6
17	1	6	311	313	6
0	2	6	1758	1749	12
2	2	6	194	194	6
4	2	6	123	116	7
6	2	6	482	489	5
8	2	6	148	149	7
10	2	6	903	914	7
12	2	6	364	368	5
14	2	6	115	115	10
16	2	6	317	325	6
1	3	6	333	326	5
3	3	6	46	23	24
5	3	6	935	924	7
7	3	6	142	141	8
9	3	6	754	769	6
11	3	6	1238	1281	9
13	3	6	57	58	23
15	3	6	166	163	8
17	3	6	476	470	6
0	4	6	2310	2322	12
2	4	6	68	50	13
4	4	6	307	302	5
6	4	6	562	562	5
8	4	6	119	131	9
10	4	6	1318	1345	10
12	4	6	110	102	11
14	4	6	45	39	45
16	4	6	244	240	7
1	5	6	326	336	5
3	5	6	307	314	5
5	5	6	591	571	5
7	5	6	91	89	11
9	5	6	324	328	5
11	5	6	263	277	6
13	5	6	71	69	17
15	5	6	364	341	6
0	6	6	39	61	39
2	6	6	149	139	7
4	6	6	213	201	6
6	6	6	1046	1066	8
8	6	6	293	309	6
10	6	6	148	148	8
12	6	6	219	215	7
14	6	6	606	600	6
16	6	6	899	900	8
1	7	6	464	465	5
3	7	6	20	28	19
5	7	6	2470	2490	13
7	7	6	107	119	10
9	7	6	309	321	6
11	7	6	369	379	6
13	7	6	246	242	7
15	7	6	752	755	7
0	8	6	251	239	6
2	8	6	274	280	6
4	8	6	331	332	5
6	8	6	283	275	6
8	8	6	340	348	6
10	8	6	239	237	7
12	8	6	82	1	15
14	8	6	314	302	7
1	9	6	434	431	5
3	9	6	36	1	35
5	9	6	73	85	16
7	9	6	586	600	6
9	9	6	303	300	6
11	9	6	759	758	6
13	9	6	84	95	16
0	10	6	2157	2184	14
2	10	6	275	211	6
4	10	6	173	188	7
6	10	6	537	550	6
8	10	6	119	110	11
10	10	6	1315	1297	10
12	10	6	325	308	6
1	11	6	223	225	6
3	11	6	331	336	6
5	11	6	495	501	5
7	11	6	158	175	9
9	11	6	349	356	6
11	11	6	834	834	7
0	12	6	525	533	6
2	12	6	179	169	8
4	12	6	199	185	7
6	12	6	827	824	7
8	12	6	91	100	15
10	12	6	339	331	6
1	13	6	33	26	32
3	13	6	48	8	37
5	13	6	1238	1245	10
7	13	6	81	76	16
0	14	6	160	154	9
2	14	6	383	386	6
4	14	6	294	287	7
6	14	6	204	181	8
1	1	7	95	86	10
3	1	7	168	171	7
5	1	7	142	149	8
7	1	7	272	272	6
9	1	7	112	102	10
11	1	7	652	661	6
13	1	7	211	223	7
15	1	7	272	285	7
0	2	7	634	632	6
2	2	7	348	342	5
4	2	7	69	55	14
6	2	7	512	508	5
8	2	7	263	254	6
10	2	7	150	148	8
12	2	7	398	398	6
14	2	7	187	194	8
1	3	7	273	275	5
3	3	7	10	6	10
5	3	7	437	430	5
7	3	7	340	344	5
9	3	7	117	116	10
11	3	7	924	900	7
13	3	7	70	55	17
0	4	7	1181	1148	8
2	4	7	25	22	25
4	4	7	136	123	8
6	4	7	194	194	7
8	4	7	116	106	9
10	4	7	527	551	6
12	4	7	445	431	6
14	4	7	107	113	13
1	5	7	56	21	19
3	5	7	69	65	16
5	5	7	66	68	17
7	5	7	484	496	5
9	5	7	165	179	8
11	5	7	14	19	13
13	5	7	281	274	7
0	6	7	231	233	6
2	6	7	132	144	9
4	6	7	211	210	6
6	6	7	778	784	7
8	6	7	245	251	7
10	6	7	117	122	11
12	6	7	215	202	8
1	7	7	132	131	9
3	7	7	158	157	8
5	7	7	1000	994	7
7	7	7	110	105	10
9	7	7	228	218	7
11	7	7	611	605	6
0	8	7	709	711	6
2	8	7	39	20	19
4	8	7	119	106	9
6	8	7	371	370	6
8	8	7	6	18	6
10	8	7	310	296	7
12	8	7	381	368	6
1	9	7	325	331	6
3	9	7	140	132	9
5	9	7	257	249	6
7	9	7	135	142	10
9	9	7	0	1	1
11	9	7	563	559	6
0	10	7	675	671	6
2	10	7	408	411	6
4	10	7	106	101	11
6	10	7	221	214	7
8	10	7	93	99	14
1	11	7	77	89	17
3	11	7	0	16	1
5	11	7	648	636	6
7	11	7	127	124	11
0	12	7	89	57	14
2	12	7	245	233	7
4	12	7	286	293	7
6	12	7	144	147	10
1	13	7	251	248	7
0	0	8	2604	2575	14
2	0	8	113	117	10
4	0	8	111	105	10
6	0	8	638	638	6
8	0	8	79	82	15
10	0	8	1592	1600	11
12	0	8	579	585	6
1	1	8	217	219	7
3	1	8	75	66	14
5	1	8	414	398	5
7	1	8	287	282	6
9	1	8	530	524	6
11	1	8	618	623	6
0	2	8	279	28	5
2	2	8	134	137	9
4	2	8	181	175	7
6	2	8	531	507	6
8	2	8	30	10	29
10	2	8	187	170	8
1	3	8	74	64	15
3	3	8	235	236	6
5	3	8	1858	1847	12
7	3	8	7	3	7
9	3	8	276	276	7
11	3	8	86	52	16
0	4	8	206	216	7
2	4	8	358	356	6
4	4	8	100	94	13
6	4	8	760	755	7
8	4	8	0	8	1
10	4	8	198	202	8
1	5	8	529	528	5
3	5	8	160	166	8
5	5	8	422	420	6
7	5	8	0	36	1
9	5	8	38	24	37
0	6	8	1830	1809	12
2	6	8	166	171	8
4	6	8	249	234	6
6	6	8	467	483	6
8	6	8	109	116	12
1	7	8	0	1	1
3	7	8	245	250	7
5	7	8	882	879	7
7	7	8	269	260	7
9	7	8	459	456	6
0	8	8	911	924	8
2	8	8	42	31	42
4	8	8	102	105	13
6	8	8	449	451	6
1	9	8	0	28	1
3	9	8	29	51	28
5	9	8	1275	1286	10
0	10	8	1031	1026	8
2	10	8	78	3	17
1	1	9	35	7	34
3	1	9	113	112	11
5	1	9	415	411	6
7	1	9	113	110	12
0	2	9	226	220	7
2	2	9	140	133	10
4	2	9	90	71	14
6	2	9	85	73	16
1	3	9	72	74	19
3	3	9	52	6	30
5	3	9	173	165	8
0	4	9	424	424	6
2	4	9	43	34	42
4	4	9	82	63	15
1	5	9	67	41	21
3	5	9	73	44	18
0	6	9	142	136	10

Observed and calculated structure factors for K31

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	672	752	3	0	8	0	2499	2537	8	3	19	0	177	177	8	3	9	1	52	25	13	1	1	2	595	561	4
4	0	0	1054	1116	5	2	8	0	174	161	4	1	1	1	147	150	3	5	9	1	402	428	4	3	1	2	780	767	5
6	0	0	542	566	4	4	8	0	561	547	4	3	1	1	303	302	3	7	9	1	305	308	4	5	1	2	1014	1007	6
8	0	0	1028	1036	6	6	8	0	673	669	5	5	1	1	971	1000	6	9	9	1	53	27	17	7	1	2	81	67	6
10	0	0	3617	3730	8	8	8	0	456	473	4	7	1	1	37	8	14	11	9	1	1642	1644	10	9	1	2	592	601	4
12	0	0	1408	1444	10	10	8	0	1140	1111	8	9	1	1	265	257	3	13	9	1	139	135	7	11	1	2	605	615	5
14	0	0	301	306	4	12	8	0	92	103	9	11	1	1	665	688	5	15	9	1	222	204	6	13	1	2	35	15	35
16	0	0	354	348	4	14	8	0	97	76	9	13	1	1	274	271	4	17	9	1	67	84	17	15	1	2	664	665	5
18	0	0	378	382	5	16	8	0	348	345	5	15	1	1	281	274	5	19	9	1	210	225	7	17	1	2	59	58	16
20	0	0	452	450	5	18	8	0	47	41	28	17	1	1	651	660	5	0	10	1	1358	1416	8	19	1	2	63	48	15
22	0	0	1811	1809	12	20	8	0	297	273	6	19	1	1	520	512	5	2	10	1	727	744	5	21	1	2	289	291	6
1	1	0	804	873	3	1	9	0	85	74	7	21	1	1	560	543	5	4	10	1	165	165	5	0	2	2	4314	4092	6
3	1	0	255	269	2	3	9	0	307	306	4	0	2	1	159	180	3	6	10	1	485	490	4	2	2	2	400	387	3
5	1	0	504	542	3	5	9	0	1832	1891	10	2	2	1	576	596	4	8	10	1	105	120	9	4	2	2	478	474	4
7	1	0	367	369	3	7	9	0	847	841	6	4	2	1	342	340	3	10	10	1	353	363	5	6	2	2	499	502	4
9	1	0	1388	1413	8	9	9	0	109	96	8	6	2	1	281	276	3	12	10	1	0	22	1	8	2	2	163	168	4
11	1	0	2936	2990	9	11	9	0	680	664	5	8	2	1	474	497	4	14	10	1	595	595	5	10	2	2	1331	1362	8
13	1	0	466	466	4	13	9	0	199	210	6	10	2	1	103	96	6	16	10	1	514	488	5	12	2	2	570	581	4
15	1	0	216	231	5	15	9	0	754	760	6	12	2	1	804	836	6	18	10	1	136	165	10	14	2	2	46	33	18
17	1	0	388	390	5	17	9	0	554	547	5	14	2	1	107	104	7	1	11	1	81	83	9	16	2	2	304	308	5
19	1	0	473	458	5	19	9	0	99	119	13	16	2	1	513	525	5	3	11	1	63	41	12	18	2	2	17	53	17
21	1	0	841	819	7	0	10	0	268	270	4	18	2	1	48	3	19	5	11	1	827	831	6	20	2	2	140	139	9
0	2	0	1178	1251	4	2	10	0	164	159	5	20	2	1	145	338	5	7	11	1	484	491	4	1	3	2	519	516	4
2	2	0	334	371	3	4	10	0	269	276	4	22	2	1	248	248	7	9	11	1	264	262	5	3	3	2	174	167	3
4	2	0	513	540	3	6	10	0	282	282	4	1	3	1	379	400	3	11	11	1	168	162	7	5	3	2	1166	1140	8
6	2	0	119	136	4	8	10	0	266	270	5	3	3	1	274	261	3	13	11	1	159	158	8	7	3	2	239	245	3
8	2	0	230	235	3	10	10	0	507	503	5	5	3	1	384	380	3	15	11	1	351	339	6	9	3	2	1240	1266	8
10	2	0	536	541	4	12	10	0	291	294	5	7	3	1	373	376	3	17	11	1	412	409	6	11	3	2	1487	1554	10
12	2	0	461	470	4	14	10	0	964	980	7	9	3	1	221	232	4	0	12	1	922	950	6	13	3	2	262	264	5
14	2	0	808	821	6	16	10	0	318	321	6	11	3	1	348	377	4	2	12	1	549	562	4	15	3	2	268	248	5
16	2	0	804	798	6	18	10	0	344	334	6	13	3	1	188	201	5	4	12	1	155	152	6	17	3	2	408	416	5
18	2	0	181	169	6	1	11	0	261	251	4	15	3	1	105	117	8	6	12	1	725	714	6	19	3	2	716	715	6
20	2	0	50	43	24	3	11	0	227	243	4	17	3	1	274	267	5	8	12	1	75	84	12	21	3	2	705	691	6
22	2	0	197	215	8	5	11	0	670	685	5	19	3	1	182	182	6	10	12	1	27	5	27	0	4	2	1775	1715	7
1	3	0	298	313	3	7	11	0	46	67	21	21	3	1	352	358	6	12	12	1	217	203	6	2	4	2	621	598	4
3	3	0	486	506	3	9	11	0	111	83	8	0	4	1	1225	1225	6	14	12	1	55	75	23	4	4	2	95	84	6
5	3	0	4691	4773	7	11	11	0	451	452	5	2	4	1	136	145	4	16	12	1	742	708	6	6	4	2	382	360	3
7	3	0	537	543	4	13	11	0	228	229	6	4	4	1	114	123	5	1	13	1	462	457	4	8	4	2	85	93	8
9	3	0	762	789	5	15	11	0	673	672	6	6	4	1	624	612	4	3	13	1	284	277	5	10	4	2	1935	1995	10
11	3	0	418	427	4	17	11	0	475	455	6	8	4	1	345	354	3	5	13	1	1011	1011	7	12	4	2	114	115	7
13	3	0	238	245	4	0	12	0	1413	1481	9	10	4	1	605	608	4	7	13	1	85	87	11	14	4	2	147	147	6
15	3	0	912	909	7	2	12	0	155	147	5	12	4	1	608	628	5	9	13	1	285	271	5	16	4	2	0	26	1
17	3	0	987	992	7	4	12	0	341	337	4	14	4	1	268	266	5	11	13	1	1217	1199	8	18	4	2	509	501	5
19	3	0	307	310	5	6	12	0	525	520	5	16	4	1	448	449	5	13	13	1	172	177	8	20	4	2	231	242	7
21	3	0	277	273	6	8	12	0	167	170	6	18	4	1	215	223	6	15	13	1	120	124	11	1	5	2	990	961	6
0	4	0	1962	2034	5	10	12	0	752	740	6	20	4	1	51	51	25	0	14	1	860	885	6	3	5	2	61	49	8
2	4	0	672	671	4	12	12	0	484	490	5	1	5	1	111	116	4	2	14	1	163	150	6	5	5	2	1834	1832	9
4	4	0	855	878	6	14	12	0	113	118	10	3	5	1	381	378	3	4	14	1	379	386	5	7	5	2	241	233	4
6	4	0	3816	3846	8	16	12	0	0	4	1	5	5	1	1103	1082	7	6	14	1	264	256	5	9	5	2	486	485	4
8	4	0	381	376	3	1	13	0	565	562	5	7	5	1	824	829	6	8	14	1	238	237	6	11	5	2	652	655	5
10	4	0	462	468	4	3	13	0	238	241	5	9	5	1	402	395	4	10	14	1	428	417	5	13	5	2	87	70	9
12	4	0	226	232	4	5	13	0	301	292	5	11	5	1	281	296	4	12	14	1	137	128	10	15	5	2	311	317	5
14	4	0	577	568	5	7	13	0	479	475	5	13	5	1	549	562	5	14	14	1	249	271	8	17	5	2	677	673	6
16	4	0	2045	2060	12	9	13	0	285	272	6	15	5	1	204	204	5	1	15	1	47	27	22	19	5	2	327	322	6
18	4	0	72	36	12	11	13	0	901	895	7	17	5	1	183	178	6	3	15	1	374	379	5	21	5	2	345	340	6
20	4	0	148	149	8	13	13	0	284	267	6	19	5	1	19	5	18	5	15	1	103	90	10	0	6	2	1110	1111	6
22	4	0	520	508	6	15	13	0	265	276	7	21	5	1	543	532	6	7	15	1	325	332	6	2	6	2	58	33	9
1	5	0	1447	1469	6	0	14	0	1244	1262	8	0	6	1	528	518	4	9	15	1	0	11	1	4	6	2	740	748	5
3	5	0	67	71	7	2	14	0	339	349	5	2	6	1	99	97	5	11	15	1	138	141	10	6	6	2	2495	2498	9
5	5	0	3044	3034	8	4	14	0	208	197	6	4	6	1	289	289	3	13	15	1	235	214	7	8	6	2	302	293	4
7	5	0	917	919	6	6	14	0	685	694	5	6	6	1	950	1005	6	0	16	1	401	398	5	10	6	2	175	185	5
9	5	0	71	50	9	8	14	0	178	163	7	8	6	1	539	538	4	2	16	1	173	163	7	12	6	2	345	353	4
11	5	0	407	431	4	10	14	0	1180	1160	8	10	6	1	120	111	6	4	16	1	53	63	22	14	6	2	725	716	5
13	5	0	173	186	5	12	14	0	67	73	20	12	6	1	350	348	4	6	16	1	1256	1247	9	16	6	2	1540	1556	11
15	5	0	193	206	6	14	14	0	31	27	31	14	6	1	35	15	35	8	16	1	348	345	6	18	6	2	22	37	22
17	5	0	520	502	5	1	15	0	130	321	5	16	6	1	947	956	7	10	16	1	53	64	28	20	6	2	79	52	14
19	5	0	134	133	8	3	15	0	320	315	5	18	6	1	267	269	6	12	16	1	0	24	1	1	7	2	636	647	5
21	5	0	465	452	6	5	15	0	496	511	5	20	6	1	473	460	6	1	17	1	114	113	9	3	7	2	111	114	6
0	6	0	748	784	5	7	15	0	108	117	10	1	7	1	146	137	4	3	17	1	182	179	7	5	7	2	4331	4380	10
2	6	0	190	190	3	9	15	0	200	210	7	3	7	1	458	471	4	5	17	1	834	820	7	7	7	2	159	149	5
4	6	0	216	212	3	11	15	0	420	402	6	5	7	1	832	841	6	7	17	1	236	228	7	9	7	2	427	449	4
6	6	0	460	450	4	13	15	0	359	343	6	7	7	1	212	196	4	9	17	1	263	264	7	11	7	2	89	94	9
8	6	0	645	638	5	0	16	0	553	550	5	9	7	1	331	336	4	0	18	1	307	302	6	13	7	2	350	345	5
10	6	0	1447	1473	10	2	16	0	259	261	6	11	7	1	86	109	10	2	18	1	102	109	11	15	7	2	980	993	7
12	6	0	116	130	7	4	16	0	131	122	8	13	7	1	34	52	34	4	18	1	305	302	6	17	7	2	1026	1035	7
14	6	0	376	383	4	6	16	0	708	705	6	15	7	1	149	156	7	6	18	1	293	275	6	19	7	2	134	134	9
16	6	0	474	466	5	8	16	0	110	101	10	17	7	1	275	259	6	1	19	1	422	410	6	0	8	2	419	410	4
18	6	0	357	361	5	10	16	0	122	123	10	19	7	1	162	158	8	3	19	1	402	386	6	2	8	2	541	538	4
20	6	0	34	14	33	12	16	0	457	450	6	0	8	1	389	376	3	0	0	2	3644	3360	6	4	8	2	233	240	4
1	7	0	563	567	4	1	17	0	333	321	5	2	8	1	134	119	5	2	0	2	710	690	5	6	8	2	371	369	4
1	7	0	266	265	3	1	17	0	299	291	6	4	8	1	62	71	11	4	0	2	185	172	3	8	8	2	543	555	4
5	7	0	1344	1343	9	5	17	0	1635	1618	10	6	8	1	267	291	4	6	0	2	732	697	5	10	8	2	94	99	9
7	7	0	536	511	4	7	17	0	66	55	18	8	8	1	11	41	10	8	0	2	654	646	5	12	8	2	0	13	1
9	7	0	1058	1058	7	9	17	0	0	42	1	10	8	1	188	197	6	10	0	2	1476	1473	9	14	8	2	464	469	5
11	7	0	633	604	5	0	18	0	405	394	6	12	8	1	457	462	4	12	0	2	1072	1067	7	16	8	2	870	868	7
13	7	0	266	259	5	2	18	0	262	259	6	14	8	1	488	484	5	14	0	2	1235	1257	8	18	8	2	30	26	10
15	7	0	104	313	5	4	18	0	84	71	14	16	8	1	420	422	5	16	0	2	854	874	6	20	8	2	153	167	10
17	7	0	403	394	5	6	18	0	317	310	6	18	8	1	264	265	6	18	0	2	515	503	5	1	9	2	519	508	4
19	7	0	621	610	6	8	18	0	247	258	7	20	8	1	163	150	6	20	0	2	214	209	7	3	9	2	153	155	5
21	7	0	600	572	6	1	19	0	154	153	9	1	9	1	887	882	6	22	0	2	433	427	6	5	9	2	561	561	4

Observed and calculated structure factors for K31

h	k	l	10Fo	10Fc	10s
7	9	2	504	500	4
9	9	2	521	519	5
11	9	2	1539	1548	10
13	9	2	220	232	6
15	9	2	97	73	11
17	9	2	753	741	6
19	9	2	261	267	7
0	10	2	4175	4269	10
2	10	2	552	557	4
4	10	2	649	647	5
6	10	2	112	121	8
8	10	2	275	287	5
10	10	2	1779	1779	13
12	10	2	389	401	5
14	10	2	291	299	6
16	10	2	164	166	9
18	10	2	148	165	9
1	11	2	437	450	4
3	11	2	682	680	5
5	11	2	68	48	12
7	11	2	0	15	1
9	11	2	525	529	5
11	11	2	1790	1796	11
13	11	2	44	50	38
15	11	2	93	58	12
17	11	2	55	70	28
0	12	2	1293	1290	8
2	12	2	161	155	6
4	12	2	180	179	6
6	12	2	781	786	6
8	12	2	200	203	6
10	12	2	638	634	6
12	12	2	290	286	6
14	12	2	392	388	6
16	12	2	511	497	6
1	13	2	133	128	7
3	13	2	38	20	37
5	13	2	1625	1644	10
7	13	2	45	40	25
9	13	2	18	31	18
11	13	2	133	147	9
13	13	2	128	135	10
15	13	2	540	533	6
0	14	2	312	311	5
2	14	2	328	326	5
4	14	2	646	652	5
6	14	2	483	484	5
8	14	2	198	195	7
10	14	2	87	47	13
12	14	2	0	3	1
14	14	2	259	267	7
1	15	2	628	641	5
3	15	2	200	191	6
5	15	2	1389	1378	10
7	15	2	459	443	5
9	15	2	42	39	41
11	15	2	441	429	6
13	15	2	125	125	11
0	16	2	879	883	6
2	16	2	179	160	7
4	16	2	104	96	10
6	16	2	607	597	6
8	16	2	0	3	1
10	16	2	754	739	6
1	17	2	270	259	6
3	17	2	396	385	6
5	17	2	41	33	41
7	17	2	165	170	8
9	17	2	305	296	7
0	18	2	599	586	6
2	18	2	112	98	11
4	18	2	276	274	6
6	18	2	127	338	7
1	1	3	211	189	3
3	1	3	554	523	4
5	1	3	0	11	1
7	1	3	178	171	3
9	1	3	222	225	4
11	1	3	1219	1222	9
13	1	3	158	364	4
15	1	3	125	333	5
17	1	3	110	306	5
19	1	3	503	507	5
21	1	3	521	524	6
0	2	3	2238	2055	8
2	2	3	716	659	5
4	2	3	221	207	3
6	2	3	1064	1035	7
8	2	3	640	625	5
10	2	3	68	49	11
12	2	3	631	640	5
14	2	3	305	320	5
16	2	3	889	897	6
18	2	3	170	183	7
20	2	3	250	253	7
1	3	3	539	499	4
3	3	3	260	235	3
5	3	3	987	943	6
7	3	3	716	701	5
9	3	3	191	191	5
11	3	3	1364	1396	9
13	3	3	0	5	1
15	3	3	186	204	6
17	3	3	257	263	6
19	3	3	87	101	12
21	3	3	412	399	6
0	4	3	2393	2229	8
2	4	3	0	0	-1
4	4	3	295	284	3
6	4	3	312	304	4
8	4	3	142	148	6
10	4	3	677	671	5
12	4	3	665	685	5
14	4	3	106	106	8
16	4	3	83	80	11
18	4	3	106	125	11
20	4	3	96	100	12
1	5	3	46	54	13
3	5	3	233	234	4
5	5	3	593	569	4
7	5	3	825	813	6
9	5	3	299	305	4
11	5	3	136	135	7
13	5	3	433	430	4
15	5	3	241	250	6
17	5	3	228	232	6
19	5	3	31	43	30
0	6	3	492	475	4
2	6	3	172	175	4
4	6	3	518	508	4
6	6	3	1315	1298	8
8	6	3	396	397	4
10	6	3	194	179	5
12	6	3	313	313	5
14	6	3	66	77	15
16	6	3	1025	1026	7
18	6	3	402	395	6
20	6	3	428	416	6
1	7	3	150	156	5
3	7	3	163	172	5
5	7	3	1477	1488	10
7	7	3	193	192	5
9	7	3	349	351	4
11	7	3	882	876	6
13	7	3	138	144	7
15	7	3	28	24	28
17	7	3	662	660	6
19	7	3	137	118	9
0	8	3	1047	1031	7
2	8	3	64	26	10
4	8	3	219	223	5
6	8	3	545	544	5
8	8	3	110	116	8
10	8	3	277	279	5
12	8	3	528	530	5
14	8	3	282	277	6
16	8	3	49	28	28
18	8	3	93	94	13
1	9	3	581	581	5
3	9	3	190	191	5
5	9	3	238	232	5
7	9	3	191	199	6
9	9	3	55	48	17
11	9	3	900	899	6
13	9	3	103	94	10
15	9	3	209	197	7
17	9	3	407	408	6
0	10	3	992	1024	7
2	10	3	725	736	5
4	10	3	274	263	5
6	10	3	269	272	5
8	10	3	182	186	6
10	10	3	174	178	7
12	10	3	70	64	15
14	10	3	594	583	5
16	10	3	264	278	7
1	11	3	201	195	5
3	11	3	54	5	15
5	11	3	872	879	6
7	11	3	186	197	6
9	11	3	310	316	5
11	11	3	132	92	9
13	11	3	45	15	30
15	11	3	185	182	8
17	11	3	506	517	6
0	12	3	126	121	7
2	12	3	346	344	5
4	12	3	408	410	5
6	12	3	228	230	6
8	12	3	32	11	32
10	12	3	0	33	1
12	12	3	205	200	7
14	12	3	154	170	9
16	12	3	469	441	6
1	13	3	365	359	5
3	13	3	384	395	5
5	13	3	439	441	5
7	13	3	119	124	9
9	13	3	208	216	7
11	13	3	529	511	5
13	13	3	0	46	1
15	13	3	0	32	1
0	14	3	258	249	5
2	14	3	119	112	9
4	14	3	307	304	5
6	14	3	144	139	8
8	14	3	284	296	6
10	14	3	244	262	7
12	14	3	63	35	20
1	15	3	197	190	6
3	15	3	298	299	6
5	15	3	276	280	6
7	15	3	212	209	7
9	15	3	44	63	43
11	15	3	346	322	6
0	16	3	231	226	6
2	16	3	24	20	24
4	16	3	252	259	7
6	16	3	1083	1084	8
8	16	3	307	303	6
10	16	3	185	204	8
1	17	3	190	185	7
3	17	3	193	209	8
5	17	3	559	548	6
7	17	3	0	18	1
0	18	3	175	177	8
2	18	3	190	206	8
4	18	3	135	131	9
2	0	4	395	372	4
4	0	4	560	543	4
6	0	4	347	320	4
8	0	4	393	385	4
10	0	4	2811	2818	11
12	0	4	1032	1030	7
14	0	4	440	446	5
16	0	4	8	23	7
18	0	4	414	418	5
20	0	4	333	331	6
1	1	4	447	404	4
3	1	4	58	31	10
5	1	4	154	139	5
7	1	4	90	66	7
9	1	4	1075	1079	8
11	1	4	1799	1798	12
13	1	4	285	282	5
15	1	4	141	132	7
17	1	4	66	83	16
19	1	4	442	434	6
0	2	4	337	354	3
2	2	4	259	239	4
4	2	4	365	355	4
6	2	4	466	466	4
8	2	4	98	90	8
10	2	4	387	381	4
12	2	4	418	423	4
14	2	4	602	618	5
16	2	4	778	786	6
18	2	4	172	169	8
20	2	4	0	11	1
1	3	4	189	181	4
3	3	4	437	401	4
5	3	4	3533	3434	10
7	3	4	212	205	5
9	3	4	622	615	5
11	3	4	158	155	6
13	3	4	252	244	5
15	3	4	814	808	6
17	3	4	760	778	6
19	3	4	275	273	6
0	4	4	563	554	4
2	4	4	527	481	4
4	4	4	484	487	4
6	4	4	2088	2052	10
8	4	4	145	150	6
10	4	4	359	371	4
12	4	4	171	170	6
14	4	4	612	615	5
16	4	4	1502	1537	10
18	4	4	106	112	11
1	5	4	1014	969	7
3	5	4	153	146	5
5	5	4	1557	1563	11
7	5	4	436	431	4
9	5	4	13	3	12
11	5	4	918	934	6
13	5	4	33	45	33
15	5	4	240	245	6
17	5	4	146	148	8
19	5	4	66	74	19
0	6	4	2052	2039	10
2	6	4	207	212	5
4	6	4	304	294	4
6	6	4	154	156	6
8	6	4	338	342	4
10	6	4	1313	1325	9
12	6	4	223	218	6
14	6	4	202	198	6
16	6	4	175	189	8
18	6	4	261	252	6
1	7	4	220	204	5
3	7	4	309	310	4
5	7	4	1237	1243	8
7	7	4	416	410	4
9	7	4	830	842	6
11	7	4	735	749	6
13	7	4	229	218	6
15	7	4	285	284	6
17	7	4	469	467	6
0	8	4	1832	1861	11
2	8	4	60	51	13
4	8	4	298	310	5
6	8	4	625	622	5
8	8	4	362	368	5
10	8	4	975	988	7
12	8	4	61	61	17
14	8	4	68	58	17
16	8	4	301	299	6
18	8	4	40	17	40
1	9	4	41	3	23
3	9	4	186	195	5
5	9	4	1748	1780	12
7	9	4	468	460	4
9	9	4	52	30	20
11	9	4	298	271	5
13	9	4	67	65	16
15	9	4	566	568	6
17	9	4	627	625	6
0	10	4	807	803	6
2	10	4	85	92	10
4	10	4	379	388	5
6	10	4	167	173	6
8	10	4	303	307	5
10	10	4	432	426	5
12	10	4	289	297	6
14	10	4	721	736	6
16	10	4	442	427	6
1	11	4	198	190	5
3	11	4	309	306	5
5	11	4	898	904	6
7	11	4	14	42	14
9	11	4	72	56	14
11	11	4	72	58	16
13	11	4	148	148	9
15	11	4	558	549	6
0	12	4	958	982	7
2	12	4	157	165	7
4	12	4	230	242	6
6	12	4	247	244	6
8	12	4	213	216	7
10	12	4	550	546	5
12	12	4	357	353	6
14	12	4	57	40	23
1	13	4	351	357	5
3	13	4	187	188	6
5	13	4	200	199	7
7	13	4	296	299	6
9	13	4	285	279	6
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13	13	4	140	157	10
0	14	4	1254	1260	9
2	14	4	194	207	7
4	14	4	305	311	6
6	14	4	465	481	5
8	14	4	138	147	9
10	14	4	902	916	7
12	14	4	45	39	44
1	15	4	278	292	6
3	15	4	334	338	6
5	15	4	273	266	6
7	15	4	56	25	25
9	15	4	181	199	8
0	16	4	150	172	9
2	16	4	249	252	7
4	16	4	74	54	16
6	16	4	403	395	6
8	16	4	46	34	45
1	17	4	365	362	6
3	17	4	213	200	7
1	1	5	46	34	16
3	1	5	135	125	6
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7	1	5	40	26	26
9	1	5	233	231	5
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13	1	5	143	134	7
15	1	5	193	197	7
17	1	5	703	703	6
19	1	5	420	410	6
0	2	5	898	858	6
2	2	5	189	165	5
4	2	5	357	352	4
6	2	5	518	493	4
8	2	5	249	240	5
10	2	5	207	200	6
12	2	5	697	692	6
14	2	5	28	24	28
16	2	5	138	127	8
18	2	5	116	108	10
1	3	5	141	135	5
3	3	5	258	248	4
5	3	5	595	588	5
7	3	5	66	70	12
9	3	5	118	113	7
11	3	5	212	211	6
13	3	5	227	227	6
15	3	5	63	47	15
17	3	5	499	501	5
0	4	5	223	213	4
2	4	5	153	89	5
4	4	5	59	37	13
6	4	5	615	600	5
8	4	5	297	287	5
10	4	5	397	392	5
12	4	5	425	428	5
14	4	5	277	275	6
16	4	5	522	530	5
18	4	5	234	241	7
1	5	5	153	154	6
3	5	5	216	204	5
5	5	5	507	486	5
7	5	5	574	567	5
9	5	5	303	306	5
11	5	5	272	264	5
13	5	5	399	403	5
15	5	5	174	167	7
17	5	5	137	127	10
0	6	5	398	432	4
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6	6	5	517	508	5
8	6	5	372	374	5
10	6	5	79	71	11
12	6	5	259	256	6
14	6	5	42	30	42
16	6	5	647	652	6
1	7	5	100	95	8
3	7	5	413	410	4
5	7	5	303	296	5
7	7	5	303	309	5
9	7	5	239	223	6
11	7	5	315	305	5
13	7	5	138	154	8
15	7	5	180	193	8
17	7	5	37	15	37
0	8	5	652	652	5
2	8	5	214	198	5
4	8	5	121	118	8
6	8	5	571	567	5
8	8	5	92	72	10
10	8	5	160	152	7

Observed and calculated structure factors for K31

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
12	8	5	337	321	5	3	1	6	138	126	6	4	8	6	329	329	5	13	3	7	74	57	16	3	1	8	106	91	9
14	8	5	438	452	6	5	1	6	1718	1688	12	6	8	6	290	282	6	0	4	7	1179	1151	8	5	1	8	447	448	5
16	8	5	545	546	6	7	1	6	145	158	6	8	8	6	336	347	6	2	4	7	48	47	23	7	1	8	276	269	6
1	9	5	687	674	5	9	1	6	338	335	5	10	8	6	197	207	7	4	4	7	191	179	6	9	1	8	597	605	6
3	9	5	0	5	-1	11	1	6	224	206	6	12	8	6	41	54	41	6	4	7	177	170	7	11	1	8	616	608	6
5	9	5	528	531	5	13	1	6	83	84	12	14	8	6	325	330	6	8	4	7	137	140	8	0	2	8	0	18	1
7	9	5	317	316	5	15	1	6	434	430	6	1	9	6	405	398	5	10	4	7	473	475	5	2	2	8	162	143	7
9	9	5	0	22	1	17	1	6	313	307	6	3	9	6	0	35	1	12	4	7	451	459	6	4	2	8	224	218	6
11	9	5	1521	1529	10	0	2	6	1825	1774	12	5	9	6	71	62	13	14	4	7	106	121	12	6	2	8	526	530	5
13	9	5	166	166	8	2	2	6	225	220	5	7	9	6	564	574	5	1	5	7	0	11	1	8	2	8	0	17	1
15	9	5	171	189	9	4	2	6	177	159	5	9	9	6	364	361	6	3	5	7	84	98	12	10	2	8	207	194	7
0	10	5	1133	1137	8	6	2	6	530	520	5	11	9	6	728	737	6	5	5	7	137	131	8	1	3	8	107	107	9
2	10	5	468	475	5	8	2	6	188	198	6	13	9	6	58	50	24	7	5	7	507	517	5	3	3	8	281	289	6
4	10	5	61	38	15	10	2	6	881	890	7	0	10	6	2171	2188	14	9	5	7	214	218	7	5	3	8	1876	1897	12
6	10	5	527	509	5	12	2	6	142	141	5	2	10	6	244	250	6	11	5	7	40	25	39	7	3	8	16	10	16
8	10	5	71	77	15	14	2	6	73	84	15	4	10	6	227	241	6	13	5	7	251	270	7	9	3	8	347	347	6
10	10	5	354	361	6	16	2	6	351	365	6	6	10	6	553	570	5	0	6	7	241	231	5	11	3	8	92	112	13
12	10	5	80	81	15	1	3	6	291	288	5	8	10	6	115	97	10	2	6	7	161	149	6	0	4	8	252	248	5
14	10	5	456	448	6	3	3	6	22	7	22	10	10	6	1269	1290	9	4	6	7	221	218	6	2	4	8	341	341	5
1	11	5	0	10	1	5	3	6	909	895	7	12	10	6	251	261	7	6	6	7	782	782	6	4	4	8	172	150	7
3	11	5	68	55	14	7	3	6	131	124	7	1	11	6	206	190	6	8	6	7	265	279	6	6	4	8	710	734	6
5	11	5	590	587	5	9	3	6	886	882	7	3	11	6	333	329	5	10	6	7	136	145	9	8	4	8	0	4	1
7	11	5	494	503	5	11	3	6	1235	1232	9	5	11	6	479	499	5	12	6	7	198	202	7	10	4	8	187	188	8
9	11	5	172	174	7	13	3	6	108	111	9	7	11	6	148	145	8	1	7	7	115	113	9	1	5	8	537	554	5
11	11	5	234	257	7	15	3	6	146	140	8	9	11	6	384	393	6	3	7	7	199	199	6	3	5	8	176	185	7
13	11	5	212	213	8	17	3	6	415	421	6	11	11	6	809	806	7	5	7	7	940	947	7	5	5	8	437	451	6
0	12	5	981	1000	7	0	4	6	2413	2373	12	0	12	6	530	533	5	7	7	7	110	111	10	7	5	8	38	39	37
2	12	5	528	539	5	2	4	6	34	31	34	2	12	6	139	154	9	9	7	7	273	266	6	9	5	8	83	62	14
4	12	5	0	19	1	4	4	6	124	131	5	4	12	6	130	146	9	11	7	7	570	585	6	0	6	8	1852	1891	12
6	12	5	748	761	6	6	4	6	533	525	5	6	12	6	844	847	7	0	8	7	691	694	6	2	6	8	194	198	7
8	12	5	48	53	31	8	4	6	137	120	7	8	12	6	76	66	16	2	8	7	0	21	1	4	6	8	275	279	6
10	12	5	51	43	29	10	4	6	1347	1349	10	10	12	6	342	344	6	4	8	7	173	165	7	6	6	8	471	470	6
12	12	5	159	168	9	12	4	6	138	132	8	1	13	6	31	2	30	6	8	7	370	372	6	8	6	8	138	127	9
1	13	5	196	196	5	14	4	6	32	12	12	3	13	6	0	17	1	8	8	7	50	25	27	1	7	8	67	36	17
3	13	5	180	194	7	16	4	6	180	197	8	5	13	6	1231	1259	9	10	8	7	254	246	6	3	7	8	231	233	6
5	13	5	1004	998	7	1	5	6	323	314	5	7	13	6	102	97	12	12	8	7	164	166	6	5	7	8	897	912	7
7	13	5	173	185	8	3	5	6	335	342	5	0	14	6	129	114	9	1	9	7	144	154	5	7	7	8	253	259	7
9	13	5	246	243	7	5	5	6	570	553	5	2	14	6	381	378	6	3	9	7	124	116	9	0	8	8	933	952	7
11	13	5	1283	1288	9	7	5	6	91	73	10	4	14	6	285	286	6	5	9	7	242	254	6	2	8	8	0	27	1
0	14	5	1039	1041	7	9	5	6	288	285	5	6	14	6	168	160	8	7	9	7	147	140	8	4	8	8	63	85	20
2	14	5	126	129	10	11	5	6	321	308	6	1	1	7	98	88	9	9	9	7	24	7	24	6	8	8	447	456	6
4	14	5	293	312	6	13	5	6	69	69	16	3	1	7	189	185	6	11	9	7	548	558	6	1	9	8	38	52	38
6	14	5	416	415	6	15	5	6	307	303	6	5	1	7	146	132	7	0	10	7	645	661	6	3	9	8	74	84	17
8	14	5	153	151	9	0	6	6	104	91	8	7	1	7	288	279	5	2	10	7	423	433	6	5	9	8	1256	1308	9
10	14	5	436	434	6	2	6	6	101	93	9	9	1	7	142	144	8	4	10	7	125	130	10	0	10	8	1011	1041	8
1	15	5	77	67	15	4	6	6	306	302	5	11	1	7	704	705	6	6	10	7	204	201	7	2	10	8	43	21	42
3	15	5	321	317	6	6	6	6	999	1014	7	13	1	7	278	276	6	8	10	7	96	103	12	1	1	9	69	12	17
5	15	5	23	43	22	8	6	6	324	315	5	15	1	7	256	260	7	1	11	7	114	112	10	3	1	9	152	139	8
7	15	5	297	314	7	10	6	6	74	75	14	0	2	7	676	660	6	3	11	7	37	12	37	5	1	9	410	410	6
0	16	5	326	332	6	12	6	6	189	200	7	2	2	7	358	364	5	5	11	7	613	622	6	0	2	9	246	220	6
2	16	5	203	208	8	14	6	6	669	676	6	4	2	7	42	45	28	7	11	7	138	139	10	2	2	9	130	116	8
4	16	5	0	59	1	16	6	6	834	835	7	6	2	7	520	513	5	0	12	7	23	35	22	4	2	9	140	124	9
0	0	6	2760	2616	11	1	7	6	528	533	5	8	2	7	259	253	6	2	12	7	219	222	7	6	2	9	81	66	14
2	0	6	166	161	5	3	7	6	63	88	16	10	2	7	71	95	15	4	12	7	287	287	6	1	3	9	100	105	11
4	0	6	549	557	5	5	7	6	2507	2510	13	12	2	7	438	439	6	0	0	8	2662	2670	14	3	3	9	25	11	24
6	0	6	707	703	6	7	7	6	110	98	9	14	2	7	180	182	7	2	0	8	168	157	7	5	3	9	165	159	8
8	0	6	430	436	5	9	7	6	151	156	5	1	3	7	263	265	5	4	0	8	200	182	6	0	4	9	441	453	6
10	0	6	957	941	7	11	7	6	420	437	5	3	3	7	16	15	16	6	0	8	688	727	6	2	4	9	16	53	35
12	0	6	808	813	6	13	7	6	218	222	7	5	3	7	426	431	5	8	0	8	69	34	15	4	4	9	59	70	23
14	0	6	739	728	6	15	7	6	700	710	6	7	3	7	403	389	5	10	0	8	1588	1615	11	1	5	9	40	31	40
16	0	6	924	916	7	0	8	6	279	279	5	9	3	7	150	145	8	12	0	8	558	561	6	3	5	9	41	51	40
1	1	6	226	200	5	2	8	6	264	265	5	11	3	7	876	892	7	1	1	8	214	194	6	0	6	9	162	160	8

Observed and calculated structure factors for K32

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	667	680	3	4	8	0	367	368	3	3	1	1	481	470	3	7	9	1	319	326	4	7	1	2	171	166	3
4	0	0	1257	1260	5	6	8	0	543	568	5	5	1	1	882	896	6	9	9	1	60	43	11	9	1	2	657	648	5
6	0	0	537	557	4	8	8	0	443	445	4	7	1	1	129	116	3	11	9	1	1614	1679	11	11	1	2	669	665	5
8	0	0	839	837	6	10	8	0	1324	1314	10	9	1	1	482	475	4	13	9	1	62	49	12	13	1	2	75	57	8
10	0	0	3730	3632	10	12	8	0	169	184	5	11	1	1	832	848	6	15	9	1	88	77	9	15	1	2	626	629	5
12	0	0	1326	1372	9	14	8	0	172	168	5	13	1	1	382	376	4	17	9	1	182	183	6	17	1	2	77	67	9
14	0	0	199	191	4	16	8	0	304	299	5	15	1	1	63	47	11	19	9	1	194	191	6	19	1	2	22	19	21
16	0	0	199	201	5	18	8	0	0	36	1	17	1	1	739	734	6	0	10	1	1199	1217	9	21	1	2	343	345	5
18	0	0	592	588	5	20	8	0	329	313	5	19	1	1	474	483	5	2	10	1	782	773	6	0	2	2	4261	4085	8
20	0	0	199	206	6	1	9	0	60	33	9	21	1	1	900	879	7	4	10	1	284	281	4	2	2	2	144	141	3
22	0	0	1612	1627	11	3	9	0	406	414	4	0	2	1	91	120	4	6	10	1	438	438	4	4	2	2	524	509	3
1	1	0	699	736	3	5	9	0	1813	1857	9	2	2	1	480	487	3	8	10	1	183	183	4	6	2	2	470	456	4
3	1	0	191	181	2	7	9	0	856	854	7	4	2	1	514	519	4	10	10	1	232	233	5	8	2	2	285	272	3
5	1	0	424	435	3	9	9	0	44	9	17	6	2	1	270	253	3	12	10	1	23	15	22	10	2	2	1256	1270	9
7	1	0	468	473	4	11	9	0	667	630	5	8	2	1	613	622	5	14	10	1	618	616	5	12	2	2	535	533	4
9	1	0	1666	1695	8	13	9	0	267	274	4	10	2	1	268	288	3	16	10	1	235	254	5	14	2	2	116	120	6
11	1	0	2884	2844	10	15	9	0	500	507	5	12	2	1	957	968	7	18	10	1	272	275	6	16	2	2	362	354	4
13	1	0	304	305	4	17	9	0	458	468	5	14	2	1	172	169	5	1	11	1	203	212	4	18	2	2	44	47	22
15	1	0	282	288	4	19	9	0	255	259	6	16	2	1	679	688	5	3	11	1	272	273	4	20	2	2	53	58	21
17	1	0	296	293	4	0	10	0	279	294	3	18	2	1	47	46	20	5	11	1	674	697	5	1	3	2	378	374	3
19	1	0	608	605	5	2	10	0	42	50	17	20	2	1	148	154	7	7	11	1	544	540	5	3	3	2	299	289	3
21	1	0	728	745	6	4	10	0	451	473	4	22	2	1	200	210	6	9	11	1	333	335	4	5	3	2	998	984	7
0	2	0	1356	1358	4	6	10	0	274	277	4	1	3	1	336	339	3	11	11	1	380	376	4	7	3	2	133	128	4
2	2	0	241	258	2	8	10	0	294	318	4	3	3	1	242	235	3	13	11	1	119	122	7	9	3	2	1573	1646	9
4	2	0	716	716	5	10	10	0	507	508	4	5	3	1	348	336	3	15	11	1	71	73	11	11	3	2	1290	1354	10
6	2	0	143	149	3	12	10	0	135	128	6	7	3	1	488	485	4	17	11	1	464	467	5	13	3	2	474	476	4
8	2	0	300	293	3	14	10	0	1182	1208	9	9	3	1	222	227	3	0	12	1	1097	1114	8	15	3	2	151	143	5
10	2	0	675	692	5	16	10	0	186	192	6	11	3	1	224	229	4	2	12	1	479	469	4	17	3	2	303	302	4
12	2	0	296	302	4	18	10	0	562	554	5	13	3	1	275	275	4	4	12	1	128	107	5	19	3	2	828	826	6
14	2	0	842	863	6	1	11	0	293	287	4	15	3	1	46	19	15	6	12	1	622	619	5	21	3	2	505	495	5
16	2	0	694	697	5	3	11	0	291	288	4	17	3	1	301	308	4	8	12	1	172	169	5	0	4	2	1863	1858	7
18	2	0	56	50	15	5	11	0	881	892	6	19	3	1	214	198	5	10	12	1	197	191	5	2	4	2	658	644	4
20	2	0	185	183	6	7	11	0	153	167	5	21	3	1	307	310	5	12	12	1	289	283	5	4	4	2	45	15	10
22	2	0	353	336	5	9	11	0	37	55	27	0	4	1	1080	1059	6	14	12	1	37	29	37	6	4	2	270	257	3
1	3	0	351	343	3	11	11	0	470	485	5	2	4	1	63	73	6	16	12	1	691	705	6	8	4	2	109	119	5
3	3	0	576	586	4	13	11	0	155	164	6	4	4	1	263	266	3	1	13	1	361	362	4	10	4	2	1928	1998	10
5	3	0	4884	4725	9	15	11	0	873	882	7	6	4	1	813	775	6	3	13	1	379	386	4	12	4	2	286	291	4
7	3	0	512	493	4	17	11	0	411	415	5	8	4	1	503	507	4	5	13	1	950	942	7	14	4	2	244	247	4
9	3	0	1010	1022	6	0	12	0	1510	1566	10	10	4	1	246	223	3	7	13	1	71	62	10	16	4	2	48	42	17
11	3	0	297	292	3	2	12	0	263	267	4	12	4	1	740	743	5	9	13	1	313	319	5	18	4	2	487	484	5
13	3	0	355	362	4	4	12	0	214	211	4	14	4	1	265	267	4	11	13	1	1066	1069	8	20	4	2	311	312	5
15	3	0	801	806	6	6	12	0	602	606	5	16	4	1	652	654	5	13	13	1	147	144	7	1	5	2	975	942	7
17	3	0	910	934	7	8	12	0	152	153	6	18	4	1	268	264	5	15	13	1	299	287	5	3	5	2	97	100	5
19	3	0	227	222	5	10	12	0	633	638	5	20	4	1	108	102	9	0	14	1	657	668	5	5	5	2	1827	1819	8
21	3	0	441	439	5	12	12	0	512	498	5	1	5	1	113	115	4	2	14	1	294	292	4	7	5	2	221	211	3
0	4	0	2030	2065	6	14	12	0	95	69	9	3	5	1	536	547	4	4	14	1	412	418	4	9	5	2	177	184	4
2	4	0	572	579	4	16	12	0	110	117	10	5	5	1	1510	1506	7	6	14	1	278	279	5	11	5	2	619	626	5
4	4	0	1110	1116	6	1	13	0	414	418	4	7	5	1	892	880	6	8	14	1	320	318	5	13	5	2	38	16	21
6	4	0	3613	3605	9	3	13	0	162	166	5	9	5	1	619	593	4	10	14	1	174	175	6	15	5	2	241	244	5
8	4	0	485	477	4	5	13	0	410	405	4	11	5	1	272	292	4	12	14	1	177	188	6	17	5	2	732	732	6
10	4	0	439	425	4	7	13	0	477	469	5	13	5	1	585	584	5	14	14	1	411	401	5	19	5	2	419	405	5
12	4	0	268	266	4	9	13	0	550	547	5	15	5	1	143	137	6	1	15	1	38	36	32	21	5	2	472	454	5
14	4	0	899	904	6	11	13	0	897	904	7	17	5	1	237	234	5	3	15	1	284	284	5	0	6	2	1097	1058	7
16	4	0	1935	1971	12	13	13	0	295	305	5	19	5	1	40	15	27	5	15	1	244	248	5	2	6	2	145	149	4
18	4	0	151	106	6	15	13	0	213	225	6	21	5	1	757	747	6	7	15	1	345	349	5	4	6	2	1126	1114	8
20	4	0	247	244	6	0	14	0	1448	1475	11	0	6	1	531	504	4	9	15	1	92	74	9	6	6	2	2273	2289	9
1	5	0	1397	1401	6	2	14	0	406	407	4	2	6	1	183	176	3	11	15	1	122	107	8	8	6	2	272	262	3
3	5	0	40	38	11	4	14	0	214	216	5	4	6	1	202	195	3	13	15	1	130	138	8	10	6	2	64	14	9
5	5	0	3169	3141	8	6	14	0	715	731	6	6	6	1	825	850	6	0	16	1	241	243	5	12	6	2	346	355	4
7	5	0	812	802	6	8	14	0	118	126	7	8	6	1	536	516	4	2	16	1	244	243	5	14	6	2	999	1011	7
9	5	0	188	198	4	10	14	0	1284	1331	10	10	6	1	132	138	5	4	16	1	51	7	18	16	6	2	1399	1432	10
11	5	0	322	345	4	12	14	0	86	82	12	12	6	1	328	325	4	6	16	1	1253	1274	9	18	6	2	48	51	20
13	5	0	348	353	4	14	14	0	21	33	20	14	6	1	53	17	13	8	16	1	298	299	5	20	6	2	101	101	10
15	5	0	257	269	4	1	15	0	220	217	5	16	6	1	1036	1026	7	10	16	1	82	81	12	1	7	2	752	726	5
17	5	0	487	483	5	3	15	0	422	422	4	18	6	1	283	285	5	12	16	1	83	80	12	3	7	2	65	1	7
19	5	0	231	235	5	5	15	0	538	545	5	20	6	1	428	432	5	1	17	1	76	75	12	5	7	2	4392	4458	11
21	5	0	298	293	6	7	15	0	31	7	11	1	7	1	157	148	3	3	17	1	323	327	5	7	7	2	207	204	4
0	6	0	866	874	6	9	15	0	100	87	9	3	7	1	592	590	4	5	17	1	700	698	6	9	7	2	486	490	4
2	6	0	173	171	3	11	15	0	373	375	5	5	7	1	405	398	3	7	17	1	228	226	6	11	7	2	123	130	6
4	6	0	451	458	4	13	15	0	429	421	5	7	7	1	212	211	4	9	17	1	411	412	5	13	7	2	358	351	4
6	6	0	582	571	4	0	16	0	592	608	5	9	7	1	457	473	4	0	18	1	302	310	5	15	7	2	909	899	7
8	6	0	667	663	5	2	16	0	189	177	6	11	7	1	16	13	15	2	18	1	86	72	11	17	7	2	935	931	7
10	6	0	1295	1311	9	4	16	0	271	276	5	13	7	1	50	61	15	4	18	1	338	335	5	19	7	2	48	40	23
12	6	0	276	281	4	6	16	0	856	840	7	15	7	1	63	49	12	6	18	1	337	340	5	0	8	2	512	518	4
14	6	0	475	478	4	8	16	0	66	66	14	17	7	1	214	208	5	1	19	1	325	316	5	2	8	2	442	431	4
16	6	0	574	578	5	10	16	0	32	46	31	19	7	1	134	132	7	3	19	1	391	403	5	4	8	2	162	177	4
18	6	0	372	377	5	12	16	0	395	411	5	0	8	1	678	651	5	0	0	2	3375	3280	7	6	8	2	426	410	4
20	6	0	37	53	36	1	17	0	283	282	5	2	8	1	0	30	1	2	0	2	561	585	4	8	8	2	579	581	5
1	7	0	727	706	5	3	17	0	302	301	5	4	8	1	124	136	5	4	0	2	411	410	3	10	8	2	26	21	26
3	7	0	118	122	4	5	17	0	1839	1872	14	6	8	1	293	298	3	6	0	2	789	740	5	12	8	2	191	185	5
5	7	0	1358	1354	8	7	17	0	62	63	17	8	8	1	142	145	5	8	0	2	542	525	4	14	8	2	553	552	5
7	7	0	470	450	4	9	17	0	50	63	24	10	8	1	95	77	7	10	0	2	1326	1308	9	16	8	2	886	877	7
9	7	0	1216	1243	9	0	18	0	311	321	5	12	8	1	513	511	4	12	0	2	920	921	7	18	8	2	73	67	13
11	7	0	575	527	5	2	18	0	309	317	5	14	8	1	585	585	5	14	0	2	1305	1328	9	1	9	2	418	407	4
13	7	0	372	375	4	4	18	0	56	43	19	16	8	1	754	733	6	16	0	2	654	661	5	3	9	2	46	30	14
15	7	0	216	221	5	6	18	0	232	241	6	18	8	1	368	359	5	18	0	2	815	824	6	5	9	2	467	447	4
17	7	0	231	236	5	8	18	0	343	339	5	20	8	1	227	240	6	20	0	2	70	56	13	7	9	2	393	391	4
19	7	0	693	692	6	1	19	0	200	199	6	1	9	1	968	950	7	1	1	2	498	507	4	9	9	2	776	772	6
0	8	0	2519	2537	9	3	19	0	41	60	40	3	9	1	159	143	4	3	1	2	793	779	6	11	9	2	1571	1565	11
2	8	0	172	172	3	1	1	1	174	165	2	5	9	1	342	361	3	5	1	2	1040	1029	6	13	9	2	79	79	10

Observed and calculated structure factors for K32

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	341	335	5	20	2	3	93	90	10	17	11	3	563	566	5	12	4	4	181	170	5	12	14	4	38	47	38
17	9	2	608	609	5	1	3	3	569	545	4	0	12	3	237	228	4	14	4	4	870	870	7	1	15	4	180	180	6
19	9	2	305	301	5	3	3	3	245	249	3	2	12	3	262	260	4	16	4	4	1401	1407	10	3	15	4	413	416	5
0	10	2	4525	4403	12	5	3	3	1068	1053	8	4	12	3	352	352	4	18	4	4	162	161	6	5	15	4	268	261	5
2	10	2	675	681	5	7	3	3	738	729	6	6	12	3	125	115	7	1	5	4	970	975	7	7	15	4	126	114	8
4	10	2	769	764	5	9	3	3	178	176	4	8	12	3	108	93	7	3	5	4	157	154	4	9	15	4	93	90	11
6	10	2	84	90	8	11	3	3	1296	1312	10	10	12	3	158	172	6	5	5	4	1486	1543	10	0	16	4	163	162	7
8	10	2	273	277	4	13	3	3	65	72	11	12	12	3	285	276	5	7	5	4	386	385	4	2	16	4	161	166	7
10	10	2	1870	1847	11	15	3	3	97	110	8	14	12	3	109	117	9	9	5	4	182	179	5	4	16	4	214	204	6
12	10	2	315	308	4	17	3	3	249	246	5	16	12	3	407	396	5	11	5	4	897	913	7	6	16	4	470	465	5
14	10	2	376	372	5	19	3	3	113	123	9	1	13	3	252	247	4	13	5	4	196	198	5	8	16	4	0	1	1
16	10	2	244	247	5	21	3	3	405	392	5	3	13	3	471	483	5	15	5	4	263	263	5	1	17	4	376	359	5
18	10	2	291	279	5	0	4	3	2191	2109	8	5	13	3	322	325	4	17	5	4	96	98	10	3	17	4	204	197	6
1	11	2	357	363	4	2	4	3	62	60	7	7	13	3	136	135	6	19	5	4	164	159	7	1	1	5	85	78	7
3	11	2	707	709	6	4	4	3	380	378	3	9	13	3	254	251	5	0	6	4	2112	2147	10	3	1	5	238	245	4
5	11	2	62	66	11	6	4	3	229	216	3	11	13	3	356	349	5	2	6	4	186	189	4	5	1	5	677	681	5
7	11	2	0	3	1	8	4	3	278	281	3	13	13	3	29	13	28	4	6	4	447	432	4	7	1	5	29	29	28
9	11	2	642	641	6	10	4	3	378	369	4	15	13	3	223	199	6	6	6	4	141	136	5	9	1	5	381	395	4
11	11	2	1721	1767	12	12	4	3	791	799	6	0	14	3	0	9	1	8	6	4	366	366	4	11	1	5	257	247	4
13	11	2	34	39	34	14	4	3	118	116	6	2	14	3	257	251	5	10	6	4	1205	1228	9	13	1	5	204	211	5
15	11	2	241	235	6	16	4	3	231	226	5	4	14	3	354	362	4	12	6	4	370	373	4	15	1	5	20	12	20
17	11	2	78	79	13	18	4	3	169	171	6	6	14	3	158	167	6	14	6	4	274	278	5	17	1	5	749	744	6
0	12	2	1315	1327	9	20	4	3	29	47	29	8	14	3	372	372	5	16	6	4	235	231	5	19	1	5	371	383	5
2	12	2	6	18	5	1	5	3	76	66	6	10	14	3	20	1	20	18	6	4	288	276	5	0	2	5	756	748	6
4	12	2	18	4	18	3	5	3	363	365	3	12	14	3	75	68	14	1	7	4	273	265	4	2	2	5	84	67	7
6	12	2	860	847	6	5	5	3	873	879	6	1	15	3	142	148	7	3	7	4	207	195	4	4	2	5	484	494	4
8	12	2	129	140	6	7	5	3	882	865	6	3	15	3	212	207	5	5	7	4	1250	1272	8	6	2	5	459	458	4
10	12	2	782	794	6	9	5	3	472	476	4	5	15	3	442	452	5	7	7	4	379	372	4	8	2	5	332	329	4
12	12	2	227	226	5	11	5	3	114	113	6	7	15	3	206	212	6	9	7	4	954	975	7	10	2	5	92	82	7
14	12	2	584	573	5	13	5	3	449	439	4	9	15	3	121	125	9	11	7	4	706	716	6	12	2	5	754	760	6
16	12	2	377	374	5	15	5	3	63	52	12	11	15	3	343	314	5	13	7	4	123	121	4	14	2	5	92	92	9
1	13	2	224	227	5	17	5	3	296	295	5	0	16	3	89	98	11	15	7	4	209	219	5	16	2	5	248	246	5
3	13	2	91	91	8	19	5	3	56	53	17	2	16	3	85	81	11	17	7	4	354	357	5	18	2	5	71	73	14
5	13	2	1855	1853	12	0	6	3	493	496	4	4	16	3	204	210	6	0	8	4	1794	1881	10	1	3	5	139	134	5
7	13	2	44	37	21	2	6	3	104	94	5	6	16	3	1127	1124	8	2	8	4	75	28	9	3	3	5	208	207	4
9	13	2	184	186	6	4	6	3	426	407	4	8	16	3	239	246	6	4	8	4	147	153	5	5	3	5	540	549	5
11	13	2	130	132	7	6	6	3	1168	1173	9	10	16	3	75	74	14	6	8	4	524	521	4	7	3	5	101	106	7
13	13	2	102	103	9	8	6	3	384	374	4	1	17	3	139	137	8	8	8	4	355	354	4	9	3	5	89	81	8
15	13	2	498	498	5	10	6	3	163	174	5	3	17	3	329	332	5	10	8	4	1138	1150	8	11	3	5	297	294	4
0	14	2	421	421	4	12	6	3	297	287	4	5	17	3	430	413	5	12	8	4	113	111	8	13	3	5	292	282	4
2	14	2	310	322	5	14	6	3	112	113	7	7	17	3	44	25	32	14	8	4	147	146	7	15	3	5	30	18	29
4	14	2	730	739	6	16	6	3	1091	1105	8	0	18	3	209	208	6	16	8	4	244	245	6	17	3	5	510	510	5
6	14	2	458	450	4	18	6	3	408	408	5	2	18	3	163	177	7	18	8	4	33	27	32	0	4	5	88	94	7
8	14	2	190	201	6	20	6	3	403	396	5	2	0	4	182	401	3	1	9	4	27	1	26	2	4	5	66	39	9
10	14	2	154	156	7	1	7	3	199	192	4	4	0	4	723	729	5	3	9	4	286	290	4	4	4	5	134	135	5
12	14	2	67	64	13	3	7	3	296	304	3	6	0	4	437	426	4	5	9	4	1762	1760	11	6	4	5	678	659	5
14	14	2	394	400	5	5	7	3	1143	1148	9	8	0	4	240	238	4	7	9	4	487	487	4	8	4	5	163	170	4
1	15	2	518	516	5	7	7	3	167	161	5	10	0	4	2619	2606	11	9	9	4	75	61	10	10	4	5	126	120	6
3	15	2	293	295	5	9	7	3	474	481	4	12	0	4	924	937	7	11	9	4	223	219	5	12	4	5	526	521	5
5	15	2	1465	1473	10	11	7	3	816	818	6	14	0	4	140	354	4	13	9	4	123	123	8	14	4	5	263	263	5
7	15	2	492	494	5	13	7	3	129	128	6	16	0	4	207	204	5	15	9	4	352	355	5	16	4	5	682	673	6
9	15	2	170	163	6	15	7	3	150	153	6	18	0	4	561	567	5	17	9	4	571	563	5	18	4	5	286	285	5
11	15	2	380	376	5	17	7	3	617	621	5	20	0	4	113	108	9	0	10	4	864	852	7	1	5	5	161	152	5
13	15	2	145	133	8	19	7	3	93	98	11	1	1	4	235	233	3	2	10	4	63	79	11	3	5	5	314	315	4
0	16	2	1004	1011	8	0	8	3	900	871	6	3	1	4	107	97	5	4	10	4	523	523	4	5	5	5	722	717	6
2	16	2	143	128	7	2	8	3	135	136	5	5	1	4	317	296	3	6	10	4	213	208	5	7	5	5	613	600	5
4	16	2	20	14	19	4	8	3	365	364	3	7	1	4	66	53	9	8	10	4	324	324	4	9	5	5	438	444	4
6	16	2	487	488	5	6	8	3	600	586	5	9	1	4	1276	1294	10	10	10	4	453	453	5	11	5	5	264	246	5
8	16	2	68	73	14	8	8	3	42	23	18	11	1	4	1599	1611	11	12	10	4	187	176	6	13	5	5	394	397	3
10	16	2	721	717	6	10	8	3	89	87	8	13	1	4	174	163	5	14	10	4	938	928	7	15	5	5	94	89	10
1	17	2	246	240	5	12	8	3	589	601	5	15	1	4	210	213	5	16	10	4	360	350	5	17	5	5	190	171	6
3	17	2	390	389	5	14	8	3	378	379	4	17	1	4	55	26	16	1	11	4	156	153	5	0	6	5	394	425	4
5	17	2	159	156	7	16	8	3	214	202	6	19	1	4	559	555	5	3	11	4	365	353	4	2	6	5	109	106	6
7	17	2	53	6	21	18	8	3	195	190	6	0	2	4	345	365	3	5	11	4	1112	1132	8	4	6	5	85	71	8
9	17	2	413	398	5	1	9	3	602	587	5	2	2	4	175	173	4	7	11	4	70	77	11	6	6	5	410	413	4
0	18	2	768	763	6	3	9	3	91	83	7	4	2	4	447	446	4	9	11	4	20	11	19	8	6	5	338	342	4
2	18	2	0	13	1	5	9	3	354	340	4	6	2	4	445	470	4	11	11	4	24	24	24	10	6	5	88	88	9
4	18	2	198	202	6	7	9	3	226	229	4	8	2	4	118	108	5	13	11	4	97	103	10	12	6	5	237	233	5
6	18	2	422	417	5	9	9	3	82	66	8	10	2	4	470	469	4	15	11	4	750	754	6	14	6	5	15	17	15
1	1	3	268	268	3	11	9	3	850	877	6	12	2	4	308	312	4	0	12	4	983	988	7	16	6	5	695	691	6
3	1	3	666	648	5	13	9	3	35	21	35	14	2	4	651	649	5	2	12	4	277	269	4	1	7	5	90	82	7
5	1	3	180	181	3	15	9	3	111	97	8	16	2	4	700	716	6	4	12	4	111	111	7	3	7	5	489	493	4
7	1	3	259	266	3	17	9	3	522	520	5	18	2	4	27	28	26	6	12	4	275	271	5	5	7	5	27	3	26
9	1	3	407	417	4	0	10	3	786	797	6	20	2	4	119	131	9	8	12	4	194	206	5	7	7	5	322	319	4
11	1	3	1372	1377	10	2	10	3	784	774	6	1	3	4	237	250	3	10	12	4	431	416	5	9	7	5	329	323	4
13	1	3	440	450	4	4	10	3	383	379	4	3	3	4	485	479	4	12	12	4	339	334	5	11	7	5	380	371	4
15	1	3	111	108	7	6	10	3	199	194	5	5	3	4	3321	3320	10	14	12	4	34	9	34	13	7	5	161	162	6
17	1	3	353	362	5	8	10	3	242	250	4	7	3	4	168	172	4	1	13	4	216	209	5	15	7	5	28	33	28
19	1	3	458	473	5	10	10	3	50	33	16	9	3	4	785	797	6	3	13	4	100	96	8	17	7	5	57	49	20
21	1	3	872	855	7	12	10	3	90	89	9	11	3	4	58	36	12	5	13	4	256	252	5	0	8	5	786	788	6
0	2	3	2239	2186	7	14	10	3	596	604	5	13	3	4	331	325	4	7	13	4	265	270	5	2	8	5	113	109	6
2	2	3	557	541	4	16	10	3	43	41	30	15	3	4	704	696	5	9	13	4	518	526	5	4	8	5	24	3	24
4	2	3	22	6	21	1	11	3	316	308	4	17	3	4	703	721	6	11	13	4	713	708	6	6	8	5	540	530	5
6	2	3	1116	1087	8	3	11	3	210	217	4	19	3	4	191	195	6	13	13	4	172	173	7	8	8	5	123	128	7
8	2	3	725	718	5	5	11	3	757	756	6	0	4	4	455	487	4	0	14	4	1412	1424	10	10	8	5	60	42	13
10	2	3	347	349	4	7	11	3	238	240	4	2	4	4	387	379	4	2	14	4	249	251	5	12	8	5	385	380	5
12	2	3	724	737	6	9	11	3	394	398	4	4	4	4	673	688	5	4	14	4	325	318	5	14	8	5	490	503	5
14	2	3	370	364	4	11	11	3	94	102	9	6	4	4	1809	1829	10	6	14	4	499	502	5	16	8	5	771	773	6
16	2	3	1091	1092	7	13	11	3	50	48	19	8	4	4	215	213	4	8	14	4	109	105	9	1	9	5	698	695	5
18	2	3	234	223	5	15	11	3	66	66	15	10	4	4	279	282	4	10	14	4	1029	1056	8	3	9	5	76	74	9

Observed and calculated structure factors for K32

h	k	l	10Fo	10Fc	10s
5	9	5	480	472	4
7	9	5	342	331	4
9	9	5	38	36	30
11	9	5	1526	1525	10
13	9	5	115	105	9
15	9	5	87	95	12
0	10	5	983	960	7
2	10	5	512	509	4
4	10	5	151	143	6
6	10	5	460	446	5
8	10	5	138	136	7
10	10	5	239	238	5
12	10	5	60	68	17
14	10	5	463	471	5
1	11	5	104	93	8
3	11	5	230	223	5
5	11	5	482	477	5
7	11	5	525	531	5
9	11	5	237	225	5
11	11	5	414	411	5
13	11	5	192	187	6
0	12	5	1094	1092	8
2	12	5	480	472	5
4	12	5	62	52	14
6	12	5	669	671	5
8	12	5	103	108	9
10	12	5	115	97	9
12	12	5	247	235	6
1	13	5	314	313	5
3	13	5	281	281	5
5	13	5	939	932	7
7	13	5	168	167	7
9	13	5	297	290	5
11	13	5	1188	1172	9
0	14	5	863	859	7
2	14	5	254	251	5
4	14	5	153	145	5
6	14	5	427	429	5
8	14	5	216	221	6
1	15	5	115	112	9
3	15	5	241	242	6
5	15	5	49	72	26
7	15	5	325	322	5
0	16	5	214	212	6
2	16	5	275	265	6
4	16	5	114	114	10
0	0	6	2537	2535	11
2	0	6	75	80	9
4	0	6	638	650	5
6	0	6	670	687	5
8	0	6	357	357	4
10	0	6	837	855	7
12	0	6	731	741	6
14	0	6	787	775	6
16	0	6	809	808	7
1	1	6	141	140	5
3	1	6	172	166	5
5	1	6	1676	1693	11
7	1	6	63	61	11
9	1	6	163	164	4
11	1	6	204	207	5
13	1	6	56	52	15
15	1	6	408	411	5
17	1	6	323	320	5
0	2	6	1677	1698	11
2	2	6	204	204	4
4	2	6	213	203	4
6	2	6	499	512	5
8	2	6	244	251	5
10	2	6	779	772	6
12	2	6	300	300	5
14	2	6	40	18	31
16	2	6	404	412	5
1	3	6	197	187	4
3	3	6	115	121	6
5	3	6	757	767	6
7	3	6	51	50	14
9	3	6	1106	1117	8
11	3	6	1072	1075	8
13	3	6	253	252	5
15	3	6	62	52	15
0	4	6	2379	2403	11
2	4	6	69	63	10
4	4	6	337	338	4
6	4	6	479	495	5
8	4	6	108	111	7
10	4	6	1349	1356	10
12	4	6	276	271	5
14	4	6	64	69	15
16	4	6	195	189	6
1	5	6	240	245	4
3	5	6	298	293	4
5	5	6	488	473	4
7	5	6	77	72	10
9	5	6	203	213	5
11	5	6	353	360	5
13	5	6	100	96	9
15	5	6	219	220	6
0	6	6	200	199	5
2	6	6	14	24	14
4	6	6	568	571	5
6	6	6	826	819	6
8	6	6	297	301	5
10	6	6	139	145	7
12	6	6	160	163	6
14	6	6	875	864	7
1	7	6	608	594	5
3	7	6	162	163	6
5	7	6	2391	2449	12
7	7	6	115	118	8
9	7	6	375	387	5
11	7	6	485	480	5
13	7	6	212	215	6
15	7	6	607	598	5
0	8	6	358	345	4
2	8	6	198	190	5
4	8	6	284	282	5
6	8	6	280	280	5
8	8	6	156	151	4
10	8	6	112	123	8
12	8	6	193	186	6
14	8	6	393	388	5
1	9	6	312	303	5
3	9	6	112	117	7
5	9	6	50	45	16
7	9	6	480	473	5
9	9	6	527	524	5
11	9	6	722	714	6
13	9	6	57	59	18
0	10	6	2142	2169	13
2	10	6	337	336	5
4	10	6	355	345	5
6	10	6	572	571	5
8	10	6	83	86	11
10	10	6	1253	1248	8
12	10	6	166	169	7
1	11	6	88	88	10
3	11	6	360	351	5
5	11	6	463	464	5
7	11	6	103	105	9
9	11	6	471	462	5
11	11	6	722	718	6
0	12	6	490	491	5
2	12	6	50	36	21
4	12	6	47	42	22
6	12	6	905	918	7
8	12	6	0	20	1
10	12	6	430	415	5
1	13	6	36	49	35
3	13	6	72	62	13
5	13	6	1386	1392	10
7	13	6	153	165	8
0	14	6	61	40	17
2	14	6	376	371	5
4	14	6	335	338	5
1	1	7	114	82	7
3	1	7	263	253	4
5	1	7	85	70	9
7	1	7	260	258	5
9	1	7	239	240	5
11	1	7	726	737	6
13	1	7	337	346	5
15	1	7	128	130	9
0	2	7	648	646	5
2	2	7	305	303	4
4	2	7	44	38	20
6	2	7	456	456	5
8	2	7	302	297	5
10	2	7	87	92	10
12	2	7	540	536	5
14	2	7	209	201	6
1	3	7	186	191	5
3	3	7	41	26	23
5	3	7	377	381	4
7	3	7	447	448	4
9	3	7	163	167	6
11	3	7	752	745	6
13	3	7	53	36	19
0	4	7	1001	988	7
2	4	7	104	103	8
4	4	7	265	272	5
6	4	7	95	86	8
8	4	7	213	214	5
10	4	7	244	233	5
12	4	7	486	488	5
14	4	7	140	129	7
1	5	7	0	20	1
3	5	7	203	199	5
5	5	7	328	321	4
7	5	7	508	516	5
9	5	7	340	345	5
11	5	7	0	32	1
13	5	7	277	272	6
0	6	7	205	204	5
2	6	7	112	108	7
4	6	7	180	181	6
6	6	7	654	669	6
8	6	7	251	257	5
10	6	7	156	156	7
12	6	7	188	194	6
1	7	7	78	80	10
3	7	7	271	278	5
5	7	7	696	678	6
7	7	7	126	121	8
9	7	7	367	362	5
11	7	7	501	503	5
0	8	7	534	531	5
2	8	7	115	111	8
4	8	7	296	292	5
6	8	7	343	335	5
8	8	7	48	36	22
10	8	7	73	69	14
1	9	7	402	394	5
3	9	7	45	32	22
5	9	7	251	250	5
7	9	7	110	115	9
9	9	7	47	17	25
0	10	7	540	549	5
2	10	7	438	435	5
4	10	7	178	176	6
6	10	7	198	189	6
8	10	7	135	132	8
1	11	7	168	170	7
3	11	7	146	140	8
5	11	7	556	547	5
7	11	7	169	173	7
0	12	7	39	48	38
2	12	7	158	164	7
4	12	7	241	250	6
0	0	8	2481	2493	13
2	0	8	155	149	6
4	0	8	263	261	5
6	0	8	715	720	6
8	0	8	0	16	1
10	0	8	1389	1417	10
1	1	8	91	87	10
3	1	8	130	129	7
5	1	8	514	529	5
7	1	8	164	177	7
9	1	8	724	705	6
11	1	8	470	475	5
0	2	8	0	8	1
2	2	8	80	69	11
4	2	8	267	273	5
6	2	8	503	495	5
8	2	8	59	42	16
10	2	8	258	251	6
1	3	8	141	136	7
3	3	8	322	325	5
5	3	8	1770	1761	13
7	3	8	0	18	1
9	3	8	441	442	5
11	3	8	149	164	8
0	4	8	269	271	5
2	4	8	272	268	5
4	4	8	263	262	5
6	4	8	582	606	5
8	4	8	0	39	1
10	4	8	112	113	9
1	5	8	533	537	5
3	5	8	149	148	7
5	5	8	421	425	5
7	5	8	0	13	1
9	5	8	185	176	7
0	6	8	1815	1861	14
2	6	8	196	196	6
4	6	8	360	359	5
6	6	8	440	445	5
8	6	8	172	171	7
1	7	8	53	63	21
3	7	8	133	137	8
5	7	8	872	895	7
7	7	8	208	219	6
0	8	8	931	935	7
2	8	8	51	41	21
4	8	8	7	4	7
6	8	8	370	378	5
1	9	8	42	40	41
3	9	8	158	158	8
5	9	8	1254	1251	9
0	10	8	1048	1029	7
2	10	8	140	142	8
1	1	9	67	62	15
3	1	9	186	191	6
5	1	9	292	292	5
0	2	9	95	98	11
2	2	9	44	35	26
4	2	9	251	251	6
6	2	9	48	4	25
1	3	9	162	160	7
3	3	9	5	15	4
5	3	9	56	68	21
0	4	9	448	438	5
2	4	9	48	49	25
4	4	9	82	73	11
1	5	9	24	10	24
3	5	9	91	110	12

Observed and calculated structure factors for R33

h	k	l	10Fo	10Fc	10s
2	0	0	602	613	2
4	0	0	1220	1214	4
6	0	0	669	690	4
8	0	0	1062	1046	5
10	0	0	4021	3889	7
12	0	0	1413	1424	7
14	0	0	257	245	3
16	0	0	366	364	3
18	0	0	610	604	4
20	0	0	372	380	3
22	0	0	1713	1704	11
1	1	0	713	769	2
3	1	0	266	261	2
5	1	0	609	613	4
7	1	0	443	437	3
9	1	0	1664	1645	6
11	1	0	3033	2918	7
13	1	0	346	346	3
15	1	0	213	227	3
17	1	0	319	324	3
19	1	0	585	591	4
21	1	0	812	823	5
0	2	0	1197	1246	3
2	2	0	312	329	2
4	2	0	613	631	4
6	2	0	100	105	2
8	2	0	248	250	2
10	2	0	610	626	4
12	2	0	347	342	3
14	2	0	851	855	5
16	2	0	775	772	5
18	2	0	42	3	11
20	2	0	154	150	4
22	2	0	317	310	4
1	3	0	127	123	2
3	3	0	497	495	3
7	3	0	501	478	3
9	3	0	985	979	6
11	3	0	415	410	3
13	3	0	167	177	3
15	3	0	955	967	7
17	3	0	972	970	6
19	3	0	267	264	3
21	3	0	322	311	4
0	4	0	2280	2349	4
2	4	0	692	686	4
4	4	0	1052	1047	5
6	4	0	3637	3716	7
8	4	0	533	524	3
10	4	0	591	592	4
12	4	0	288	281	3
14	4	0	822	828	5
16	4	0	2088	2060	9
18	4	0	114	109	5
20	4	0	264	259	4
22	4	0	462	464	4
1	5	0	1483	1496	5
3	5	0	64	56	2
5	5	0	3172	3165	6
7	5	0	906	896	6
9	5	0	65	67	4
11	5	0	364	377	3
13	5	0	277	281	3
15	5	0	282	284	3
17	5	0	466	472	4
19	5	0	168	176	4
21	5	0	335	335	4
0	6	0	999	1007	5
2	6	0	107	107	2
4	6	0	279	292	2
6	6	0	468	458	3
8	6	0	615	609	4
10	6	0	1489	1495	7
12	6	0	292	286	3
14	6	0	409	409	3
16	6	0	473	470	4
18	6	0	399	400	3
20	6	0	107	34	6
1	7	0	710	701	4
3	7	0	193	197	2
5	7	0	1513	1516	6
7	7	0	449	445	3
9	7	0	1229	1240	7
11	7	0	609	570	4
13	7	0	184	191	3
15	7	0	106	105	3
17	7	0	259	251	3
19	7	0	725	726	5
21	7	0	677	664	5
0	8	0	2671	2701	7
2	8	0	123	119	2
4	8	0	486	489	3
6	8	0	586	587	4
8	8	0	527	526	4
10	8	0	1187	1182	8
12	8	0	179	187	3
14	8	0	106	109	5
16	8	0	240	248	4
18	8	0	13	5	12
20	8	0	360	345	4
1	9	0	204	188	2
3	9	0	329	336	3
5	9	0	1901	1931	7
7	9	0	946	935	6
9	9	0	148	140	3
11	9	0	577	562	4
13	9	0	301	288	3
15	9	0	650	649	4
17	9	0	531	541	4
19	9	0	285	281	4
0	10	0	370	385	3
2	10	0	58	64	5
4	10	0	378	389	3
6	10	0	254	245	2
8	10	0	340	349	3
10	10	0	612	605	5
12	10	0	177	182	3
14	10	0	1166	1156	8
16	10	0	308	310	4
18	10	0	519	523	4
1	11	0	322	320	3
3	11	0	286	291	2
5	11	0	928	940	6
7	11	0	121	132	4
9	11	0	128	128	4
11	11	0	446	460	4
13	11	0	194	197	4
15	11	0	894	896	6
17	11	0	458	464	4
0	12	0	1446	1454	8
2	12	0	207	196	3
4	12	0	343	334	3
6	12	0	644	655	4
8	12	0	191	190	3
10	12	0	642	642	5
12	12	0	545	547	4
14	12	0	156	160	4
16	12	0	81	80	8
1	13	0	568	570	4
3	13	0	242	245	3
5	13	0	424	423	3
7	13	0	533	543	4
9	13	0	374	370	3
11	13	0	965	960	7
13	13	0	322	325	4
15	13	0	309	307	4
0	14	0	1486	1504	9
2	14	0	397	399	3
4	14	0	218	201	3
6	14	0	717	724	5
8	14	0	144	149	4
10	14	0	1361	1372	10
12	14	0	117	89	6
14	14	0	52	21	12
1	15	0	332	319	3
3	15	0	383	378	3
5	15	0	472	462	4
7	15	0	38	5	15
9	15	0	224	220	4
11	15	0	403	403	4
13	15	0	423	430	4
0	16	0	571	578	4
2	16	0	219	217	3
4	16	0	134	131	4
6	16	0	834	832	5
8	16	0	66	81	9
10	16	0	66	53	9
12	16	0	467	464	4
1	17	0	245	237	4
3	17	0	344	342	3
5	17	0	1855	1869	10
7	17	0	36	23	20
9	17	0	31	4	30
0	18	0	307	312	4
2	18	0	272	276	4
4	18	0	118	110	5
6	18	0	299	254	4
8	18	0	303	292	4
1	19	0	230	228	4
3	19	0	129	114	5
1	1	1	192	175	1
3	1	1	470	457	3
5	1	1	716	727	4
7	1	1	139	127	2
9	1	1	391	384	3
11	1	1	834	854	5
13	1	1	308	304	3
15	1	1	60	40	6
17	1	1	684	699	5
19	1	1	471	485	4
21	1	1	860	845	6
0	2	1	247	203	2
2	2	1	438	460	3
4	2	1	452	454	3
6	2	1	207	186	2
8	2	1	700	700	4
10	2	1	342	364	3
12	2	1	919	920	6
14	2	1	98	95	4
16	2	1	725	744	5
18	2	1	44	52	11
20	2	1	172	178	4
22	2	1	224	229	4
1	3	1	327	328	2
3	3	1	243	236	2
5	3	1	260	248	2
7	3	1	501	499	3
9	3	1	309	312	2
11	3	1	299	309	2
13	3	1	289	292	3
15	3	1	35	34	13
17	3	1	139	140	3
19	3	1	217	220	4
21	3	1	182	188	4
0	4	1	970	986	4
2	4	1	51	59	3
4	4	1	276	265	2
6	4	1	808	771	5
8	4	1	505	497	3
10	4	1	293	273	2
12	4	1	681	683	4
14	4	1	291	280	3
16	4	1	632	636	4
18	4	1	217	220	4
20	4	1	85	79	7
1	5	1	147	144	1
3	5	1	573	570	3
5	5	1	1581	1581	5
7	5	1	873	860	6
9	5	1	479	478	3
11	5	1	165	186	3
13	5	1	670	673	4
15	5	1	134	119	4
17	5	1	240	230	3
19	5	1	61	60	9
21	5	1	784	781	5
0	6	1	317	297	2
2	6	1	216	213	2
4	6	1	263	254	2
6	6	1	952	953	6
8	6	1	492	482	4
10	6	1	17	10	17
12	6	1	141	329	3
14	6	1	36	17	13
16	6	1	1085	1086	7
18	6	1	244	243	4
20	6	1	422	423	4
1	7	1	58	41	3
3	7	1	623	621	4
5	7	1	522	518	4
7	7	1	141	138	3
9	7	1	493	510	4
11	7	1	47	14	7
13	7	1	42	42	10
15	7	1	34	14	18
17	7	1	190	190	4
19	7	1	191	175	4
0	8	1	691	679	4
2	8	1	24	14	11
4	8	1	77	81	3
6	8	1	331	350	3
8	8	1	125	127	3
10	8	1	87	79	4
12	8	1	461	462	3
14	8	1	545	542	4
16	8	1	699	695	5
18	8	1	296	290	4
20	8	1	233	237	4
1	9	1	952	941	6
3	9	1	135	127	3
5	9	1	527	555	4
7	9	1	302	301	3
9	9	1	68	68	5
11	9	1	1699	1725	8
13	9	1	51	48	9
15	9	1	60	57	9
17	9	1	134	139	5
19	9	1	169	183	5
0	10	1	1352	1377	7
2	10	1	797	793	5
4	10	1	289	298	3
6	10	1	455	450	3
8	10	1	124	121	3
10	10	1	322	321	3
12	10	1	49	36	9
14	10	1	671	667	5
16	10	1	364	375	3
18	10	1	301	286	4
1	11	1	272	280	3
3	11	1	241	239	3
5	11	1	631	642	4
7	11	1	457	455	3
9	11	1	393	392	3
11	11	1	370	374	3
13	11	1	99	100	5
15	11	1	102	109	6
17	11	1	168	173	4
0	12	1	1145	1166	8
2	12	1	532	532	4
4	12	1	95	96	4
6	12	1	693	684	5
8	12	1	148	141	4
10	12	1	193	195	3
12	12	1	273	271	3
14	12	1	98	97	6
16	12	1	760	770	5
1	13	1	395	385	3
3	13	1	332	337	3
5	13	1	1047	1051	7
7	13	1	84	86	5
9	13	1	356	357	3
11	13	1	1178	1172	8
13	13	1	144	130	4
15	13	1	208	198	4
0	14	1	714	733	5
2	14	1	274	266	3
4	14	1	480	481	4
6	14	1	225	211	3
8	14	1	297	295	3
10	14	1	242	245	4
12	14	1	117	127	5
14	14	1	395	392	4
1	15	1	67	61	7
3	15	1	286	293	3
5	15	1	292	290	3
7	15	1	288	288	3
9	15	1	67	71	8
11	15	1	219	209	4
13	15	1	139	137	5
0	16	1	332	340	3
2	16	1	270	267	3
4	16	1	45	35	12
6	16	1	1273	1259	8
8	16	1	366	365	3
10	16	1	0	14	1
12	16	1	87	92	8
1	17	1	77	66	7
3	17	1	268	264	4
5	17	1	795	790	6
7	17	1	274	266	4
9	17	1	389	388	4
0	18	1	241	247	4
2	18	1	41	54	16
4	18	1	390	397	4
6	18	1	389	389	4
1	19	1	377	388	4
3	19	1	409	415	4
2	0	2	659	684	4
4	0	2	353	349	2
6	0	2	708	677	4
8	0	2	701	694	5
10	0	2	1555	1531	7
12	0	2	946	946	6
14	0	2	1376	1367	8
16	0	2	825	835	5
18	0	2	800	802	5
20	0	2	131	136	5
22	0	2	255	267	4
1	1	2	501	515	3
3	1	2	704	714	4
5	1	2	1205	1193	5
7	1	2	174	171	2
9	1	2	670	660	4
11	1	2	604	601	4
13	1	2	89	85	4
15	1	2	728	738	5
17	1	2	79	72	6
19	1	2	18	15	18
21	1	2	280	264	4
2	2	2	301	307	2
4	2	2	455	452	3
6	2	2	397	388	3
8	2	2	220	211	2
10	2	2	1341	1161	7
12	2	2	564	571	4
14	2	2	107	103	4
16	2	2	293	289	3
18	2	2	57	37	8
20	2	2	59	43	10
1	3	2	439	439	1
3	3	2	216	209	2
5	3	2	1200	1198	5
7	3	2	178	179	2
9	3	2	1535	1572	7
11	3	2	1436	1452	7
13	3	2	462	455	3
15	3	2	252	245	3
17	3	2	334	333	3
19	3	2	829	838	5
21	3	2	640	639	4
0	4	2	2128	2082	5
2	4	2	735	727	5
4	4	2	67	49	3
6	4	2	350	334	2
8	4	2	188	198	2
10	4	2	2128	2199	7
12	4	2	265	271	3
14	4	2	224	224	3
16	4	2	91	60	5
18	4	2	536	529	4
20	4	2	367	361	4
1	5	2	1054	1030	5
3	5	2	85	88	2
5	5	2	1797	1784	6
7	5	2	167	157	2
9	5	2	491	493	3
11	5	2	689	675	4
13	5	2	86	70	5
15	5	2	287	283	3
17	5	2	781	772	5
19	5	2	434	425	4
21	5	2	455	449	4
0	6	2	1208	1205	5
2	6	2	70	73	3
4	6	2	930	923	6
6	6	2	2421	2416	7
8	6	2	256	248	2
10	6	2	107	103	4
12	6	2	406	405	3
14	6	2	896	898	6
16	6	2	1497	1516	9
18	6	2	59	39	10
20	6	2	59	46	11
1	7	2	714	704	5
3	7	2	78	72	3
5	7	2	4556	4597	8
7	7	2	210	192	2
9	7	2	483	501	3
11	7	2	72	72	5
13	7	2	196	193	3
15	7	2	1035	1031	6
17	7	2	949	961	6
19	7	2	103	104	6
0	8	2	338	345	3
2	8	2	510	504	3
4	8	2	245	248	2
6	8	2	199	192	3
8	8	2	629	630	4
10	8	2	71	76	6
12	8	2	160	160	3
14	8	2	584	580	4
16	8	2	919	927	6
18	8	2	86	83	7
1	9	2	551	540	4
3	9	2	117	103	3
5	9	2	519	510	4
7	9	2	481	468	3
9	9	2	586	597	4
11	9	2	1606	1612	8
13	9	2	115	119	5

Observed and calculated structure factors for K33

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	249	245	4	20	2	3	104	102	6	17	11	3	481	479	4	12	4	4	179	179	3	12	14	4	44	45	15
17	9	2	700	691	5	1	3	3	507	505	3	0	12	3	281	288	3	14	4	4	804	822	5	1	15	4	284	272	3
19	9	2	268	262	4	3	3	3	270	270	2	2	12	3	318	314	3	16	4	4	1480	1489	10	3	15	4	386	384	3
0	10	2	4438	4460	9	5	3	3	1103	1089	6	4	12	3	354	355	3	18	4	4	170	162	4	5	15	4	204	201	4
2	10	2	596	592	4	7	3	3	762	751	5	6	12	3	182	181	3	1	5	4	1025	1011	6	7	15	4	138	128	5
4	10	2	709	703	4	9	3	3	229	229	2	8	12	3	68	64	7	3	5	4	167	153	2	9	15	4	206	201	4
6	10	2	43	34	8	11	3	3	1344	1369	8	10	12	3	195	195	4	5	5	4	1571	1592	7	0	16	4	160	153	4
8	10	2	319	322	3	13	3	3	89	79	5	12	12	3	272	264	4	7	5	4	426	429	3	2	16	4	191	195	4
10	10	2	1894	1936	9	15	3	3	105	110	5	14	12	3	180	188	4	9	5	4	87	80	4	4	16	4	90	77	7
12	10	2	361	362	3	17	3	3	234	227	3	16	12	3	474	474	4	11	5	4	903	912	6	6	16	4	458	465	4
14	10	2	334	336	3	19	3	3	143	138	5	1	13	3	283	277	3	13	5	4	136	130	4	8	16	4	0	6	1
16	10	2	146	149	5	21	3	3	439	441	4	3	13	3	452	451	3	15	5	4	286	289	3	1	17	4	321	313	4
18	10	2	283	272	4	0	4	3	2118	2035	6	5	13	3	443	444	4	17	5	4	91	94	7	3	17	4	227	219	4
1	11	2	340	339	3	2	4	3	58	63	4	7	13	3	121	120	4	19	5	4	118	107	6	1	1	5	73	71	4
3	11	2	701	706	5	4	4	3	386	379	3	9	13	3	300	299	3	0	6	4	2214	2207	7	3	1	5	220	227	2
5	11	2	116	112	4	6	4	3	213	208	2	11	13	3	462	455	4	2	6	4	134	136	3	5	1	5	588	594	4
7	11	2	27	18	19	8	4	3	263	265	2	13	13	3	25	6	24	4	6	4	325	318	3	7	1	5	29	34	16
9	11	2	651	667	5	10	4	3	397	389	3	15	13	3	130	110	6	6	6	4	201	204	3	9	1	5	312	320	3
11	11	2	1770	1774	9	12	4	3	732	748	5	0	14	3	83	75	6	8	6	4	318	310	3	11	1	5	256	253	3
13	11	2	67	54	7	14	4	3	122	114	4	2	14	3	231	232	3	10	6	4	1361	1352	8	13	1	5	143	152	4
15	11	2	232	218	4	16	4	3	246	231	3	4	14	3	397	410	3	12	6	4	365	372	3	15	1	5	41	11	13
17	11	2	105	98	6	18	4	3	141	127	4	6	14	3	202	215	4	14	6	4	210	206	3	17	1	5	717	718	5
0	12	2	1404	1411	8	20	4	3	26	15	25	8	14	3	353	355	3	16	6	4	179	159	4	19	1	5	368	383	4
2	12	2	49	49	8	1	5	3	51	49	4	10	14	3	101	83	6	18	6	4	301	292	4	0	2	5	602	598	4
4	12	2	108	109	4	3	5	3	357	369	3	12	14	3	19	9	19	1	7	4	284	272	2	2	2	5	111	70	3
6	12	2	861	860	6	5	5	3	951	951	6	1	15	3	244	238	3	3	7	4	259	256	2	4	2	5	428	431	3
8	12	2	192	192	3	7	5	3	851	852	5	3	15	3	213	207	4	5	7	4	1354	1361	8	6	2	5	434	433	3
10	12	2	796	803	6	9	5	3	357	361	3	5	15	3	466	480	4	7	7	4	364	361	3	8	2	5	359	354	3
12	12	2	265	255	4	11	5	3	233	201	3	7	15	3	155	151	4	9	7	4	941	966	7	10	2	5	158	121	3
14	12	2	476	467	4	13	5	3	514	512	4	9	15	3	141	134	5	11	7	4	730	733	5	12	2	5	734	742	5
16	12	2	407	408	4	15	5	3	39	32	14	11	15	3	419	399	4	13	7	4	330	326	3	14	2	5	39	17	13
1	13	2	106	101	4	17	5	3	296	293	3	0	16	3	189	180	4	15	7	4	282	281	4	16	2	5	288	290	4
3	13	2	24	9	24	19	5	3	107	99	6	2	16	3	94	94	6	17	7	4	356	359	4	18	2	5	138	142	5
5	13	2	1820	1848	9	0	6	3	651	660	4	4	16	3	187	189	4	0	8	4	1953	1981	8	1	3	5	118	118	3
7	13	2	84	75	6	2	6	3	92	86	3	6	16	3	1103	1105	7	2	8	4	28	9	13	3	3	5	213	213	3
9	13	2	65	49	7	4	6	3	495	473	3	8	16	3	303	305	4	4	8	4	240	241	3	5	3	5	475	483	3
11	13	2	53	64	10	6	6	3	1256	1251	7	10	16	3	137	145	5	6	8	4	538	539	4	7	3	5	107	110	4
13	13	2	142	143	5	8	6	3	355	350	3	1	17	3	139	144	5	8	8	4	411	416	3	9	3	5	143	141	3
15	13	2	592	595	4	10	6	3	62	71	6	3	17	3	281	278	4	10	8	4	1178	1200	7	11	3	5	236	234	3
0	14	2	467	465	4	12	6	3	307	299	3	5	17	3	505	510	4	12	8	4	112	112	5	13	3	5	302	300	3
2	14	2	309	307	3	14	6	3	75	69	6	7	17	3	50	5	12	14	8	4	100	98	5	15	3	5	34	27	19
4	14	2	725	729	5	16	6	3	1135	1147	8	0	18	3	264	256	4	16	8	4	200	204	4	17	3	5	534	537	4
6	14	2	450	434	4	18	6	3	372	376	4	2	18	3	159	162	5	18	8	4	85	63	7	0	4	5	79	66	4
8	14	2	206	200	3	20	6	3	378	383	4	2	0	4	346	347	3	1	9	4	109	100	4	2	4	5	50	14	7
10	14	2	161	168	4	1	7	3	102	94	3	4	0	4	665	671	4	3	9	4	224	227	3	4	4	5	124	124	3
12	14	2	117	57	5	3	7	3	290	302	2	6	0	4	331	315	3	5	9	4	1786	1798	8	6	4	5	660	663	5
14	14	2	385	381	4	5	7	3	1256	1231	7	8	0	4	152	156	3	7	9	4	527	532	4	8	4	5	351	361	3
1	15	2	614	617	5	7	7	3	244	229	2	10	0	4	2826	2821	8	9	9	4	57	55	8	10	4	5	167	155	3
3	15	2	261	263	3	9	7	3	487	497	4	12	0	4	962	966	6	11	9	4	175	169	4	12	4	5	456	464	4
5	15	2	1513	1520	9	11	7	3	796	791	5	14	0	4	412	415	3	13	9	4	128	124	5	14	4	5	278	274	3
7	15	2	528	521	4	13	7	3	148	152	4	16	0	4	57	52	9	15	9	4	464	465	4	16	4	5	646	654	4
9	15	2	52	23	11	15	7	3	118	123	5	18	0	4	589	577	4	17	9	4	625	619	5	18	4	5	250	246	4
11	15	2	393	389	4	17	7	3	614	613	4	20	0	4	245	244	4	0	10	4	903	904	6	1	5	5	173	166	3
13	15	2	158	149	5	19	7	3	146	136	5	1	1	4	278	270	2	2	10	4	18	12	18	3	5	5	311	308	3
0	16	2	954	961	7	0	8	3	821	814	5	3	1	4	80	69	3	4	10	4	455	462	3	5	5	5	760	765	5
2	16	2	166	162	4	2	8	3	118	124	3	5	1	4	158	147	2	6	10	4	229	225	3	7	5	5	581	585	4
4	16	2	139	138	5	4	8	3	331	329	3	7	1	4	21	19	20	8	10	4	362	356	3	9	5	5	346	356	3
6	16	2	482	487	4	6	8	3	540	526	4	9	1	4	1221	1258	7	10	10	4	500	515	4	11	5	5	308	313	3
8	16	2	7	37	6	8	8	3	73	44	5	11	1	4	1673	1680	8	12	10	4	221	215	4	13	5	5	451	455	4
10	16	2	741	738	5	10	8	3	68	56	6	13	1	4	189	191	3	14	10	4	867	872	6	15	5	5	86	72	7
1	17	2	217	214	4	12	8	3	543	553	4	15	1	4	159	151	4	16	10	4	439	435	4	17	5	5	179	168	4
3	17	2	424	420	4	14	8	3	318	322	3	17	1	4	30	3	29	1	11	4	212	203	3	0	6	5	271	303	3
5	17	2	178	176	4	16	8	3	213	198	4	19	1	4	556	544	4	3	11	4	362	357	3	2	6	5	106	108	4
7	17	2	87	82	7	18	8	3	112	121	6	0	2	4	304	324	2	5	11	4	1115	1138	7	4	6	5	7	22	6
9	17	2	147	137	4	1	9	3	585	584	4	2	2	4	211	211	2	7	11	4	39	34	12	6	6	5	473	466	3
0	18	2	753	741	5	3	9	3	121	124	3	4	2	4	396	396	3	9	11	4	73	71	7	8	6	5	123	131	3
2	18	2	64	64	9	5	9	3	165	154	3	6	2	4	472	491	3	11	11	4	35	25	18	10	6	5	20	11	19
4	18	2	296	294	4	7	9	3	218	218	3	8	2	4	79	82	4	13	11	4	115	124	5	12	6	5	251	240	3
6	18	2	404	400	4	9	9	3	105	107	4	10	2	4	413	429	3	15	11	4	751	751	5	14	6	5	62	36	8
1	1	3	254	251	2	11	9	3	938	929	6	12	2	4	334	339	3	0	12	4	907	911	6	16	6	5	733	736	5
3	1	3	648	652	4	13	9	3	66	23	7	14	2	4	637	633	4	2	12	4	228	224	3	1	7	5	71	42	5
5	1	3	279	282	2	15	9	3	97	80	6	16	2	4	757	767	5	4	12	4	212	207	3	3	7	5	479	494	3
7	1	3	263	267	2	17	9	3	488	487	4	18	2	4	24	17	24	6	12	4	316	315	3	5	7	5	110	96	4
9	1	3	339	343	3	0	10	3	941	956	6	20	2	4	110	98	6	8	12	4	248	249	3	7	7	5	280	281	3
11	1	3	1373	1376	7	2	10	3	784	791	5	1	3	4	216	212	2	10	12	4	432	429	4	9	7	5	333	333	3
13	1	3	393	391	3	4	10	3	391	397	3	3	3	4	415	411	3	12	12	4	368	370	4	11	7	5	377	376	3
15	1	3	112	109	5	6	10	3	219	214	3	5	3	4	3601	3485	8	14	12	4	54	57	12	13	7	5	167	162	4
17	1	3	332	324	3	8	10	3	196	197	3	7	3	4	157	155	3	1	13	4	330	334	3	15	7	5	64	68	9
19	1	3	459	475	4	10	10	3	108	122	5	9	3	4	735	756	4	3	13	4	152	157	4	17	7	5	62	64	10
21	1	3	824	808	5	12	10	3	125	136	4	11	3	4	127	130	4	5	13	4	281	281	3	0	8	5	811	821	5
0	2	3	2497	2386	6	14	10	3	649	655	5	13	3	4	326	335	3	7	13	4	322	325	3	2	8	5	121	120	4
2	2	3	536	526	3	16	10	3	152	166	5	15	3	4	819	830	6	9	13	4	379	381	3	4	8	5	45	24	9
4	2	3	85	74	3	1	11	3	376	374	3	17	3	4	748	747	5	11	13	4	768	766	5	6	8	5	582	582	4
6	2	3	1151	1126	6	3	11	3	184	186	3	19	3	4	229	231	4	13	13	4	174	187	5	8	8	5	130	120	4
8	2	3	792	779	5	5	11	3	712	705	5	0	4	4	661	686	4	0	14	4	1433	1443	9	10	8	5	48	44	11
10	2	3	158	372	3	7	11	3	160	150	3	2	4	4	453	442	3	2	14	4	229	231	4	12	8	5	325	331	3
12	2	3	686	697	5	9	11	3	433	445	4	4	4	4	608	637	4	4	14	4	314	318	3	14	8	5	474	476	4
14	2	3	316	307	3	11	11	3	150	97	4	6	4	4	1914	1895	7	6	14	4	482	498	4	16	8	5	752	739	5
16	2	3	1106	1112	7	13	11	3	83	75	6	8	4	4	232	233	3	8	14	4	132	118	5	1	9	5	667	678	4
18	2	3	151	144	4	15	11	3	37	39	21	10	4	4	408	420	3	10	14	4	1077	1079	7	3	9	5	56	46	7

Observed and calculated structure factors for K33

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	9	5	602	592	4	11	1	6	239	235	3	10	8	6	105	89	6	0	4	7	981	963	7	5	1	8	427	428	3
7	9	5	329	321	3	13	1	6	32	18	25	12	8	6	189	171	4	2	4	7	112	102	4	7	1	8	207	201	4
9	9	5	62	64	7	15	1	6	478	478	4	14	8	6	410	408	4	4	4	7	266	254	3	9	1	8	683	680	5
11	9	5	1546	1548	10	17	1	6	313	316	4	1	9	6	395	389	3	6	4	7	98	92	5	11	1	8	519	524	4
13	9	5	108	116	6	0	2	6	1737	1734	8	3	9	6	75	79	6	8	4	7	210	210	4	0	2	8	20	10	20
15	9	5	75	83	9	2	2	6	203	192	3	5	9	6	0	4	1	10	4	7	258	255	4	2	2	8	95	96	6
0	10	5	1065	1077	7	4	2	6	162	169	3	7	9	6	508	523	4	12	4	7	449	460	4	4	2	8	240	241	4
2	10	5	502	511	4	6	2	6	457	464	4	9	9	6	417	411	3	14	4	7	130	133	6	6	2	8	512	508	4
4	10	5	148	137	4	8	2	6	226	225	3	11	9	6	742	744	5	1	5	7	23	11	22	8	2	8	0	24	1
6	10	5	471	468	4	10	2	6	881	841	5	13	9	6	0	32	1	3	5	7	180	185	4	10	2	8	228	226	4
8	10	5	81	87	6	12	2	6	311	319	3	0	10	6	2220	2215	9	5	5	7	344	347	3	1	3	8	117	115	5
10	10	5	317	312	3	14	2	6	7	0	7	2	10	6	279	277	3	7	5	7	504	513	4	3	3	8	288	295	3
12	10	5	34	39	25	16	2	6	350	351	4	4	10	6	101	290	3	9	5	7	253	259	4	5	3	8	1835	1836	10
14	10	5	502	500	4	1	3	6	222	215	3	6	10	6	502	517	4	11	5	7	91	79	7	7	3	8	91	19	6
1	11	5	127	131	4	3	3	6	75	71	5	8	10	6	110	109	6	13	5	7	310	310	4	9	3	8	416	418	4
3	11	5	189	191	4	5	3	6	882	884	6	10	10	6	1314	1331	8	0	6	7	295	294	3	11	3	8	111	109	6
5	11	5	448	439	4	7	3	6	75	72	5	12	10	6	214	209	4	2	6	7	118	118	4	0	4	8	177	168	4
7	11	5	474	479	4	9	3	6	1044	1059	7	1	11	6	67	78	8	4	6	7	213	217	3	2	4	8	286	287	3
9	11	5	260	261	4	11	3	6	1119	1134	7	3	11	6	330	321	3	6	6	7	716	707	5	4	4	8	247	237	4
11	11	5	403	405	4	13	3	6	238	228	4	5	11	6	406	409	4	8	6	7	246	250	4	6	4	8	623	627	4
13	11	5	183	174	4	15	3	6	129	120	5	7	11	6	94	92	6	10	6	7	91	93	6	8	4	8	51	36	11
0	12	5	1144	1131	7	17	3	6	349	353	4	9	11	6	493	495	4	12	6	7	202	203	4	10	4	8	203	199	4
2	12	5	512	515	4	0	4	6	2516	2490	8	11	11	6	729	734	5	1	7	7	49	56	11	1	5	8	535	537	4
4	12	5	71	67	7	2	4	6	90	88	4	0	12	6	559	573	4	3	7	7	264	264	3	3	5	8	149	154	4
6	12	5	720	720	5	4	4	6	332	341	3	2	12	6	78	86	7	5	7	7	751	743	5	5	5	8	465	465	4
8	12	5	97	86	6	6	4	6	516	512	4	4	12	6	101	111	6	7	7	7	149	141	4	7	5	8	56	30	10
10	12	5	99	96	6	8	4	6	144	151	4	6	12	6	887	900	6	9	7	7	353	352	3	9	5	8	116	114	6
12	12	5	225	223	4	10	4	6	1451	1447	9	8	12	6	45	51	15	11	7	7	496	500	4	0	6	8	1867	1874	10
1	13	5	334	328	3	12	4	6	247	240	3	10	12	6	437	439	4	0	8	7	504	503	4	2	6	8	165	165	4
3	13	5	243	247	4	14	4	6	53	50	11	1	13	6	39	34	16	2	8	7	102	101	5	4	6	8	295	293	4
5	13	5	995	1004	7	16	4	6	240	235	4	3	13	6	32	3	31	4	8	7	262	255	4	6	6	8	475	474	4
7	13	5	195	193	4	1	5	6	306	306	3	5	13	6	1368	1373	8	6	8	7	314	307	3	8	6	8	125	129	5
9	13	5	312	314	4	3	5	6	311	319	3	7	13	6	189	192	4	8	8	7	46	35	13	1	7	8	62	70	9
11	13	5	1261	1245	7	5	5	6	472	475	3	0	14	6	65	17	9	10	8	7	65	60	9	3	7	8	165	169	4
0	14	5	915	906	6	7	5	6	97	103	5	2	14	6	357	360	4	1	9	7	371	367	3	5	7	8	910	923	6
2	14	5	232	219	4	9	5	6	261	264	3	4	14	6	323	323	4	3	9	7	67	62	8	7	7	8	212	204	4
4	14	5	374	380	3	11	5	6	322	321	3	6	14	6	136	122	5	5	9	7	161	157	4	0	8	8	987	979	6
6	14	5	377	382	4	13	5	6	50	59	11	1	1	7	95	84	5	7	9	7	131	128	5	2	8	8	63	58	9
8	14	5	199	197	4	15	5	6	250	250	4	3	1	7	241	238	3	9	9	7	24	19	24	4	8	8	64	45	9
1	15	5	33	47	24	0	6	6	92	88	5	5	1	7	35	12	14	0	10	7	618	625	4	6	8	8	384	385	4
3	15	5	245	249	4	2	6	6	29	21	18	7	1	7	254	252	3	2	10	7	427	436	4	1	9	8	24	3	24
5	15	5	117	108	6	4	6	6	448	442	4	9	1	7	188	192	4	4	10	7	197	189	4	3	9	8	133	119	5
7	15	5	271	280	4	6	6	6	906	904	6	11	1	7	749	746	5	6	10	7	206	190	4	5	9	8	1220	1249	7
0	16	5	297	292	4	8	6	6	293	296	3	13	1	7	299	303	4	8	10	7	93	92	7	0	10	8	1041	1046	7
2	16	5	293	288	4	10	6	6	41	24	13	15	1	7	118	123	6	1	11	7	192	199	4	2	10	8	93	86	7
4	16	5	137	140	5	12	6	6	198	199	4	0	2	7	755	746	5	3	11	7	108	105	6	1	1	9	53	48	11
0	0	6	2724	2645	8	14	6	6	794	795	5	2	2	7	320	316	3	5	11	7	509	507	4	3	1	9	195	183	4
2	0	6	132	130	3	1	7	6	568	572	4	4	2	7	20	15	19	7	11	7	119	121	6	5	1	9	256	254	4
4	0	6	611	624	4	3	7	6	139	138	4	6	2	7	487	482	4	0	12	7	86	95	7	0	2	9	72	57	8
6	0	6	701	704	4	5	7	6	2555	2535	9	8	2	7	302	299	3	2	12	7	201	197	4	2	2	9	57	58	11
8	0	6	432	437	3	7	7	6	97	98	5	10	2	7	111	107	5	4	12	7	248	248	4	4	2	9	185	181	4
10	0	6	947	949	6	9	7	6	403	406	3	12	2	7	503	505	4	0	0	8	2612	2582	10	6	2	9	16	14	24
12	0	6	727	731	5	11	7	6	410	425	3	14	2	7	143	145	5	2	0	8	143	143	4	1	3	9	135	135	5
14	0	6	780	789	5	13	7	6	242	232	4	1	3	7	209	200	3	4	0	8	243	241	4	3	3	9	20	34	20
16	0	6	877	895	6	15	7	6	684	688	5	3	3	7	27	21	26	6	0	8	679	666	5	5	3	9	47	51	15
1	1	6	165	159	3	0	8	6	236	239	3	5	3	7	438	436	3	8	0	8	18	22	18	0	4	9	389	384	4
3	1	6	128	118	3	2	8	6	222	219	3	7	3	7	430	436	4	10	0	8	1529	1531	11	2	4	9	12	43	11
5	1	6	1765	1751	8	4	8	6	337	334	3	9	3	7	188	185	4	12	0	8	505	503	4	4	4	9	66	77	9
7	1	6	75	71	5	6	8	6	275	271	3	11	3	7	807	803	5	1	1	8	108	116	5	1	5	9	30	18	29
9	1	6	366	356	3	8	8	6	371	371	3	13	3	7	22	29	21	3	1	8	120	115	5	3	5	9	84	87	7

Observed and calculated structure factors for K34

h	k	l	10Fo	10Fc	10s
2	0	0	640	663	3
4	0	0	1311	1289	4
6	0	0	556	579	4
8	0	0	945	929	6
10	0	0	3862	3761	8
12	0	0	1398	1424	8
14	0	0	267	262	3
16	0	0	241	236	4
18	0	0	649	641	5
20	0	0	326	328	4
22	0	0	1593	1607	10
1	1	0	294	282	2
5	1	0	549	561	3
7	1	0	195	190	3
9	1	0	1650	1647	7
11	1	0	2929	2840	8
13	1	0	281	283	3
15	1	0	221	229	4
17	1	0	332	331	4
19	1	0	616	618	5
21	1	0	747	756	5
0	2	0	1210	1226	3
2	2	0	327	348	2
4	2	0	610	615	4
6	2	0	83	73	4
8	2	0	231	236	2
10	2	0	621	628	4
12	2	0	352	346	3
14	2	0	853	855	6
16	2	0	727	729	5
18	2	0	88	73	8
20	2	0	180	173	5
22	2	0	316	315	5
1	3	0	394	386	3
3	3	0	609	611	4
7	3	0	476	465	3
9	3	0	1052	1051	7
11	3	0	287	291	3
13	3	0	345	351	3
15	3	0	897	901	7
17	3	0	952	947	6
19	3	0	266	263	4
21	3	0	409	393	4
0	4	0	2268	2285	5
2	4	0	722	718	5
4	4	0	1042	1040	5
6	4	0	3866	3645	7
8	4	0	553	554	4
10	4	0	554	562	4
12	4	0	335	339	3
14	4	0	868	877	6
16	4	0	1951	1962	10
18	4	0	165	162	5
20	4	0	296	280	4
22	4	0	438	435	5
1	5	0	1542	1535	5
3	5	0	42	28	7
5	5	0	3281	3121	6
7	5	0	897	896	5
9	5	0	82	91	5
11	5	0	378	392	3
13	5	0	339	350	3
15	5	0	296	300	4
17	5	0	438	440	4
19	5	0	187	193	5
21	5	0	310	313	5
0	6	0	878	890	6
2	6	0	142	140	3
4	6	0	167	373	3
6	6	0	541	533	4
8	6	0	709	700	5
10	6	0	1407	1405	8
12	6	0	306	312	3
14	6	0	448	445	4
16	6	0	558	546	4
18	6	0	373	384	4
20	6	0	49	2	20
1	7	0	711	699	4
3	7	0	184	188	3
5	7	0	1488	1469	7
7	7	0	478	486	4
9	7	0	1246	1245	8
11	7	0	533	495	4
13	7	0	438	441	4
15	7	0	289	291	4
17	7	0	228	236	5
19	7	0	747	754	5
0	8	0	2643	2628	7
2	8	0	154	151	3
4	8	0	489	483	3
6	8	0	621	625	4
8	8	0	466	474	4
10	8	0	1404	1386	9
12	8	0	219	218	4
14	8	0	116	120	6
16	8	0	281	277	4
18	8	0	0	22	1
20	8	0	366	360	5
1	9	0	162	143	3
3	9	0	403	414	3
5	9	0	1813	1842	8
7	9	0	927	923	6
9	9	0	101	95	6
11	9	0	604	600	5
13	9	0	251	254	4
15	9	0	572	582	4
17	9	0	500	497	4
19	9	0	322	318	5
0	10	0	291	313	3
2	10	0	52	55	10
4	10	0	361	364	3
6	10	0	287	287	3
8	10	0	368	386	3
10	10	0	566	569	4
12	10	0	178	184	5
14	10	0	1175	1188	8
16	10	0	247	232	5
18	10	0	583	583	5
1	11	0	379	374	3
3	11	0	272	271	3
5	11	0	892	902	6
7	11	0	138	146	5
9	11	0	111	120	6
11	11	0	527	542	4
13	11	0	140	149	6
15	11	0	918	934	6
17	11	0	480	483	4
0	12	0	1402	1429	9
2	12	0	263	257	3
4	12	0	297	294	3
6	12	0	631	643	5
8	12	0	232	233	4
10	12	0	579	591	4
12	12	0	532	539	4
14	12	0	136	146	7
16	12	0	135	121	7
1	13	0	551	550	4
3	13	0	248	252	4
5	13	0	372	372	4
7	13	0	550	572	4
9	13	0	384	384	4
11	13	0	886	900	6
13	13	0	338	348	4
15	13	0	284	288	5
0	14	0	1417	1410	8
2	14	0	420	417	4
4	14	0	244	217	4
6	14	0	798	809	6
8	14	0	113	112	7
10	14	0	1364	1369	9
12	14	0	49	62	19
14	14	0	59	43	16
1	15	0	297	293	4
3	15	0	440	442	4
5	15	0	475	484	4
7	15	0	0	2	1
9	15	0	174	167	5
11	15	0	425	422	4
13	15	0	479	472	4
0	16	0	532	541	5
2	16	0	225	223	5
4	16	0	143	141	6
6	16	0	866	856	6
8	16	0	72	72	12
10	16	0	52	30	17
12	16	0	461	466	4
1	17	0	266	262	5
3	17	0	318	320	4
5	17	0	1813	1822	12
7	17	0	30	11	30
9	17	0	21	15	21
0	18	0	351	351	4
2	18	0	320	319	5
4	18	0	76	75	11
6	18	0	202	195	6
8	18	0	348	337	5
1	19	0	260	259	5
3	19	0	94	91	10
1	1	1	184	171	2
3	1	1	489	485	3
5	1	1	776	791	5
7	1	1	181	170	2
9	1	1	449	450	3
11	1	1	785	806	5
13	1	1	330	330	3
15	1	1	0	23	1
17	1	1	715	724	5
19	1	1	442	461	4
21	1	1	893	873	6
0	2	1	116	59	2
2	2	1	192	417	3
4	2	1	515	516	3
6	2	1	285	258	2
8	2	1	698	710	4
10	2	1	386	404	3
12	2	1	920	933	7
14	2	1	102	102	6
16	2	1	705	708	5
18	2	1	47	50	16
20	2	1	113	116	8
22	2	1	264	252	5
1	3	1	310	317	2
3	3	1	236	232	2
5	3	1	288	271	2
7	3	1	490	496	3
9	3	1	294	302	3
11	3	1	235	250	3
13	3	1	298	306	3
15	3	1	34	13	25
17	3	1	355	353	4
19	3	1	228	218	5
21	3	1	343	348	5
0	4	1	1034	1043	5
2	4	1	30	32	12
4	4	1	308	306	2
6	4	1	811	773	5
8	4	1	491	487	4
10	4	1	229	202	3
12	4	1	694	708	5
14	4	1	294	293	3
16	4	1	630	632	5
18	4	1	233	239	5
20	4	1	131	127	7
1	5	1	140	141	2
3	5	1	584	590	4
5	5	1	1572	1559	6
7	5	1	856	842	6
9	5	1	550	539	4
11	5	1	284	306	3
13	5	1	661	673	5
15	5	1	200	193	4
17	5	1	246	248	4
19	5	1	94	91	9
21	5	1	798	790	6
0	6	1	386	371	3
2	6	1	251	235	2
4	6	1	228	221	2
6	6	1	891	880	6
8	6	1	491	487	4
10	6	1	29	24	28
12	6	1	316	307	3
14	6	1	27	10	27
16	6	1	1041	1037	7
18	6	1	228	227	5
20	6	1	401	404	4
1	7	1	62	38	6
3	7	1	612	618	4
5	7	1	447	444	3
7	7	1	165	153	3
9	7	1	546	552	4
11	7	1	50	17	11
13	7	1	114	73	5
15	7	1	76	69	9
17	7	1	185	184	5
19	7	1	163	166	6
0	8	1	644	637	4
2	8	1	53	31	7
4	8	1	151	155	3
6	8	1	302	316	3
8	8	1	120	124	5
10	8	1	102	95	6
12	8	1	447	452	4
14	8	1	555	546	4
16	8	1	716	711	5
18	8	1	317	314	4
20	8	1	189	197	6
1	9	1	946	952	6
3	9	1	134	131	4
5	9	1	461	488	4
7	9	1	269	271	3
9	9	1	54	63	11
11	9	1	1669	1671	10
13	9	1	55	34	12
15	9	1	31	28	30
17	9	1	154	156	6
19	9	1	152	169	6
0	10	1	1293	1306	8
2	10	1	778	780	6
4	10	1	324	330	3
6	10	1	417	433	3
8	10	1	128	126	5
10	10	1	284	278	4
12	10	1	39	22	20
14	10	1	687	674	5
16	10	1	296	306	4
18	10	1	331	331	5
1	11	1	309	311	3
3	11	1	252	250	3
5	11	1	641	656	5
7	11	1	449	453	4
9	11	1	410	410	4
11	11	1	395	394	4
13	11	1	121	128	6
15	11	1	47	51	20
17	11	1	381	384	4
0	12	1	1117	1137	7
2	12	1	517	518	4
4	12	1	113	110	5
6	12	1	656	651	5
8	12	1	120	125	6
10	12	1	209	207	4
12	12	1	262	259	4
14	12	1	98	96	8
16	12	1	706	713	5
1	13	1	382	375	3
3	13	1	350	361	3
5	13	1	984	1004	7
7	13	1	63	56	10
9	13	1	354	364	4
11	13	1	1109	1119	8
13	13	1	119	108	7
15	13	1	246	239	5
0	14	1	681	702	5
2	14	1	286	283	4
4	14	1	494	495	4
6	14	1	212	206	4
8	14	1	289	279	4
10	14	1	181	191	5
12	14	1	125	138	7
14	14	1	432	415	4
1	15	1	63	68	11
3	15	1	312	313	4
5	15	1	279	278	4
7	15	1	278	285	4
9	15	1	83	91	10
11	15	1	190	176	5
13	15	1	134	129	7
0	16	1	277	275	4
2	16	1	269	267	4
4	16	1	45	40	21
6	16	1	1269	1257	8
8	16	1	371	370	4
10	16	1	48	53	22
12	16	1	66	70	14
1	17	1	62	59	13
3	17	1	288	274	4
5	17	1	746	750	6
7	17	1	258	249	5
9	17	1	408	411	5
0	18	1	266	275	5
2	18	1	37	57	37
4	18	1	398	411	4
6	18	1	406	405	5
1	19	1	376	373	5
3	19	1	431	434	5
0	0	2	3184	3480	5
2	0	2	686	707	4
4	0	2	346	341	2
6	0	2	754	729	5
8	0	2	710	702	5
10	0	2	1510	1469	8
12	0	2	963	971	7
14	0	2	1402	1397	9
16	0	2	720	726	5
18	0	2	915	908	7
20	0	2	97	107	9
22	0	2	203	208	6
1	1	2	559	561	3
3	1	2	788	798	5
5	1	2	1118	1104	6
7	1	2	186	179	3
9	1	2	685	694	4
11	1	2	682	684	4
13	1	2	40	48	16
15	1	2	713	711	5
17	1	2	101	102	7
19	1	2	136	34	6
21	1	2	319	319	5
2	2	2	344	340	2
4	2	2	505	501	3
6	2	2	434	423	3
8	2	2	299	301	3
10	2	2	1300	1309	8
12	2	2	538	547	4
14	2	2	125	121	5
16	2	2	341	339	4
18	2	2	44	40	19
20	2	2	0	2	1
1	3	2	426	420	3
3	3	2	212	207	2
5	3	2	1116	1093	6
7	3	2	228	226	2
9	3	2	1583	1607	7
11	3	2	1344	1347	8
13	3	2	527	536	4
15	3	2	215	208	4
17	3	2	330	334	4
19	3	2	863	870	6
21	3	2	535	555	5
0	4	2	1938	1937	6
2	4	2	728	715	5
4	4	2	36	8	10
6	4	2	227	211	2
8	4	2	129	135	4
10	4	2	2124	2138	8
12	4	2	282	290	3
14	4	2	256	249	4
16	4	2	45	36	16
18	4	2	521	513	4
20	4	2	369	364	4
1	5	2	1024	999	6
3	5	2	22	32	22
5	5	2	1821	1759	7
7	5	2	199	186	3
9	5	2	447	449	3
11	5	2	669	671	5
13	5	2	109	104	6
15	5	2	244	241	4
17	5	2	808	781	6
19	5	2	451	440	4
21	5	2	482	473	4
0	6	2	1127	1122	6
2	6	2	18	50	10
4	6	2	951	947	6
6	6	2	2437	2374	8
8	6	2	236	233	3
10	6	2	53	36	11
12	6	2	457	457	4
14	6	2	955	944	6
16	6	2	1443	1433	9
18	6	2	97	89	8
20	6	2	59	57	16
1	7	2	787	778	6
3	7	2	19	13	18
5	7	2	4646	4473	8
7	7	2	225	205	3
9	7	2	511	514	4
11	7	2	187	188	4
13	7	2	362	364	3
15	7	2	977	998	6
17	7	2	894	909	6
19	7	2	77	88	12
0	8	2	406	414	3
2	8	2	559	542	4
4	8	2	189	191	3
6	8	2	375	359	3
8	8	2	677	688	5
10	8	2	100	99	6
12	8	2	189	179	4
14	8	2	567	571	4
16	8	2	892	885	6
18	8	2	127	120	7
1	9	2	570	562	4
3	9	2	90	77	6
5	9	2	504	488	4
7	9	2	480	481	4
9	9	2	628	633	4
11	9	2	1619	1618	10
13	9	2	93	85	7
15	9	2	292	293	4

Observed and calculated structure factors for K34

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
17	9	2	700	694	5	1	3	3	528	516	3	0	12	3	239	242	4	14	4	4	847	851	6	1	15	4	251	243	5
19	9	2	269	273	5	3	3	3	264	258	2	2	12	3	298	290	4	16	4	4	1390	1403	9	3	15	4	431	431	4
0	10	2	4438	4361	9	5	3	3	1107	1085	7	4	12	3	366	367	4	18	4	4	198	208	5	5	15	4	241	211	5
2	10	2	642	649	5	7	3	3	747	741	4	6	12	3	140	136	5	1	5	4	1066	1063	6	7	15	4	137	123	7
4	10	2	719	724	5	9	3	3	231	224	3	8	12	3	81	68	8	3	5	4	182	162	3	9	15	4	167	158	6
6	10	2	100	101	6	11	3	3	1336	1331	9	10	12	3	182	197	5	5	5	4	1495	1544	8	0	16	4	116	113	8
8	10	2	269	270	3	13	3	3	81	87	8	12	12	3	267	261	4	7	5	4	443	440	3	2	16	4	217	203	5
10	10	2	1870	1874	10	15	3	3	87	87	7	14	12	3	171	174	6	9	5	4	98	99	6	4	16	4	95	89	9
12	10	2	356	351	4	17	3	3	224	227	5	16	12	3	404	409	5	11	5	4	935	943	6	6	16	4	480	481	5
14	10	2	364	358	4	19	3	3	135	144	7	1	13	3	261	260	4	13	5	4	193	183	4	8	16	4	17	5	17
16	10	2	223	227	5	21	3	3	405	410	5	3	13	3	465	462	4	15	5	4	296	297	4	1	17	4	342	337	5
18	10	2	289	278	5	0	4	3	2119	2080	7	5	13	3	392	392	4	17	5	4	49	57	18	3	17	4	208	206	6
1	11	2	332	325	3	2	4	3	88	88	4	7	13	3	144	145	5	19	5	4	128	128	7	1	1	5	84	78	6
3	11	2	752	754	6	4	4	3	411	411	3	9	13	3	302	301	4	0	6	4	2093	2134	8	3	1	5	260	259	3
5	11	2	89	89	6	6	4	3	222	214	3	11	13	3	395	396	4	2	6	4	150	167	4	5	1	5	621	622	4
7	11	2	69	21	9	8	4	3	263	265	3	13	13	3	46	30	20	4	6	4	370	373	3	7	1	5	59	64	10
9	11	2	642	641	5	10	4	3	350	332	3	15	13	3	156	152	7	6	6	4	152	161	4	9	1	5	367	376	3
11	11	2	1713	1699	10	12	4	3	767	777	5	0	14	3	48	49	17	8	6	4	388	389	3	11	1	5	221	220	4
13	11	2	30	33	29	14	4	3	131	130	5	2	14	3	246	247	4	10	6	4	1285	1288	8	13	1	5	160	163	5
15	11	2	279	270	5	16	4	3	231	226	4	4	14	3	424	427	4	12	6	4	404	401	4	15	1	5	17	41	31
17	11	2	97	95	9	18	4	3	144	147	6	6	14	3	212	219	5	14	6	4	245	240	4	17	1	5	730	741	5
0	12	2	1370	1360	9	20	4	3	72	59	12	8	14	3	336	337	4	16	6	4	226	213	5	19	1	5	372	373	5
2	12	2	19	15	19	1	5	3	50	45	8	10	14	3	91	30	9	18	6	4	279	282	5	0	2	5	666	663	5
4	12	2	100	104	7	3	5	3	377	384	3	12	14	3	26	16	25	1	7	4	278	265	3	2	2	5	52	28	10
6	12	2	899	911	6	5	5	3	959	946	6	1	15	3	240	240	4	3	7	4	258	257	3	4	2	5	465	482	4
8	12	2	162	178	5	7	5	3	839	836	5	3	15	3	222	218	5	5	7	4	1322	1332	9	6	2	5	487	479	4
10	12	2	797	817	5	9	5	3	413	413	3	5	15	3	449	457	4	7	7	4	408	399	3	8	2	5	181	180	3
12	12	2	289	277	4	11	5	3	147	137	4	7	15	3	145	146	6	9	7	4	951	968	6	10	2	5	159	159	5
14	12	2	528	505	4	13	5	3	517	512	4	9	15	3	153	157	6	11	7	4	673	676	5	12	2	5	745	753	5
16	12	2	384	398	5	15	5	3	109	98	7	11	15	3	372	356	5	13	7	4	376	373	4	14	2	5	34	33	34
1	13	2	142	138	5	17	5	3	300	305	4	0	16	3	106	100	8	15	7	4	271	272	5	16	2	5	270	265	5
3	13	2	82	74	8	19	5	3	131	128	7	2	16	3	96	86	8	17	7	4	352	351	5	18	2	5	160	145	6
5	13	2	1799	1811	10	0	6	3	617	623	4	4	16	3	190	186	5	0	8	4	1891	1918	9	1	3	5	117	117	5
7	13	2	78	80	8	2	6	3	79	72	5	6	16	3	1074	1087	7	2	8	4	0	4	1	3	3	5	207	201	3
9	13	2	88	86	8	4	6	3	460	444	3	8	16	3	308	298	5	4	8	4	239	236	4	5	3	5	492	496	4
11	13	2	100	100	8	6	6	3	1223	1213	8	10	16	3	98	98	9	6	8	4	584	578	4	7	3	5	103	102	6
13	13	2	145	93	6	8	6	3	363	363	3	1	17	3	121	126	7	8	8	4	382	384	4	9	3	5	134	130	5
15	13	2	569	561	5	10	6	3	85	83	6	3	17	3	276	273	5	10	8	4	1190	1203	7	11	3	5	268	273	4
0	14	2	439	438	4	12	6	3	272	270	4	5	17	3	464	455	4	12	8	4	137	139	6	13	3	5	321	319	4
2	14	2	340	142	4	14	6	3	67	67	10	7	17	3	66	13	13	14	8	4	111	114	7	15	3	5	63	44	12
4	14	2	702	717	5	16	6	3	1112	1114	8	0	18	3	251	238	5	16	8	4	237	232	5	17	3	5	549	551	5
6	14	2	423	412	4	18	6	3	363	361	4	2	18	3	163	170	6	18	8	4	22	43	21	0	4	5	91	97	6
8	14	2	211	205	5	20	6	3	362	370	5	2	0	4	369	371	3	1	9	4	85	78	7	2	4	5	0	15	1
10	14	2	185	192	5	1	7	3	112	103	4	4	0	4	716	736	4	3	9	4	300	301	3	4	4	5	150	158	4
12	14	2	47	51	20	3	7	3	319	323	3	6	0	4	433	421	3	5	9	4	1738	1746	9	6	4	5	673	659	5
14	14	2	375	387	5	5	7	3	1196	1188	8	8	0	4	294	288	3	7	9	4	524	529	4	8	4	5	151	359	3
1	15	2	629	616	5	7	7	3	216	215	3	10	0	4	2688	2714	9	9	9	4	16	14	16	10	4	5	113	108	6
3	15	2	273	268	4	9	7	3	542	544	4	12	0	4	942	963	7	11	9	4	180	187	5	12	4	5	480	484	4
5	15	2	1502	1492	9	11	7	3	803	803	5	14	0	4	415	420	4	13	9	4	101	95	8	14	4	5	295	289	4
7	15	2	531	537	4	13	7	3	133	132	5	16	0	4	162	167	5	15	9	4	408	411	4	16	4	5	644	650	5
9	15	2	57	60	15	15	7	3	175	174	5	18	0	4	620	609	5	17	9	4	593	592	5	18	4	5	257	263	5
11	15	2	410	409	4	17	7	3	609	621	5	20	0	4	214	202	5	0	10	4	868	865	6	1	5	5	178	165	4
13	15	2	142	129	7	19	7	3	150	138	6	1	1	4	276	268	3	2	10	4	0	5	1	3	5	5	150	340	3
0	16	2	916	921	6	0	8	3	882	863	6	3	1	4	48	41	9	4	10	4	429	440	4	5	5	5	758	752	5
2	16	2	136	141	6	2	8	3	143	146	4	5	1	4	247	202	3	6	10	4	217	203	4	7	5	5	576	568	4
4	16	2	105	106	8	4	8	3	383	387	3	7	1	4	29	8	28	8	10	4	388	380	4	9	5	5	400	408	4
6	16	2	478	480	4	6	8	3	578	571	4	9	1	4	1249	1261	9	10	10	4	497	494	4	11	5	5	253	249	4
8	16	2	94	94	9	8	8	3	65	34	9	11	1	4	1589	1613	9	12	10	4	233	225	5	13	5	5	462	465	4
10	16	2	706	710	5	10	8	3	51	47	12	13	1	4	140	136	5	14	10	4	923	906	6	15	5	5	136	132	7
1	17	2	224	199	5	12	8	3	556	555	4	15	1	4	156	162	5	16	10	4	378	379	5	17	5	5	184	184	5
3	17	2	428	426	4	14	8	3	338	335	4	17	1	4	0	1	1	1	11	4	236	234	4	0	6	5	329	359	3
5	17	2	183	172	6	16	8	3	226	203	5	19	1	4	565	560	5	3	11	4	337	342	4	2	6	5	133	135	5
7	17	2	58	66	15	18	8	3	158	144	6	0	2	4	301	311	3	5	11	4	1104	1117	7	4	6	5	47	47	11
9	17	2	324	321	5	1	9	3	591	593	4	2	2	4	235	226	3	7	11	4	54	53	12	6	6	5	445	418	4
0	18	2	753	737	6	3	9	3	108	112	5	4	2	4	382	379	3	9	11	4	73	61	10	8	6	5	316	323	4
2	18	2	76	58	11	5	9	3	219	208	4	6	2	4	506	518	4	11	11	4	75	82	10	10	6	5	0	12	1
4	18	2	278	278	5	7	9	3	198	190	4	8	2	4	73	66	7	13	11	4	88	84	9	12	6	5	229	227	4
6	18	2	429	441	5	9	9	3	95	102	7	10	2	4	411	430	3	15	11	4	800	789	6	14	6	5	50	21	16
1	1	3	275	266	2	11	9	3	877	885	6	12	2	4	346	348	3	0	12	4	899	894	6	16	6	5	685	697	5
3	1	3	678	664	4	13	9	3	45	9	17	14	2	4	632	636	5	2	12	4	275	274	4	1	7	5	44	33	14
5	1	3	248	251	2	15	9	3	81	56	10	16	2	4	731	737	5	4	12	4	158	171	5	3	7	5	484	493	4
7	1	3	231	228	3	17	9	3	510	504	4	18	2	4	62	49	13	6	12	4	300	307	4	5	7	5	56	45	11
9	1	3	391	400	3	0	10	3	889	910	6	20	2	4	114	118	8	8	12	4	281	284	4	7	7	5	298	293	4
11	1	3	1358	1346	8	2	10	3	780	791	5	1	3	4	271	270	3	10	12	4	398	384	4	9	7	5	371	366	4
13	1	3	411	416	4	4	10	3	430	431	4	3	3	4	496	485	4	12	12	4	364	364	4	11	7	5	382	385	4
15	1	3	47	49	15	6	10	3	227	208	4	5	3	4	3358	3364	8	14	12	4	54	45	18	13	7	5	195	191	5
17	1	3	342	339	4	8	10	3	207	209	4	7	3	4	136	145	4	1	13	4	318	322	4	15	7	5	22	25	21
19	1	3	433	450	4	10	10	3	87	85	8	9	3	4	803	812	5	3	13	4	159	159	5	17	7	5	65	74	15
21	1	3	853	838	6	12	10	3	110	122	7	11	3	4	43	32	15	5	13	4	257	244	4	0	8	5	783	793	5
0	2	3	2266	2314	6	14	10	3	662	668	5	13	3	4	317	320	4	7	13	4	353	349	4	2	8	5	107	104	6
2	2	3	513	496	3	16	10	3	105	108	8	15	3	4	761	774	5	9	13	4	394	396	4	4	8	5	0	25	1
4	2	3	26	11	26	1	11	3	384	389	3	17	3	4	723	727	5	11	13	4	719	722	5	6	8	5	571	558	4
6	2	3	1102	1090	7	3	11	3	207	211	4	19	3	4	227	225	5	13	13	4	195	206	6	8	8	5	116	120	6
8	2	3	780	777	5	5	11	3	736	735	5	0	4	4	595	617	4	0	14	4	1356	1379	9	10	8	5	52	56	14
10	2	3	413	422	3	7	11	3	141	150	5	2	4	4	489	475	3	2	14	4	284	246	4	12	8	5	327	322	4
12	2	3	691	696	5	9	11	3	462	472	4	4	4	4	604	632	4	4	14	4	329	327	4	14	8	5	181	480	4
14	2	3	315	309	4	11	11	3	94	97	8	6	4	4	1833	1839	8	6	14	4	541	559	4	16	8	5	764	751	5
16	2	3	1093	1090	7	13	11	3	52	56	17	8	4	4	268	274	3	8	14	4	71	84	12	1	9	5	688	686	5
18	2	3	136	143	6	15	11	3	108	94	8	10	4	4	383	386	3	10	14	4	1067	1085	8	3	9	5	80	57	7
20	2	3	46	46	23	17	11	3	499	502	4	12	4	4	225	218	4	12	14	4	10	29	9	5	9	5	559	543	4

Observed and calculated structure factors for K34

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	9	5	312	296	4	13	1	6	56	67	14	12	8	6	189	181	5	4	4	7	100	287	4	11	1	8	487	485	5
9	9	5	60	54	12	15	1	6	464	462	4	14	8	6	412	402	4	6	4	7	91	86	8	0	2	8	52	13	15
11	9	5	1498	1506	9	17	1	6	311	306	5	1	9	6	404	399	4	8	4	7	220	216	5	2	2	8	83	98	10
13	9	5	98	103	9	0	2	6	1644	1688	9	3	9	6	75	82	10	10	4	7	216	210	5	4	2	8	233	233	5
15	9	5	72	60	12	2	2	6	220	211	4	5	9	6	45	30	18	12	4	7	464	475	4	6	2	8	532	527	5
0	10	5	1016	1015	7	4	2	6	218	203	4	7	9	6	534	534	4	14	4	7	145	147	7	8	2	8	0	18	1
2	10	5	491	503	4	6	2	6	487	491	4	9	9	6	433	429	4	1	5	7	0	18	1	10	2	8	236	231	5
4	10	5	170	164	5	8	2	6	282	275	4	11	9	6	738	739	5	3	5	7	210	211	4	1	1	8	166	149	5
6	10	5	454	446	4	10	2	6	798	803	5	13	9	6	74	66	12	5	5	7	355	357	4	3	1	8	324	326	4
8	10	5	94	87	8	12	2	6	108	104	4	0	10	6	2131	2142	11	7	5	7	500	499	4	5	1	8	1782	1776	12
10	10	5	274	273	4	14	2	6	26	15	26	2	10	6	104	103	4	9	5	7	300	300	4	7	1	8	16	32	35
12	10	5	0	46	1	16	2	6	192	191	5	4	10	6	310	311	4	11	5	7	37	41	36	9	1	8	455	448	4
14	10	5	500	505	4	1	3	6	241	221	4	6	10	6	572	580	5	13	5	7	316	320	5	11	1	8	158	172	7
1	11	5	154	160	5	3	3	6	82	75	7	8	10	6	100	92	8	0	6	7	285	268	4	0	4	8	213	218	5
3	11	5	185	200	5	5	3	6	845	835	6	10	10	6	1268	1279	8	2	6	7	108	105	7	2	4	8	321	316	4
5	11	5	441	439	4	7	3	6	98	104	6	12	10	6	207	195	6	4	6	7	210	203	5	4	4	8	241	229	5
7	11	5	474	477	4	9	3	6	1075	1087	7	1	11	6	50	67	17	6	6	7	696	690	5	6	4	8	594	598	5
9	11	5	275	273	4	11	3	6	1059	1078	7	3	11	6	177	172	4	8	6	7	241	253	5	8	4	8	72	77	12
11	11	5	430	434	4	13	3	6	289	288	4	5	11	6	436	440	4	10	6	7	107	107	8	10	4	8	169	172	6
13	11	5	194	199	6	15	3	6	93	90	9	7	11	6	123	117	7	12	6	7	189	186	6	1	5	8	573	574	5
0	12	5	1135	1124	8	17	3	6	167	160	5	9	11	6	474	469	4	1	7	7	50	49	16	3	5	8	151	144	6
2	12	5	506	508	4	0	4	6	2376	2430	10	11	11	6	671	678	5	3	7	7	273	279	4	5	5	8	441	435	4
4	12	5	71	58	10	2	4	6	93	79	6	0	12	6	538	543	5	5	7	7	714	713	5	7	5	8	38	32	38
6	12	5	699	704	5	4	4	6	359	363	3	2	12	6	62	61	13	7	7	7	137	140	6	9	5	8	133	133	7
8	12	5	73	72	11	6	4	6	462	463	4	4	12	6	118	111	7	9	7	7	400	387	4	0	6	8	1806	1844	12
10	12	5	117	109	8	8	4	6	101	106	7	6	12	6	940	942	6	11	7	7	507	502	4	2	6	8	182	187	6
12	12	5	204	208	6	10	4	6	1412	1419	9	8	12	6	57	45	17	0	8	7	523	517	5	4	6	8	328	327	5
1	13	5	323	323	4	12	4	6	269	266	4	10	12	6	460	449	4	2	8	7	118	125	7	6	6	8	470	461	4
3	13	5	262	267	5	14	4	6	72	70	12	1	13	6	38	5	31	4	8	7	312	302	4	8	6	8	192	183	6
5	13	5	965	969	6	16	4	6	194	182	6	3	13	6	42	34	26	6	8	7	327	328	4	1	7	8	151	67	6
7	13	5	176	168	6	1	5	6	283	275	4	5	13	6	1336	1343	8	8	8	7	46	47	21	3	7	8	170	174	6
9	13	5	331	321	5	3	5	6	342	343	3	7	13	6	203	199	6	10	8	7	52	38	19	5	7	8	909	905	6
11	13	5	1208	1209	8	5	5	6	462	446	4	0	14	6	56	49	17	1	9	7	393	386	4	7	7	8	227	228	5
0	14	5	883	876	6	7	5	6	75	85	9	2	14	6	198	197	5	3	9	7	34	50	34	0	8	8	948	934	7
2	14	5	231	237	5	9	5	6	239	239	4	4	14	6	107	114	5	5	9	7	184	179	6	2	8	8	18	62	18
4	14	5	394	395	4	11	5	6	141	137	4	1	1	7	88	87	8	7	9	7	96	101	9	4	8	8	46	39	22
6	14	5	171	172	4	13	5	6	44	41	21	3	1	7	271	265	4	9	9	7	0	11	1	6	8	8	414	418	4
8	14	5	183	190	6	15	5	6	220	219	5	5	1	7	29	28	28	0	10	7	614	612	5	1	9	8	33	1	33
1	15	5	34	37	34	0	6	6	146	146	5	7	1	7	236	233	4	2	10	7	437	439	4	3	9	8	178	173	6
3	15	5	265	266	5	2	6	6	42	36	17	9	1	7	234	234	5	4	10	7	213	210	5	5	9	8	1209	1236	8
5	15	5	108	112	9	4	6	6	456	462	4	11	1	7	721	726	5	6	10	7	205	195	5	0	10	8	1035	1039	6
7	15	5	272	276	5	6	6	6	872	878	6	13	1	7	318	317	5	8	10	7	105	101	9	2	10	8	111	99	8
0	16	5	253	255	5	8	6	6	274	275	4	15	1	7	89	87	10	1	11	7	211	211	5	1	1	9	60	61	16
2	16	5	295	290	5	10	6	6	118	81	6	0	2	7	701	705	5	3	11	7	131	129	7	3	1	9	200	204	6
4	16	5	155	143	7	12	6	6	222	226	5	2	2	7	298	290	4	5	11	7	534	529	5	5	1	9	266	261	5
0	0	6	2497	2620	9	14	6	6	812	818	6	4	2	7	29	17	29	7	11	7	132	117	7	0	2	9	73	69	12
2	0	6	146	140	5	1	7	6	628	623	5	6	2	7	453	449	4	0	12	7	68	71	13	2	2	9	29	29	29
4	0	6	608	616	4	3	7	6	167	169	5	8	2	7	321	316	4	2	12	7	166	175	6	4	2	9	229	220	5
6	0	6	694	694	5	5	7	6	2434	2466	11	10	2	7	142	129	6	4	12	7	270	261	5	6	2	9	0	26	1
8	0	6	437	443	4	7	7	6	108	110	7	12	2	7	514	512	4	0	0	8	2418	2514	11	1	3	9	152	151	7
10	0	6	921	923	6	9	7	6	413	417	4	14	2	7	157	157	6	2	0	8	148	139	6	3	3	9	42	30	29
12	0	6	760	768	5	11	7	6	502	506	4	1	3	7	198	193	4	4	0	8	277	274	4	5	3	9	59	43	16
14	0	6	810	817	6	13	7	6	232	219	5	3	3	7	34	16	33	6	0	8	720	732	5	0	4	9	423	419	4
16	0	6	834	834	6	15	7	6	707	661	5	5	3	7	420	416	4	8	0	8	21	9	21	2	4	9	19	27	19
1	1	6	185	178	4	0	8	6	282	269	4	7	3	7	428	437	4	10	0	8	1453	1475	8	4	4	9	87	92	10
3	1	6	182	175	4	2	8	6	251	244	4	9	3	7	179	182	5	1	1	8	145	117	6	1	5	9	26	14	25
5	1	6	1675	1710	10	4	8	6	104	295	4	11	3	7	776	771	5	3	1	8	83	91	10	3	5	9	114	120	9
7	1	6	86	60	7	6	8	6	258	261	4	13	3	7	0	24	1	5	1	8	465	471	4						
9	1	6	380	382	4	8	8	6	410	412	4	0	4	7	994	977	6	7	1	8	205	217	5						
11	1	6	210	196	4	10	8	6	72	71	11	2	4	7	131	124	6	9	1	8	693	678	5						

Observed and calculated structure factors for K35

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	623	647	3	4	8	0	623	611	4	3	1	1	237	229	2	3	9	1	12	7	12	22	0	2	611	615	5
4	0	0	949	942	5	6	8	0	654	662	4	5	1	1	1019	1018	6	5	9	1	452	483	4	1	1	2	468	487	3
6	0	0	694	703	4	8	8	0	566	586	4	7	1	1	57	66	7	7	9	1	335	339	3	3	1	2	616	627	4
8	0	0	1313	1279	7	10	8	0	1112	1119	8	9	1	1	117	111	4	9	9	1	38	31	21	5	1	2	1120	1133	7
10	0	0	4189	4006	10	12	8	0	53	43	14	11	1	1	623	639	5	11	9	1	1716	1725	11	7	1	2	89	87	5
12	0	0	1513	1518	9	14	8	0	66	61	12	13	1	1	212	206	4	13	9	1	198	183	5	9	1	2	556	540	4
14	0	0	360	344	4	16	8	0	333	331	5	15	1	1	403	408	4	15	9	1	296	290	5	11	1	2	487	483	4
16	0	0	577	565	5	18	8	0	0	10	1	17	1	1	660	668	5	17	9	1	69	51	15	13	1	2	94	88	7
18	0	0	316	317	5	20	8	0	303	294	6	19	1	1	589	592	5	19	9	1	251	244	6	15	1	2	756	760	5
20	0	0	602	609	5	1	9	0	181	169	4	21	1	1	381	395	5	0	10	1	1545	1570	9	17	1	2	18	9	17
22	0	0	2101	2099	14	3	9	0	191	191	4	0	2	1	101	118	3	2	10	1	733	730	5	19	1	2	75	75	12
1	1	0	239	230	2	5	9	0	1980	2000	9	2	2	1	618	644	4	4	10	1	118	120	6	21	1	2	237	235	6
5	1	0	575	576	4	7	9	0	889	897	6	4	2	1	196	204	2	6	10	1	534	544	4	0	2	2	4059	4193	7
7	1	0	426	429	3	9	9	0	214	202	4	6	2	1	273	256	3	8	10	1	84	80	8	2	2	2	310	314	2
9	1	0	1401	1380	8	11	9	0	636	629	5	8	2	1	477	482	3	10	10	1	472	471	4	4	2	2	357	358	3
11	1	0	3242	3110	10	13	9	0	230	225	5	10	2	1	301	289	3	12	10	1	0	1	1	6	2	2	453	440	3
13	1	0	632	642	5	15	9	0	949	960	6	12	2	1	789	807	5	14	10	1	614	627	5	8	2	2	41	18	13
15	1	0	234	234	4	17	9	0	689	687	5	14	2	1	95	86	8	16	10	1	691	692	5	10	2	2	1509	1500	9
17	1	0	423	426	4	19	9	0	45	47	14	16	2	1	479	481	4	18	10	1	115	124	10	12	2	2	668	665	5
19	1	0	460	459	5	0	10	0	274	285	4	18	2	1	44	51	23	1	11	1	46	22	16	14	2	2	84	82	8
21	1	0	938	950	7	2	10	0	213	213	4	20	2	1	469	471	5	3	11	1	69	74	10	16	2	2	237	226	5
0	2	0	1284	1305	4	4	10	0	227	238	4	22	2	1	302	300	6	5	11	1	920	946	6	18	2	2	89	84	10
2	2	0	323	335	2	6	10	0	276	275	4	1	3	1	384	393	3	7	11	1	497	497	4	20	2	2	271	276	5
4	2	0	525	544	3	8	10	0	197	200	4	3	3	1	262	264	2	9	11	1	239	245	4	22	2	2	696	680	6
6	2	0	217	216	2	10	10	0	508	487	4	5	3	1	392	388	3	11	11	1	79	69	10	1	3	2	499	505	3
8	2	0	290	281	3	12	10	0	377	386	4	7	3	1	340	339	3	13	11	1	168	181	6	3	3	2	170	167	3
10	2	0	552	552	4	14	10	0	908	929	6	9	3	1	253	255	3	15	11	1	524	519	5	5	3	2	1242	1221	7
12	2	0	542	548	4	16	10	0	414	415	5	11	3	1	463	473	4	17	11	1	418	411	5	7	3	2	228	215	3
14	2	0	868	871	6	18	10	0	194	217	7	13	3	1	188	190	5	0	12	1	878	892	6	9	3	2	1146	1152	7
16	2	0	875	877	6	1	11	0	191	186	4	15	3	1	174	171	5	2	12	1	603	617	5	11	3	2	1694	1693	10
18	2	0	161	161	4	3	11	0	267	269	4	17	3	1	267	261	5	4	12	1	166	168	5	13	3	2	99	97	7
20	2	0	0	5	1	5	11	0	685	702	5	19	3	1	186	191	6	6	12	1	802	802	6	15	3	2	284	287	4
22	2	0	159	154	8	7	11	0	45	54	17	21	3	1	440	443	5	8	12	1	59	50	13	17	3	2	489	488	4
1	3	0	191	191	2	9	11	0	83	89	9	0	4	1	1310	1306	6	10	12	1	107	103	8	19	3	2	715	730	6
3	3	0	310	320	3	11	11	0	358	375	4	2	4	1	210	211	2	12	12	1	202	200	6	21	3	2	848	861	6
7	3	0	552	540	4	13	11	0	348	354	5	4	4	1	23	25	23	14	12	1	99	91	9	0	4	2	1831	1853	7
9	3	0	640	625	4	15	11	0	618	628	5	6	4	1	582	551	4	16	12	1	809	808	6	2	4	2	672	666	4
11	3	0	646	640	5	17	11	0	474	485	5	8	4	1	291	288	3	1	13	1	508	507	4	4	4	2	175	168	3
13	3	0	293	275	4	0	12	0	1490	1513	10	10	4	1	868	848	6	3	13	1	218	219	5	6	4	2	570	555	4
15	3	0	1065	1070	8	2	12	0	61	55	12	12	4	1	585	593	4	5	13	1	1117	1127	8	8	4	2	195	202	3
17	3	0	1096	1095	7	4	12	0	471	478	4	14	4	1	281	277	4	7	13	1	131	125	7	10	4	2	2117	2121	10
19	3	0	363	370	5	6	12	0	534	547	4	16	4	1	368	370	4	9	13	1	268	269	5	12	4	2	74	75	9
21	3	0	139	140	8	8	12	0	163	156	5	18	4	1	218	217	5	11	13	1	1356	1349	9	14	4	2	77	78	9
0	4	0	2092	2064	6	10	12	0	856	855	6	20	4	1	136	138	8	13	13	1	224	215	6	16	4	2	151	151	6
2	4	0	643	656	4	12	12	0	535	540	5	22	4	1	377	384	6	15	13	1	15	11	14	18	4	2	622	616	5
4	4	0	859	856	6	14	12	0	156	177	7	1	5	1	91	93	4	0	14	1	1058	1076	7	20	4	2	256	251	6
6	4	0	4203	3962	8	16	12	0	105	82	10	3	5	1	304	312	2	2	14	1	93	87	9	1	5	2	1068	1064	7
8	4	0	297	290	3	1	13	0	642	639	5	5	5	1	960	937	6	4	14	1	370	374	4	3	5	2	122	119	4
10	4	0	512	500	4	3	13	0	241	239	4	7	5	1	841	837	5	6	14	1	269	263	5	5	5	2	1948	1901	8
12	4	0	144	146	5	5	13	0	242	251	5	9	5	1	290	290	3	8	14	1	183	195	6	7	5	2	209	193	3
14	4	0	489	480	4	7	13	0	448	461	4	11	5	1	312	328	4	10	14	1	593	600	5	9	5	2	627	626	4
16	4	0	2247	2239	12	9	13	0	176	170	6	13	5	1	583	582	4	12	14	1	101	107	12	11	5	2	736	735	5
18	4	0	33	53	33	11	13	0	916	953	6	15	5	1	413	416	4	14	14	1	252	248	6	13	5	2	57	60	14
20	4	0	95	83	10	13	13	0	215	212	6	17	5	1	179	173	6	1	15	1	54	53	17	15	5	2	418	421	4
22	4	0	605	608	5	15	13	0	300	296	5	19	5	1	23	30	22	3	15	1	420	428	4	17	5	2	684	679	5
1	5	0	1473	1454	6	0	14	0	1318	1310	9	21	5	1	478	472	5	5	15	1	19	23	19	19	5	2	305	298	5
3	5	0	175	167	3	2	14	0	352	353	4	0	6	1	472	460	3	7	15	1	360	352	5	21	5	2	294	285	6
5	5	0	3305	3131	8	4	14	0	183	183	6	2	6	1	51	52	9	9	15	1	25	4	25	0	6	2	1114	1121	7
7	5	0	979	956	6	6	14	0	596	621	5	4	6	1	371	373	3	11	15	1	193	171	6	2	6	2	0	42	1
9	5	0	145	142	4	8	14	0	238	234	5	6	6	1	1088	1089	6	13	15	1	286	279	6	4	6	2	613	629	4
11	5	0	405	432	4	10	14	0	1119	1173	8	8	6	1	537	528	4	0	16	1	504	512	5	6	6	2	2683	2582	9
13	5	0	20	34	19	12	14	0	108	116	10	10	6	1	95	77	7	2	16	1	148	151	7	8	6	2	384	372	3
15	5	0	235	231	5	14	14	0	11	29	30	12	6	1	380	383	4	4	16	1	96	102	10	10	6	2	279	281	4
17	5	0	531	532	5	1	15	0	420	417	4	14	6	1	48	54	18	6	16	1	1298	1306	9	12	6	2	295	301	4
19	5	0	105	103	9	3	15	0	241	234	5	16	6	1	982	996	7	8	16	1	375	381	5	14	6	2	641	633	5
21	5	0	536	532	5	5	15	0	528	535	5	18	6	1	287	279	5	10	16	1	131	142	8	16	6	2	1703	1711	10
0	6	0	854	869	5	7	15	0	150	153	7	20	6	1	512	506	5	12	16	1	0	17	1	18	6	2	143	147	7
2	6	0	127	131	3	9	15	0	329	328	5	1	7	1	143	136	4	1	17	1	173	160	6	20	6	2	69	53	16
4	6	0	29	40	25	11	15	0	450	445	5	3	7	1	395	398	3	3	17	1	117	111	8	1	7	2	538	526	4
6	6	0	304	287	3	13	15	0	298	301	6	5	7	1	1076	1093	7	5	17	1	941	959	7	3	7	2	268	272	3
8	6	0	547	539	4	0	16	0	512	534	5	7	7	1	190	184	4	7	17	1	254	246	6	5	7	2	4831	4528	10
10	6	0	1653	1665	9	2	16	0	301	292	5	9	7	1	270	279	4	9	17	1	208	212	6	7	7	2	166	162	4
12	6	0	100	99	7	4	16	0	66	77	15	11	7	1	151	169	5	0	18	1	325	328	5	9	7	2	397	398	4
14	6	0	316	314	4	6	16	0	671	683	6	13	7	1	58	56	12	2	18	1	138	138	8	11	7	2	68	36	10
16	6	0	344	354	4	8	16	0	95	93	11	15	7	1	306	293	4	4	18	1	322	320	5	13	7	2	412	416	4
18	6	0	445	451	5	10	16	0	152	153	7	17	7	1	301	295	5	6	18	1	243	252	6	15	7	2	1120	1129	7
20	6	0	56	76	20	12	16	0	480	493	5	19	7	1	202	208	6	8	18	1	211	216	6	17	7	2	1174	1180	8
1	7	0	560	552	4	1	17	0	313	309	5	21	7	1	142	137	9	1	19	1	496	494	5	19	7	2	182	194	7
3	7	0	302	308	3	3	17	0	329	329	5	0	8	1	312	295	3	3	19	1	407	402	5	0	8	2	351	350	3
5	7	0	1404	1371	8	5	17	0	1662	1656	11	2	8	1	215	213	3	0	0	2	3186	3422	7	2	8	2	525	522	4
7	7	0	515	509	4	7	17	0	137	142	8	4	8	1	211	200	3	2	0	2	645	664	4	4	8	2	346	352	3
9	7	0	1055	1057	7	9	17	0	31	11	30	6	8	1	283	292	3	4	0	2	170	162	3	6	8	2	332	328	3
11	7	0	724	680	5	0	18	0	442	441	5	8	8	1	0	6	1	6	0	2	721	695	4	8	8	2	487	496	4
13	7	0	181	177	5	2	18	0	199	203	6	10	8	1	333	338	4	8	0	2	676	663	4	10	8	2	201	198	5
15	7	0	332	335	4	4	18	0	109	115	10	12	8	1	474	472	4	10	0	2	1583	1546	9	12	8	2	61	48	12
17	7	0	511	513	5	6	18	0	375	363	5	14	8	1	475	478	4	12	0	2	1138	1134	8	14	8	2	477	482	4
19	7	0	609	620	5	8	18	0	198	196	7	16	8	1	274	272	5	14	0	2	1295	1291	9	16	8	2	887	895	6
21	7	0	657	648	6	1	19	0	121	122	9	18	8	1	234	242	6	16	0	2	1040	1043	7	18	8	2	139	112	8
0	8	0	2784	2694	9	3	19	0	197	216	7	20	8	1	453	447	5	18	0	2	323	320	5	20	8	2	108	118	11
2	8	0	111	107	5	1	1	1	122	109	2	1	9	1	857	856	6	20	0	2	263	261	6	1	9	2	537	525	4

Observed and calculated structure factors for K35

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
3	9	2	195	183	4	8	2	3	604	600	4	3	11	3	121	113	6	15	3	4	931	939	6	7	13	4	288	285	5
5	9	2	567	572	4	10	2	3	240	235	4	5	11	3	973	977	7	17	3	4	855	854	6	9	13	4	189	184	6
7	9	2	529	520	4	12	2	3	639	639	5	7	11	3	190	191	5	19	3	4	322	319	5	11	13	4	804	790	6
9	9	2	426	433	4	14	2	3	314	304	4	9	11	3	104	100	4	0	4	4	578	608	4	13	13	4	113	116	10
11	9	2	1573	1573	9	16	2	3	853	853	6	11	11	3	179	178	6	2	4	4	504	496	4	0	14	4	1281	1294	9
13	9	2	371	380	4	18	2	3	173	172	6	13	11	3	43	2	29	4	4	4	404	424	4	2	14	4	206	212	6
15	9	2	79	30	11	20	2	3	375	372	5	15	11	3	341	341	5	6	4	4	2110	2121	10	4	14	4	309	298	5
17	9	2	844	855	6	1	3	3	462	463	3	17	11	3	521	516	5	8	4	4	97	98	7	6	14	4	400	406	5
19	9	2	304	301	6	3	3	3	253	249	3	0	12	3	63	69	12	10	4	4	413	419	4	8	14	4	223	215	6
0	10	2	4475	4390	11	5	3	3	950	932	5	2	12	3	390	389	4	12	4	4	135	132	6	10	14	4	910	913	6
2	10	2	449	451	4	7	3	3	712	699	5	4	12	3	416	426	4	14	4	4	527	528	4	12	14	4	84	73	13
4	10	2	542	542	4	9	3	3	210	206	4	6	12	3	308	306	4	16	4	4	1656	1671	10	1	15	4	388	378	5
6	10	2	44	47	17	11	3	3	1461	1469	8	8	12	3	0	30	1	18	4	4	56	61	20	3	15	4	279	270	5
8	10	2	354	363	4	13	3	3	14	39	13	10	12	3	60	58	15	20	4	4	37	44	36	5	15	4	292	286	5
10	10	2	1895	1883	11	15	3	3	245	255	5	12	12	3	178	178	6	1	5	4	917	904	6	7	15	4	13	11	13
12	10	2	479	480	4	17	3	3	266	265	5	14	12	3	172	194	7	3	5	4	86	76	7	9	15	4	296	295	6
14	10	2	224	237	5	19	3	3	119	119	9	16	12	3	541	523	5	5	5	4	1612	1629	9	0	16	4	158	163	7
16	10	2	88	63	11	21	3	3	469	470	5	1	13	3	438	424	4	7	5	4	411	407	4	2	16	4	291	281	5
18	10	2	133	143	9	0	4	3	2261	2247	8	3	13	3	343	343	4	9	5	4	53	56	14	4	16	4	0	1	1
1	11	2	460	464	4	2	4	3	99	25	5	5	13	3	533	549	5	11	5	4	920	913	6	6	16	4	380	380	5
3	11	2	617	631	5	4	4	3	237	225	3	7	13	3	102	112	9	13	5	4	104	104	8	8	16	4	44	30	19
5	11	2	101	97	7	6	4	3	336	324	3	9	13	3	207	209	6	15	5	4	283	280	5	1	17	4	333	333	6
7	11	2	40	21	21	8	4	3	107	107	6	11	13	3	645	644	5	17	5	4	177	179	7	3	17	4	245	235	6
9	11	2	537	538	4	10	4	3	864	856	5	13	13	3	48	59	28	19	5	4	47	54	32	5	17	4	1293	1268	9
11	11	2	1899	1885	12	12	4	3	614	622	5	15	13	3	70	62	16	0	6	4	2018	2068	9	1	1	5	0	4	1
13	11	2	90	93	9	14	4	3	107	117	8	0	14	3	413	416	4	2	6	4	143	162	5	3	1	5	68	77	9
15	11	2	82	50	12	16	4	3	37	12	16	2	14	3	69	54	12	4	6	4	180	178	4	5	1	5	822	828	5
17	11	2	97	99	12	18	4	3	92	91	11	4	14	3	292	291	5	6	6	4	255	256	4	7	1	5	67	60	10
0	12	2	1394	1381	9	20	4	3	183	176	7	6	14	3	132	136	7	8	6	4	264	256	4	9	1	5	125	123	6
2	12	2	207	204	5	1	5	3	76	80	6	8	14	3	275	259	5	10	6	4	1430	1446	9	11	1	5	105	105	8
4	12	2	260	252	4	3	5	3	164	169	4	10	14	3	427	431	5	12	6	4	174	174	5	13	1	5	72	75	12
6	12	2	733	741	6	5	5	3	463	446	3	12	14	3	40	24	40	14	6	4	144	141	7	15	1	5	297	296	5
8	12	2	300	297	4	7	5	3	819	814	5	1	15	3	207	204	6	16	6	4	95	102	11	17	1	5	674	689	5
10	12	2	624	637	5	9	5	3	204	206	4	3	15	3	343	346	5	18	6	4	299	298	5	19	1	5	460	464	5
12	12	2	324	319	5	11	5	3	163	164	5	5	15	3	209	212	6	1	7	4	224	206	4	0	2	5	799	823	6
14	12	2	348	333	5	13	5	3	448	453	4	7	15	3	241	231	5	3	7	4	317	326	4	2	2	5	227	215	4
16	12	2	584	581	5	15	5	3	438	440	4	9	15	3	14	48	13	5	7	4	1205	1225	8	4	2	5	228	226	4
1	13	2	28	22	28	17	5	3	222	225	6	11	15	3	356	341	5	7	7	4	384	381	4	6	2	5	470	473	4
3	13	2	62	60	12	19	5	3	54	5	20	0	16	3	332	327	5	9	7	4	815	826	5	8	2	5	219	217	4
5	13	2	1679	1683	12	0	6	3	537	534	4	2	16	3	0	6	1	11	7	4	800	793	6	10	2	5	344	346	4
7	13	2	28	47	28	2	6	3	198	199	3	4	16	3	304	305	5	13	7	4	137	136	7	12	2	5	654	649	5
9	13	2	84	85	10	4	6	3	570	571	4	6	16	3	1133	1135	8	15	7	4	290	291	5	14	2	5	43	5	25
11	13	2	94	95	10	6	6	3	1346	1358	9	8	16	3	334	337	5	17	7	4	555	551	5	16	2	5	81	80	12
13	13	2	208	214	6	8	6	3	376	371	4	10	16	3	276	279	6	0	8	4	1895	1950	10	18	2	5	151	154	8
15	13	2	609	617	5	10	6	3	130	145	6	1	17	3	238	229	6	2	8	4	0	3	1	1	3	5	122	120	6
0	14	2	270	266	5	12	6	3	157	149	4	3	17	3	155	161	8	4	8	4	344	343	4	3	3	5	246	241	4
2	14	2	306	301	4	14	6	3	51	50	18	5	17	3	673	667	6	6	8	4	597	597	5	5	3	5	561	566	4
4	14	2	677	681	5	16	6	3	1050	1062	7	7	17	3	38	13	38	8	8	4	442	453	4	7	3	5	59	53	12
6	14	2	508	516	5	18	6	3	420	414	5	0	18	3	153	160	8	10	8	4	977	984	6	9	3	5	155	134	5
8	14	2	180	178	6	20	6	3	449	452	5	2	18	3	217	233	7	12	8	4	32	5	32	11	3	5	148	146	6
10	14	2	29	29	29	1	7	3	140	133	5	4	18	3	158	135	8	14	8	4	45	42	28	13	3	5	222	217	5
12	14	2	0	21	1	3	7	3	89	101	7	0	0	4	6557	6886	11	16	8	4	311	286	5	15	3	5	89	94	11
14	14	2	240	252	6	5	7	3	1697	1674	9	2	0	4	268	268	3	18	8	4	69	64	16	17	3	5	489	484	5
1	15	2	690	691	5	7	7	3	232	233	4	4	0	4	367	375	3	1	9	4	87	79	8	19	3	5	163	161	8
3	15	2	193	195	6	9	7	3	300	298	4	6	0	4	188	172	4	3	9	4	89	77	8	0	4	5	244	245	4
5	15	2	1449	1457	10	11	7	3	922	927	6	8	0	4	554	559	4	5	9	4	1822	1849	11	2	4	5	131	108	5
7	15	2	409	414	5	13	7	3	159	158	6	10	0	4	2976	3019	11	7	9	4	496	488	4	4	4	5	25	6	25
9	15	2	99	116	10	15	7	3	146	140	7	12	0	4	1084	1097	8	9	9	4	118	121	7	6	4	5	579	569	4
11	15	2	433	444	5	17	7	3	686	683	5	14	0	4	465	465	4	11	9	4	228	226	5	8	4	5	241	251	4
13	15	2	178	176	7	19	7	3	179	168	7	16	0	4	182	172	6	13	9	4	70	74	14	10	4	5	526	527	4
0	16	2	926	920	7	0	8	3	1092	1090	7	18	0	4	395	390	5	15	9	4	716	725	6	12	4	5	382	380	4
2	16	2	212	211	6	2	8	3	52	48	12	20	0	4	474	473	5	17	9	4	735	737	6	14	4	5	281	286	5
4	16	2	165	164	6	4	8	3	125	127	6	1	1	4	432	435	3	0	10	4	790	789	6	16	4	5	476	472	5
6	16	2	620	617	5	6	8	3	520	522	4	3	1	4	40	24	14	2	10	4	110	115	7	18	4	5	227	229	6
8	16	2	76	68	14	8	8	3	152	155	5	5	1	4	88	64	6	4	10	4	357	370	4	1	5	5	131	128	6
10	16	2	842	831	6	10	8	3	388	395	4	7	1	4	72	77	8	6	10	4	179	166	5	3	5	5	150	149	5
1	17	2	310	294	5	12	8	3	508	512	4	9	1	4	1012	1006	6	8	10	4	256	245	5	5	5	5	407	191	4
3	17	2	166	362	5	14	8	3	268	264	5	11	1	4	1836	1881	11	10	10	4	393	388	4	7	5	5	545	555	4
5	17	2	68	39	16	16	8	3	146	163	7	13	1	4	385	387	4	12	10	4	351	347	5	9	5	5	222	225	5
7	17	2	232	248	6	18	8	3	10	36	10	15	1	4	98	107	9	14	10	4	672	677	5	11	5	5	275	284	5
9	17	2	305	304	6	1	9	3	596	574	5	17	1	4	114	123	9	16	10	4	506	496	5	13	5	5	420	411	5
0	18	2	605	602	5	3	9	3	223	216	4	19	1	4	422	415	5	1	11	4	153	153	6	15	5	5	313	314	5
2	18	2	129	132	9	5	9	3	171	167	5	0	2	4	361	378	3	3	11	4	334	333	4	17	5	5	102	112	11
4	18	2	299	301	6	7	9	3	206	200	4	2	2	4	220	215	3	5	11	4	883	902	7	0	6	5	336	364	4
6	18	2	292	293	6	9	9	3	64	53	11	4	2	4	342	342	3	7	11	4	57	62	16	2	6	5	25	27	25
1	1	3	149	136	3	11	9	3	966	968	6	6	2	4	394	416	3	9	11	4	62	63	14	4	6	5	55	40	13
3	1	3	468	471	3	13	9	3	123	116	7	8	2	4	126	129	5	11	11	4	0	2	1	6	6	5	557	565	4
5	1	3	37	26	14	15	9	3	280	267	5	10	2	4	384	385	4	13	11	4	233	237	6	8	6	5	354	351	4
7	1	3	448	441	3	17	9	3	359	370	5	12	2	4	468	462	4	15	11	4	499	495	5	10	6	5	33	45	33
9	1	3	101	100	6	0	10	3	1162	1161	8	14	2	4	649	642	5	0	12	4	1001	1017	7	12	6	5	271	265	5
11	1	3	1162	1174	8	2	10	3	707	707	5	16	2	4	821	837	6	2	12	4	73	69	11	14	6	5	73	57	13
13	1	3	318	314	4	4	10	3	219	212	4	18	2	4	338	335	5	4	12	4	365	369	4	16	6	5	670	666	5
15	1	3	450	455	4	6	10	3	332	326	4	20	2	4	30	29	29	6	12	4	279	277	5	18	6	5	134	138	9
17	1	3	310	311	5	8	10	3	124	138	7	1	3	4	86	79	6	8	12	4	178	187	6	1	7	5	89	84	8
19	1	3	563	572	5	10	10	3	277	282	5	3	3	4	275	259	3	10	12	4	655	654	5	3	7	5	359	360	4
21	1	3	390	382	5	12	10	3	82	80	10	5	3	4	3571	3559	10	12	12	4	406	405	5	5	7	5	442	439	4
0	2	3	2024	2037	7	14	10	3	595	602	5	7	3	4	174	187	5	14	12	4	88	95	13	7	7	5	283	282	4
2	2	3	739	725	5	16	10	3	472	471	5	9	3	4	473	477	4	1	13	4	420	419	4	9	7	5	191	189	5
4	2	3	355	352	3	18	10	3	76	70	15	11	3	4	309	319	4	3	13	4	196	193	6	11	7	5	264	261	5
6	2	3	1040	1014	6	1	11	3	153	153	5	13	3	4	268	269	4	5	13	4	175	176	6	13	7	5	143	146	7

Observed and calculated structure factors for K35

h	k	l	10Fo	10Fc	10s
15	7	5	297	281	5
17	7	5	44	10	44
0	8	5	577	587	5
2	8	5	262	246	4
4	8	5	189	187	5
6	8	5	565	564	5
8	8	5	51	45	17
10	8	5	239	236	5
12	8	5	326	315	5
14	8	5	448	444	5
16	8	5	437	433	5
1	9	5	664	668	5
1	9	5	8	8	8
5	9	5	585	576	5
7	9	5	322	315	4
9	9	5	23	6	22
11	9	5	1563	1571	9
13	9	5	201	192	6
15	9	5	239	231	6
0	10	5	1244	1233	8
2	10	5	441	447	4
4	10	5	34	3	33
6	10	5	543	541	5
8	10	5	36	47	35
10	10	5	440	444	5
12	10	5	55	71	22
14	10	5	462	458	5
1	11	5	55	37	16
3	11	5	8	27	8
5	11	5	672	655	5
7	11	5	486	492	5
9	11	5	157	153	7
11	11	5	174	179	7
13	11	5	219	223	6
0	12	5	939	944	6
2	12	5	566	554	5
4	12	5	19	6	19
6	12	5	819	815	6
8	12	5	18	38	18
10	12	5	103	110	11
12	12	5	157	161	7
1	13	5	449	434	5
3	13	5	144	131	7
5	13	5	1068	1076	7
7	13	5	206	202	6
9	13	5	222	222	6
11	13	5	1411	1382	9
0	14	5	1184	1162	8
2	14	5	75	73	14
4	14	5	290	283	5
6	14	5	431	421	5
8	14	5	115	112	10
10	14	5	573	572	5
1	15	5	58	48	20
3	15	5	358	348	5
5	15	5	105	100	11
7	15	5	329	326	5
0	16	5	430	414	5
2	16	5	184	190	7
4	16	5	8	10	7
0	0	6	2437	2556	11
2	0	6	153	154	5
4	0	6	502	509	4
6	0	6	679	691	5
8	0	6	429	430	4
10	0	6	953	953	6
12	0	6	794	799	5
14	0	6	718	712	5
16	0	6	1001	1008	7
1	1	6	165	167	5
3	1	6	29	29	28
5	1	6	1675	1704	11
7	1	6	158	156	5
9	1	6	289	288	4
11	1	6	284	274	5
13	1	6	45	49	25
15	1	6	491	478	5
17	1	6	337	329	5
0	2	6	1747	1788	11
2	2	6	152	157	5
4	2	6	110	77	7
6	2	6	438	448	4
8	2	6	97	95	8
10	2	6	950	967	6
12	2	6	391	392	5
14	2	6	117	116	9
16	2	6	289	289	5
1	3	6	291	295	4
3	3	6	24	14	23
5	3	6	915	924	6
7	3	6	101	103	8
9	3	6	769	764	5
11	3	6	1267	1295	8
13	3	6	18	2	17
15	3	6	172	168	7
17	3	6	454	458	5
0	4	6	2349	2386	11
2	4	6	93	88	8
4	4	6	275	271	4
6	4	6	598	609	5
8	4	6	202	201	5
10	4	6	1381	1394	8
12	4	6	101	98	10
14	4	6	52	63	23
16	4	6	287	279	6
1	5	6	393	384	4
3	5	6	281	279	4
5	5	6	611	605	5
7	5	6	110	125	8
9	5	6	361	363	4
11	5	6	247	241	5
13	5	6	99	92	10
15	5	6	388	382	5
0	6	6	64	51	12
2	6	6	114	109	7
4	6	6	194	190	5
6	6	6	1047	1054	6
8	6	6	345	344	4
10	6	6	159	164	6
12	6	6	190	182	6
14	6	6	588	591	5
16	6	6	936	934	6
1	7	6	416	416	4
3	7	6	44	29	20
5	7	6	2553	2549	12
7	7	6	131	127	7
9	7	6	312	299	5
11	7	6	307	316	5
13	7	6	291	284	5
15	7	6	801	800	6
0	8	6	248	229	5
2	8	6	257	247	5
4	8	6	369	379	4
6	8	6	263	260	5
8	8	6	298	305	5
10	8	6	263	262	5
12	8	6	21	11	20
14	8	6	123	318	5
1	9	6	426	418	4
3	9	6	20	17	19
5	9	6	162	76	6
7	9	6	572	579	5
9	9	6	282	281	5
11	9	6	732	736	5
13	9	6	137	139	8
0	10	6	2206	2216	13
2	10	6	157	157	7
4	10	6	135	145	7
6	10	6	484	484	4
8	10	6	156	150	7
10	10	6	1345	1345	8
12	10	6	346	333	5
1	11	6	213	217	6
3	11	6	294	285	5
5	11	6	476	492	5
7	11	6	153	142	7
9	11	6	187	178	5
11	11	6	868	854	6
0	12	6	596	588	5
2	12	6	173	174	7
4	12	6	185	184	6
6	12	6	776	776	6
8	12	6	136	133	8
10	12	6	352	346	6
1	13	6	68	73	16
3	13	6	44	43	40
5	13	6	1252	1248	9
7	13	6	103	96	11
0	14	6	150	143	8
2	14	6	141	149	5
4	14	6	295	284	6
6	14	6	189	185	7
1	15	6	475	476	5
1	1	7	93	86	8
3	1	7	158	156	6
5	1	7	141	131	7
7	1	7	275	272	5
9	1	7	86	79	10
11	1	7	658	665	5
13	1	7	201	211	6
15	1	7	297	302	6
0	2	7	663	660	5
2	2	7	350	348	4
4	2	7	81	74	10
6	2	7	522	519	4
8	2	7	261	249	5
10	2	7	130	154	8
12	2	7	177	185	5
14	2	7	173	180	7
1	3	7	288	275	4
3	3	7	0	5	1
5	3	7	456	453	4
7	3	7	334	335	5
9	3	7	115	125	8
11	3	7	924	914	6
13	3	7	49	55	27
15	3	7	154	151	8
0	4	7	1131	1138	8
2	4	7	0	5	1
4	4	7	100	96	9
6	4	7	200	199	5
8	4	7	74	99	12
10	4	7	597	591	5
12	4	7	417	416	5
14	4	7	118	114	10
1	5	7	35	23	35
3	5	7	85	60	10
5	5	7	65	64	14
7	5	7	490	489	4
9	5	7	155	152	7
11	5	7	63	44	16
13	5	7	281	281	6
0	6	7	263	258	5
2	6	7	154	148	6
4	6	7	242	229	5
6	6	7	783	785	6
8	6	7	247	250	5
10	6	7	100	102	10
12	6	7	205	209	6
1	7	7	139	135	7
3	7	7	141	136	7
5	7	7	1039	1032	7
7	7	7	117	104	8
9	7	7	197	200	6
11	7	7	602	606	5
13	7	7	115	107	10
0	8	7	712	709	6
2	8	7	53	39	17
4	8	7	79	76	12
6	8	7	353	349	5
8	8	7	41	48	41
10	8	7	333	335	5
12	8	7	356	357	5
1	9	7	312	309	5
3	9	7	117	133	9
5	9	7	217	220	6
7	9	7	142	152	8
9	9	7	16	13	15
11	9	7	560	563	5
0	10	7	700	699	5
2	10	7	399	405	5
4	10	7	104	103	10
6	10	7	207	208	6
8	10	7	71	77	16
10	10	7	169	173	8
1	11	7	85	87	13
3	11	7	61	46	19
5	11	7	641	642	5
7	11	7	122	128	10
0	12	7	74	51	14
2	12	7	246	244	6
4	12	7	273	271	6
6	12	7	155	163	8
1	13	7	258	244	6
0	0	8	2510	2632	13
2	0	8	68	83	14
4	0	8	84	81	11
6	0	8	579	580	5
8	0	8	133	138	8
10	0	8	1642	1659	10
12	0	8	589	587	5
1	1	8	200	194	6
3	1	8	99	94	10
5	1	8	382	385	5
7	1	8	253	247	5
9	1	8	547	540	5
11	1	8	644	633	5
0	2	8	12	6	12
2	2	8	110	121	9
4	2	8	183	187	6
6	2	8	490	479	5
8	2	8	17	38	37
10	2	8	204	184	6
12	2	8	304	312	6
1	3	8	27	36	27
3	3	8	182	178	6
5	3	8	1885	1892	11
7	3	8	0	14	1
9	3	8	246	246	6
11	3	8	0	4	1
0	4	8	183	185	6
2	4	8	328	327	5
4	4	8	125	110	8
6	4	8	720	750	5
8	4	8	0	32	1
10	4	8	213	210	6
1	5	8	495	500	5
3	5	8	140	147	8
5	5	8	467	468	5
7	5	8	50	29	24
9	5	8	0	8	1
0	6	8	1800	1818	11
2	6	8	132	133	8
4	6	8	174	185	7
6	6	8	494	495	5
8	6	8	83	58	12
10	6	8	942	941	7
1	7	8	0	12	1
3	7	8	258	244	5
5	7	8	860	863	6
7	7	8	234	235	6
9	7	8	466	455	5
0	8	8	981	968	7
2	8	8	72	57	15
4	8	8	107	100	10
6	8	8	412	413	5
8	8	8	249	252	6
1	9	8	0	6	1
3	9	8	0	2	1
5	9	8	1276	1288	8
0	10	8	979	979	7
2	10	8	25	9	25
1	1	9	41	14	40
3	1	9	110	107	10
5	1	9	396	402	5
7	1	9	119	119	9
0	2	9	225	203	6
2	2	9	136	143	8
4	2	9	14	33	34
6	2	9	87	69	12
1	3	9	70	56	16
3	3	9	11	6	30
5	3	9	160	164	8
0	4	9	405	403	5
2	4	9	0	43	1
4	4	9	44	63	43
1	5	9	44	41	43
3	5	9	56	35	21
0	6	9	106	112	10
2	6	9	24	17	24

Observed and calculated structure factors for K36

h	k	l	10Fo	10Fc	10s
2	0	0	606	638	3
4	0	0	903	913	4
6	0	0	757	762	5
8	0	0	1252	1224	6
10	0	0	4183	4044	8
12	0	0	1494	1506	8
14	0	0	307	301	3
16	0	0	599	600	5
18	0	0	300	302	4
20	0	0	573	568	5
22	0	0	2146	2136	12
1	1	0	186	176	2
5	1	0	575	571	4
7	1	0	464	461	3
9	1	0	1454	1421	7
11	1	0	1229	1125	8
13	1	0	653	657	5
15	1	0	253	262	4
17	1	0	426	427	4
19	1	0	464	470	4
21	1	0	964	975	7
0	2	0	1290	1346	3
2	2	0	292	309	2
4	2	0	553	574	4
6	2	0	238	244	2
8	2	0	307	304	3
10	2	0	588	590	4
12	2	0	525	534	4
14	2	0	861	866	6
16	2	0	860	866	6
18	2	0	365	364	4
20	2	0	0	19	1
22	2	0	152	159	7
1	3	0	150	156	2
3	3	0	318	322	2
7	3	0	562	545	4
9	3	0	647	630	4
11	3	0	664	675	5
13	3	0	277	270	3
15	3	0	1052	1070	7
17	3	0	1084	1094	7
19	3	0	141	354	4
21	3	0	136	146	7
0	4	0	2032	2062	5
2	4	0	592	605	4
4	4	0	887	870	5
8	4	0	273	265	3
10	4	0	492	486	4
12	4	0	145	147	4
14	4	0	506	508	4
16	4	0	2294	2285	10
18	4	0	76	84	10
20	4	0	71	77	12
22	4	0	627	628	5
1	5	0	1186	1406	5
3	5	0	152	144	3
5	5	0	3241	3170	6
7	5	0	946	938	5
9	5	0	122	113	4
11	5	0	384	408	3
13	5	0	47	47	14
15	5	0	222	229	4
17	5	0	542	541	4
19	5	0	110	110	8
21	5	0	514	518	5
0	6	0	925	928	6
2	6	0	138	140	3
4	6	0	42	47	9
6	6	0	289	275	3
8	6	0	528	516	4
10	6	0	1656	1659	8
12	6	0	93	105	7
14	6	0	337	329	4
16	6	0	342	358	4
18	6	0	448	446	4
20	6	0	67	81	14
1	7	0	568	560	4
3	7	0	247	254	2
5	7	0	1191	1367	7
7	7	0	505	491	4
9	7	0	1069	1059	7
11	7	0	742	708	5
13	7	0	137	133	5
15	7	0	106	106	4
17	7	0	534	526	4
19	7	0	596	598	5
21	7	0	669	665	5
0	8	0	2723	2718	7
2	8	0	101	93	4
4	8	0	561	566	4
6	8	0	603	614	4
8	8	0	582	585	4
10	8	0	1171	1144	7
12	8	0	19	11	20
14	8	0	81	70	8
16	8	0	359	319	4
18	8	0	8	13	8
20	8	0	307	289	5
1	9	0	196	181	3
3	9	0	178	170	3
5	9	0	1995	2053	8
7	9	0	903	896	6
9	9	0	209	199	4
11	9	0	627	603	5
13	9	0	263	251	4
15	9	0	921	950	6
17	9	0	696	693	5
19	9	0	42	43	32
0	10	0	315	319	3
2	10	0	166	164	4
4	10	0	288	295	3
6	10	0	253	250	3
8	10	0	136	147	5
10	10	0	484	492	4
12	10	0	158	165	4
14	10	0	927	943	6
16	10	0	426	422	4
18	10	0	198	204	6
1	11	0	150	146	4
3	11	0	280	284	3
5	11	0	752	757	5
7	11	0	54	67	12
9	11	0	79	85	8
11	11	0	317	332	4
13	11	0	346	358	4
15	11	0	648	651	5
17	11	0	440	446	4
0	12	0	1518	1553	9
2	12	0	52	49	12
4	12	0	456	452	4
6	12	0	557	562	4
8	12	0	126	122	6
10	12	0	867	875	6
12	12	0	517	526	4
14	12	0	144	147	7
16	12	0	94	93	10
1	13	0	625	620	5
3	13	0	212	209	4
5	13	0	320	317	4
7	13	0	434	439	4
9	13	0	230	220	4
11	13	0	988	996	7
13	13	0	198	199	5
15	13	0	294	295	5
0	14	0	1384	1398	10
2	14	0	335	333	4
4	14	0	189	187	5
6	14	0	582	582	5
8	14	0	233	223	4
10	14	0	1172	1195	8
12	14	0	121	128	8
14	14	0	0	4	1
1	15	0	405	399	4
3	15	0	229	220	4
5	15	0	512	523	4
7	15	0	135	146	6
9	15	0	301	305	4
11	15	0	430	424	4
13	15	0	274	277	5
0	16	0	569	573	5
2	16	0	268	267	4
4	16	0	92	106	9
6	16	0	685	690	5
8	16	0	90	84	10
10	16	0	150	153	7
12	16	0	476	485	5
1	17	0	301	290	4
3	17	0	337	335	4
5	17	0	1761	1732	12
7	17	0	134	134	7
9	17	0	31	39	30
0	18	0	404	409	4
2	18	0	176	177	6
4	18	0	151	147	6
6	18	0	372	362	5
8	18	0	179	176	6
1	19	0	89	103	11
3	19	0	189	196	6
1	1	1	136	128	2
3	1	1	207	206	2
5	1	1	1006	1004	5
7	1	1	66	81	6
9	1	1	126	108	4
11	1	1	681	694	5
13	1	1	245	237	3
15	1	1	418	413	4
17	1	1	656	667	5
19	1	1	584	578	5
21	1	1	430	430	4
0	2	1	74	87	3
2	2	1	658	685	4
4	2	1	220	223	2
6	2	1	203	193	2
8	2	1	431	444	3
10	2	1	281	271	3
12	2	1	805	820	6
14	2	1	96	96	6
16	2	1	510	517	4
18	2	1	21	24	21
20	2	1	467	472	4
22	2	1	278	275	5
1	3	1	405	412	3
3	3	1	281	277	2
5	3	1	396	388	3
7	3	1	163	163	3
9	3	1	250	243	3
11	3	1	460	469	3
13	3	1	181	184	4
15	3	1	167	175	5
17	3	1	250	249	4
19	3	1	225	210	5
21	3	1	440	439	4
0	4	1	1239	1245	5
2	4	1	224	220	2
4	4	1	40	35	9
6	4	1	616	582	4
8	4	1	118	121	3
10	4	1	830	820	5
12	4	1	593	602	4
14	4	1	255	251	4
16	4	1	419	408	4
18	4	1	220	212	5
20	4	1	139	138	7
22	4	1	364	363	5
1	5	1	84	90	4
3	5	1	264	272	2
5	5	1	1010	990	6
7	5	1	886	875	6
9	5	1	299	287	3
11	5	1	347	356	3
13	5	1	543	551	4
15	5	1	397	406	4
17	5	1	180	175	5
19	5	1	44	35	24
21	5	1	483	484	4
0	6	1	450	445	3
2	6	1	56	41	6
4	6	1	361	354	3
6	6	1	1105	1110	7
8	6	1	532	535	4
10	6	1	99	90	6
12	6	1	182	180	4
14	6	1	59	55	11
16	6	1	1012	1029	7
18	6	1	115	101	4
20	6	1	494	504	5
1	7	1	168	162	3
3	7	1	426	432	3
5	7	1	1025	1040	7
7	7	1	192	179	3
9	7	1	259	253	3
11	7	1	146	166	4
13	7	1	17	24	17
15	7	1	293	282	4
17	7	1	298	285	4
19	7	1	195	186	6
21	7	1	121	116	8
0	8	1	382	364	3
2	8	1	221	204	3
4	8	1	225	213	3
6	8	1	290	300	3
8	8	1	31	4	31
10	8	1	293	302	3
12	8	1	492	494	4
14	8	1	478	484	4
16	8	1	333	312	4
18	8	1	243	255	5
20	8	1	460	457	5
1	9	1	871	860	5
3	9	1	17	20	16
5	9	1	448	462	4
7	9	1	371	377	1
9	9	1	85	47	7
11	9	1	1740	1755	10
13	9	1	188	188	5
15	9	1	306	301	4
17	9	1	68	71	13
19	9	1	245	228	5
0	10	1	1529	1562	8
2	10	1	746	746	5
4	10	1	91	95	6
6	10	1	556	565	4
8	10	1	114	105	6
10	10	1	463	471	4
12	10	1	19	5	19
14	10	1	600	606	5
16	10	1	680	681	5
18	10	1	100	126	9
1	11	1	36	13	20
3	11	1	36	38	21
5	11	1	924	921	6
7	11	1	514	517	4
9	11	1	232	235	4
11	11	1	74	84	10
13	11	1	133	151	6
15	11	1	524	508	5
17	11	1	432	434	5
0	12	1	893	908	6
2	12	1	597	611	4
4	12	1	141	141	5
6	12	1	783	795	5
8	12	1	54	70	13
10	12	1	94	88	8
12	12	1	243	232	5
14	12	1	93	93	9
16	12	1	827	822	6
1	13	1	494	488	4
3	13	1	244	241	4
5	13	1	1107	1127	7
7	13	1	140	144	6
9	13	1	284	279	4
11	13	1	1338	1340	9
13	13	1	245	229	5
15	13	1	62	47	15
0	14	1	1033	1064	7
2	14	1	111	99	6
4	14	1	336	342	4
6	14	1	304	294	4
8	14	1	235	221	5
10	14	1	583	589	5
12	14	1	123	127	9
14	14	1	263	245	5
1	15	1	16	17	16
3	15	1	386	394	4
5	15	1	50	54	16
7	15	1	359	356	4
9	15	1	0	15	1
11	15	1	180	161	6
13	15	1	267	265	5
0	16	1	513	507	4
2	16	1	169	175	6
4	16	1	115	88	7
6	16	1	1307	1303	8
8	16	1	367	366	4
10	16	1	113	121	8
12	16	1	31	43	31
1	17	1	183	174	6
3	17	1	150	141	6
5	17	1	960	951	7
7	17	1	272	258	5
9	17	1	209	217	6
0	18	1	319	322	5
2	18	1	142	144	7
4	18	1	313	300	5
6	18	1	240	231	5
8	18	1	191	188	6
1	19	1	490	483	4
3	19	1	389	391	5
2	0	2	602	612	4
4	0	2	187	174	2
6	0	2	696	663	4
8	0	2	575	562	4
10	0	2	1556	1528	8
12	0	2	1122	1126	7
14	0	2	1256	1242	8
16	0	2	1051	1043	7
18	0	2	290	291	4
20	0	2	233	231	5
22	0	2	638	633	5
1	1	2	436	435	3
3	1	2	612	610	3
5	1	2	1172	1151	6
7	1	2	99	93	4
9	1	2	543	529	4
11	1	2	460	455	4
13	1	2	87	90	7
15	1	2	742	756	5
17	1	2	48	14	16
19	1	2	85	98	10
21	1	2	248	234	5
2	2	2	294	296	2
4	2	2	340	344	1
6	2	2	437	420	1
8	2	2	38	1	11
10	2	2	1502	1509	8
12	2	2	661	663	5
14	2	2	67	79	9
16	2	2	209	215	4
18	2	2	73	71	11
20	2	2	258	256	5
22	2	2	684	688	6
1	3	2	495	493	1
3	3	2	243	236	2
5	3	2	1232	1229	6
7	3	2	181	173	3
9	3	2	1174	1181	8
11	3	2	1708	1716	8
13	3	2	53	55	12
15	3	2	281	272	4
17	3	2	479	487	4
19	3	2	721	715	5
21	3	2	844	861	6
0	4	2	1932	1929	6
2	4	2	661	654	4
4	4	2	211	204	2
6	4	2	627	624	4
8	4	2	205	205	3
10	4	2	2126	2134	8
12	4	2	101	107	6
14	4	2	93	94	7
16	4	2	188	187	5
18	4	2	600	599	5
20	4	2	274	269	5
1	5	2	1089	1060	6
3	5	2	190	182	2
5	5	2	1967	1927	7
7	5	2	198	179	3
9	5	2	610	601	4
11	5	2	742	736	5
13	5	2	0	4	1
15	5	2	434	436	4
17	5	2	657	664	5
19	5	2	302	294	5
21	5	2	284	283	5
0	6	2	1150	1146	6
2	6	2	90	101	4
4	6	2	679	688	4
6	6	2	2626	2556	8
8	6	2	394	392	3
10	6	2	264	266	3
12	6	2	276	275	4
14	6	2	667	667	5
16	6	2	1722	1737	11
18	6	2	176	169	6
20	6	2	87	77	10
1	7	2	486	481	3
3	7	2	243	244	3
5	7	2	4692	4607	8
7	7	2	174	164	4
9	7	2	395	395	3
11	7	2	115	103	6
13	7	2	396	396	4
15	7	2	1116	1122	7
17	7	2	1189	1202	8
19	7	2	179	182	6
0	8	2	339	336	3
2	8	2	474	474	4
4	8	2	345	351	3
6	8	2	179	167	3
8	8	2	429	437	3
10	8	2	206	190	4
12	8	2	51	48	14
14	8	2	476	489	4
16	8	2	929	924	6
18	8	2	133	131	7
20	8	2	97	104	10
1	9	2	492	483	4
3	9	2	179	176	4
5	9	2	570	562	4
7	9	2	505	500	4

Observed and calculated structure factors for K36

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
9	9	2	458	461	4	14	2	3	300	310	4	9	11	3	290	288	4	0	4	4	600	618	4	13	13	4	108	108	9
11	9	2	1583	1570	10	16	2	3	894	904	6	11	11	3	153	151	6	2	4	4	463	449	3	0	14	4	1340	1362	9
13	9	2	346	362	4	18	2	3	190	193	5	13	11	3	33	14	32	4	4	4	428	446	3	2	14	4	191	201	5
15	9	2	27	5	26	20	2	3	382	382	5	15	11	3	339	328	5	6	4	4	2149	2137	8	4	14	4	296	299	5
17	9	2	817	840	6	1	3	3	486	480	3	17	11	3	517	529	5	8	4	4	73	67	8	6	14	4	381	379	4
19	9	2	296	289	5	3	3	3	243	236	2	0	12	3	83	93	8	10	4	4	399	404	4	8	14	4	227	212	5
0	10	2	4470	4465	9	5	3	3	967	942	6	2	12	3	398	395	4	12	4	4	139	137	5	10	14	4	935	934	6
2	10	2	464	459	4	7	3	3	722	715	5	4	12	3	394	402	4	14	4	4	549	554	4	12	14	4	75	81	12
4	10	2	556	569	4	9	3	3	217	205	3	6	12	3	312	312	4	16	4	4	1703	1710	11	1	15	4	370	364	4
6	10	2	15	11	15	11	3	3	1454	1473	9	8	12	3	18	25	17	18	4	4	38	31	38	3	15	4	261	261	5
8	10	2	349	356	3	13	3	3	46	32	14	10	12	3	65	46	12	20	4	4	39	43	39	5	15	4	278	276	5
10	10	2	1937	1923	10	15	3	3	263	260	4	12	12	3	209	202	5	1	5	4	890	873	5	7	15	4	15	14	14
12	10	2	461	457	4	17	3	3	262	267	4	14	12	3	191	197	6	3	5	4	101	94	5	9	15	4	276	278	5
14	10	2	250	251	4	19	3	3	135	129	7	16	12	3	541	533	5	5	5	4	1616	1655	8	0	16	4	191	193	6
16	10	2	39	41	18	21	3	3	481	483	5	1	13	3	407	409	4	7	5	4	408	405	3	2	16	4	265	261	5
18	10	2	149	144	6	0	4	3	2249	2218	7	3	13	3	364	366	4	9	5	4	50	35	13	4	16	4	0	22	1
1	11	2	465	466	4	2	4	3	51	37	7	5	13	3	530	545	4	11	5	4	884	896	6	6	16	4	390	387	5
3	11	2	599	599	4	4	4	3	226	227	3	7	13	3	86	94	9	13	5	4	77	81	9	8	16	4	30	19	29
5	11	2	45	63	15	6	4	3	108	102	3	9	13	3	221	213	5	15	5	4	282	276	4	1	17	4	317	321	5
7	11	2	39	37	20	8	4	3	129	128	4	11	13	3	642	634	5	17	5	4	202	192	5	3	17	4	250	238	5
9	11	2	574	573	4	10	4	3	852	849	6	13	13	3	85	81	11	19	5	4	58	53	17	5	17	4	1333	1325	8
11	11	2	1951	1932	11	12	4	3	628	628	5	15	13	3	48	50	22	0	6	4	2092	2125	8	1	1	5	19	15	18
13	11	2	113	107	7	14	4	3	101	97	7	0	14	3	402	393	4	2	6	4	145	161	4	3	1	5	65	61	8
15	11	2	66	48	13	16	4	3	36	29	35	2	14	3	56	62	14	4	6	4	184	180	4	5	1	5	825	819	5
17	11	2	86	74	11	18	4	3	103	88	8	4	14	3	263	261	4	6	6	4	272	266	3	7	1	5	74	74	8
0	12	2	1423	1420	9	20	4	3	168	171	6	6	14	3	108	114	7	8	6	4	250	232	4	9	1	5	117	121	6
2	12	2	209	199	4	1	5	3	90	86	5	8	14	3	288	282	4	10	6	4	1458	1457	10	11	1	5	129	140	6
4	12	2	220	206	4	3	5	3	151	148	3	10	14	3	403	410	4	12	6	4	172	176	5	13	1	5	108	102	7
6	12	2	714	719	5	5	5	3	495	475	4	12	14	3	55	46	19	14	6	4	158	153	5	15	1	5	299	300	4
8	12	2	276	278	4	7	5	3	843	844	6	14	14	3	310	312	5	16	6	4	99	94	8	17	1	5	692	689	5
10	12	2	660	664	5	9	5	3	204	207	4	1	15	3	187	177	5	18	6	4	301	298	5	19	1	5	446	448	5
12	12	2	297	303	4	11	5	3	189	179	4	3	15	3	327	326	4	1	7	4	212	207	3	0	2	5	784	798	5
14	12	2	152	350	4	13	5	3	433	429	4	5	15	3	250	258	5	3	7	4	283	287	3	2	2	5	242	234	3
16	12	2	568	561	5	15	5	3	431	432	4	7	15	3	243	241	5	5	7	4	1236	1240	7	4	2	5	241	244	3
1	13	2	39	22	20	17	5	3	234	230	5	9	15	3	31	30	31	7	7	4	377	370	3	6	2	5	432	431	4
3	13	2	80	83	8	19	5	3	32	2	11	11	15	3	353	350	5	9	7	4	818	833	5	8	2	5	199	194	4
5	13	2	1741	1752	10	0	6	3	539	527	4	0	16	3	341	343	4	11	7	4	832	829	6	10	2	5	332	334	4
7	13	2	51	40	15	2	6	3	207	198	3	2	16	3	38	37	34	13	7	4	106	103	7	12	2	5	654	654	5
9	13	2	65	66	11	4	6	3	565	552	4	4	16	3	285	291	5	15	7	4	266	272	4	14	2	5	81	14	9
11	13	2	57	75	15	6	6	3	1352	1364	8	6	16	3	1144	1148	8	17	7	4	560	566	5	16	2	5	129	103	7
13	13	2	238	237	5	8	6	3	362	367	3	8	16	3	331	335	5	0	8	4	1923	1990	9	18	2	5	125	135	8
15	13	2	626	624	5	10	6	3	148	157	5	10	16	3	281	269	5	2	8	4	0	2	1	1	3	5	134	131	4
0	14	2	292	282	4	12	6	3	349	353	4	1	17	3	257	249	5	4	8	4	309	312	3	3	3	5	264	253	3
2	14	2	269	273	4	14	6	3	48	51	15	3	17	3	184	197	6	6	8	4	556	551	4	5	3	5	574	582	4
4	14	2	702	713	5	16	6	3	1096	1094	7	5	17	3	668	673	5	8	8	4	445	447	4	7	3	5	67	68	9
6	14	2	517	513	4	18	6	3	434	431	4	7	17	3	0	2	1	10	8	4	1016	1009	7	9	3	5	123	124	6
8	14	2	173	163	5	20	6	3	440	455	5	0	18	3	161	165	7	12	8	4	21	6	20	11	3	5	151	152	5
10	14	2	169	43	5	1	7	3	164	149	3	2	18	3	232	237	5	14	8	4	49	46	18	13	3	5	219	208	4
12	14	2	35	14	35	3	7	3	110	122	5	4	18	3	115	115	8	16	8	4	268	270	5	15	3	5	121	99	7
14	14	2	271	281	5	5	7	3	1629	1632	8	2	0	4	268	279	3	18	8	4	76	64	13	17	3	5	468	476	4
1	15	2	649	660	5	7	7	3	229	231	4	4	0	4	352	363	3	1	9	4	97	88	6	19	3	5	176	182	6
3	15	2	213	211	5	9	7	3	288	281	3	6	0	4	154	122	4	3	9	4	65	56	9	0	4	5	210	209	4
5	15	2	1491	1497	9	11	7	3	907	921	6	8	0	4	513	521	4	5	9	4	1859	1888	10	2	4	5	122	122	5
7	15	2	406	407	4	13	7	3	175	173	5	10	0	4	3055	3043	9	7	9	4	491	493	4	4	4	5	0	11	1
9	15	2	85	87	10	15	7	3	131	129	6	12	0	4	1085	1094	7	9	9	4	119	121	6	6	4	5	602	589	4
11	15	2	437	424	4	17	7	3	682	666	5	14	0	4	420	432	4	11	9	4	214	211	5	8	4	5	264	264	4
13	15	2	177	183	6	19	7	3	147	139	7	16	0	4	211	190	5	13	9	4	102	104	8	10	4	5	509	510	4
0	16	2	984	984	7	0	8	3	1036	1039	6	18	0	4	374	375	4	15	9	4	721	717	5	12	4	5	398	396	4
2	16	2	214	213	5	2	8	3	67	48	7	20	0	4	437	443	5	17	9	4	740	738	5	14	4	5	265	260	4
4	16	2	161	168	6	4	8	3	115	112	5	1	1	4	415	418	3	0	10	4	806	817	5	16	4	5	512	510	5
6	16	2	601	595	5	6	8	3	513	515	4	3	1	4	108	71	4	2	10	4	95	85	6	18	4	5	242	231	5
8	16	2	84	82	11	8	8	3	156	155	4	5	1	4	99	83	5	4	10	4	408	413	4	1	5	5	134	132	5
10	16	2	863	846	6	10	8	3	173	177	4	7	1	4	38	44	16	6	10	4	172	183	5	3	5	5	119	125	5
1	17	2	305	299	4	12	8	3	524	526	4	9	1	4	1017	1038	7	8	10	4	207	210	4	5	5	5	451	433	4
3	17	2	365	365	4	14	8	3	270	270	4	11	1	4	1875	1896	9	10	10	4	399	401	4	7	5	5	588	586	4
5	17	2	28	22	27	16	8	3	136	146	7	13	1	4	414	412	4	12	10	4	332	329	4	9	5	5	218	219	4
7	17	2	233	240	5	18	8	3	24	51	24	15	1	4	126	133	6	14	10	4	679	690	5	11	5	5	315	313	4
9	17	2	336	328	5	1	9	3	571	573	4	17	1	4	124	128	7	16	10	4	519	510	5	13	5	5	387	386	4
0	18	2	629	634	5	3	9	3	217	221	3	19	1	4	430	434	4	1	11	4	117	117	6	15	5	5	295	307	5
2	18	2	111	124	9	5	9	3	216	203	4	0	2	4	390	404	3	3	11	4	340	346	4	17	5	5	117	113	8
4	18	2	113	310	5	7	9	3	235	233	4	2	2	4	204	196	3	5	11	4	939	961	6	0	6	5	122	354	3
6	18	2	292	303	5	9	9	3	65	58	10	4	2	4	367	366	3	7	11	4	70	50	10	2	6	5	0	15	1
1	1	3	163	151	3	11	9	3	975	983	6	6	2	4	373	398	3	9	11	4	49	62	17	4	6	5	34	27	29
3	1	3	461	455	3	13	9	3	137	124	6	8	2	4	139	146	4	11	11	4	43	45	23	6	6	5	592	586	4
5	1	3	36	6	13	15	9	3	287	279	4	10	2	4	400	412	4	13	11	4	248	247	5	8	6	5	355	362	4
7	1	3	446	451	3	17	9	3	382	388	5	12	2	4	448	450	4	15	11	4	523	518	5	10	6	5	114	52	6
9	1	3	88	92	6	0	10	3	1113	1131	7	14	2	4	642	640	5	0	12	4	1022	1039	7	12	6	5	263	263	4
11	1	3	1185	1222	9	2	10	3	690	713	5	16	2	4	837	838	6	2	12	4	65	62	11	14	6	5	60	62	15
13	1	3	334	333	3	4	10	3	190	190	4	18	2	4	337	337	4	4	12	4	144	353	4	16	6	5	693	697	5
15	1	3	459	460	4	6	10	3	336	332	3	20	2	4	0	6	1	6	12	4	292	286	4	18	6	5	152	158	7
17	1	3	317	316	4	8	10	3	143	153	5	1	3	4	58	54	8	8	12	4	150	158	6	1	7	5	114	99	5
19	1	3	560	564	5	10	10	3	269	271	4	3	3	4	282	263	3	10	12	4	665	663	5	3	7	5	373	384	4
21	1	3	419	422	5	12	10	3	85	85	9	5	3	4	3529	3607	8	12	12	4	405	396	4	5	7	5	433	407	4
0	2	3	2076	2069	6	14	10	3	572	578	5	7	3	4	193	194	4	14	12	4	68	74	14	7	7	5	281	281	4
2	2	3	742	741	5	16	10	3	448	445	4	9	3	4	481	481	4	1	13	4	407	400	4	9	7	5	179	169	5
4	2	3	338	330	3	18	10	3	50	65	21	11	3	4	344	350	3	3	13	4	164	172	5	11	7	5	271	268	4
6	2	3	1082	1058	7	1	11	3	149	150	5	13	3	4	257	263	4	5	13	4	223	221	5	13	7	5	127	120	7
8	2	3	582	584	4	3	11	3	94	92	7	15	3	4	939	942	6	7	13	4	269	271	4	15	7	5	283	278	5
10	2	3	207	203	4	5	11	3	947	940	6	17	3	4	855	859	6	9	13	4	234	225	5	17	7	5	42	6	32
12	2	3	658	660	5	7	11	3	219	214	4	19	3	4	309	308	5	11	13	4	814	815	6	0	8	5	610	634	5

Observed and calculated structure factors for K36

h	k	l	10Fo	10Fc	10s
2	8	5	258	250	4
4	8	5	204	206	4
6	8	5	578	566	4
8	8	5	67	49	11
10	8	5	218	210	5
12	8	5	346	342	4
14	8	5	442	441	4
16	8	5	489	472	5
1	9	5	666	671	5
3	9	5	23	19	23
5	9	5	584	575	4
7	9	5	354	347	4
9	9	5	0	24	1
11	9	5	1611	1608	9
13	9	5	209	197	5
15	9	5	241	241	5
0	10	5	1220	1238	8
2	10	5	464	466	4
4	10	5	27	17	26
6	10	5	576	562	4
8	10	5	69	71	11
10	10	5	455	451	4
12	10	5	72	64	12
14	10	5	443	449	5
1	11	5	60	48	12
3	11	5	0	2	1
5	11	5	654	646	5
7	11	5	506	508	4
9	11	5	145	149	7
11	11	5	177	184	6
13	11	5	188	197	6
0	12	5	945	951	7
2	12	5	556	552	5
4	12	5	0	18	1
6	12	5	811	807	6
8	12	5	58	53	15
10	12	5	109	102	8
12	12	5	192	192	6
1	13	5	431	422	4
3	13	5	155	150	6
5	13	5	1079	1084	7
7	13	5	229	220	5
9	13	5	241	235	5
11	13	5	1191	1187	9
0	14	5	1150	1166	7
2	14	5	90	88	10
4	14	5	271	267	5
6	14	5	450	446	4
8	14	5	130	135	8
10	14	5	571	571	5
1	15	5	81	80	11
3	15	5	315	319	5
5	15	5	99	87	10
7	15	5	120	127	5
0	16	5	410	403	5
2	16	5	204	205	6
4	16	5	57	40	18
0	0	6	2492	2574	9
2	0	6	133	137	5
4	0	6	516	518	4
6	0	6	696	708	5
8	0	6	384	391	4
10	0	6	952	963	6
12	0	6	787	795	6
14	0	6	684	684	5
16	0	6	1038	1032	7
1	1	6	143	139	5
3	1	6	39	21	19
5	1	6	1720	1733	10
7	1	6	139	152	5
9	1	6	288	285	4
11	1	6	310	297	4
13	1	6	34	38	34
15	1	6	479	479	4
17	1	6	348	339	5
0	2	6	1789	1810	9
2	2	6	152	152	5
4	2	6	77	68	8
6	2	6	438	438	4
8	2	6	94	85	7
10	2	6	973	968	7
12	2	6	392	391	4
14	2	6	118	112	7
16	2	6	284	289	5
1	3	6	289	283	4
3	3	6	29	17	29
5	3	6	927	932	6
7	3	6	101	86	7
9	3	6	783	786	5
11	3	6	1301	1313	8
13	3	6	17	25	36
15	3	6	165	162	6
17	3	6	463	460	5
0	4	6	2399	2442	9
2	4	6	91	90	7
4	4	6	248	249	4
6	4	6	638	646	5
8	4	6	228	212	4
10	4	6	1425	1420	9
12	4	6	120	115	7
14	4	6	55	51	16
16	4	6	316	316	5
1	5	6	381	384	3
3	5	6	248	248	4
5	5	6	618	616	5
7	5	6	127	129	6
9	5	6	359	359	4
11	5	6	247	246	5
13	5	6	128	119	7
15	5	6	389	394	5
0	6	6	68	47	9
2	6	6	83	73	7
4	6	6	234	232	4
6	6	6	1042	1042	7
8	6	6	366	364	4
10	6	6	147	145	6
12	6	6	180	172	6
14	6	6	624	619	5
16	6	6	945	941	7
1	7	6	386	392	4
3	7	6	20	18	20
5	7	6	2567	2602	11
7	7	6	130	129	6
9	7	6	309	295	4
11	7	6	271	279	5
13	7	6	277	270	5
15	7	6	802	799	6
0	8	6	248	236	4
2	8	6	235	224	4
4	8	6	378	382	4
6	8	6	276	278	4
8	8	6	270	271	4
10	8	6	259	263	5
12	8	6	43	13	25
14	8	6	327	326	5
1	9	6	405	398	4
3	9	6	42	26	20
5	9	6	67	70	11
7	9	6	555	565	4
9	9	6	310	301	4
11	9	6	749	746	6
13	9	6	128	137	8
0	10	6	2258	2281	11
2	10	6	174	171	5
4	10	6	151	164	6
6	10	6	454	457	4
8	10	6	136	135	7
10	10	6	1379	1375	8
12	10	6	332	324	5
1	11	6	222	219	5
3	11	6	266	264	5
5	11	6	477	476	4
7	11	6	133	133	7
9	11	6	409	402	4
11	11	6	892	889	6
0	12	6	609	605	5
2	12	6	178	175	6
4	12	6	158	159	6
6	12	6	774	777	5
8	12	6	119	118	8
10	12	6	373	358	5
1	13	6	94	75	9
3	13	6	54	49	18
5	13	6	1319	1318	9
7	13	6	104	95	9
0	14	6	113	116	8
2	14	6	325	325	5
4	14	6	321	308	5
6	14	6	209	200	6
1	15	6	451	455	5
1	1	7	96	87	7
3	1	7	142	141	5
5	1	7	122	121	6
7	1	7	291	291	4
9	1	7	66	66	11
11	1	7	702	698	5
13	1	7	236	232	5
15	1	7	323	312	5
0	2	7	700	690	5
2	2	7	361	368	4
4	2	7	74	74	10
6	2	7	554	549	4
8	2	7	241	235	5
10	2	7	139	138	6
12	2	7	405	403	4
14	2	7	168	177	7
1	3	7	278	276	4
3	3	7	25	12	25
5	3	7	461	451	4
7	3	7	364	360	4
9	3	7	143	134	6
11	3	7	937	924	6
13	3	7	70	63	13
15	3	7	166	166	7
0	4	7	1147	1133	7
2	4	7	15	1	14
4	4	7	104	100	7
6	4	7	188	187	5
8	4	7	108	108	8
10	4	7	596	592	5
12	4	7	427	423	4
14	4	7	99	102	10
1	5	7	21	25	21
3	5	7	43	51	20
5	5	7	91	85	8
7	5	7	508	509	4
9	5	7	157	151	6
11	5	7	50	57	20
13	5	7	258	265	5
0	6	7	261	257	4
2	6	7	149	155	6
4	6	7	225	225	5
6	6	7	793	796	6
8	6	7	241	250	5
10	6	7	122	113	7
12	6	7	213	215	6
1	7	7	120	134	7
3	7	7	148	151	6
5	7	7	1012	1014	6
7	7	7	119	112	7
9	7	7	201	199	6
11	7	7	603	602	5
13	7	7	117	123	9
0	8	7	682	685	5
2	8	7	36	39	35
4	8	7	76	69	11
6	8	7	358	350	4
8	8	7	60	50	15
10	8	7	318	321	5
12	8	7	373	367	5
1	9	7	321	317	4
3	9	7	129	130	7
5	9	7	239	236	5
7	9	7	162	167	6
9	9	7	23	11	23
11	9	7	577	582	5
0	10	7	680	686	5
2	10	7	406	409	4
4	10	7	97	92	9
6	10	7	212	213	5
8	10	7	82	84	11
10	10	7	169	167	7
1	11	7	88	86	10
3	11	7	35	19	35
5	11	7	622	623	5
7	11	7	141	143	7
0	12	7	36	40	36
2	12	7	248	250	5
4	12	7	270	262	5
6	12	7	164	169	7
1	13	7	257	244	5
0	0	8	2606	2689	11
2	0	8	90	88	8
4	0	8	65	70	13
6	0	8	546	553	4
8	0	8	120	117	7
10	0	8	1655	1686	10
12	0	8	596	597	5
1	1	8	197	187	5
3	1	8	132	119	7
5	1	8	403	403	4
7	1	8	241	235	5
9	1	8	558	560	5
11	1	8	658	645	5
0	2	8	17	22	16
2	2	8	120	112	7
4	2	8	201	202	5
6	2	8	481	478	4
8	2	8	53	47	19
10	2	8	199	202	6
12	2	8	299	305	5
1	3	8	7	22	6
3	3	8	185	184	6
5	3	8	1906	1941	12
7	3	8	0	10	1
9	3	8	256	250	5
11	3	8	26	18	26
0	4	8	164	175	6
2	4	8	309	306	4
4	4	8	145	122	6
6	4	8	759	769	5
8	4	8	46	54	24
10	4	8	197	206	6
1	5	8	496	485	4
3	5	8	167	163	6
5	5	8	481	482	4
7	5	8	9	31	9
9	5	8	38	24	38
0	6	8	1884	1871	12
2	6	8	143	138	6
4	6	8	195	191	6
6	6	8	505	503	4
8	6	8	54	45	18
10	6	8	967	962	7
1	7	8	0	9	1
3	7	8	226	222	5
5	7	8	886	893	6
7	7	8	231	231	5
9	7	8	476	469	5
0	8	8	1020	1008	7
2	8	8	52	47	19
4	8	8	93	85	10
6	8	8	386	382	5
8	8	8	258	239	5
1	9	8	28	1	28
3	9	8	0	17	1
5	9	8	1304	1312	8
0	10	8	1008	1008	7
2	10	8	26	6	25
1	1	9	32	8	31
3	1	9	87	97	10
5	1	9	408	398	5
7	1	9	121	128	8
0	2	9	190	184	6
2	2	9	144	147	7
4	2	9	58	47	16
6	2	9	45	45	27
1	3	9	64	65	15
3	3	9	0	2	1
5	3	9	172	173	6
0	4	9	403	398	5
2	4	9	79	62	11
4	4	9	44	54	27
1	5	9	60	41	16
3	5	9	36	17	36
0	6	9	110	110	9
2	6	9	34	22	33

Observed and calculated structure factors for K38

h	k	l	10Fo	10Fc	10s
2	0	0	648	686	3
4	0	0	1048	1063	4
6	0	0	635	655	4
8	0	0	1044	1042	6
10	0	0	1855	1832	7
12	0	0	1425	1442	8
14	0	0	257	252	3
16	0	0	404	397	4
18	0	0	376	378	4
20	0	0	441	444	4
22	0	0	1919	1891	12
1	1	0	213	208	2
5	1	0	514	520	3
7	1	0	425	435	3
9	1	0	1498	1478	6
11	1	0	1062	1016	8
13	1	0	490	495	4
15	1	0	265	275	3
17	1	0	371	387	4
19	1	0	484	488	4
21	1	0	870	864	6
0	2	0	1273	1323	3
2	2	0	305	317	2
4	2	0	578	594	4
6	2	0	198	194	2
8	2	0	280	274	3
10	2	0	610	598	4
12	2	0	445	451	3
14	2	0	839	839	6
16	2	0	789	798	5
18	2	0	190	193	5
20	2	0	45	63	23
22	2	0	232	222	5
1	3	0	250	253	2
3	3	0	451	454	3
7	3	0	547	541	4
9	3	0	787	772	5
11	3	0	488	493	4
13	3	0	283	282	3
15	3	0	939	946	6
17	3	0	1004	1010	7
19	3	0	290	285	4
21	3	0	262	270	5
0	4	0	2012	2045	4
2	4	0	621	616	4
4	4	0	930	924	5
8	4	0	177	366	3
10	4	0	448	443	3
12	4	0	204	207	3
14	4	0	617	616	5
16	4	0	2121	2134	10
18	4	0	0	0	1
20	4	0	134	130	7
22	4	0	534	533	5
1	5	0	1407	1425	5
3	5	0	78	76	4
5	5	0	1226	1105	6
7	5	0	904	891	5
9	5	0	51	28	9
11	5	0	375	390	3
13	5	0	182	185	4
15	5	0	218	224	4
17	5	0	515	519	4
19	5	0	159	154	5
21	5	0	459	456	4
0	6	0	845	852	6
2	6	0	179	181	2
4	6	0	219	221	2
6	6	0	440	423	3
8	6	0	610	591	4
10	6	0	1516	1505	8
12	6	0	135	140	5
14	6	0	178	182	4
16	6	0	443	448	4
18	6	0	386	389	4
20	6	0	62	39	14
1	7	0	586	580	4
3	7	0	230	235	2
5	7	0	1389	1358	7
7	7	0	510	499	4
9	7	0	1101	1089	6
11	7	0	676	640	5
13	7	0	242	234	4
15	7	0	281	286	4
17	7	0	418	408	4
19	7	0	602	598	5
21	7	0	619	600	5
0	8	0	2613	2593	7
2	8	0	159	149	3
4	8	0	521	522	4
6	8	0	629	626	4
8	8	0	492	498	4
10	8	0	1173	1161	7
12	8	0	95	97	6
14	8	0	97	94	7
16	8	0	333	327	4
18	8	0	0	23	1
20	8	0	295	276	5
1	9	0	117	92	4
3	9	0	285	283	3
5	9	0	1919	1949	8
7	9	0	868	858	6
9	9	0	103	103	6
11	9	0	655	632	4
13	9	0	244	232	4
15	9	0	775	789	5
17	9	0	576	571	5
19	9	0	120	124	8
0	10	0	299	313	3
2	10	0	103	110	5
4	10	0	327	329	3
6	10	0	252	256	3
8	10	0	216	229	4
10	10	0	497	506	4
12	10	0	281	281	4
14	10	0	982	1005	7
16	10	0	319	326	4
18	10	0	329	339	5
1	11	0	231	217	3
3	11	0	263	272	3
5	11	0	759	768	5
7	11	0	90	87	7
9	11	0	86	83	7
11	11	0	397	407	4
13	11	0	280	272	4
15	11	0	695	703	5
17	11	0	429	429	4
0	12	0	1521	1547	9
2	12	0	144	141	5
4	12	0	342	343	3
6	12	0	555	558	4
8	12	0	153	148	5
10	12	0	797	782	6
12	12	0	503	500	4
14	12	0	102	112	8
16	12	0	31	5	30
1	13	0	548	554	4
3	13	0	213	207	4
5	13	0	351	350	4
7	13	0	457	455	4
9	13	0	330	323	4
11	13	0	945	944	7
13	13	0	249	253	5
15	13	0	271	270	5
0	14	0	1371	1386	10
2	14	0	349	351	4
4	14	0	213	204	4
6	14	0	640	647	5
8	14	0	175	174	5
10	14	0	1188	1210	8
12	14	0	104	109	9
14	14	0	36	5	36
1	15	0	330	313	4
3	15	0	314	309	4
5	15	0	518	525	4
7	15	0	107	108	8
9	15	0	205	203	5
11	15	0	402	391	4
13	15	0	328	330	5
0	16	0	599	595	5
2	16	0	244	240	4
4	16	0	159	151	6
6	16	0	745	741	5
8	16	0	95	85	9
10	16	0	137	117	7
12	16	0	460	463	4
1	17	0	309	298	4
3	17	0	305	299	4
5	17	0	1727	1735	12
7	17	0	75	56	12
9	17	0	62	60	14
0	18	0	362	365	4
2	18	0	233	242	5
4	18	0	90	92	10
6	18	0	339	330	5
8	18	0	254	246	5
1	19	0	147	146	7
3	19	0	157	151	7
1	1	1	157	145	2
3	1	1	307	299	2
5	1	1	987	990	5
7	1	1	17	24	17
9	1	1	260	248	2
11	1	1	739	739	5
13	1	1	281	282	3
15	1	1	302	298	3
17	1	1	660	678	5
19	1	1	510	514	5
21	1	1	583	593	5
0	2	1	129	146	2
2	2	1	595	614	4
4	2	1	344	343	2
6	2	1	246	228	2
8	2	1	481	486	3
10	2	1	96	90	5
12	2	1	838	868	6
14	2	1	111	120	5
16	2	1	552	562	4
18	2	1	28	22	28
20	2	1	357	361	4
22	2	1	253	247	5
1	3	1	372	390	2
3	3	1	271	264	2
5	3	1	390	390	3
7	3	1	401	396	3
9	3	1	223	224	3
11	3	1	364	377	3
13	3	1	196	198	4
15	3	1	116	119	6
17	3	1	269	268	4
19	3	1	182	184	5
21	3	1	380	373	4
0	4	1	1181	1192	5
2	4	1	176	172	2
4	4	1	120	114	3
6	4	1	672	642	4
8	4	1	380	374	3
10	4	1	622	609	4
12	4	1	637	646	4
14	4	1	249	246	4
16	4	1	491	495	4
18	4	1	230	235	4
20	4	1	75	62	11
22	4	1	285	283	5
1	5	1	99	108	3
3	5	1	352	363	2
5	5	1	1170	1146	6
7	5	1	880	866	5
9	5	1	405	401	3
11	5	1	313	323	3
13	5	1	537	535	4
15	5	1	218	209	4
17	5	1	193	192	5
19	5	1	54	18	15
21	5	1	541	548	5
0	6	1	509	503	3
2	6	1	85	82	4
4	6	1	298	291	2
6	6	1	1009	1010	7
8	6	1	534	532	4
10	6	1	135	126	4
12	6	1	372	369	3
14	6	1	28	13	27
16	6	1	984	1003	6
18	6	1	295	291	4
20	6	1	483	478	4
1	7	1	172	164	3
3	7	1	469	476	3
5	7	1	806	806	6
7	7	1	207	199	3
9	7	1	315	313	3
11	7	1	96	109	6
13	7	1	45	45	15
15	7	1	165	165	5
17	7	1	273	257	4
19	7	1	151	151	6
0	8	1	466	448	3
2	8	1	134	119	4
4	8	1	90	90	5
6	8	1	293	297	3
8	8	1	54	51	10
10	8	1	161	170	4
12	8	1	502	502	4
14	8	1	497	505	4
16	8	1	459	461	4
18	8	1	295	286	4
20	8	1	381	379	4
1	9	1	899	888	6
3	9	1	43	35	12
5	9	1	392	408	3
7	9	1	347	357	3
9	9	1	35	37	24
11	9	1	1689	1702	9
13	9	1	149	142	5
15	9	1	237	226	4
17	9	1	101	119	8
19	9	1	205	214	6
0	10	1	1389	1417	8
2	10	1	743	756	5
4	10	1	150	152	4
6	10	1	510	508	4
8	10	1	132	136	5
10	10	1	371	369	4
12	10	1	0	14	1
14	10	1	588	586	4
16	10	1	501	500	4
18	10	1	152	156	6
1	11	1	57	69	10
3	11	1	60	66	10
5	11	1	816	838	5
7	11	1	528	527	4
9	11	1	253	252	4
11	11	1	176	183	5
13	11	1	146	148	6
15	11	1	358	348	4
17	11	1	435	449	4
0	12	1	951	971	6
2	12	1	565	560	4
4	12	1	140	140	5
6	12	1	711	719	5
8	12	1	119	104	6
10	12	1	0	13	1
12	12	1	242	247	4
14	12	1	66	61	12
16	12	1	755	756	6
1	13	1	439	438	4
3	13	1	293	295	4
5	13	1	1011	1036	7
7	13	1	116	116	6
9	13	1	281	282	4
11	13	1	1216	1213	8
13	13	1	194	193	5
15	13	1	124	141	8
0	14	1	874	904	6
2	14	1	159	161	5
4	14	1	367	369	4
6	14	1	298	293	4
8	14	1	269	254	4
10	14	1	428	425	4
12	14	1	145	150	7
14	14	1	288	283	5
1	15	1	24	10	23
3	15	1	346	357	4
5	15	1	138	115	6
7	15	1	367	361	4
9	15	1	26	16	25
11	15	1	146	131	7
13	15	1	217	217	6
0	16	1	405	405	4
2	16	1	182	185	5
4	16	1	67	54	11
6	16	1	1255	1272	8
8	16	1	329	329	4
10	16	1	16	51	35
12	16	1	42	61	32
1	17	1	136	132	6
3	17	1	219	209	5
5	17	1	825	834	6
7	17	1	248	240	5
9	17	1	286	285	5
0	18	1	320	318	5
2	18	1	103	116	9
4	18	1	308	299	5
6	18	1	267	261	5
8	18	1	104	119	9
1	19	1	416	409	5
3	19	1	394	388	5
2	0	2	615	623	4
4	0	2	228	217	2
6	0	2	702	686	4
8	0	2	577	561	4
10	0	2	1491	1454	7
12	0	2	1048	1050	7
14	0	2	1246	1238	7
16	0	2	882	877	6
18	0	2	467	479	4
20	0	2	183	188	5
22	0	2	460	460	4
1	1	2	491	491	3
3	1	2	697	711	4
5	1	2	1065	1065	6
7	1	2	89	90	4
9	1	2	589	577	4
11	1	2	560	556	4
13	1	2	50	52	12
15	1	2	681	690	5
17	1	2	52	35	14
19	1	2	49	48	18
21	1	2	282	275	5
2	2	2	345	343	2
4	2	2	430	432	1
6	2	2	474	459	3
8	2	2	152	128	1
10	2	2	1424	1398	7
12	2	2	590	594	4
14	2	2	0	12	1
16	2	2	283	286	4
18	2	2	51	41	14
20	2	2	159	147	6
22	2	2	582	582	5
1	3	2	487	483	3
3	3	2	235	230	2
5	3	2	1134	1143	6
7	3	2	190	182	3
9	3	2	1279	1303	7
11	3	2	1554	1570	8
13	3	2	232	230	3
15	3	2	243	228	4
17	3	2	418	419	4
19	3	2	721	723	5
21	3	2	709	708	5
0	4	2	1847	1833	5
2	4	2	619	615	4
4	4	2	134	119	3
6	4	2	470	457	3
8	4	2	133	137	4
10	4	2	2021	2036	8
12	4	2	142	152	5
14	4	2	150	148	5
16	4	2	83	79	8
18	4	2	528	522	4
20	4	2	276	270	5
1	5	2	999	987	6
3	5	2	122	123	3
5	5	2	1899	1871	7
7	5	2	231	214	3
9	5	2	491	502	4
11	5	2	675	669	5
13	5	2	14	19	30
15	5	2	351	348	4
17	5	2	662	669	5
19	5	2	123	126	4
21	5	2	348	341	5
0	6	2	1108	1114	6
2	6	2	87	97	4
4	6	2	805	816	5
6	6	2	2518	2466	7
8	6	2	313	317	3
10	6	2	148	156	4
12	6	2	316	318	3
14	6	2	749	761	5
16	6	2	1585	1597	10
18	6	2	59	70	14
20	6	2	78	72	11
1	7	2	588	581	4
3	7	2	128	131	4
5	7	2	4537	4490	8
7	7	2	181	174	3
9	7	2	435	435	3
11	7	2	12	7	11
13	7	2	349	350	3
15	7	2	994	1023	7
17	7	2	1066	1076	7
19	7	2	113	115	8
0	8	2	388	400	3
2	8	2	470	476	4
4	8	2	253	262	3
6	8	2	402	395	3
8	8	2	494	499	4
10	8	2	121	117	5
12	8	2	0	18	1
14	8	2	493	493	4
16	8	2	863	890	6
18	8	2	60	43	16
20	8	2	170	147	6
1	9	2	470	463	4
3	9	2	135	137	4
5	9	2	536	532	4
7	9	2	467	471	4
9	9	2	559	560	4

Observed and calculated structure factors for K38

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1534	1555	10	16	2	3	939	948	6	11	11	3	63	65	12	4	4	4	488	507	4	2	14	4	215	208	5
13	9	2	232	240	4	18	2	3	210	218	5	13	11	3	25	14	25	6	4	4	2021	2030	8	4	14	4	317	313	4
15	9	2	118	110	7	20	2	3	298	287	5	15	11	3	190	181	6	8	4	4	133	135	5	6	14	4	424	435	4
17	9	2	730	730	6	1	3	3	513	506	3	17	11	3	535	541	5	10	4	4	340	344	3	8	14	4	158	159	6
19	9	2	283	271	5	3	3	3	236	230	2	0	12	3	134	135	5	12	4	4	157	160	5	10	14	4	935	949	6
0	10	2	4388	4384	8	5	3	3	981	965	7	2	12	3	341	345	4	14	4	4	626	640	5	12	14	4	91	63	10
2	10	2	559	553	4	7	3	3	711	709	4	4	12	3	397	395	4	16	4	4	1559	1566	9	1	15	4	280	283	5
4	10	2	642	656	5	9	3	3	197	191	3	6	12	3	237	230	4	18	4	4	83	86	10	3	15	4	320	323	4
6	10	2	61	65	10	11	3	3	1195	1406	9	8	12	3	35	19	34	20	4	4	84	86	11	5	15	4	280	268	4
8	10	2	297	302	3	13	3	3	41	6	16	10	12	3	15	15	14	1	5	4	929	924	6	7	15	4	60	39	15
10	10	2	1854	1855	10	15	3	3	209	208	4	12	12	3	246	227	4	3	5	4	141	133	4	9	15	4	192	197	6
12	10	2	398	394	4	17	3	3	253	260	4	14	12	3	158	156	6	5	5	4	1552	1573	8	0	16	4	179	189	6
14	10	2	280	294	4	19	3	3	104	105	8	16	12	3	482	465	4	7	5	4	197	401	3	2	16	4	231	232	5
16	10	2	144	144	6	21	3	3	428	421	4	1	13	3	359	344	4	9	5	4	36	30	21	4	16	4	70	76	13
18	10	2	184	182	6	0	4	3	2242	2288	6	3	13	3	398	403	4	11	5	4	897	906	6	6	16	4	414	412	4
1	11	2	447	451	4	2	4	3	55	3	7	5	13	3	437	446	4	13	5	4	9	43	9	8	16	4	0	22	1
3	11	2	640	655	5	4	4	3	289	281	3	7	13	3	96	103	8	15	5	4	253	260	4	1	17	4	359	345	5
5	11	2	24	17	24	6	4	3	284	283	3	9	13	3	216	213	5	17	5	4	153	158	6	3	17	4	204	204	6
7	11	2	28	7	27	8	4	3	170	174	4	11	13	3	515	509	5	19	5	4	89	89	10	5	17	4	1318	1308	9
9	11	2	565	572	4	10	4	3	669	674	4	13	13	3	48	55	22	0	6	4	2070	2090	8	1	1	5	3	33	2
11	11	2	1871	1853	10	12	4	3	675	687	5	15	13	3	63	44	15	2	6	4	189	201	3	3	1	5	117	121	5
13	11	2	72	59	11	14	4	3	102	96	6	0	14	3	243	238	4	4	6	4	297	294	3	5	1	5	790	785	5
15	11	2	57	40	15	16	4	3	108	104	7	2	14	3	120	120	6	6	6	4	190	188	4	7	1	5	54	49	11
17	11	2	41	52	40	18	4	3	128	126	6	4	14	3	289	296	4	8	6	4	306	305	3	9	1	5	212	219	4
0	12	2	1336	1345	9	20	4	3	109	100	8	6	14	3	130	130	6	10	6	4	1124	1147	8	11	1	5	175	170	5
2	12	2	135	136	5	1	5	3	90	79	4	8	14	3	311	306	4	12	6	4	219	221	4	13	1	5	143	142	5
4	12	2	148	145	5	3	5	3	217	216	3	10	14	3	247	254	5	14	6	4	205	202	5	15	1	5	203	208	5
6	12	2	763	765	5	5	5	3	622	592	4	12	14	3	42	50	10	16	6	4	150	155	6	17	1	5	691	700	5
8	12	2	212	202	4	7	5	3	859	848	5	1	15	3	159	161	6	18	6	4	274	264	5	19	1	5	400	398	5
10	12	2	670	676	5	9	5	3	301	302	3	3	15	3	285	289	4	1	7	4	222	208	3	0	2	5	809	807	6
12	12	2	273	264	4	11	5	3	153	145	5	5	15	3	313	317	4	3	7	4	268	268	3	2	2	5	199	180	3
14	12	2	409	410	4	13	5	3	405	407	4	7	15	3	247	237	5	5	7	4	1230	1243	9	4	2	5	331	336	3
16	12	2	491	492	4	15	5	3	257	259	4	9	15	3	67	64	13	7	7	4	386	386	3	6	2	5	455	453	4
1	13	2	118	126	6	17	5	3	265	252	4	11	15	3	332	324	5	9	7	4	848	861	6	8	2	5	227	225	4
3	13	2	0	0	1	19	5	3	48	18	18	0	16	3	243	248	5	11	7	4	780	782	5	10	2	5	191	196	4
5	13	2	1725	1745	10	0	6	3	491	489	4	2	16	3	54	42	16	13	7	4	193	188	5	12	2	5	682	694	5
7	13	2	0	29	1	2	6	3	181	168	3	4	16	3	260	260	5	15	7	4	252	258	4	14	2	5	34	36	34
9	13	2	43	50	20	4	6	3	514	499	4	6	16	3	1118	1123	7	17	7	4	468	477	4	16	2	5	159	147	6
11	13	2	128	122	6	6	6	3	1285	1288	8	8	16	3	298	294	5	0	8	4	1864	1902	8	18	2	5	95	90	10
13	13	2	183	175	5	8	6	3	380	372	3	10	16	3	194	198	6	2	8	4	39	34	16	1	3	5	125	131	5
15	13	2	552	557	5	10	6	3	189	180	4	1	17	3	197	201	6	4	8	4	279	275	3	3	3	5	247	239	3
0	14	2	331	332	4	12	6	3	344	338	3	3	17	3	237	240	5	6	8	4	563	564	4	5	3	5	566	577	4
2	14	2	304	302	4	14	6	3	70	79	10	5	17	3	562	557	5	8	8	4	374	382	4	7	3	5	97	82	6
4	14	2	683	696	5	16	6	3	1058	1072	7	7	17	3	29	11	29	10	8	4	1015	1021	7	9	3	5	105	101	6
6	14	2	489	492	4	18	6	3	413	417	4	0	18	3	178	175	6	12	8	4	46	45	17	11	3	5	218	206	4
8	14	2	195	190	5	20	6	3	438	437	4	2	18	3	218	216	5	14	8	4	83	72	9	13	3	5	216	218	5
10	14	2	0	26	1	1	7	3	189	168	3	4	18	3	115	119	8	16	8	4	271	279	5	15	3	5	46	50	19
12	14	2	35	4	34	3	7	3	178	186	3	2	0	4	345	354	3	18	8	4	0	34	1	17	3	5	481	487	4
14	14	2	306	310	5	5	7	3	1457	1450	8	4	0	4	504	514	3	1	9	4	34	27	25	0	4	5	173	176	4
1	15	2	603	614	5	7	7	3	195	198	4	6	0	4	275	266	3	3	9	4	168	166	4	2	4	5	95	95	6
3	15	2	229	222	4	9	7	3	345	345	3	8	0	4	378	381	3	5	9	4	1808	1816	9	4	4	5	37	38	18
5	15	2	1435	1444	9	11	7	3	869	879	6	10	0	4	2839	2832	9	7	9	4	464	469	4	6	4	5	617	606	4
7	15	2	437	434	4	13	7	3	149	148	5	12	0	4	1014	1017	6	9	9	4	41	33	19	8	4	5	295	293	3
9	15	2	26	10	25	15	7	3	0	22	1	14	0	4	397	397	4	11	9	4	241	231	4	10	4	5	384	377	4
11	15	2	414	409	4	17	7	3	643	646	5	16	0	4	0	4	1	13	9	4	108	90	7	12	4	5	430	432	4
13	15	2	144	141	7	19	7	3	117	108	8	18	0	4	411	415	4	15	9	4	577	580	5	14	4	5	263	252	4
0	16	2	975	968	6	0	8	3	1011	999	6	20	0	4	342	330	5	17	9	4	646	636	5	16	4	5	558	559	5
2	16	2	179	172	5	2	8	3	10	19	10	1	1	4	384	378	3	0	10	4	813	828	6	18	4	5	262	250	5
4	16	2	92	96	9	4	8	3	201	200	3	3	1	4	60	53	7	2	10	4	46	38	14	1	5	5	137	136	5
6	16	2	570	573	5	6	8	3	551	545	4	5	1	4	183	157	3	4	10	4	424	435	4	3	5	5	190	182	4
8	16	2	31	17	30	8	8	3	111	109	6	7	1	4	9	32	8	6	10	4	193	192	4	5	5	5	517	510	4
10	16	2	784	778	6	10	8	3	269	273	4	9	1	4	1096	1094	7	8	10	4	260	261	4	7	5	5	589	589	4
1	17	2	270	270	5	12	8	3	557	561	4	11	1	4	1764	1784	9	10	10	4	425	423	4	9	5	5	294	297	4
3	17	2	380	375	4	14	8	3	299	298	4	13	1	4	298	297	4	12	10	4	272	273	4	11	5	5	280	277	4
5	17	2	37	41	36	16	8	3	36	16	16	15	1	4	159	159	5	14	10	4	747	755	5	13	5	5	369	365	4
7	17	2	139	153	7	18	8	3	101	102	9	17	1	4	79	81	10	16	10	4	448	440	4	15	5	5	154	166	6
9	17	2	345	339	5	1	9	3	572	571	4	19	1	4	459	454	4	1	11	4	147	147	5	17	5	5	142	132	7
0	18	2	660	649	5	3	9	3	174	170	4	0	2	4	352	366	3	3	11	4	330	329	4	0	6	5	368	198	4
2	18	2	89	81	9	5	9	3	274	263	3	2	2	4	210	207	3	5	11	4	947	988	7	2	6	5	32	42	12
4	18	2	279	282	5	7	9	3	232	234	4	4	2	4	174	373	3	7	11	4	0	19	1	4	6	5	0	10	1
6	18	2	347	350	5	9	9	3	68	51	9	6	2	4	418	437	3	9	11	4	58	56	13	6	6	5	517	519	4
1	1	3	202	193	2	11	9	3	904	924	6	8	2	4	112	110	5	11	11	4	0	1	1	8	6	5	353	359	3
3	1	3	521	515	3	13	9	3	92	92	8	10	2	4	415	410	4	13	11	4	179	181	5	10	6	5	69	75	10
5	1	3	39	39	11	15	9	3	227	214	5	12	2	4	401	404	3	15	11	4	569	571	5	12	6	5	270	259	4
7	1	3	197	194	3	17	9	3	427	443	4	14	2	4	632	624	5	0	12	4	986	1014	6	14	6	5	31	29	31
9	1	3	216	208	3	0	10	3	981	990	7	16	2	4	773	786	5	2	12	4	144	146	5	16	6	5	679	676	5
11	1	3	1279	1266	8	2	10	3	715	737	5	18	2	4	184	187	5	4	12	4	248	250	4	1	7	5	118	96	5
13	1	3	176	369	3	4	10	3	256	253	3	20	2	4	11	31	10	6	12	4	264	264	4	3	7	5	408	417	3
15	1	3	147	354	4	6	10	3	288	269	3	1	3	4	146	149	3	8	12	4	179	184	5	5	7	5	269	260	4
17	1	3	324	323	4	8	10	3	170	189	5	3	3	4	384	374	3	10	12	4	567	570	5	7	7	5	299	295	4
19	1	3	502	505	4	10	10	3	170	171	5	5	3	4	3406	1451	8	12	12	4	364	358	4	9	7	5	218	212	4
21	1	3	579	572	5	12	10	3	84	82	8	7	3	4	202	206	3	14	12	4	56	42	16	11	7	5	314	302	4
0	2	3	2137	2074	6	14	10	3	560	567	5	9	3	4	595	597	4	1	13	4	337	333	4	13	7	5	135	136	6
2	2	3	702	677	4	16	10	3	280	281	5	11	3	4	206	200	4	3	13	4	153	152	5	15	7	5	186	194	6
4	2	3	217	209	2	18	10	3	85	93	11	13	3	4	258	262	4	5	13	4	232	231	4	17	7	5	34	15	34
6	2	3	1092	1058	7	1	11	3	194	193	4	15	3	4	830	829	5	7	13	4	277	272	4	0	8	5	658	669	5
8	2	3	617	611	4	3	11	3	8	15	7	17	3	4	792	784	5	9	13	4	332	327	4	2	8	5	216	203	4
10	2	3	37	31	19	5	11	3	864	874	6	19	3	4	255	252	5	11	13	4	757	761	5	4	8	5	138	138	5
12	2	3	669	680	5	7	11	3	224	226	4	0	4	4	521	555	4	13	13	4	132	143	7	6	8	5	547	547	4
14	2	3	327	322	3	9	11	3	311	314	4	2	4	4	447	440	1	0	14	4	1425	1349	9	8	8	5	66	69	10

Observed and calculated structure factors for K38

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
10	8	5	133	129	6	3	1	6	114	105	5	6	8	6	286	280	4	2	4	7	55	33	13	5	1	8	440	445	4
12	8	5	352	355	4	5	1	6	1689	1690	9	8	8	6	298	306	4	4	4	7	164	157	5	7	1	8	231	222	5
14	8	5	446	448	4	7	1	6	136	141	5	10	8	6	220	216	5	6	4	7	158	161	5	9	1	8	601	595	5
16	8	5	571	567	4	9	1	6	122	123	4	12	8	6	82	66	10	8	4	7	139	140	6	11	1	8	575	577	5
1	9	5	667	673	5	11	1	6	250	245	4	14	8	6	348	340	5	10	4	7	453	460	4	0	2	8	54	4	15
3	9	5	25	6	25	13	1	6	58	60	14	1	9	6	367	365	4	12	4	7	440	447	4	2	2	8	111	105	7
5	9	5	532	520	4	15	1	6	436	432	4	3	9	6	56	48	13	14	4	7	115	103	8	4	2	8	219	220	5
7	9	5	339	340	4	17	1	6	124	115	5	5	9	6	49	36	16	1	5	7	36	16	26	6	2	8	500	486	4
9	9	5	10	25	10	0	2	6	1744	1749	9	7	9	6	530	536	4	3	5	7	84	93	8	8	2	8	50	35	19
11	9	5	1542	1551	9	2	2	6	198	192	4	9	9	6	379	370	4	5	5	7	144	147	6	10	2	8	212	208	6
13	9	5	167	170	6	4	2	6	140	131	5	11	9	6	730	721	5	7	5	7	496	514	4	1	3	8	83	77	10
15	9	5	203	196	5	6	2	6	481	483	4	13	9	6	60	59	15	9	5	7	223	213	5	3	3	8	255	261	5
0	10	5	1128	1124	8	8	2	6	165	164	5	0	10	6	2159	2196	11	11	5	7	31	38	30	5	3	8	1866	1841	11
2	10	5	474	484	4	10	2	6	864	882	6	2	10	6	254	244	4	13	5	7	248	246	5	7	3	8	0	7	1
4	10	5	0	34	1	12	2	6	343	340	4	4	10	6	246	240	4	0	6	7	231	222	4	9	3	8	317	321	5
6	10	5	514	513	4	14	2	6	85	67	10	6	10	6	511	516	4	2	6	7	143	144	6	11	3	8	56	68	17
8	10	5	91	99	8	16	2	6	145	146	5	8	10	6	92	97	9	4	6	7	211	211	5	0	4	8	212	222	5
10	10	5	363	361	4	1	3	6	263	259	4	10	10	6	1298	1296	8	6	6	7	745	739	5	2	4	8	298	294	4
12	10	5	84	77	10	3	3	6	43	47	15	12	10	6	256	255	5	8	6	7	260	257	5	4	4	8	182	168	5
14	10	5	439	440	4	5	3	6	866	868	6	1	11	6	175	179	5	10	6	7	134	139	7	6	4	8	696	705	5
1	11	5	29	11	28	7	3	6	83	83	8	3	11	6	312	308	4	12	6	7	202	213	6	8	4	8	10	20	10
3	11	5	89	75	8	9	3	6	879	886	6	5	11	6	466	474	4	1	7	7	118	117	7	10	4	8	162	161	7
5	11	5	591	584	5	11	3	6	1198	1214	7	7	11	6	150	130	6	3	7	7	197	195	5	1	5	8	514	508	4
7	11	5	516	516	4	13	3	6	65	84	12	9	11	6	410	407	4	5	7	7	881	881	6	3	5	8	164	164	6
9	11	5	168	160	5	15	3	6	120	119	8	11	11	6	832	812	6	7	7	7	104	110	8	5	5	8	447	442	4
11	11	5	257	256	5	17	3	6	394	409	5	0	12	6	532	534	4	9	7	7	256	249	5	7	5	8	35	31	34
13	11	5	194	197	6	0	4	6	2348	2380	9	2	12	6	126	134	7	11	7	7	564	560	5	9	5	8	90	77	10
0	12	5	962	985	7	2	4	6	48	47	14	4	12	6	118	126	7	0	8	7	639	642	5	0	6	8	1818	1837	11
2	12	5	525	527	4	4	4	6	301	301	3	6	12	6	817	826	6	2	8	7	25	12	25	2	6	8	179	183	6
4	12	5	30	26	30	6	4	6	565	565	4	8	12	6	81	68	11	4	8	7	151	141	6	4	6	8	263	264	5
6	12	5	744	743	5	8	4	6	139	143	6	10	12	6	356	354	5	6	8	7	360	349	4	6	6	8	461	464	4
8	12	5	68	66	12	10	4	6	1348	1356	9	1	13	6	0	9	1	8	8	7	33	24	11	8	6	8	104	113	9
10	12	5	56	36	16	12	4	6	143	147	6	3	13	6	23	11	22	10	8	7	228	230	5	1	7	8	39	24	38
12	12	5	206	206	5	14	4	6	16	4	15	5	13	6	1305	1305	8	12	8	7	374	378	5	3	7	8	190	190	6
1	13	5	382	377	4	16	4	6	252	246	5	7	13	6	111	102	8	1	9	7	338	333	4	5	7	8	880	878	6
3	13	5	209	203	5	1	5	6	118	115	3	0	14	6	71	91	13	3	9	7	97	103	8	7	7	8	221	231	5
5	13	5	997	1007	7	3	5	6	281	279	4	2	14	6	343	347	5	5	9	7	246	246	5	9	7	8	505	501	5
7	13	5	192	201	5	5	5	6	559	553	4	4	14	6	301	303	5	7	9	7	143	157	6	0	8	8	932	952	7
9	13	5	255	248	5	7	5	6	78	90	9	6	14	6	182	175	6	9	9	7	0	3	1	2	8	8	36	26	35
11	13	5	1275	1278	8	9	5	6	311	300	4	1	1	7	79	79	8	11	9	7	550	562	5	4	8	8	68	65	11
0	14	5	1029	1037	7	11	5	6	105	103	4	3	1	7	174	174	5	0	10	7	619	623	5	6	8	8	383	395	5
2	14	5	152	140	6	13	5	6	106	99	8	5	1	7	129	122	6	2	10	7	413	420	4	1	9	8	0	33	1
4	14	5	301	292	4	15	5	6	126	123	5	7	1	7	292	285	4	4	10	7	128	118	7	3	9	8	73	69	12
6	14	5	437	444	4	0	6	6	104	103	6	9	1	7	123	125	7	6	10	7	197	196	5	5	9	8	1254	1270	9
8	14	5	166	168	6	2	6	6	58	52	11	11	1	7	701	696	5	8	10	7	101	104	9	0	10	8	990	1002	7
10	14	5	440	434	4	4	6	6	144	140	4	13	1	7	267	272	5	1	11	7	98	108	9	2	10	8	70	52	13
1	15	5	116	99	8	6	6	6	964	962	6	15	1	7	253	260	5	3	11	7	37	22	37	1	1	9	0	9	1
3	15	5	299	294	5	8	6	6	121	124	4	0	2	7	643	644	5	5	11	7	587	593	5	3	1	9	124	121	8
5	15	5	36	38	35	10	6	6	43	41	21	2	2	7	353	349	4	7	11	7	151	154	7	5	1	9	190	368	5
7	15	5	348	334	5	12	6	6	176	174	5	4	2	7	54	37	13	0	12	7	0	11	1	7	1	9	112	108	8
0	16	5	333	327	5	14	6	6	686	685	5	6	2	7	509	503	4	2	12	7	230	225	5	0	2	9	183	167	6
2	16	5	213	218	5	16	6	6	833	823	6	8	2	7	257	243	4	4	12	7	251	258	5	2	2	9	117	116	8
4	16	5	62	70	16	1	7	6	475	480	4	10	2	7	80	78	10	6	12	7	107	114	9	4	2	9	112	113	8
0	0	6	2536	2546	9	3	7	6	74	71	9	12	2	7	438	444	4	1	13	7	224	220	5	6	2	9	45	37	28
2	0	6	118	116	5	5	7	6	2474	2499	10	14	2	7	183	180	6	0	0	8	2554	2572	11	1	3	9	102	95	9
4	0	6	540	557	4	7	7	6	111	110	7	1	3	7	247	242	4	2	0	8	136	139	6	1	3	9	0	3	1
6	0	6	692	697	5	9	7	6	334	334	4	3	3	7	29	22	29	4	0	8	161	152	6	5	3	9	144	135	7
8	0	6	372	375	4	11	7	6	368	370	4	5	3	7	415	411	4	6	0	8	634	635	5	0	4	9	421	418	4
10	0	6	902	914	6	13	7	6	236	224	5	7	3	7	395	386	4	8	0	8	47	39	21	2	4	9	67	58	14
12	0	6	764	769	6	15	7	6	705	709	5	9	3	7	141	142	6	10	0	8	1560	1553	10	4	4	9	57	58	18
14	0	6	698	706	5	0	8	6	275	276	4	11	3	7	861	844	6	12	0	8	541	542	5	1	5	9	47	24	21
16	0	6	937	924	6	2	8	6	221	221	4	13	3	7	77	61	11	1	1	8	161	158	6	3	5	9	38	41	37
1	1	6	165	156	4	4	8	6	333	336	4	0	4	7	1083	1081	7	3	1	8	106	110	8	0	6	9	128	131	8

Observed and calculated structure factors for K39

h	k	l	10Fo	10Fc	10s
2	0	0	696	705	4
4	0	0	1137	1147	5
6	0	0	599	608	4
8	0	0	968	945	6
10	0	0	3702	3742	10
12	0	0	1424	1427	10
14	0	0	236	223	5
16	0	0	327	312	5
18	0	0	444	442	5
20	0	0	377	374	6
22	0	0	1817	1807	11
3	1	0	229	221	2
5	1	0	489	492	3
7	1	0	435	431	3
9	1	0	1551	1540	8
11	1	0	2986	2957	10
13	1	0	431	426	4
15	1	0	281	281	5
17	1	0	357	364	5
19	1	0	540	535	5
21	1	0	816	818	6
0	2	0	1283	1310	4
2	2	0	295	317	2
4	2	0	598	612	4
6	2	0	167	160	3
8	2	0	280	277	3
10	2	0	617	623	4
12	2	0	404	405	4
14	2	0	845	842	6
16	2	0	776	768	6
18	2	0	107	111	10
20	2	0	102	102	11
22	2	0	266	261	7
1	3	0	305	298	3
3	3	0	512	524	4
7	3	0	548	533	4
9	3	0	872	862	5
11	3	0	418	408	4
13	3	0	292	292	4
15	3	0	896	898	6
17	3	0	977	989	7
19	3	0	268	263	6
21	3	0	345	337	6
0	4	0	2033	2059	6
2	4	0	625	622	4
4	4	0	990	980	7
6	4	0	3854	3779	8
8	4	0	424	417	3
10	4	0	435	434	4
12	4	0	244	246	4
14	4	0	710	711	5
16	4	0	2066	2072	13
18	4	0	56	38	21
20	4	0	182	176	8
22	4	0	478	497	6
1	5	0	1434	1439	7
3	5	0	54	54	9
5	5	0	3177	1098	8
7	5	0	880	872	6
9	5	0	33	42	33
11	5	0	365	384	4
13	5	0	246	251	5
15	5	0	239	234	5
17	5	0	510	506	5
19	5	0	175	181	7
21	5	0	413	416	6
0	6	0	833	839	6
2	6	0	195	192	3
4	6	0	104	108	3
6	6	0	501	484	4
8	6	0	644	637	4
10	6	0	1419	1435	8
12	6	0	183	184	5
14	6	0	431	416	4
16	6	0	498	502	5
18	6	0	387	371	5
20	6	0	0	11	1
1	7	0	615	609	4
3	7	0	209	203	3
5	7	0	1377	1360	9
7	7	0	506	497	4
9	7	0	1128	1133	7
11	7	0	637	604	5
13	7	0	283	283	5
15	7	0	264	267	5
17	7	0	165	356	5
19	7	0	641	635	6
21	7	0	605	592	6
0	8	0	2588	2567	9
2	8	0	163	170	4
4	8	0	488	483	4
6	8	0	611	619	5
8	8	0	472	472	4
10	8	0	1202	1206	8
12	8	0	133	131	6
14	8	0	131	122	8
16	8	0	331	329	5
18	8	0	12	33	12
20	8	0	303	289	6
1	9	0	79	75	8
3	9	0	354	353	4
5	9	0	1882	1904	10
7	9	0	856	856	6
9	9	0	67	66	13
11	9	0	653	638	5
13	9	0	245	237	5
15	9	0	681	697	6
17	9	0	538	530	5
19	9	0	182	180	7
0	10	0	300	312	4
2	10	0	49	64	16
4	10	0	352	363	4
6	10	0	275	268	4
8	10	0	247	264	5
10	10	0	506	508	5
12	10	0	232	241	5
14	10	0	1057	1077	7
16	10	0	280	276	6
18	10	0	399	408	6
1	11	0	267	257	4
3	11	0	261	268	4
5	11	0	785	797	6
7	11	0	113	110	7
9	11	0	70	81	13
11	11	0	431	448	5
13	11	0	224	227	6
15	11	0	761	767	6
17	11	0	426	430	6
0	12	0	1526	1551	11
2	12	0	194	195	5
4	12	0	312	299	4
6	12	0	572	576	5
8	12	0	152	167	7
10	12	0	725	733	6
12	12	0	508	504	5
14	12	0	89	107	13
16	12	0	63	41	20
1	13	0	524	523	5
3	13	0	193	200	6
5	13	0	368	371	5
7	13	0	473	480	5
9	13	0	394	394	5
11	13	0	932	930	7
13	13	0	280	280	6
15	13	0	253	255	7
0	14	0	1377	1388	9
2	14	0	358	367	5
4	14	0	209	216	6
6	14	0	686	688	5
8	14	0	149	145	7
10	14	0	1245	1250	9
12	14	0	110	92	11
14	14	0	48	14	15
1	15	0	300	286	5
3	15	0	357	359	5
5	15	0	523	533	5
7	15	0	77	80	13
9	15	0	156	165	8
11	15	0	403	397	6
13	15	0	387	373	6
0	16	0	598	606	5
2	16	0	216	227	6
4	16	0	178	178	7
6	16	0	785	798	6
8	16	0	90	86	13
10	16	0	68	91	19
12	16	0	454	459	6
1	17	0	303	301	6
3	17	0	294	291	6
5	17	0	1771	1787	12
7	17	0	0	16	1
9	17	0	78	59	16
0	18	0	354	355	6
2	18	0	281	278	6
4	18	0	68	75	18
6	18	0	289	293	6
8	18	0	298	287	6
1	19	0	173	177	9
3	19	0	130	126	10
1	1	1	158	148	3
3	1	1	359	356	3
5	1	1	958	972	6
7	1	1	37	23	17
9	1	1	321	327	3
11	1	1	771	776	5
13	1	1	320	318	4
15	1	1	226	215	5
17	1	1	693	694	5
19	1	1	488	496	5
21	1	1	692	686	6
0	2	1	157	163	3
2	2	1	558	572	4
4	2	1	398	403	3
6	2	1	256	245	3
8	2	1	520	527	4
10	2	1	39	36	21
12	2	1	898	901	6
14	2	1	145	135	6
16	2	1	592	605	5
18	2	1	68	33	14
20	2	1	285	292	6
22	2	1	225	228	7
1	3	1	368	373	3
3	3	1	262	251	3
5	3	1	373	369	3
7	3	1	430	427	3
9	3	1	223	224	4
11	3	1	324	323	4
13	3	1	215	221	5
15	3	1	69	93	13
17	3	1	289	282	5
19	3	1	187	186	7
21	3	1	348	349	6
0	4	1	1162	1159	6
2	4	1	129	137	4
4	4	1	178	169	3
6	4	1	725	690	5
8	4	1	413	408	3
10	4	1	489	475	4
12	4	1	657	677	5
14	4	1	253	252	5
16	4	1	545	545	5
18	4	1	245	247	6
20	4	1	0	8	1
1	5	1	107	103	5
3	5	1	414	417	3
5	5	1	1287	1261	8
7	5	1	887	875	6
9	5	1	470	468	4
11	5	1	280	306	4
13	5	1	536	544	5
15	5	1	82	91	11
17	5	1	212	197	6
19	5	1	73	2	15
21	5	1	626	614	5
0	6	1	523	513	4
2	6	1	116	117	5
4	6	1	260	255	3
6	6	1	957	956	6
8	6	1	535	527	4
10	6	1	138	134	6
12	6	1	357	355	4
14	6	1	33	4	32
16	6	1	1002	1012	7
18	6	1	287	290	6
20	6	1	467	462	6
1	7	1	169	158	4
3	7	1	502	508	4
5	7	1	655	661	5
7	7	1	218	206	4
9	7	1	166	170	4
11	7	1	77	78	11
13	7	1	59	58	15
15	7	1	73	84	14
17	7	1	254	238	6
19	7	1	144	140	9
0	8	1	532	510	4
2	8	1	87	80	7
4	8	1	27	6	26
6	8	1	293	298	4
8	8	1	65	75	12
10	8	1	76	90	11
12	8	1	503	504	4
14	8	1	526	522	5
16	8	1	555	556	5
18	8	1	121	111	6
20	8	1	123	131	6
1	9	1	928	914	7
3	9	1	92	67	7
5	9	1	165	183	4
7	9	1	346	345	4
9	9	1	42	37	25
11	9	1	1706	1703	12
13	9	1	116	123	8
15	9	1	179	174	7
17	9	1	129	134	9
19	9	1	209	208	7
0	10	1	1346	1351	8
2	10	1	753	759	5
4	10	1	183	197	5
6	10	1	492	481	4
8	10	1	141	147	6
10	10	1	324	317	5
12	10	1	19	20	38
14	10	1	589	594	5
16	10	1	415	416	5
18	10	1	187	194	8
1	11	1	132	122	7
3	11	1	127	125	7
5	11	1	780	794	5
7	11	1	540	538	5
9	11	1	284	282	5
11	11	1	258	254	5
13	11	1	140	155	8
15	11	1	268	253	6
17	11	1	454	453	6
0	12	1	1001	1029	7
2	12	1	537	536	5
4	12	1	124	130	7
6	12	1	698	690	5
8	12	1	117	110	8
10	12	1	82	81	12
12	12	1	257	254	6
14	12	1	50	53	27
16	12	1	749	741	6
1	13	1	432	420	4
3	13	1	320	328	5
5	13	1	991	1005	7
7	13	1	99	100	10
9	13	1	297	292	5
11	13	1	1173	1174	8
13	13	1	170	174	8
15	13	1	198	193	7
0	14	1	813	826	6
2	14	1	196	196	6
4	14	1	381	389	5
6	14	1	286	292	5
8	14	1	277	264	6
10	14	1	330	334	6
12	14	1	168	167	8
14	14	1	126	315	6
1	15	1	33	12	32
3	15	1	348	348	5
5	15	1	151	169	8
7	15	1	375	367	5
9	15	1	50	35	29
11	15	1	136	127	9
13	15	1	197	200	8
0	16	1	345	348	5
2	16	1	199	208	6
4	16	1	34	38	33
6	16	1	1316	1296	9
8	16	1	337	332	6
10	16	1	61	4	20
12	16	1	60	64	24
1	17	1	102	111	11
3	17	1	244	243	6
5	17	1	792	796	6
7	17	1	221	229	7
9	17	1	319	326	6
0	18	1	311	315	6
2	18	1	112	111	11
4	18	1	313	316	6
6	18	1	291	290	7
1	19	1	400	390	6
3	19	1	393	407	6
0	0	2	3288	3328	6
2	0	2	605	625	4
4	0	2	272	265	3
6	0	2	735	703	5
8	0	2	572	555	4
10	0	2	1412	1398	10
12	0	2	1007	1017	7
14	0	2	1254	1262	8
16	0	2	789	801	6
18	0	2	599	593	5
20	0	2	159	150	8
22	0	2	380	380	6
1	1	2	496	510	3
3	1	2	753	753	5
5	1	2	1021	1033	6
7	1	2	111	109	5
9	1	2	618	607	4
11	1	2	612	608	5
13	1	2	0	40	1
15	1	2	664	668	5
17	1	2	71	52	14
19	1	2	48	19	26
21	1	2	305	312	6
0	2	2	4150	4100	7
2	2	2	359	354	3
4	2	2	474	469	3
6	2	2	473	464	4
8	2	2	212	201	4
10	2	2	1337	1347	8
12	2	2	558	567	4
14	2	2	60	39	14
16	2	2	342	319	5
18	2	2	0	19	1
20	2	2	78	79	15
1	3	2	472	460	3
3	3	2	240	239	3
5	3	2	1102	1084	8
7	3	2	187	179	4
9	3	2	1416	1411	9
11	3	2	1468	1489	10
13	3	2	326	320	4
15	3	2	199	195	6
17	3	2	388	387	5
19	3	2	759	764	6
21	3	2	637	637	6
0	4	2	1835	1804	7
2	4	2	619	615	4
4	4	2	79	66	6
6	4	2	199	168	3
8	4	2	100	118	7
10	4	2	1952	2012	10
12	4	2	189	196	5
14	4	2	191	179	5
16	4	2	44	21	28
18	4	2	504	502	5
20	4	2	330	288	6
1	5	2	960	965	6
3	5	2	98	96	5
5	5	2	1874	1848	9
7	5	2	235	221	4
9	5	2	464	458	4
11	5	2	659	654	5
13	5	2	0	31	1
15	5	2	322	318	5
17	5	2	689	692	5
19	5	2	368	359	6
21	5	2	388	379	6
0	6	2	1101	1101	7
2	6	2	94	102	6
4	6	2	893	903	6
6	6	2	2464	2418	9
8	6	2	300	290	4
10	6	2	142	87	6
12	6	2	350	346	4
14	6	2	848	847	6
16	6	2	1532	1538	9
18	6	2	32	32	31
20	6	2	68	78	19
1	7	2	660	646	5
3	7	2	79	70	7
5	7	2	4403	4454	10
7	7	2	189	182	5
9	7	2	450	457	4
11	7	2	65	64	13
13	7	2	332	339	5
15	7	2	964	979	7
17	7	2	1013	1027	7
19	7	2	83	82	15
0	8	2	429	442	4
2	8	2	474	477	4
4	8	2	220	226	4
6	8	2	402	395	4
8	8	2	540	546	5
10	8	2	278	76	4
12	8	2	72	67	13
14	8	2	510	514	5
16	8	2	883	881	6
18	8	2	50	0	10
20	8	2	190	177	8
1	9	2	486	470	4
3	9	2	116	103	7
5	9	2	516	513	4
7	9	2	462	455	4
9	9	2	621	619	5

Observed and calculated structure factors for K39

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1574	1575	10	16	2	3	976	991	7	13	11	3	47	17	27	6	4	4	1940	1955	10	6	14	4	464	462	5
13	9	2	186	188	6	18	2	3	213	220	7	15	11	3	105	97	11	8	4	4	160	172	6	8	14	4	128	126	10
15	9	2	179	181	7	20	2	3	208	218	8	17	11	3	541	550	6	10	4	4	307	320	4	10	14	4	975	977	7
17	9	2	704	698	6	1	3	3	526	521	4	0	12	3	169	164	6	12	4	4	169	170	6	12	14	4	38	52	38
19	9	2	286	285	7	3	3	3	240	235	3	2	12	3	337	322	5	14	4	4	705	715	5	1	15	4	254	252	6
0	10	2	4435	4389	11	5	3	3	1005	987	7	4	12	3	380	385	5	16	4	4	1492	1502	10	3	15	4	371	163	6
2	10	2	622	612	5	7	3	3	724	716	5	6	12	3	185	188	6	18	4	4	110	110	11	5	15	4	257	263	6
4	10	2	702	698	5	9	3	3	176	182	5	8	12	3	35	31	35	1	5	4	952	955	7	7	15	4	65	61	20
6	10	2	95	83	8	11	3	3	1359	1370	9	10	12	3	76	89	14	3	5	4	157	143	5	9	15	4	159	160	9
8	10	2	278	278	5	13	3	3	45	14	21	12	12	3	253	245	6	5	5	4	1501	1545	10	0	16	4	174	184	8
10	10	2	1826	1845	12	15	3	3	172	175	6	14	12	3	140	147	10	7	5	4	403	403	4	2	16	4	222	216	7
12	10	2	382	370	5	17	3	3	266	262	6	16	12	3	447	443	6	9	5	4	73	73	11	4	16	4	110	106	12
14	10	2	308	316	5	19	3	3	110	112	11	1	13	3	318	314	5	11	5	4	913	910	6	6	16	4	447	443	6
16	10	2	182	193	8	21	3	3	391	405	6	3	13	3	422	434	5	13	5	4	88	98	11	8	16	4	62	20	20
18	10	2	216	204	7	0	4	3	2224	2167	8	5	13	3	407	403	5	15	5	4	258	254	6	1	17	4	367	356	6
1	11	2	422	422	4	2	4	3	0	15	1	7	13	3	124	115	8	17	5	4	120	131	10	3	17	4	204	192	8
3	11	2	674	692	5	4	4	3	320	315	3	9	13	3	232	228	6	19	5	4	125	117	10	5	17	4	1332	1334	9
5	11	2	32	11	32	6	4	3	266	260	4	11	13	3	464	456	5	0	6	4	2080	2084	10	1	1	5	51	43	16
7	11	2	50	6	18	8	4	3	202	201	4	13	13	3	35	37	35	2	6	4	208	208	4	3	1	5	170	159	5
9	11	2	615	594	5	10	4	3	554	565	4	15	13	3	111	98	11	4	6	4	346	343	4	5	1	5	730	752	5
11	11	2	1814	1826	13	12	4	3	726	730	5	0	14	3	160	155	7	6	6	4	166	168	6	7	1	5	0	22	1
13	11	2	63	47	17	14	4	3	103	100	9	2	14	3	158	158	7	8	6	4	352	343	4	9	1	5	278	276	5
15	11	2	122	104	10	16	4	3	148	146	7	4	14	3	322	317	5	10	6	4	1284	1294	8	11	1	5	183	191	6
17	11	2	56	52	25	18	4	3	139	146	8	6	14	3	139	139	8	12	6	4	292	274	5	13	1	5	158	168	7
0	12	2	1334	1323	10	20	4	3	47	53	46	8	14	3	316	320	6	14	6	4	215	228	6	15	1	5	141	143	8
2	12	2	84	89	10	1	5	3	79	78	7	10	14	3	154	164	8	16	6	4	192	190	7	17	1	5	707	711	6
4	12	2	111	113	8	3	5	3	253	260	3	12	14	3	22	55	22	18	6	4	248	258	7	19	1	5	378	385	6
6	12	2	811	810	6	5	5	3	698	687	5	1	15	3	159	165	8	1	7	4	238	218	4	0	2	5	812	800	6
8	12	2	188	184	6	7	5	3	863	856	6	3	15	3	283	273	5	3	7	4	246	247	4	2	2	5	152	145	6
10	12	2	710	708	5	9	5	3	355	361	4	5	15	3	364	368	6	5	7	4	1232	1251	9	4	2	5	380	388	4
12	12	2	268	262	6	11	5	3	145	131	6	7	15	3	235	235	6	7	7	4	396	393	4	6	2	5	465	460	4
14	12	2	459	461	5	13	5	3	399	407	4	9	15	3	86	85	14	9	7	4	872	890	6	8	2	5	255	253	5
16	12	2	455	463	6	15	5	3	153	151	7	11	15	3	142	322	6	11	7	4	739	754	6	10	2	5	95	103	9
1	13	2	166	161	6	17	5	3	259	257	6	0	16	3	201	186	7	13	7	4	232	232	6	12	2	5	716	716	6
3	13	2	22	47	22	19	5	3	54	38	25	2	16	3	73	53	16	15	7	4	237	246	6	14	2	5	48	51	26
5	13	2	1761	1783	13	0	6	3	484	487	4	4	16	3	243	247	6	17	7	4	444	442	5	16	2	5	181	179	7
7	13	2	0	11	1	2	6	3	159	147	4	6	16	3	1122	1135	8	0	8	4	1830	1872	11	18	2	5	69	81	19
9	13	2	98	95	10	4	6	3	487	466	4	8	16	3	286	288	6	2	8	4	25	42	25	1	3	5	138	132	6
11	13	2	122	130	9	6	6	3	1239	1252	8	10	16	3	148	154	9	4	8	4	251	245	5	3	3	5	234	228	5
13	13	2	139	138	9	8	6	3	378	378	4	1	17	3	196	181	7	6	8	4	561	561	5	5	3	5	552	566	5
15	13	2	543	543	6	10	6	3	191	183	5	3	17	3	277	269	6	8	8	4	363	364	5	7	3	5	89	89	9
0	14	2	389	364	5	12	6	3	318	319	5	5	17	3	511	509	6	10	8	4	1049	1052	7	9	3	5	88	94	10
2	14	2	313	319	5	14	6	3	73	91	13	7	17	3	24	25	23	12	8	4	62	73	17	11	3	5	243	237	5
4	14	2	710	708	6	16	6	3	1069	1081	7	0	18	3	199	195	8	14	8	4	89	97	13	13	3	5	234	237	6
6	14	2	506	493	5	18	6	3	416	414	5	2	18	3	202	215	7	16	8	4	286	275	6	15	3	5	18	26	17
8	14	2	201	195	6	20	6	3	424	420	6	4	18	3	149	136	9	18	8	4	14	28	14	17	3	5	508	495	5
10	14	2	54	72	23	1	7	3	215	178	4	2	0	4	172	180	3	1	9	4	20	19	20	0	4	5	146	156	6
12	14	2	36	20	36	3	7	3	213	217	4	4	0	4	590	598	4	3	9	4	236	230	5	2	4	5	80	77	10
14	14	2	140	140	6	5	7	3	1347	1345	8	6	0	4	334	333	4	5	9	4	1765	1778	12	4	4	5	75	69	11
1	15	2	598	600	5	7	7	3	171	181	5	8	0	4	317	314	4	7	9	4	470	470	5	6	4	5	632	622	5
1	15	2	251	244	6	9	7	3	392	388	4	10	0	4	2665	2730	11	9	9	4	41	3	40	8	4	5	311	311	4
5	15	2	1443	1455	10	11	7	3	849	862	6	12	0	4	959	983	7	11	9	4	238	228	5	10	4	5	299	289	5
7	15	2	467	470	5	13	7	3	149	139	7	14	0	4	375	375	5	13	9	4	83	86	13	12	4	5	463	458	5
9	15	2	61	44	20	15	7	3	51	41	23	16	0	4	79	80	14	15	9	4	497	505	5	14	4	5	243	252	6
11	15	2	416	406	6	17	7	3	639	643	6	18	0	4	458	454	5	17	9	4	599	607	6	16	4	5	598	591	5
13	15	2	121	134	11	19	7	3	109	104	12	20	0	4	258	257	7	0	10	4	837	845	6	18	4	5	266	261	7
0	16	2	982	969	7	0	8	3	977	959	6	1	1	4	344	336	3	2	10	4	0	6	1	1	5	5	146	138	6
2	16	2	151	146	8	2	8	3	60	53	12	3	1	4	66	55	9	4	10	4	446	450	5	3	5	5	224	219	5
4	16	2	78	75	14	4	8	3	258	261	4	5	1	4	214	198	4	6	10	4	202	199	6	5	5	5	584	569	5
6	16	2	543	545	5	6	8	3	571	565	5	7	1	4	40	12	22	8	10	4	288	285	5	7	5	5	591	594	5
8	16	2	63	28	19	8	8	3	106	86	7	9	1	4	1135	1153	7	10	10	4	440	433	5	9	5	5	341	345	5
10	16	2	763	757	6	10	8	3	209	207	5	11	1	4	1702	1718	12	12	10	4	255	255	6	11	5	5	267	260	5
1	17	2	250	255	6	12	8	3	566	576	5	13	1	4	247	245	5	14	10	4	801	811	6	13	5	5	375	369	5
3	17	2	387	383	6	14	8	3	313	314	5	15	1	4	167	179	7	16	10	4	399	401	6	15	5	5	73	82	16
5	17	2	102	89	12	16	8	3	78	64	16	17	1	4	44	48	40	1	11	4	159	162	7	17	5	5	144	139	9
7	17	2	125	114	10	18	8	3	129	135	10	19	1	4	497	489	5	3	11	4	330	326	5	0	6	5	381	415	4
9	17	2	366	352	6	1	9	3	574	579	5	0	2	4	329	350	3	5	11	4	1004	1016	7	2	6	5	64	65	13
0	18	2	694	688	6	3	9	3	151	149	6	2	2	4	206	206	4	7	11	4	24	8	23	4	6	5	24	29	23
2	18	2	80	72	16	5	9	3	301	296	4	4	2	4	391	383	4	9	11	4	64	48	16	6	6	5	478	474	5
4	18	2	256	267	7	7	9	3	236	236	5	6	2	4	437	456	4	11	11	4	33	20	12	8	6	5	354	355	5
6	18	2	189	185	6	9	9	3	74	56	12	8	2	4	102	108	8	13	11	4	139	144	9	10	6	5	82	82	11
1	1	3	222	215	3	11	9	3	893	914	6	10	2	4	410	424	4	15	11	4	630	631	6	12	6	5	258	249	6
3	1	3	562	556	4	13	9	3	94	80	10	12	2	4	373	378	4	0	12	4	1002	997	7	14	6	5	44	16	16
5	1	3	80	75	7	15	9	3	190	173	7	14	2	4	636	626	5	2	12	4	205	199	6	16	6	5	682	676	6
7	1	3	350	351	3	17	9	3	461	469	6	16	2	4	758	760	6	4	12	4	203	201	6	1	7	5	104	94	8
9	1	3	279	281	4	0	10	3	919	934	6	18	2	4	121	114	10	6	12	4	274	267	5	3	7	5	423	437	4
11	1	3	1294	1301	9	2	10	3	740	747	5	20	2	4	73	62	17	8	12	4	205	207	6	5	7	5	169	168	6
13	1	3	389	403	4	4	10	3	297	296	4	1	3	4	185	191	4	10	12	4	508	515	5	7	7	5	304	306	5
15	1	3	278	272	5	6	10	3	256	246	5	3	3	4	428	425	4	12	12	4	348	348	6	9	7	5	266	247	5
17	1	3	327	328	5	8	10	3	199	207	6	5	3	4	3370	3375	10	14	12	4	40	32	19	11	7	5	331	325	5
19	1	3	479	483	5	10	10	3	124	123	8	7	3	4	188	199	5	1	13	4	309	302	5	13	7	5	152	153	8
21	1	3	675	661	6	12	10	3	98	79	10	9	3	4	651	667	5	3	13	4	147	138	7	15	7	5	134	134	9
0	2	3	2145	2093	8	14	10	3	578	576	5	11	3	4	130	133	7	5	13	4	249	243	6	17	7	5	48	31	47
2	2	3	653	633	4	16	10	3	192	201	8	13	3	4	276	271	5	7	13	4	295	284	6	0	8	5	704	708	5
4	2	3	135	135	4	1	11	3	248	233	5	15	3	4	778	778	6	9	13	4	389	387	5	2	8	5	190	178	5
6	2	3	1084	1067	7	3	11	3	87	74	10	17	3	4	764	761	6	11	13	4	757	741	6	4	8	5	94	86	9
8	2	3	646	636	5	5	11	3	821	839	6	19	3	4	223	231	7	13	13	4	164	158	9	6	8	5	549	541	5
10	2	3	93	92	8	7	11	3	237	230	5	0	4	4	521	532	4	0	14	4	1324	1349	9	8	8	5	80	84	12
12	2	3	683	689	5	9	11	3	331	339	5	2	4	4	429	428	4	2	14	4	211	216	6	10	8	5	83	74	12
14	2	3	326	334	5	11	11	3	117	10	9	4	4	4	542	561	4	4	14	4	317	323	6	12	8	5	364	359	5

Observed and calculated structure factors for K39

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
14	8	5	459	458	5	5	1	6	1632	1659	12	6	8	6	276	276	5	0	4	7	1051	1046	7	1	1	8	98	108	11
16	8	5	645	636	6	7	1	6	114	116	8	8	8	6	315	328	5	2	4	7	49	54	24	5	1	8	462	457	5
1	9	5	673	675	5	9	1	6	332	336	5	10	8	6	174	185	8	4	4	7	201	198	6	7	1	8	210	212	7
3	9	5	24	24	23	11	1	6	224	226	6	12	8	6	111	100	11	6	4	7	130	131	8	9	1	8	634	619	5
5	9	5	498	493	5	13	1	6	75	69	15	14	8	6	362	353	6	8	4	7	152	157	8	11	1	8	546	531	6
7	9	5	348	336	5	15	1	6	425	421	6	1	9	6	358	354	5	10	4	7	377	377	5	0	2	8	0	10	1
9	9	5	57	32	17	17	1	6	315	314	6	3	9	6	53	71	22	12	4	7	450	458	6	2	2	8	98	99	10
11	9	5	1510	1519	10	0	2	6	1702	1702	12	5	9	6	0	16	1	14	4	7	113	109	12	4	2	8	225	228	6
13	9	5	137	159	9	2	2	6	193	201	5	7	9	6	519	521	5	1	5	7	48	8	22	6	2	8	489	486	5
15	9	5	169	162	9	4	2	6	172	161	6	9	9	6	416	413	5	3	5	7	103	121	10	8	2	8	56	36	22
0	10	5	1061	1063	7	6	2	6	489	491	5	11	9	6	711	719	6	5	5	7	192	201	7	10	2	8	218	213	7
2	10	5	480	487	5	8	2	6	207	207	6	13	9	6	28	18	27	7	5	7	502	515	5	1	3	8	100	99	11
4	10	5	75	68	13	10	2	6	804	833	6	0	10	6	2166	2161	14	9	5	7	244	252	6	3	3	8	288	290	6
6	10	5	492	490	5	12	2	6	314	318	5	2	10	6	293	282	5	11	5	7	47	31	33	5	3	8	1770	1771	12
8	10	5	86	105	12	14	2	6	55	34	22	4	10	6	270	276	6	13	5	7	240	244	7	7	3	8	30	4	29
10	10	5	315	312	6	16	2	6	377	367	6	6	10	6	534	540	5	0	6	7	213	214	6	9	3	8	372	362	6
12	10	5	73	77	16	1	3	6	256	242	5	8	10	6	88	84	13	2	6	7	126	133	8	11	3	8	107	104	12
14	10	5	451	444	6	3	3	6	68	67	13	10	10	6	1262	1266	9	4	6	7	194	199	7	0	4	8	209	234	7
1	11	5	38	29	17	5	3	6	818	831	6	12	10	6	219	222	7	6	6	7	716	710	6	2	4	8	292	285	6
3	11	5	117	116	9	7	3	6	77	79	12	1	11	6	146	145	8	8	6	7	261	259	6	4	4	8	204	195	7
5	11	5	546	545	5	9	3	6	942	950	7	3	11	6	332	328	5	10	6	7	141	145	9	6	4	8	661	655	6
7	11	5	522	528	5	11	3	6	1140	1152	8	5	11	6	475	468	5	12	6	7	211	205	7	8	4	8	32	3	32
9	11	5	185	184	7	13	3	6	135	142	8	7	11	6	128	125	9	1	7	7	100	103	10	10	4	8	153	145	9
11	11	5	316	317	6	15	3	6	97	95	12	9	11	6	429	425	6	3	7	7	204	214	7	1	5	8	513	517	5
13	11	5	203	207	7	17	3	6	392	389	6	11	11	6	773	771	6	5	7	7	813	809	6	3	5	8	161	159	8
0	12	5	1016	1029	7	0	4	6	2326	2343	12	0	12	6	506	506	5	7	7	7	118	109	10	5	5	8	422	419	5
2	12	5	523	513	5	2	4	6	40	40	31	2	12	6	107	105	11	9	7	7	294	284	6	7	5	8	60	26	21
4	12	5	57	38	19	4	4	6	327	324	5	4	12	6	105	108	11	11	7	7	543	540	5	9	5	8	128	104	10
6	12	5	711	722	6	6	4	6	526	531	5	6	12	6	865	862	7	0	8	7	618	600	5	0	6	8	1830	1807	12
8	12	5	64	68	19	8	4	6	112	116	9	8	12	6	58	53	25	2	8	7	50	42	26	2	6	8	180	191	8
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1	13	5	370	359	5	14	4	6	35	24	14	3	13	6	41	39	41	8	8	7	21	12	20	8	6	8	136	140	10
3	13	5	238	230	6	16	4	6	211	211	7	5	13	6	1317	1320	9	10	8	7	171	171	8	1	7	8	40	37	40
5	13	5	962	978	7	1	5	6	285	284	5	7	13	6	114	122	12	12	8	7	374	367	6	3	7	8	171	170	8
7	13	5	197	195	7	3	5	6	100	296	5	0	14	6	147	77	9	1	9	7	353	352	6	5	7	8	880	876	7
9	13	5	267	259	6	5	5	6	513	513	5	2	14	6	360	362	6	3	9	7	92	88	12	7	7	8	213	230	7
11	13	5	1261	1248	8	7	5	6	85	73	11	4	14	6	312	311	6	5	9	7	249	253	6	0	8	8	932	913	7
0	14	5	994	980	7	9	5	6	264	261	5	6	14	6	170	161	8	7	9	7	134	146	9	2	8	8	28	26	27
2	14	5	187	166	7	11	5	6	119	319	5	1	1	7	73	74	13	9	9	7	28	3	28	4	8	8	41	48	40
4	14	5	116	313	6	13	5	6	83	92	14	3	1	7	201	197	6	11	9	7	566	564	6	6	8	8	392	392	6
6	14	5	441	441	6	15	5	6	293	286	6	5	1	7	102	105	10	0	10	7	588	598	6	1	9	8	0	34	1
8	14	5	168	173	8	0	6	6	122	123	8	7	1	7	275	274	6	2	10	7	422	419	5	3	9	8	111	109	11
10	14	5	167	160	6	2	6	6	8	34	8	9	1	7	178	161	7	4	10	7	153	135	8	5	9	8	1227	1236	8
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3	15	5	282	287	6	6	6	6	917	911	7	13	1	7	304	299	6	8	10	7	102	110	13	2	10	8	84	80	15
5	15	5	40	11	39	8	6	6	301	307	5	15	1	7	216	216	8	1	11	7	116	127	11	1	1	9	41	22	40
7	15	5	140	135	6	10	6	6	32	17	32	0	2	7	641	631	5	3	11	7	51	55	29	3	1	9	145	139	9
0	16	5	290	288	7	12	6	6	173	174	8	2	2	7	335	336	5	5	11	7	583	577	6	5	1	9	347	339	6
2	16	5	251	240	7	14	6	6	743	740	6	4	2	7	39	17	39	7	11	7	153	158	10	0	2	9	157	152	9
4	16	5	71	82	19	16	6	6	778	765	6	6	2	7	478	478	5	0	12	7	9	4	9	2	2	9	87	94	14
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2	0	6	118	106	7	3	7	6	121	116	8	10	2	7	50	25	26	4	12	7	252	258	7	6	2	9	39	27	38
4	0	6	571	578	5	5	7	6	2418	2446	13	12	2	7	469	471	5	1	13	7	217	211	7	1	3	9	131	120	10
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12	0	6	755	767	6	13	7	6	213	207	7	5	3	7	390	396	5	6	0	8	667	668	6	2	4	9	50	54	33
14	0	6	722	721	6	15	7	6	659	663	6	7	3	7	409	405	5	8	0	8	0	5	1	4	4	9	66	61	20
16	0	6	864	866	7	0	8	6	304	291	5	9	3	7	148	147	8	10	0	8	1476	1473	10	1	5	9	53	15	29
1	1	6	160	154	6	2	8	6	214	216	6	11	3	7	808	808	6	12	0	8	517	517	6	3	5	9	63	56	22
3	1	6	139	136	7	4	8	6	123	112	5	13	3	7	59	53	23	1	1	8	140	138	8	0	6	9	143	136	9

Observed and calculated structure factors for K40

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	678	710	2	6	8	0	687	695	5	5	1	1	1059	1071	4	5	9	1	438	450	3	3	1	2	665	679	4
4	0	0	945	952	3	8	8	0	528	533	4	7	1	1	61	55	4	7	9	1	328	336	3	5	1	2	1033	1038	5
6	0	0	614	639	4	10	8	0	1065	1056	6	9	1	1	142	136	2	9	9	1	35	12	14	7	1	2	48	44	5
8	0	0	1220	1214	5	12	8	0	64	67	7	11	1	1	604	625	4	11	9	1	1675	1715	8	9	1	2	559	551	3
10	0	0	1865	3924	7	14	8	0	51	52	9	13	1	1	224	219	3	13	9	1	206	196	3	11	1	2	530	535	4
12	0	0	1458	1465	7	16	8	0	372	368	3	15	1	1	432	425	3	15	9	1	302	300	3	13	1	2	41	43	10
14	0	0	359	347	3	18	8	0	0	15	1	17	1	1	651	659	5	17	9	1	64	46	10	15	1	2	715	721	5
16	0	0	536	531	4	20	8	0	275	267	4	19	1	1	597	595	4	19	9	1	256	254	4	17	1	2	43	28	12
18	0	0	283	277	3	1	9	0	117	99	3	21	1	1	373	375	4	0	10	1	1540	1553	7	19	1	2	96	97	6
20	0	0	579	583	5	3	9	0	213	210	2	0	2	1	188	198	2	2	10	1	758	745	5	21	1	2	270	257	4
22	0	0	2065	2069	11	5	9	0	1986	1983	7	2	2	1	626	655	4	4	10	1	90	90	4	2	2	2	365	365	2
1	1	0	276	273	2	7	9	0	859	855	6	4	2	1	234	241	2	6	10	1	564	553	4	4	2	2	413	408	3
5	1	0	590	588	3	9	9	0	163	156	3	6	2	1	268	255	2	8	10	1	102	99	4	6	2	2	513	498	3
7	1	0	372	372	2	11	9	0	716	684	5	8	2	1	446	454	3	10	10	1	464	459	3	8	2	2	59	53	5
9	1	0	1328	1309	6	13	9	0	229	219	3	10	2	1	334	329	3	12	10	1	0	8	1	10	2	2	1432	1452	7
11	1	0	1176	1135	7	15	9	0	923	944	6	12	2	1	775	788	5	14	10	1	604	610	5	12	2	2	614	620	4
13	1	0	620	627	4	17	9	0	647	647	4	14	2	1	115	107	4	16	10	1	679	682	5	14	2	2	125	118	4
15	1	0	206	212	3	19	9	0	0	17	1	16	2	1	451	457	4	18	10	1	100	100	7	16	2	2	248	249	3
17	1	0	444	447	3	0	10	0	291	294	3	18	2	1	40	36	14	1	11	1	0	4	1	18	2	2	101	101	6
19	1	0	410	419	4	2	10	0	263	264	2	20	2	1	465	470	4	3	11	1	66	62	6	20	2	2	243	254	4
21	1	0	962	949	6	4	10	0	211	219	3	22	2	1	295	293	4	5	11	1	936	950	6	22	2	2	657	656	5
0	2	0	1213	1262	3	6	10	0	269	263	3	1	3	1	408	421	3	7	11	1	506	508	4	1	3	2	577	566	4
2	2	0	388	396	3	8	10	0	219	230	3	3	3	1	276	278	2	9	11	1	227	229	3	3	3	2	127	125	2
4	2	0	476	491	3	10	10	0	509	514	4	5	3	1	423	420	3	11	11	1	101	53	5	5	3	2	1249	1229	5
6	2	0	175	178	2	12	10	0	390	403	3	7	3	1	335	333	2	13	11	1	156	162	4	7	3	2	266	261	2
8	2	0	246	242	2	14	10	0	894	894	6	9	3	1	225	231	2	15	11	1	539	528	4	9	3	2	1075	1077	6
10	2	0	511	514	3	16	10	0	419	412	4	11	3	1	451	467	3	17	11	1	433	431	4	11	3	2	1691	1713	7
12	2	0	570	580	4	18	10	0	225	231	4	13	3	1	168	170	3	0	12	1	870	889	5	13	3	2	111	105	4
14	2	0	829	830	5	1	11	0	212	205	3	15	3	1	179	176	3	2	12	1	605	609	4	15	3	2	315	317	3
16	2	0	884	896	6	3	11	0	239	241	3	17	3	1	248	246	3	4	12	1	175	169	3	17	3	2	494	502	4
18	2	0	348	347	3	5	11	0	635	637	4	19	3	1	193	187	4	6	12	1	800	796	5	19	3	2	683	687	5
20	2	0	51	25	11	7	11	0	25	25	25	21	3	1	426	425	4	8	12	1	73	73	6	21	3	2	860	858	6
22	2	0	180	151	5	9	11	0	92	97	5	0	4	1	1318	1319	4	10	12	1	108	106	5	0	4	2	1744	1738	5
1	3	0	228	232	2	11	11	0	412	413	4	2	4	1	222	209	2	12	12	1	210	205	4	2	4	2	620	614	4
3	3	0	363	371	2	13	11	0	322	335	3	4	4	1	56	28	4	14	12	1	98	89	6	4	4	2	167	161	2
7	3	0	601	585	4	15	11	0	587	599	4	6	4	1	563	532	4	16	12	1	809	805	5	6	4	2	526	510	3
9	3	0	643	638	4	17	11	0	488	497	4	8	4	1	299	302	2	1	13	1	512	510	4	8	4	2	145	150	3
11	3	0	584	580	4	0	12	0	1491	1519	8	10	4	1	871	859	5	3	13	1	225	227	3	10	4	2	2025	2048	7
13	3	0	240	234	3	2	12	0	79	77	5	12	4	1	589	591	4	5	13	1	1095	1117	7	12	4	2	37	49	12
15	3	0	1033	1032	7	4	12	0	425	422	3	14	4	1	266	271	3	7	13	1	129	132	4	14	4	2	89	90	5
17	3	0	1056	1058	7	6	12	0	504	504	4	16	4	1	365	361	3	9	13	1	254	258	4	16	4	2	107	108	5
19	3	0	378	379	3	8	12	0	165	164	4	18	4	1	216	214	4	11	13	1	1351	1346	10	18	4	2	572	578	4
21	3	0	166	163	5	10	12	0	863	857	6	20	4	1	145	142	5	13	13	1	237	231	4	20	4	2	243	242	4
0	4	0	2016	2029	4	12	12	0	492	500	4	22	4	1	387	387	4	15	13	1	0	33	1	1	5	2	995	994	5
2	4	0	712	700	4	14	12	0	141	143	5	1	5	1	109	104	2	0	14	1	1059	1077	7	3	5	2	85	91	3
4	4	0	777	771	5	16	12	0	63	70	10	3	5	1	302	306	2	2	14	1	97	87	5	5	5	2	1920	1891	6
8	4	0	318	311	2	1	13	0	638	644	4	5	5	1	925	890	5	4	14	1	155	158	3	7	5	2	248	239	2
10	4	0	511	510	4	3	13	0	279	281	3	7	5	1	826	832	5	6	14	1	282	280	3	9	5	2	561	557	4
12	4	0	180	184	3	5	13	0	276	279	3	9	5	1	312	308	3	8	14	1	234	219	4	11	5	2	703	696	5
14	4	0	419	422	3	7	13	0	469	479	4	11	5	1	296	312	3	10	14	1	600	600	4	13	5	2	71	65	6
16	4	0	2232	2246	9	9	13	0	168	164	4	13	5	1	569	573	4	12	14	1	117	123	6	15	5	2	406	401	3
18	4	0	59	61	9	11	13	0	971	963	6	15	5	1	419	425	3	14	14	1	228	230	4	17	5	2	638	645	5
20	4	0	139	102	5	13	13	0	250	245	4	17	5	1	178	171	4	1	15	1	39	28	15	19	5	2	266	268	4
22	4	0	632	621	5	15	13	0	328	321	4	19	5	1	56	43	10	3	15	1	404	414	4	21	5	2	294	285	4
1	5	0	1496	1474	4	0	14	0	1279	1288	9	21	5	1	448	447	4	5	15	1	35	25	19	0	6	2	1164	1149	5
3	5	0	115	105	2	2	14	0	329	333	3	0	6	1	544	524	3	7	15	1	359	358	3	2	6	2	0	6	1
5	5	0	3122	3065	5	4	14	0	219	209	3	2	6	1	64	49	4	9	15	1	30	18	29	4	6	2	602	596	4
7	5	0	988	998	6	6	14	0	659	669	5	4	6	1	354	344	2	11	15	1	162	156	5	6	6	2	2639	2601	7
9	5	0	183	165	2	8	14	0	238	232	4	6	6	1	1096	1096	6	13	15	1	265	268	4	8	6	2	335	333	3
11	5	0	434	462	3	10	14	0	1140	1143	7	8	6	1	574	556	4	0	16	1	510	513	4	10	6	2	310	314	3
13	5	0	66	70	6	12	14	0	97	98	6	10	6	1	116	105	3	2	16	1	151	144	4	12	6	2	306	314	3
15	5	0	179	182	4	14	14	0	35	5	27	12	6	1	379	374	3	4	16	1	104	107	6	14	6	2	597	603	4
17	5	0	515	515	4	1	15	0	394	391	3	14	6	1	38	12	13	6	16	1	1294	1311	8	16	6	2	1723	1723	9
19	5	0	92	85	6	3	15	0	264	253	3	16	6	1	958	977	6	8	16	1	371	376	4	18	6	2	147	141	5
21	5	0	555	549	4	5	15	0	533	532	4	18	6	1	293	296	4	10	16	1	145	138	5	20	6	2	54	37	11
0	6	0	791	802	5	7	15	0	188	186	4	20	6	1	504	503	4	12	16	1	21	19	20	1	7	2	574	558	4
2	6	0	179	180	2	9	15	0	299	294	4	1	7	1	175	165	2	1	17	1	157	161	5	3	7	2	238	236	2
4	6	0	81	79	3	11	15	0	434	434	4	3	7	1	407	415	3	3	17	1	121	122	5	7	7	2	165	129	3
6	6	0	372	357	3	13	15	0	305	308	4	5	7	1	1097	1086	6	5	17	1	963	958	6	9	7	2	411	413	3
8	6	0	579	563	4	0	16	0	576	579	4	7	7	1	197	192	3	7	17	1	260	256	4	11	7	2	18	4	17
10	6	0	1589	1617	7	2	16	0	320	315	3	9	7	1	245	248	3	9	17	1	206	210	4	13	7	2	390	387	3
12	6	0	50	54	8	4	16	0	80	85	7	11	7	1	168	178	3	0	18	1	342	335	4	15	7	2	1076	1094	7
14	6	0	346	345	3	6	16	0	659	679	5	13	7	1	32	30	17	2	18	1	147	138	5	17	7	2	1133	1155	7
16	6	0	384	398	3	8	16	0	135	130	5	15	7	1	287	293	3	4	18	1	304	307	4	19	7	2	211	204	4
18	6	0	436	430	4	10	16	0	196	178	4	17	7	1	331	310	3	6	18	1	232	234	4	0	8	2	349	357	3
20	6	0	54	68	12	12	16	0	495	499	4	19	7	1	196	198	4	8	18	1	198	208	5	2	8	2	557	554	4
1	7	0	519	505	3	1	17	0	363	360	4	21	7	1	136	135	6	1	19	1	493	491	4	4	8	2	291	297	3
3	7	0	340	350	2	3	17	0	333	334	4	0	8	1	295	277	2	3	19	1	388	392	4	6	8	2	378	377	3
5	7	0	1403	1367	6	5	17	0	1647	1667	10	2	8	1	210	196	2	2	0	2	708	715	4	8	8	2	489	498	4
7	7	0	559	558	4	7	17	0	126	125	6	4	8	1	229	206	2	4	0	2	75	67	3	10	8	2	198	192	3
9	7	0	1008	991	6	9	17	0	43	47	17	6	8	1	272	281	2	6	0	2	676	648	4	12	8	2	83	84	6
11	7	0	730	699	5	0	18	0	437	443	4	8	8	1	17	5	16	8	0	2	678	674	4	14	8	2	425	434	4
13	7	0	197	190	3	2	18	0	230	226	4	10	8	1	337	342	3	10	0	2	1560	1555	7	16	8	2	872	904	6
15	7	0	344	356	3	4	18	0	109	104	6	12	8	1	481	483	4	12	0	2	1158	1168	7	18	8	2	113	112	6
17	7	0	533	528	4	6	18	0	396	391	4	14	8	1	480	486	4	14	0	2	1205	1213	8	20	8	2	129	124	6
19	7	0	584	581	4	8	18	0	221	217	5	16	8	1	269	260	3	16	0	2	1040	1048	7	1	9	2	532	525	4
21	7	0	664	648	5	1	19	0	119	119	6	18	8	1	240	233	4	18	0	2	319	315	3	3	9	2	234	227	3
0	8	0	2643	2611	6	3	19	0	242	240	4	20	8	1	462	453	4	20	0	2	283	286	4	5	9	2	621	617	4
2	8	0	161	150	2	1	1	1	148	129	1	1	9	1	868	862	5	22	0	2	628	614	5	7	9	2	552	546	4
4	8	0	631	626	4	3	1	1	215	212	2	3	9	1	59	12	6	1	1	2	508	520	3	9	9	2	424	422	3

Observed and calculated structure factors for K40

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1591	1586	9	16	2	3	837	837	6	11	11	3	206	197	4	4	4	4	358	369	3	2	14	4	195	197	4
13	9	2	333	346	3	18	2	3	193	187	4	13	11	3	45	14	13	6	4	4	2186	2160	7	4	14	4	319	319	4
15	9	2	60	55	9	20	2	3	370	373	4	15	11	3	361	348	4	8	4	4	101	106	4	6	14	4	438	442	4
17	9	2	852	849	6	1	3	3	486	477	3	17	11	3	529	535	4	10	4	4	420	426	3	8	14	4	222	218	4
19	9	2	286	284	4	3	3	3	244	240	2	0	12	3	61	56	8	12	4	4	163	167	4	10	14	4	891	892	6
0	10	2	4369	4365	8	5	3	3	913	903	6	2	12	3	382	384	3	14	4	4	489	487	4	12	14	4	63	57	10
2	10	2	479	475	3	7	3	3	702	698	4	4	12	3	431	432	3	16	4	4	1671	1677	10	1	15	4	359	358	4
4	10	2	592	593	4	9	3	3	197	188	3	6	12	3	304	300	3	18	4	4	63	55	9	3	15	4	291	290	4
6	10	2	87	100	5	11	3	3	1455	1462	8	8	12	3	26	16	25	20	4	4	58	61	12	5	15	4	286	281	4
8	10	2	348	345	3	13	3	3	49	51	9	10	12	3	77	63	7	1	5	4	935	921	5	7	15	4	37	14	22
10	10	2	1877	1858	9	15	3	3	257	262	3	12	12	3	186	177	4	3	5	4	144	131	3	9	15	4	266	266	4
12	10	2	435	437	4	17	3	3	278	269	3	14	12	3	192	195	5	5	5	4	1587	1581	7	0	16	4	197	197	4
14	10	2	256	258	4	19	3	3	112	109	6	16	12	3	528	515	4	7	5	4	444	443	3	2	16	4	294	299	4
16	10	2	102	96	6	21	3	3	456	457	4	1	13	3	434	428	4	9	5	4	78	77	5	4	16	4	40	5	18
18	10	2	128	130	6	0	4	3	2306	2265	6	3	13	3	351	358	3	11	5	4	929	937	6	6	16	4	182	176	4
1	11	2	503	507	3	2	4	3	40	31	7	5	13	3	521	533	4	13	5	4	70	71	7	8	16	4	61	57	11
3	11	2	648	659	4	4	4	3	230	223	2	7	13	3	115	109	5	15	5	4	240	239	4	1	17	4	379	378	4
5	11	2	107	95	4	6	4	3	346	336	3	9	13	3	203	198	4	17	5	4	174	172	4	3	17	4	247	235	4
7	11	2	34	6	14	8	4	3	103	110	4	11	13	3	650	632	5	19	5	4	57	34	11	5	17	4	1280	1277	8
9	11	2	497	504	4	10	4	3	882	873	6	13	13	3	73	76	8	0	6	4	1985	2022	7	1	1	5	17	13	17
11	11	2	1930	1920	9	12	4	3	596	617	4	15	13	3	106	62	6	2	6	4	186	196	3	3	1	5	58	64	6
13	11	2	87	80	6	14	4	3	112	109	5	0	14	3	405	409	3	4	6	4	208	210	3	5	1	5	859	868	6
15	11	2	49	43	13	16	4	3	19	0	19	2	14	3	44	52	12	6	6	4	197	197	3	7	1	5	60	56	7
17	11	2	76	78	9	18	4	3	76	88	8	4	14	3	273	274	3	8	6	4	275	271	3	9	1	5	134	138	4
0	12	2	1369	1354	8	20	4	3	174	179	5	6	14	3	125	123	5	10	6	4	1399	1415	8	11	1	5	103	94	5
2	12	2	258	249	3	1	5	3	73	70	4	8	14	3	289	285	4	12	6	4	126	132	4	13	1	5	84	88	6
4	12	2	266	256	3	3	5	3	159	165	2	10	14	3	427	429	4	14	6	4	163	163	4	15	1	5	305	309	3
6	12	2	742	753	5	5	5	3	432	410	3	12	14	3	46	43	14	16	6	4	129	137	5	17	1	5	688	685	5
8	12	2	257	261	3	7	5	3	809	809	5	1	15	3	195	185	4	18	6	4	289	280	4	19	1	5	462	465	4
10	12	2	590	596	4	9	5	3	226	222	3	3	15	3	333	333	4	1	7	4	184	169	3	0	2	5	850	867	6
12	12	2	332	329	3	11	5	3	156	150	3	5	15	3	219	216	4	3	7	4	355	365	3	2	2	5	222	217	3
14	12	2	318	318	4	13	5	3	449	445	3	7	15	3	235	236	4	5	7	4	1225	1229	8	4	2	5	256	254	3
16	12	2	598	596	4	15	5	3	448	448	4	9	15	3	43	35	15	7	7	4	433	422	3	6	2	5	461	470	3
1	13	2	72	76	6	17	5	3	231	221	4	11	15	3	348	331	4	9	7	4	768	774	5	8	2	5	204	199	3
3	13	2	49	53	10	19	5	3	36	7	20	0	16	3	330	323	4	11	7	4	809	809	5	10	2	5	371	372	3
5	13	2	1649	1666	9	0	6	3	484	481	3	2	16	3	41	3	15	13	7	4	151	149	4	12	2	5	630	632	5
7	13	2	75	84	7	2	6	3	221	199	2	4	16	3	313	314	4	15	7	4	308	312	4	14	2	5	18	22	17
9	13	2	48	46	10	4	6	3	560	547	4	6	16	3	1141	1139	7	17	7	4	566	563	4	16	2	5	63	60	9
11	13	2	132	144	5	6	6	3	1360	1366	7	8	16	3	334	336	4	0	8	4	1844	1887	8	18	2	5	133	146	5
13	13	2	224	219	4	8	6	3	388	392	3	10	16	3	271	278	4	2	8	4	37	43	11	1	3	5	145	134	3
15	13	2	591	602	5	10	6	3	162	169	3	1	17	3	235	234	4	4	8	4	353	358	3	3	3	5	264	257	3
0	14	2	286	278	3	12	6	3	344	344	3	3	17	3	175	174	5	6	8	4	620	628	4	5	3	5	588	594	4
2	14	2	329	331	3	14	6	3	73	71	7	5	17	3	667	660	5	8	8	4	402	409	3	7	3	5	37	51	12
4	14	2	663	670	5	16	6	3	1045	1049	7	7	17	3	0	11	1	10	8	4	935	933	6	9	3	5	122	118	4
6	14	2	530	526	4	18	6	3	428	431	4	0	18	3	156	166	5	12	8	4	21	26	21	11	3	5	147	155	4
8	14	2	220	215	4	20	6	3	446	450	4	2	18	3	239	235	4	14	8	4	35	33	20	13	3	5	204	199	4
10	14	2	42	26	15	1	7	3	165	154	3	4	18	3	120	117	6	16	8	4	127	121	4	15	3	5	96	99	6
12	14	2	29	38	29	3	7	3	104	110	4	2	0	4	317	317	2	18	8	4	50	43	14	17	3	5	477	473	4
14	14	2	235	237	4	5	7	3	1702	1675	7	4	0	4	384	386	3	1	9	4	55	24	7	19	3	5	163	163	5
1	15	2	705	717	5	7	7	3	225	229	3	6	0	4	218	209	2	3	9	4	95	91	5	0	4	5	253	257	3
3	15	2	180	170	4	9	7	3	276	273	3	8	0	4	499	506	4	5	9	4	1832	1840	8	2	4	5	115	111	4
5	15	2	1437	1445	10	11	7	3	931	936	6	10	0	4	2966	2962	8	7	9	4	460	452	3	4	4	5	23	10	22
7	15	2	437	440	4	13	7	3	184	178	4	12	0	4	1064	1065	7	9	9	4	79	85	6	6	4	5	565	558	4
9	15	2	123	130	5	15	7	3	143	139	4	14	0	4	469	474	4	11	9	4	268	269	3	8	4	5	263	259	3
11	15	2	468	466	4	17	7	3	706	692	5	16	0	4	140	140	4	13	9	4	74	71	8	10	4	5	544	540	4
13	15	2	157	156	5	19	7	3	166	154	5	18	0	4	358	360	4	15	9	4	705	712	5	12	4	5	379	385	3
0	16	2	919	921	6	0	8	3	1145	1111	7	20	0	4	448	452	4	17	9	4	711	702	5	14	4	5	282	281	4
2	16	2	190	196	4	2	8	3	52	40	7	1	1	4	488	487	3	0	10	4	815	804	5	16	4	5	464	467	4
4	16	2	134	131	5	4	8	3	126	121	3	3	1	4	21	4	21	2	10	4	163	160	3	18	4	5	226	231	4
6	16	2	681	681	5	6	8	3	537	532	4	5	1	4	62	57	5	4	10	4	342	354	3	1	5	5	149	134	3
8	16	2	69	74	9	8	8	3	150	155	4	7	1	4	114	117	3	6	10	4	173	175	4	3	5	5	148	144	3
10	16	2	836	826	6	10	8	3	402	403	3	9	1	4	944	957	6	8	10	4	276	276	3	5	5	5	376	165	3
1	17	2	304	306	4	12	8	3	508	516	4	11	1	4	1878	1909	8	10	10	4	420	416	3	7	5	5	562	555	4
3	17	2	409	406	4	14	8	3	267	268	3	13	1	4	385	382	3	12	10	4	359	359	3	9	5	5	239	237	3
5	17	2	0	27	1	16	8	3	171	182	4	15	1	4	106	91	5	14	10	4	644	645	5	11	5	5	280	273	3
7	17	2	272	278	4	18	8	3	34	24	33	17	1	4	148	146	5	16	10	4	501	498	4	13	5	5	408	404	3
9	17	2	301	301	4	1	9	3	576	583	4	19	1	4	182	188	4	1	11	4	175	169	4	15	5	5	324	322	4
0	18	2	585	578	5	3	9	3	223	224	3	0	2	4	328	356	2	3	11	4	320	315	3	17	5	5	126	110	6
2	18	2	145	148	5	5	9	3	200	202	3	2	2	4	260	256	2	5	11	4	836	855	5	0	6	5	374	403	3
4	18	2	324	325	4	7	9	3	201	195	3	4	2	4	308	304	3	7	11	4	80	86	6	2	6	5	23	25	22
6	18	2	312	315	4	9	9	3	46	34	9	6	2	4	413	443	3	9	11	4	68	68	8	4	6	5	20	17	20
1	1	3	156	146	2	11	9	3	957	959	6	8	2	4	97	98	4	11	11	4	0	29	1	6	6	5	585	576	4
3	1	3	456	462	3	13	9	3	126	131	5	10	2	4	396	357	3	13	11	4	221	224	4	8	6	5	363	373	3
5	1	3	120	71	2	15	9	3	281	276	4	12	2	4	478	485	4	15	11	4	473	474	4	10	6	5	61	64	8
7	1	3	427	434	3	17	9	3	350	362	4	14	2	4	600	609	5	0	12	4	1009	1026	6	12	6	5	265	257	3
9	1	3	117	119	3	0	10	3	1121	1149	8	16	2	4	847	856	6	2	12	4	85	88	6	14	6	5	38	40	18
11	1	3	1164	1161	7	2	10	3	716	722	5	18	2	4	327	324	4	4	12	4	325	326	3	16	6	5	656	654	5
13	1	3	319	323	3	4	10	3	186	187	3	20	2	4	40	46	20	6	12	4	245	246	3	18	6	5	156	151	5
15	1	3	470	471	4	6	10	3	341	334	3	1	3	4	102	109	3	8	12	4	202	196	4	1	7	5	108	101	4
17	1	3	305	309	3	8	10	3	154	157	4	3	3	4	315	298	2	10	12	4	657	656	4	3	7	5	364	375	3
19	1	3	574	579	4	10	10	3	272	271	3	5	3	4	3572	3502	7	12	12	4	369	376	4	5	7	5	434	434	3
21	1	3	375	364	4	12	10	3	71	72	7	7	3	4	217	223	3	14	12	4	72	65	9	7	7	5	293	289	3
0	2	3	2022	1976	5	14	10	3	588	588	4	9	3	4	480	489	3	1	13	4	432	421	3	9	7	5	182	168	4
2	2	3	735	720	4	16	10	3	458	460	4	11	3	4	279	272	3	3	13	4	228	227	4	11	7	5	259	259	4
4	2	3	330	317	2	18	10	3	41	48	18	13	3	4	234	236	3	5	13	4	200	201	4	13	7	5	124	126	5
6	2	3	1010	1010	6	1	11	3	130	130	4	15	3	4	899	912	6	7	13	4	305	300	4	15	7	5	290	286	4
8	2	3	588	589	4	3	11	3	105	106	4	17	3	4	826	827	6	9	13	4	191	182	4	17	7	5	42	22	18
10	2	3	257	263	3	5	11	3	975	983	7	19	3	4	331	328	4	11	13	4	804	800	5	0	8	5	562	576	4
12	2	3	625	630	4	7	11	3	200	200	3	0	4	4	583	592	4	13	13	4	127	142	6	2	8	5	244	242	3
14	2	3	329	327	3	9	11	3	284	286	3	2	4	4	540	526	4	0	14	4	1274	1284	8	4	8	5	199	198	3

Observed and calculated structure factors for K40

h	k	l	10Fo	10Fc	10s
6	8	5	566	558	4
8	8	5	55	51	9
10	8	5	241	243	4
12	8	5	330	329	4
14	8	5	459	449	4
16	8	5	426	426	4
1	9	5	673	675	4
3	9	5	32	12	18
5	9	5	564	558	4
7	9	5	326	316	3
9	9	5	32	8	23
11	9	5	1580	1573	10
13	9	5	209	203	4
15	9	5	250	241	4
0	10	5	1219	1229	7
2	10	5	451	459	4
4	10	5	19	23	18
6	10	5	557	550	4
8	10	5	66	61	8
10	10	5	441	438	4
12	10	5	76	78	8
14	10	5	440	447	4
1	11	5	56	55	9
3	11	5	14	19	14
5	11	5	664	662	5
7	11	5	495	502	4
9	11	5	150	142	4
11	11	5	157	169	5
13	11	5	205	209	4
0	12	5	937	948	6
2	12	5	554	554	4
4	12	5	45	5	13
6	12	5	811	813	6
8	12	5	47	52	13
10	12	5	116	115	6
12	12	5	169	167	5
1	13	5	440	438	4
3	13	5	141	139	5
5	13	5	1083	1074	7
7	13	5	214	211	4
9	13	5	216	217	4
11	13	5	1400	1392	9
0	14	5	1157	1177	7
2	14	5	78	74	8
4	14	5	277	275	4
6	14	5	436	437	4
8	14	5	134	130	6
10	14	5	586	578	5
1	15	5	62	67	10
3	15	5	340	340	4
5	15	5	110	102	7
7	15	5	331	330	4
0	16	5	407	410	4
2	16	5	192	187	5
4	16	5	55	28	13
0	0	6	2564	2555	8
2	0	6	191	187	3
4	0	6	460	460	3
6	0	6	702	712	5
8	0	6	449	447	4
10	0	6	952	968	6
12	0	6	810	817	5
14	0	6	664	662	5
16	0	6	1012	1017	7
1	1	6	191	187	3
3	1	6	58	53	7
5	1	6	1639	1660	8
7	1	6	183	184	3
9	1	6	294	294	3
11	1	6	246	241	3
13	1	6	82	73	7
15	1	6	471	456	4
17	1	6	310	310	4
0	2	6	1743	1766	8
2	2	6	188	192	3
4	2	6	103	102	4
6	2	6	476	479	4
8	2	6	113	119	5
10	2	6	925	938	6
12	2	6	363	367	3
14	2	6	130	141	5
16	2	6	321	305	4
1	3	6	332	328	3
3	3	6	32	41	16
5	3	6	935	939	6
7	3	6	133	135	4
9	3	6	718	723	5
11	3	6	1292	1312	8
13	3	6	32	3	28
15	3	6	213	193	4
17	3	6	467	471	4
0	4	6	2107	2336	8
2	4	6	63	60	7
4	4	6	278	279	3
6	4	6	570	580	4
8	4	6	176	173	4
10	4	6	1355	1358	8
12	4	6	81	75	7
14	4	6	52	58	12
16	4	6	255	251	4
1	5	6	344	346	3
3	5	6	311	305	3
5	5	6	606	599	4
7	5	6	99	97	5
9	5	6	315	321	3
11	5	6	266	267	4
13	5	6	90	83	7
15	5	6	173	169	4
0	6	6	122	33	4
2	6	6	139	131	4
4	6	6	179	173	4
6	6	6	1072	1075	6
8	6	6	336	330	3
10	6	6	190	186	4
12	6	6	208	200	4
14	6	6	575	580	4
16	6	6	959	942	6
1	7	6	435	436	3
3	7	6	0	2	1
5	7	6	2534	2526	9
7	7	6	108	106	5
9	7	6	312	310	3
11	7	6	335	344	4
13	7	6	276	264	4
15	7	6	774	780	5
0	8	6	247	235	3
2	8	6	266	267	3
4	8	6	343	347	3
6	8	6	289	293	3
8	8	6	300	306	4
10	8	6	258	261	4
12	8	6	0	13	1
14	8	6	293	287	4
1	9	6	438	423	3
3	9	6	25	7	25
5	9	6	92	98	6
7	9	6	592	600	4
9	9	6	286	277	4
11	9	6	752	746	5
13	9	6	124	120	6
0	10	6	2195	2208	10
2	10	6	183	178	4
4	10	6	182	178	4
6	10	6	520	524	4
8	10	6	129	130	5
10	10	6	1344	1334	8
12	10	6	311	312	4
1	11	6	247	249	4
3	11	6	300	298	4
5	11	6	491	498	4
7	11	6	163	166	5
9	11	6	349	358	4
11	11	6	883	880	6
0	12	6	573	571	4
2	12	6	212	210	4
4	12	6	201	191	4
6	12	6	786	790	5
8	12	6	101	103	7
10	12	6	323	317	4
1	13	6	11	33	31
3	13	6	33	35	33
5	13	6	1252	1242	7
7	13	6	75	71	9
0	14	6	208	145	4
2	14	6	371	373	4
4	14	6	278	273	4
6	14	6	204	192	4
1	15	6	497	495	4
1	1	7	91	91	5
3	1	7	144	145	4
5	1	7	156	161	4
7	1	7	276	274	3
9	1	7	81	85	7
11	1	7	655	662	5
13	1	7	226	222	4
15	1	7	315	318	4
0	2	7	647	639	4
2	2	7	350	353	3
4	2	7	65	60	7
6	2	7	521	524	4
8	2	7	244	239	4
10	2	7	170	173	4
12	2	7	180	177	4
14	2	7	194	191	5
1	3	7	286	283	3
3	3	7	12	8	12
5	3	7	446	438	4
7	3	7	336	340	3
9	3	7	120	121	5
11	3	7	925	917	6
13	3	7	88	69	7
0	4	7	1154	1162	7
2	4	7	20	5	20
4	4	7	95	99	6
6	4	7	216	208	4
8	4	7	100	101	6
10	4	7	600	607	4
12	4	7	408	417	4
14	4	7	111	113	6
1	5	7	19	22	19
3	5	7	66	54	7
5	5	7	42	42	13
7	5	7	489	490	4
9	5	7	164	161	4
11	5	7	29	28	29
13	5	7	267	276	4
0	6	7	225	227	4
2	6	7	146	151	4
4	6	7	220	214	4
6	6	7	800	799	5
8	6	7	261	267	4
10	6	7	124	120	5
12	6	7	201	205	4
1	7	7	144	142	4
3	7	7	144	149	5
5	7	7	1045	1039	7
7	7	7	112	107	6
9	7	7	198	194	4
11	7	7	612	611	4
13	7	7	133	123	5
0	8	7	734	732	5
2	8	7	38	34	16
4	8	7	82	76	7
6	8	7	381	362	4
8	8	7	62	48	10
10	8	7	348	341	4
12	8	7	370	365	4
1	9	7	318	319	4
3	9	7	137	137	5
5	9	7	254	248	4
7	9	7	142	147	5
9	9	7	0	4	1
11	9	7	557	558	4
0	10	7	682	695	5
2	10	7	404	414	4
4	10	7	91	85	7
6	10	7	223	209	4
8	10	7	88	88	7
1	11	7	87	77	7
3	11	7	38	40	20
5	11	7	649	646	5
7	11	7	140	133	5
0	12	7	79	64	8
2	12	7	247	242	4
4	12	7	282	280	4
6	12	7	176	158	5
1	13	7	251	254	4
0	0	8	2607	2616	10
2	0	8	112	114	6
4	0	8	93	85	6
6	0	8	610	605	5
8	0	8	104	104	6
10	0	8	1639	1641	11
12	0	8	575	579	4
1	1	8	226	226	4
3	1	8	90	87	6
5	1	8	383	386	4
7	1	8	272	275	4
9	1	8	517	517	4
11	1	8	657	654	5
0	2	8	45	3	13
2	2	8	151	144	5
4	2	8	168	167	4
6	2	8	509	500	4
8	2	8	25	19	25
10	2	8	172	173	5
12	2	8	324	325	4
1	3	8	50	52	12
3	3	8	198	202	4
5	3	8	1881	1881	10
7	3	8	0	3	1
9	3	8	247	254	4
11	3	8	27	33	27
0	4	8	184	197	4
2	4	8	337	346	4
4	4	8	99	83	6
6	4	8	772	776	5
8	4	8	0	36	1
10	4	8	230	215	4
1	5	8	507	508	4
3	5	8	190	182	4
5	5	8	440	444	4
7	5	8	51	47	13
9	5	8	0	1	1
0	6	8	1802	1812	10
2	6	8	155	151	5
4	6	8	212	206	4
6	6	8	466	465	4
8	6	8	74	64	9
10	6	8	936	933	6
1	7	8	34	7	13
3	7	8	275	267	4
5	7	8	878	873	5
7	7	8	260	260	4
9	7	8	430	429	4
0	8	8	943	936	6
2	8	8	48	32	14
4	8	8	114	106	6
6	8	8	426	435	4
1	9	8	30	35	29
3	9	8	0	6	1
5	9	8	1277	1293	8
0	10	8	992	1002	6
2	10	8	9	36	9
1	1	9	19	9	18
3	1	9	104	101	6
5	1	9	433	431	4
7	1	9	124	120	6
0	2	9	233	227	4
2	2	9	133	140	5
4	2	9	53	52	13
6	2	9	84	70	8
1	3	9	65	61	9
3	3	9	0	3	1
5	3	9	180	183	5
0	4	9	417	416	4
2	4	9	47	51	14
4	4	9	63	61	11
1	5	9	52	43	13
3	5	9	0	28	1
0	6	9	143	136	5
2	6	9	18	16	18

Observed and calculated structure factors for K41

h	k	l	10Fo	10Fc	10s
2	0	0	681	688	4
4	0	0	1250	1254	6
6	0	0	549	562	4
8	0	0	733	736	6
10	0	0	3571	3592	11
12	0	0	1351	1356	11
14	0	0	119	111	6
16	0	0	185	175	5
18	0	0	571	557	5
20	0	0	105	109	11
22	0	0	1667	1701	13
3	1	0	154	148	2
5	1	0	395	399	3
7	1	0	518	504	4
9	1	0	1751	1742	9
11	1	0	2907	2879	11
13	1	0	287	293	4
15	1	0	336	331	4
17	1	0	303	296	5
19	1	0	594	615	5
21	1	0	756	761	7
0	2	0	1439	1398	4
2	2	0	226	235	2
4	2	0	748	743	5
6	2	0	155	159	3
8	2	0	314	307	3
10	2	0	717	731	5
12	2	0	288	291	4
14	2	0	880	866	6
16	2	0	705	690	6
18	2	0	76	72	11
20	2	0	195	204	6
22	2	0	359	360	6
1	3	0	336	330	2
3	3	0	643	626	5
5	3	0	4838	4681	10
7	3	0	535	509	4
9	3	0	1052	1034	7
11	3	0	288	281	4
13	3	0	344	342	4
15	3	0	757	739	6
17	3	0	965	950	8
19	3	0	175	174	7
21	3	0	502	502	6
0	4	0	2049	2008	7
2	4	0	546	541	4
4	4	0	1131	1124	7
6	4	0	1748	1607	10
8	4	0	501	480	4
10	4	0	388	382	4
12	4	0	277	273	4
14	4	0	948	935	7
16	4	0	2018	2017	13
18	4	0	77	74	11
20	4	0	257	247	6
1	5	0	1398	1362	7
3	5	0	31	3	9
5	5	0	1291	1131	10
7	5	0	804	777	6
9	5	0	234	245	4
11	5	0	320	334	4
13	5	0	391	400	4
15	5	0	247	246	5
17	5	0	497	497	5
19	5	0	278	277	6
21	5	0	286	282	6
0	6	0	848	851	6
2	6	0	212	207	3
4	6	0	517	521	4
6	6	0	621	589	4
8	6	0	694	685	5
10	6	0	1247	1227	9
12	6	0	286	296	4
14	6	0	511	502	5
16	6	0	618	617	5
18	6	0	366	364	5
20	6	0	85	93	12
1	7	0	689	678	5
3	7	0	69	74	5
5	7	0	1312	1315	9
7	7	0	475	458	4
9	7	0	1253	1230	8
11	7	0	598	554	5
13	7	0	349	346	4
15	7	0	168	181	6
17	7	0	257	254	5
19	7	0	662	665	6
0	8	0	2522	2472	10
2	8	0	187	186	3
4	8	0	289	295	3
6	8	0	556	549	5
8	8	0	409	410	4
10	8	0	1314	1291	9
12	8	0	160	172	6
14	8	0	208	207	5
16	8	0	313	314	5
18	8	0	52	58	21
20	8	0	298	302	6
1	9	0	24	1	23
3	9	0	424	432	4
5	9	0	1876	1860	10
7	9	0	830	826	6
9	9	0	72	57	9
11	9	0	628	614	5
13	9	0	284	280	5
15	9	0	430	437	5
17	9	0	457	465	5
19	9	0	264	258	6
0	10	0	295	317	4
2	10	0	123	125	5
4	10	0	505	528	4
6	10	0	235	238	4
8	10	0	260	265	4
10	10	0	476	482	5
12	10	0	113	119	7
14	10	0	1227	1235	10
16	10	0	148	155	7
18	10	0	555	566	6
1	11	0	259	247	4
3	11	0	281	277	4
5	11	0	858	898	7
7	11	0	184	192	5
9	11	0	25	23	25
11	11	0	469	476	5
13	11	0	135	138	7
15	11	0	874	880	7
17	11	0	350	358	6
0	12	0	1655	1650	12
2	12	0	300	298	4
4	12	0	151	140	5
6	12	0	587	594	5
8	12	0	117	118	7
10	12	0	640	638	5
12	12	0	474	474	5
14	12	0	0	18	1
16	12	0	116	116	10
1	13	0	377	378	4
3	13	0	125	123	6
5	13	0	464	468	4
7	13	0	419	437	5
9	13	0	630	639	5
11	13	0	954	952	8
13	13	0	290	292	6
15	13	0	173	193	7
0	14	0	1531	1509	10
2	14	0	368	368	4
4	14	0	225	231	5
6	14	0	660	689	5
8	14	0	55	76	16
10	14	0	1290	1302	10
12	14	0	78	99	16
14	14	0	43	18	42
1	15	0	151	147	6
3	15	0	426	429	5
5	15	0	544	562	5
7	15	0	0	20	1
9	15	0	50	16	18
11	15	0	335	337	5
13	15	0	394	399	6
0	16	0	672	662	6
2	16	0	155	155	6
4	16	0	333	342	5
6	16	0	853	885	7
8	16	0	57	69	17
10	16	0	17	43	36
12	16	0	387	385	6
1	17	0	290	282	5
3	17	0	256	260	6
5	17	0	1926	1912	15
7	17	0	112	107	9
9	17	0	112	105	9
0	18	0	286	282	6
2	18	0	309	310	6
4	18	0	42	35	33
6	18	0	238	250	6
8	18	0	324	330	6
1	19	0	163	170	8
3	19	0	40	36	40
1	1	1	190	181	2
3	1	1	498	482	3
5	1	1	921	932	7
7	1	1	103	86	4
9	1	1	512	509	4
11	1	1	915	917	7
13	1	1	407	412	4
15	1	1	53	50	13
17	1	1	757	749	6
19	1	1	466	481	5
21	1	1	967	960	7
0	2	1	148	175	2
2	2	1	479	506	3
4	2	1	576	568	4
6	2	1	210	198	3
8	2	1	591	592	4
10	2	1	279	290	3
12	2	1	994	998	7
14	2	1	224	225	5
16	2	1	727	721	6
18	2	1	122	97	7
20	2	1	135	142	8
22	2	1	167	175	8
1	3	1	341	355	2
3	3	1	238	230	2
5	3	1	394	380	3
7	3	1	505	496	4
9	3	1	168	176	4
11	3	1	197	209	4
13	3	1	262	260	4
15	3	1	40	44	19
17	3	1	287	286	5
19	3	1	199	191	6
21	3	1	300	303	6
0	4	1	1016	1017	6
2	4	1	78	77	3
4	4	1	287	272	2
6	4	1	860	817	6
8	4	1	547	541	4
10	4	1	213	185	4
12	4	1	757	772	6
14	4	1	244	251	5
16	4	1	719	724	6
18	4	1	283	279	5
20	4	1	115	112	9
1	5	1	113	113	3
3	5	1	504	521	4
5	5	1	1558	1534	8
7	5	1	941	921	7
9	5	1	656	648	5
11	5	1	283	308	4
13	5	1	528	532	5
15	5	1	158	159	6
17	5	1	236	228	5
19	5	1	42	20	26
21	5	1	785	769	7
0	6	1	564	542	4
2	6	1	173	172	3
4	6	1	139	132	3
6	6	1	850	854	6
8	6	1	521	504	4
10	6	1	212	194	4
12	6	1	325	318	4
14	6	1	140	75	6
16	6	1	1067	1066	8
18	6	1	320	320	5
20	6	1	417	433	6
1	7	1	204	193	3
3	7	1	598	604	4
5	7	1	292	289	3
7	7	1	233	226	4
9	7	1	441	436	4
11	7	1	26	4	26
13	7	1	40	42	20
15	7	1	77	67	10
17	7	1	211	206	6
19	7	1	92	106	11
0	8	1	739	704	5
2	8	1	23	35	23
4	8	1	151	151	4
6	8	1	303	312	4
8	8	1	172	170	5
10	8	1	127	113	6
12	8	1	564	557	5
14	8	1	632	613	6
16	8	1	816	818	7
18	8	1	393	387	5
20	8	1	237	238	7
1	9	1	1002	967	7
3	9	1	156	158	4
5	9	1	260	288	4
7	9	1	375	363	4
9	9	1	11	19	11
11	9	1	1715	1710	13
13	9	1	78	56	10
15	9	1	102	89	8
17	9	1	206	204	6
19	9	1	187	191	7
0	10	1	1120	1127	8
2	10	1	769	754	6
4	10	1	221	232	4
6	10	1	451	461	4
8	10	1	226	215	5
10	10	1	197	195	5
12	10	1	41	41	23
14	10	1	562	558	5
16	10	1	190	211	6
18	10	1	268	257	6
1	11	1	197	198	4
3	11	1	326	324	4
5	11	1	640	668	5
7	11	1	585	578	5
9	11	1	300	308	5
11	11	1	435	425	5
13	11	1	97	98	9
15	11	1	33	38	12
17	11	1	504	512	5
0	12	1	1098	1105	8
2	12	1	436	440	4
4	12	1	108	107	6
6	12	1	585	598	5
8	12	1	192	190	5
10	12	1	205	211	6
12	12	1	320	310	5
14	12	1	32	17	32
16	12	1	718	716	6
1	13	1	375	362	4
3	13	1	403	403	4
5	13	1	857	878	7
7	13	1	50	64	18
9	13	1	267	280	5
11	13	1	1033	1043	8
13	13	1	150	162	7
15	13	1	329	336	6
0	14	1	589	605	5
2	14	1	305	304	5
4	14	1	358	358	5
6	14	1	317	319	5
8	14	1	348	346	5
10	14	1	132	127	7
12	14	1	228	225	6
14	14	1	384	381	6
1	15	1	59	70	14
3	15	1	243	240	5
5	15	1	282	276	5
7	15	1	358	372	5
9	15	1	94	91	11
11	15	1	117	97	9
13	15	1	108	119	11
0	16	1	183	184	6
2	16	1	257	248	5
4	16	1	12	12	11
6	16	1	1258	1272	9
8	16	1	277	266	6
10	16	1	122	127	9
12	16	1	107	98	10
1	17	1	103	104	9
3	17	1	366	368	5
5	17	1	622	628	6
7	17	1	211	205	7
9	17	1	388	396	6
0	18	1	298	300	6
2	18	1	64	74	16
4	18	1	301	297	6
6	18	1	320	319	6
1	19	1	299	295	6
3	19	1	383	377	6
0	0	2	2965	3221	8
2	0	2	523	550	4
4	0	2	403	409	3
6	0	2	711	684	5
8	0	2	432	423	3
10	0	2	1271	1250	10
12	0	2	937	939	7
14	0	2	1270	1272	10
16	0	2	618	612	5
18	0	2	836	828	7
20	0	2	29	23	29
1	1	2	459	481	3
3	1	2	801	799	5
5	1	2	945	969	7
7	1	2	172	164	3
9	1	2	636	635	5
11	1	2	686	675	5
13	1	2	37	36	21
15	1	2	583	575	5
17	1	2	50	39	16
19	1	2	24	20	23
21	1	2	377	371	6
0	2	2	4022	4075	9
2	2	2	351	356	3
4	2	2	527	526	4
6	2	2	487	477	4
8	2	2	299	291	3
10	2	2	1225	1229	8
12	2	2	513	520	4
14	2	2	129	138	6
16	2	2	366	366	5
18	2	2	67	46	13
20	2	2	133	121	8
1	3	2	378	382	3
3	3	2	332	337	3
5	3	2	958	948	6
7	3	2	99	94	4
9	3	2	1658	1677	10
11	3	2	1335	1375	9
13	3	2	464	462	4
15	3	2	118	107	7
17	3	2	309	313	5
19	3	2	807	814	7
21	3	2	444	451	6
0	4	2	1848	1842	8
2	4	2	601	599	4
4	4	2	43	24	7
6	4	2	294	285	3
8	4	2	73	83	6
10	4	2	1874	1925	11
12	4	2	342	340	4
14	4	2	256	251	5
16	4	2	66	58	12
18	4	2	456	453	5
20	4	2	293	299	6
1	5	2	902	893	6
3	5	2	129	116	3
5	5	2	1906	1849	9
7	5	2	237	232	3
9	5	2	351	334	4
11	5	2	615	605	5
13	5	2	14	31	27
15	5	2	235	228	5
17	5	2	707	717	6
19	5	2	419	411	5
21	5	2	464	462	6
0	6	2	1067	1049	7
2	6	2	190	195	3
4	6	2	1208	1203	9
6	6	2	2330	2269	10
8	6	2	267	259	4
10	6	2	85	81	7
12	6	2	329	329	4
14	6	2	1046	1065	8
16	6	2	1444	1463	11
18	6	2	49	12	22
20	6	2	128	132	9
1	7	2	703	703	5
3	7	2	58	59	7
5	7	2	4686	4447	12
7	7	2	207	199	4
9	7	2	477	479	4
11	7	2	103	99	7
13	7	2	304	303	5
15	7	2	825	828	6
17	7	2	968	964	7
19	7	2	41	10	40
0	8	2	538	536	4
2	8	2	389	388	4
4	8	2	130	141	4
6	8	2	477	467	4
8	8	2	536	539	5
10	8	2	0	10	1
12	8	2	179	174	5
14	8	2	550	549	5
16	8	2	895	894	7
18	8	2	72	55	15
1	9	2	384	364	4
3	9	2	42	30	13
5	9	2	443	440	4
7	9	2	374	367	4
9	9	2	838	838	7
11	9	2	1589	1587	10
13	9	2	42	38	22
15	9	2	391	388	5

Observed and calculated structure factors for K41

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
17	9	2	564	576	6	1	3	3	572	572	4	2	12	3	238	246	5	12	4	4	171	182	6	12	14	4	85	61	13
19	9	2	299	302	6	3	3	3	236	235	3	4	12	3	341	346	4	14	4	4	885	887	7	1	15	4	124	117	8
0	10	2	4455	4409	14	5	3	3	1062	1042	7	6	12	3	108	110	7	16	4	4	1412	1417	10	3	15	4	419	416	5
2	10	2	737	734	6	7	3	3	739	731	6	8	12	3	99	101	8	18	4	4	134	133	8	5	15	4	275	272	6
4	10	2	786	805	6	9	3	3	163	150	4	10	12	3	177	176	6	1	5	4	950	955	7	7	15	4	87	98	12
6	10	2	86	86	7	11	3	3	1302	1312	9	12	12	3	298	291	5	3	5	4	183	174	4	9	15	4	57	34	20
8	10	2	229	238	5	13	3	3	73	73	9	14	12	3	74	74	14	5	5	4	1491	1507	10	0	16	4	202	198	6
10	10	2	1815	1823	13	15	3	3	103	117	8	16	12	3	387	390	6	7	5	4	375	376	4	2	16	4	154	146	7
12	10	2	276	277	5	17	3	3	258	262	5	1	13	3	241	244	5	9	5	4	223	222	4	4	16	4	255	258	6
14	10	2	380	374	5	19	3	3	100	105	10	3	13	3	480	492	5	11	5	4	890	912	7	6	16	4	498	499	5
16	10	2	277	271	6	0	4	3	2137	2091	9	5	13	3	259	259	5	13	5	4	248	246	5	8	16	4	0	0	1
18	10	2	266	265	6	2	4	3	49	53	7	7	13	3	139	135	6	15	5	4	245	241	5	1	17	4	368	357	6
1	11	2	392	387	4	4	4	3	179	178	3	9	13	3	212	207	6	17	5	4	110	110	9	3	17	4	174	161	8
3	11	2	697	698	5	6	4	3	194	187	4	11	13	3	321	313	5	19	5	4	201	186	7	1	1	5	92	94	5
5	11	2	87	91	7	8	4	3	297	305	4	13	13	3	55	40	20	0	6	4	2126	2139	11	3	1	5	247	250	4
7	11	2	18	3	18	10	4	3	363	355	4	15	13	3	255	239	7	2	6	4	186	208	4	5	1	5	689	687	5
9	11	2	658	648	5	12	4	3	801	816	6	0	14	3	80	84	11	4	6	4	461	465	4	7	1	5	0	15	1
11	11	2	1801	1812	14	14	4	3	111	107	7	2	14	3	259	261	5	6	6	4	126	129	5	9	1	5	411	423	4
13	11	2	51	46	19	16	4	3	261	261	5	4	14	3	307	304	5	8	6	4	370	378	4	11	1	5	297	288	4
15	11	2	240	238	6	18	4	3	166	179	7	6	14	3	141	136	7	10	6	4	1167	1177	8	13	1	5	226	237	5
17	11	2	45	39	30	20	4	3	69	67	16	8	14	3	196	198	5	12	6	4	379	386	5	15	1	5	19	7	19
0	12	2	1268	1282	10	1	5	3	79	63	5	10	14	3	73	58	13	14	6	4	292	298	5	17	1	5	734	744	6
2	12	2	30	30	30	3	5	3	344	355	3	12	14	3	115	105	9	16	6	4	239	239	6	0	2	5	754	759	6
4	12	2	68	61	10	5	5	3	896	883	6	1	15	3	122	120	8	18	6	4	269	265	6	2	2	5	76	70	7
6	12	2	818	831	6	7	5	3	903	889	7	3	15	3	179	174	6	1	7	4	243	233	4	4	2	5	532	533	4
8	12	2	85	90	9	9	5	3	535	529	5	5	15	3	475	490	5	3	7	4	155	157	4	6	2	5	422	410	4
10	12	2	780	792	7	11	5	3	173	114	5	7	15	3	247	244	6	5	7	4	1229	1254	9	8	2	5	313	309	4
12	12	2	215	211	6	13	5	3	395	395	4	9	15	3	133	134	8	7	7	4	380	379	4	10	2	5	88	82	8
14	12	2	635	629	6	15	5	3	89	74	9	11	15	3	332	327	6	9	7	4	959	963	7	12	2	5	754	761	6
16	12	2	356	363	6	17	5	3	283	293	6	0	16	3	89	71	11	11	7	4	751	750	6	14	2	5	141	136	7
1	13	2	263	262	5	19	5	3	48	19	26	2	16	3	102	95	9	13	7	4	298	299	5	16	2	5	260	256	6
3	13	2	126	120	6	0	6	3	426	437	4	4	16	3	217	217	6	15	7	4	186	189	6	18	2	5	62	41	17
5	13	2	1884	1883	13	2	6	3	101	85	4	6	16	3	1131	1136	8	17	7	4	379	378	6	1	3	5	148	151	4
7	13	2	38	28	37	4	6	3	358	341	3	8	16	3	219	224	7	0	8	4	1824	1842	11	3	3	5	205	199	4
9	13	2	237	242	5	6	6	3	1173	1159	8	10	16	3	0	34	1	2	8	4	32	44	25	5	3	5	575	579	5
11	13	2	125	131	8	8	6	3	351	355	4	1	17	3	170	165	7	4	8	4	98	104	6	7	3	5	102	104	6
13	13	2	113	98	9	10	6	3	207	212	4	3	17	3	174	176	6	6	8	4	522	492	5	9	3	5	38	16	26
15	13	2	464	455	6	12	6	3	297	291	5	5	17	3	367	351	6	8	8	4	317	321	4	11	3	5	311	310	5
0	14	2	473	417	4	14	6	3	137	147	7	7	17	3	42	35	41	10	8	4	1116	1126	8	13	3	5	268	266	5
2	14	2	310	308	5	16	6	3	1150	1149	9	0	18	3	223	208	7	12	8	4	100	95	8	15	3	5	54	21	17
4	14	2	763	748	6	18	6	3	445	439	5	2	18	3	167	177	8	14	8	4	178	176	6	17	3	5	489	484	5
6	14	2	476	471	5	20	6	3	193	401	6	4	18	3	127	128	10	16	8	4	269	253	6	0	4	5	53	59	10
8	14	2	184	185	6	1	7	3	238	231	3	0	0	4	6057	6452	13	18	8	4	10	9	30	2	4	5	58	45	10
10	14	2	132	139	8	3	7	3	308	319	3	2	0	4	408	425	3	1	9	4	11	25	10	4	4	5	127	131	5
12	14	2	68	65	15	5	7	3	1072	1066	8	4	0	4	712	740	6	3	9	4	301	307	4	6	4	5	691	675	5
14	14	2	402	417	6	7	7	3	130	137	5	6	0	4	436	425	4	5	9	4	1761	1752	12	8	4	5	376	387	4
1	15	2	452	456	5	9	7	3	450	458	4	8	0	4	155	163	5	7	9	4	468	471	4	10	4	5	82	87	9
3	15	2	313	307	5	11	7	3	818	811	6	10	0	4	2478	2527	12	9	9	4	110	103	7	12	4	5	534	543	5
5	15	2	1474	1448	11	13	7	3	136	131	6	12	0	4	925	926	7	11	9	4	209	208	6	14	4	5	257	245	5
7	15	2	480	480	5	15	7	3	163	170	6	14	0	4	277	283	5	13	9	4	132	134	8	16	4	5	733	731	6
9	15	2	242	238	6	17	7	3	614	611	6	16	0	4	258	257	5	15	9	4	299	293	6	18	4	5	298	301	6
11	15	2	363	358	6	19	7	3	71	61	14	18	0	4	544	537	5	17	9	4	543	551	6	1	5	5	157	157	5
13	15	2	143	120	8	0	8	3	847	832	6	20	0	4	13	33	33	0	10	4	862	868	7	3	5	5	296	301	4
0	16	2	1052	1055	8	2	8	3	145	139	4	1	1	4	216	222	3	2	10	4	115	125	6	5	5	5	732	726	6
2	16	2	115	106	8	4	8	3	369	371	4	3	1	4	115	111	4	4	10	4	541	550	5	7	5	5	630	627	5
4	16	2	25	30	24	6	8	3	577	572	5	5	1	4	357	341	3	6	10	4	237	242	5	9	5	5	467	477	5
6	16	2	439	445	5	8	8	3	48	7	14	7	1	4	82	80	6	8	10	4	286	285	5	11	5	5	267	262	5
8	16	2	125	88	9	10	8	3	63	74	12	9	1	4	1292	1310	9	10	10	4	431	446	5	13	5	5	348	351	5
10	16	2	704	700	6	12	8	3	630	626	5	11	1	4	1602	1617	12	12	10	4	154	169	7	15	5	5	110	105	9
1	17	2	238	233	6	14	8	3	411	410	5	13	1	4	172	161	5	14	10	4	950	946	8	17	5	5	159	163	8
3	17	2	371	362	6	16	8	3	246	243	6	15	1	4	251	247	5	16	10	4	142	136	6	0	6	5	401	441	4
5	17	2	172	177	7	18	8	3	215	210	7	17	1	4	15	23	15	1	11	4	126	113	6	2	6	5	99	106	6
7	17	2	34	17	34	1	9	3	596	595	5	19	1	4	561	568	6	3	11	4	339	336	4	4	6	5	101	112	6
9	17	2	430	431	6	3	9	3	64	62	9	0	2	4	334	372	3	5	11	4	1116	1147	9	6	6	5	419	420	4
0	18	2	790	764	7	5	9	3	429	429	4	2	2	4	163	162	3	7	11	4	110	102	8	8	6	5	329	314	4
2	18	2	0	1	1	7	9	3	256	258	4	4	2	4	461	456	4	9	11	4	0	10	1	10	6	5	117	124	7
4	18	2	170	170	7	9	9	3	29	31	29	6	2	4	443	471	4	11	11	4	0	5	1	12	6	5	225	217	5
6	18	2	453	436	6	11	9	3	888	880	7	8	2	4	104	110	6	13	11	4	70	87	15	14	6	5	16	41	16
1	1	3	288	292	3	13	9	3	18	31	18	10	2	4	468	486	4	15	11	4	760	750	6	16	6	5	715	711	6
3	1	3	642	645	5	15	9	3	110	105	9	12	2	4	302	304	4	0	12	4	1039	1029	8	1	7	5	119	108	6
5	1	3	171	175	3	17	9	3	544	543	5	14	2	4	654	649	6	2	12	4	289	292	5	3	7	5	497	503	4
7	1	3	282	284	3	0	10	3	681	690	5	16	2	4	717	720	6	4	12	4	46	54	20	5	7	5	72	77	9
9	1	3	440	437	4	2	10	3	736	743	6	18	2	4	56	49	18	6	12	4	252	248	5	7	7	5	320	325	4
11	1	3	1446	1441	11	4	10	3	111	128	4	20	2	4	143	150	8	8	12	4	180	177	6	9	7	5	293	293	5
13	1	3	466	470	4	6	10	3	197	195	5	1	3	4	238	248	3	10	12	4	393	403	5	11	7	5	388	378	5
15	1	3	110	111	7	8	10	3	267	271	5	3	3	4	501	505	4	12	12	4	327	311	6	13	7	5	147	142	7
17	1	3	373	378	5	10	10	3	19	6	19	5	3	4	3253	3266	11	14	12	4	40	49	39	15	7	5	17	21	16
19	1	3	467	476	5	12	10	3	62	64	14	7	3	4	185	185	4	1	13	4	168	176	6	17	7	5	58	48	19
21	1	3	946	940	8	14	10	3	541	544	5	9	3	4	787	799	6	3	13	4	64	59	12	0	8	5	803	808	6
0	2	3	2117	2155	8	16	10	3	29	17	28	11	3	4	23	27	22	5	13	4	287	290	5	2	8	5	96	109	7
2	2	3	537	539	4	1	11	3	295	295	4	13	3	4	309	303	5	7	13	4	245	248	5	4	8	5	29	9	28
4	2	3	57	64	6	3	11	3	262	261	4	15	3	4	631	639	6	9	13	4	577	597	6	6	8	5	530	528	5
6	2	3	1139	1125	9	5	11	3	704	712	6	17	3	4	748	736	6	11	13	4	726	731	6	8	8	5	151	144	6
8	2	3	698	702	5	7	11	3	267	279	5	19	3	4	167	155	7	13	13	4	161	163	8	10	8	5	73	70	12
10	2	3	385	381	4	9	11	3	160	173	5	0	4	4	423	448	3	0	14	4	1425	1434	10	12	8	5	424	423	5
12	2	3	770	774	6	11	11	3	163	159	6	2	4	4	356	342	3	2	14	4	227	224	6	14	8	5	510	517	5
14	2	3	396	406	4	13	11	3	64	56	14	4	4	4	671	699	5	4	14	4	315	320	5	16	8	5	856	843	7
16	2	3	1133	1155	8	15	11	3	109	101	10	6	4	4	1834	1830	11	6	14	4	461	472	5	1	9	5	690	696	6
18	2	3	276	275	6	17	11	3	592	591	6	8	4	4	204	207	4	8	14	4	71	65	14	3	9	5	82	85	9
20	2	3	96	92	11	0	12	3	236	226	5	10	4	4	227	230	5	10	14	4	1021	1032	8	5	9	5	440	428	4

Observed and calculated structure factors for K41

h	k	l	10Fo	10Fc	10s
7	9	5	356	355	5
9	9	5	38	24	37
11	9	5	1538	1538	12
13	9	5	109	113	9
15	9	5	111	105	10
0	10	5	917	891	7
2	10	5	495	503	5
4	10	5	124	115	7
6	10	5	468	463	5
8	10	5	159	163	6
10	10	5	214	205	6
12	10	5	87	81	11
14	10	5	428	428	6
1	11	5	75	84	10
3	11	5	257	262	5
5	11	5	570	458	5
7	11	5	540	549	5
9	11	5	216	210	6
11	11	5	425	440	5
13	11	5	157	161	8
0	12	5	1069	1068	8
2	12	5	433	439	5
4	12	5	33	48	32
6	12	5	630	641	5
8	12	5	123	127	8
10	12	5	113	115	9
12	12	5	268	258	6
1	13	5	309	308	5
3	13	5	294	293	5
5	13	5	869	874	7
7	13	5	175	173	7
9	13	5	259	262	6
11	13	5	1130	1145	9
0	14	5	830	816	7
2	14	5	259	260	6
4	14	5	316	307	5
6	14	5	444	454	5
8	14	5	236	240	6
1	15	5	131	132	8
3	15	5	203	199	7
5	15	5	91	89	11
7	15	5	321	324	6
0	16	5	155	148	8
2	16	5	256	262	6
4	16	5	89	92	13
0	0	6	2337	2476	12
2	0	6	68	65	9
4	0	6	623	632	5
6	0	6	706	709	6
8	0	6	293	302	5
10	0	6	838	831	7
12	0	6	739	739	6
14	0	6	735	736	6
16	0	6	794	798	7
1	1	6	126	115	6
3	1	6	192	185	5
5	1	6	1631	1662	12
7	1	6	40	49	22
9	1	6	355	358	5
11	1	6	204	212	6
13	1	6	61	52	14
15	1	6	372	374	5
17	1	6	354	341	6
0	2	6	1603	1663	12
2	2	6	209	207	4
4	2	6	206	211	5
6	2	6	510	521	5
8	2	6	250	258	5
10	2	6	724	728	6
12	2	6	291	293	5
14	2	6	42	35	28
16	2	6	431	430	6
1	3	6	196	194	5
3	3	6	148	144	5
5	3	6	719	734	6
7	3	6	47	42	16
9	3	6	1116	1121	8
11	3	6	1080	1075	8
13	3	6	257	248	5
15	3	6	44	31	27
0	4	6	2318	2361	12
2	4	6	55	45	11
4	4	6	316	320	4
6	4	6	491	498	5
8	4	6	94	87	8
10	4	6	1298	1313	9
12	4	6	299	298	5
14	4	6	74	77	13
16	4	6	196	194	7
1	5	6	202	199	5
3	5	6	262	267	5
5	5	6	473	461	5
7	5	6	55	48	14
9	5	6	185	189	6
11	5	6	396	388	5
13	5	6	91	111	11
15	5	6	208	203	6
0	6	6	226	213	5
2	6	6	43	47	17
4	6	6	611	614	5
6	6	6	794	800	6
8	6	6	298	294	5
10	6	6	177	191	6
12	6	6	152	155	7
14	6	6	885	882	7
1	7	6	576	578	5
3	7	6	206	195	5
5	7	6	2395	2395	14
7	7	6	119	118	7
9	7	6	374	369	5
11	7	6	470	472	5
13	7	6	190	176	7
15	7	6	539	543	6
0	8	6	173	168	5
2	8	6	173	170	6
4	8	6	247	248	5
6	8	6	305	304	5
8	8	6	116	124	5
10	8	6	135	127	7
12	8	6	171	179	7
14	8	6	388	382	6
1	9	6	275	272	5
3	9	6	112	114	8
5	9	6	123	55	7
7	9	6	440	445	5
9	9	6	562	556	5
11	9	6	727	724	6
13	9	6	70	75	16
0	10	6	2191	2149	14
2	10	6	365	368	5
4	10	6	365	368	5
6	10	6	539	552	5
8	10	6	65	53	15
10	10	6	1205	1203	9
12	10	6	163	158	8
1	11	6	88	99	10
3	11	6	342	342	5
5	11	6	456	457	5
7	11	6	118	108	8
9	11	6	454	454	5
11	11	6	724	727	6
0	12	6	432	441	5
2	12	6	35	24	35
4	12	6	0	3	1
6	12	6	907	910	7
8	12	6	0	14	1
10	12	6	388	401	6
1	13	6	62	68	16
3	13	6	86	85	11
5	13	6	1423	1410	11
7	13	6	155	153	8
0	14	6	35	23	35
2	14	6	360	152	6
4	14	6	134	141	6
6	14	6	178	164	8
1	1	7	85	85	8
3	1	7	242	251	5
5	1	7	76	75	10
7	1	7	266	270	5
9	1	7	243	249	6
11	1	7	762	758	7
13	1	7	162	160	6
15	1	7	135	131	8
0	2	7	612	617	5
2	2	7	304	301	5
4	2	7	59	59	13
6	2	7	459	462	5
8	2	7	290	285	5
10	2	7	99	99	10
12	2	7	563	556	6
14	2	7	234	227	6
1	3	7	194	186	5
3	3	7	33	29	12
5	3	7	342	350	5
7	3	7	470	457	5
9	3	7	155	152	7
11	3	7	740	727	6
13	3	7	45	44	28
0	4	7	959	953	7
2	4	7	120	103	7
4	4	7	289	282	5
6	4	7	68	60	12
8	4	7	217	224	6
10	4	7	219	210	6
12	4	7	477	482	5
14	4	7	119	122	9
1	5	7	35	30	35
3	5	7	201	199	5
5	5	7	323	323	5
7	5	7	510	516	5
9	5	7	374	378	5
11	5	7	70	35	14
13	5	7	226	238	7
0	6	7	166	166	6
2	6	7	98	101	8
4	6	7	140	144	7
6	6	7	654	650	6
8	6	7	228	239	6
10	6	7	176	181	7
12	6	7	205	194	7
1	7	7	74	84	11
3	7	7	282	278	5
5	7	7	620	615	6
7	7	7	127	115	8
9	7	7	340	348	6
11	7	7	484	483	5
0	8	7	489	494	5
2	8	7	117	121	8
4	8	7	313	307	5
6	8	7	326	316	5
8	8	7	57	42	17
10	8	7	45	42	30
1	9	7	411	406	5
3	9	7	11	18	11
5	9	7	283	291	6
7	9	7	116	121	9
9	9	7	29	45	29
0	10	7	473	484	5
2	10	7	408	403	5
4	10	7	147	138	7
6	10	7	193	192	7
8	10	7	146	139	8
1	11	7	165	164	7
3	11	7	162	161	7
5	11	7	515	509	5
7	11	7	191	188	7
0	12	7	61	39	17
2	12	7	160	156	7
4	12	7	254	251	6
0	0	8	2296	2403	15
2	0	8	161	157	7
4	0	8	282	259	5
6	0	8	714	700	6
8	0	8	50	58	25
10	0	8	1342	1337	10
1	1	8	87	89	10
3	1	8	123	124	8
5	1	8	541	546	5
7	1	8	172	168	7
9	1	8	685	688	6
11	1	8	474	468	6
0	2	8	13	11	13
2	2	8	61	63	15
4	2	8	275	272	6
6	2	8	496	491	5
8	2	8	0	42	1
10	2	8	266	254	6
1	3	8	127	130	7
3	3	8	337	333	5
5	3	8	1729	1703	12
7	3	8	25	14	25
9	3	8	436	430	6
11	3	8	156	166	8
0	4	8	273	279	5
2	4	8	250	245	6
4	4	8	258	261	6
6	4	8	602	606	5
8	4	8	45	32	27
10	4	8	82	77	13
1	5	8	503	515	5
3	5	8	148	149	7
5	5	8	393	398	5
7	5	8	11	6	10
9	5	8	209	208	7
0	6	8	1827	1827	12
2	6	8	215	203	6
4	6	8	375	369	5
6	6	8	437	432	5
8	6	8	186	176	7
1	7	8	41	40	41
3	7	8	114	108	9
5	7	8	906	876	7
7	7	8	225	218	7
0	8	8	910	911	7
2	8	8	42	24	29
4	8	8	32	26	32
6	8	8	342	346	6
1	9	8	53	51	21
3	9	8	170	167	8
5	9	8	1251	1218	10
0	10	8	1037	1016	8
2	10	8	168	160	7
1	1	9	92	78	11
3	1	9	187	183	7
5	1	9	277	278	6
0	2	9	103	96	9
2	2	9	81	30	12
4	2	9	293	282	6
6	2	9	0	33	1
1	3	9	191	180	7
3	3	9	27	11	26
5	3	9	73	68	15
0	4	9	425	419	6
2	4	9	36	55	35
4	4	9	56	64	21
1	5	9	29	14	28
3	5	9	106	97	10

Observed and calculated structure factors for K42

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	577	584	4	6	8	0	582	572	7	5	1	1	741	746	6	9	9	1	82	70	22	9	1	2	670	674	7
4	0	0	1271	1277	8	8	8	0	510	514	7	7	1	1	177	171	7	11	9	1	1693	1696	13	11	1	2	658	631	7
6	0	0	610	616	5	10	8	0	1389	1389	11	9	1	1	461	452	6	13	9	1	50	14	49	13	1	2	97	112	19
8	0	0	1051	1029	8	12	8	0	211	211	11	11	1	1	871	870	8	15	9	1	35	31	34	15	1	2	748	701	8
10	0	0	1745	1780	18	14	8	0	146	138	15	13	1	1	118	316	8	17	9	1	193	192	15	17	1	2	85	84	29
12	0	0	1376	1374	11	16	8	0	269	257	11	15	1	1	0	9	1	19	9	1	209	201	16	19	1	2	0	35	1
14	0	0	222	214	10	18	8	0	56	9	55	17	1	1	733	740	9	0	10	1	1283	1290	10	21	1	2	290	311	13
16	0	0	274	279	10	20	8	0	357	343	13	19	1	1	495	506	10	2	10	1	808	797	8	0	2	2	4307	4142	13
18	0	0	711	692	9	1	9	0	119	118	12	21	1	1	935	913	11	4	10	1	342	345	8	2	2	2	295	299	5
20	0	0	258	262	14	3	9	0	369	376	7	0	2	1	169	134	4	6	10	1	397	402	8	4	2	2	480	477	5
22	0	0	1587	1621	14	5	9	0	1870	1882	13	2	2	1	395	409	4	8	10	1	146	130	13	6	2	2	423	403	5
3	1	0	258	248	6	7	9	0	902	902	8	4	2	1	464	475	4	10	10	1	268	264	10	8	2	2	248	234	7
5	1	0	529	538	5	9	9	0	65	70	33	6	2	1	258	241	5	12	10	1	0	41	1	10	2	2	1301	1317	10
7	1	0	472	473	5	11	9	0	604	588	8	8	2	1	761	766	7	14	10	1	677	673	9	12	2	2	537	545	7
9	1	0	1722	1725	13	13	9	0	307	309	10	10	2	1	190	406	7	16	10	1	280	282	13	14	2	2	124	139	16
11	1	0	2830	2851	19	15	9	0	514	542	10	12	2	1	986	974	9	18	10	1	323	312	13	16	2	2	316	319	10
13	1	0	284	293	8	17	9	0	478	496	11	14	2	1	135	134	14	1	11	1	263	278	9	18	2	2	71	74	46
15	1	0	232	242	10	19	9	0	311	293	13	16	2	1	738	739	8	3	11	1	297	294	9	20	2	2	71	30	53
17	1	0	258	270	11	0	10	0	343	353	8	18	2	1	7	40	6	5	11	1	632	649	8	1	3	2	337	345	5
19	1	0	627	615	10	2	10	0	33	23	33	20	2	1	118	147	22	7	11	1	475	481	8	3	3	2	207	199	6
21	1	0	762	768	10	4	10	0	464	453	7	22	2	1	233	241	14	9	11	1	381	386	9	5	3	2	1101	1105	8
0	2	0	1296	1315	8	6	10	0	252	262	9	1	3	1	293	300	4	11	11	1	390	400	10	7	3	2	148	144	9
2	2	0	264	277	3	8	10	0	373	388	8	3	3	1	206	209	5	13	11	1	110	91	23	9	3	2	1663	1682	13
4	2	0	707	715	6	10	10	0	564	580	8	5	3	1	272	257	5	15	11	1	80	63	38	11	3	2	1368	1373	11
6	2	0	122	128	8	12	10	0	125	123	18	7	3	1	522	512	5	17	11	1	413	408	12	13	3	2	540	539	8
8	2	0	287	279	6	14	10	0	1213	1210	11	9	3	1	279	296	7	0	12	1	1200	1200	10	15	3	2	178	191	12
10	2	0	670	678	7	16	10	0	262	252	12	11	3	1	243	249	8	2	12	1	459	467	8	17	3	2	287	283	11
12	2	0	286	288	8	18	10	0	604	601	11	13	3	1	131	126	8	4	12	1	83	78	22	19	3	2	855	853	10
14	2	0	871	868	8	1	11	0	332	327	8	15	3	1	20	21	19	6	12	1	636	632	8	21	3	2	563	550	11
16	2	0	717	725	8	3	11	0	319	321	9	17	3	1	349	345	10	8	12	1	200	208	12	0	4	2	2054	2053	14
18	2	0	59	64	58	5	11	0	952	965	9	19	3	1	192	206	15	10	12	1	242	232	12	2	4	2	738	735	6
20	2	0	198	194	15	7	11	0	152	169	12	21	3	1	339	352	12	12	12	1	267	283	12	4	4	2	0	13	1
22	2	0	160	351	13	9	11	0	98	109	22	0	4	1	974	980	7	14	12	1	36	56	36	6	4	2	276	260	7
1	3	0	356	348	3	11	11	0	479	480	9	2	4	1	42	42	22	16	12	1	745	724	11	8	4	2	207	228	8
3	3	0	466	463	4	13	11	0	185	190	15	4	4	1	288	282	5	1	13	1	337	332	9	10	4	2	2110	2148	16
5	3	0	4853	4886	15	15	11	0	939	940	10	6	4	1	831	788	7	3	13	1	361	350	9	12	4	2	293	291	9
7	3	0	463	456	5	17	11	0	430	454	12	8	4	1	553	549	6	5	13	1	991	998	9	14	4	2	257	255	10
9	3	0	1049	1042	8	0	12	0	1467	1484	12	10	4	1	213	188	9	7	13	1	72	74	35	16	4	2	0	11	1
11	3	0	336	339	8	2	12	0	224	227	10	12	4	1	725	726	7	9	13	1	356	365	11	18	4	2	539	534	10
13	3	0	450	445	8	4	12	0	298	284	9	14	4	1	298	287	9	11	13	1	1080	1097	11	20	4	2	386	366	12
15	3	0	894	895	9	6	12	0	635	655	8	16	4	1	664	667	9	13	13	1	124	114	21	1	5	2	1016	1007	8
17	3	0	950	939	9	8	12	0	168	174	14	18	4	1	222	236	14	15	13	1	267	260	14	3	5	2	92	86	11
19	3	0	235	241	13	10	12	0	617	623	9	20	4	1	140	122	21	0	14	1	652	668	9	5	5	2	1805	1780	13
21	3	0	182	187	12	12	12	0	543	533	10	1	5	1	126	123	7	2	14	1	338	304	10	7	5	2	175	163	9
0	4	0	2248	2265	11	14	12	0	150	129	17	3	5	1	677	674	6	4	14	1	459	483	9	9	5	2	438	442	7
2	4	0	638	640	5	16	12	0	105	117	30	5	5	1	1623	1653	12	6	14	1	228	222	13	11	5	2	664	651	7
4	4	0	1148	1163	9	1	13	0	449	469	9	7	5	1	872	850	8	8	14	1	303	317	12	13	5	2	45	57	44
6	4	0	3639	3592	15	3	13	0	231	217	10	9	5	1	551	555	7	10	14	1	186	185	15	15	5	2	277	263	10
8	4	0	552	552	6	5	13	0	411	406	9	11	5	1	323	340	8	12	14	1	132	132	22	17	5	2	782	779	9
10	4	0	528	537	7	7	13	0	507	508	9	13	5	1	689	710	8	14	14	1	435	429	12	19	5	2	445	432	11
12	4	0	272	258	8	9	13	0	482	482	9	15	5	1	189	180	12	1	15	1	49	12	49	21	5	2	494	486	12
14	4	0	923	922	9	11	13	0	918	921	9	17	5	1	263	249	12	3	15	1	257	259	12	0	6	2	1142	1138	9
16	4	0	1985	1992	15	13	13	0	319	327	12	19	5	1	29	29	28	5	15	1	288	291	11	2	6	2	96	105	11
18	4	0	154	137	16	15	13	0	273	267	13	21	5	1	816	817	11	7	15	1	288	289	12	4	6	2	1046	1063	9
20	4	0	294	285	13	0	14	0	1547	1541	13	0	6	1	381	366	5	9	15	1	97	78	30	6	6	2	2397	2311	18
1	5	0	1486	1448	10	2	14	0	446	440	9	2	6	1	231	231	6	11	15	1	166	160	18	8	6	2	233	224	8
3	5	0	85	81	10	4	14	0	212	197	12	4	6	1	268	260	6	13	15	1	57	110	57	10	6	2	29	20	29
5	5	0	3219	3191	15	6	14	0	726	737	9	6	6	1	862	856	7	0	16	1	290	289	12	12	6	2	385	382	8
7	5	0	859	843	7	8	14	0	177	182	15	8	6	1	480	470	7	2	16	1	264	255	13	14	6	2	991	992	9
9	5	0	165	169	9	10	14	0	1420	1402	11	10	6	1	35	50	35	4	16	1	18	50	18	16	6	2	1431	1454	13
11	5	0	129	351	8	12	14	0	48	75	48	12	6	1	344	339	8	6	16	1	1250	1248	11	18	6	2	91	68	31
13	5	0	104	312	9	14	14	0	0	40	1	14	6	1	0	8	1	8	16	1	282	309	14	20	6	2	84	67	19
15	5	0	287	291	10	1	15	0	295	280	11	16	6	1	1049	1060	10	10	16	1	78	56	45	1	7	2	750	747	7
17	5	0	469	467	10	3	15	0	411	405	10	18	6	1	252	253	13	12	16	1	125	97	25	3	7	2	85	96	14
19	5	0	204	209	15	5	15	0	502	499	10	20	6	1	440	419	11	1	17	1	0	32	1	5	7	2	4740	4580	19
21	5	0	251	274	14	7	15	0	60	34	60	1	7	1	94	72	10	3	17	1	304	297	13	7	7	2	217	202	9
0	6	0	999	992	8	9	15	0	165	167	17	3	7	1	627	622	6	5	17	1	741	739	10	9	7	2	506	503	7
2	6	0	80	96	11	11	15	0	403	397	11	5	7	1	416	414	6	7	17	1	278	270	14	11	7	2	103	110	19
4	6	0	380	391	5	13	15	0	483	459	11	7	7	1	177	164	9	9	17	1	456	438	12	13	7	2	455	436	9
6	6	0	537	524	6	0	16	0	582	572	10	9	7	1	524	532	7	0	18	1	312	280	13	15	7	2	965	968	9
8	6	0	593	591	7	2	16	0	190	179	16	11	7	1	0	17	1	2	18	1	78	42	51	17	7	2	886	907	10
10	6	0	1384	1410	11	4	16	0	201	203	15	13	7	1	23	65	22	4	18	1	378	382	12	19	7	2	85	66	18
12	6	0	315	322	9	6	16	0	827	836	10	15	7	1	69	61	17	6	18	1	392	383	13	0	8	2	432	435	7
14	6	0	473	457	9	8	16	0	74	77	49	17	7	1	180	184	16	1	19	1	328	328	14	2	8	2	465	461	7
16	6	0	522	526	9	10	16	0	0	16	1	19	7	1	175	164	17	3	19	1	374	393	14	4	8	2	229	241	8
18	6	0	407	417	11	12	16	0	404	420	12	0	8	1	715	717	7	0	0	2	3441	3489	12	6	8	2	389	377	8
20	6	0	0	7	1	1	17	0	260	255	13	2	8	1	89	81	13	2	0	2	638	657	5	8	8	2	649	636	7
1	7	0	765	754	7	3	17	0	331	355	12	4	8	1	107	132	12	4	0	2	456	458	5	10	8	2	92	76	22
3	7	0	173	189	7	5	17	0	1895	1893	15	6	8	1	336	329	7	6	0	2	779	740	6	12	8	2	231	232	12
5	7	0	1466	1478	10	7	17	0	37	33	37	8	8	1	175	187	10	8	0	2	698	683	7	14	8	2	591	585	9
7	7	0	442	427	7	9	17	0	64	24	64	10	8	1	131	115	14	10	0	2	1420	1419	11	16	8	2	906	911	10
9	7	0	1272	1286	10	0	18	0	306	306	13	12	8	1	462	473	9	12	0	2	884	885	8	18	8	2	94	97	14
11	7	0	568	528	8	2	18	0	288	312	14	14	8	1	601	589	9	14	0	2	1354	1379	12	1	9	2	497	460	7
13	7	0	454	450	8	4	18	0	87	81	42	16	8	1	756	755	9	16	0	2	736	740	9	3	9	2	59	39	29
15	7	0	252	254	11	6	18	0	242	229	15	18	8	1	317	315	12	18	0	2	916	912	10	5	9	2	445	444	8
17	7	0	194	193	14	8	18	0	336	342	13	20	8	1	211	216	16	20	0	2	83	60	37	7	9	2	413	405	8
19	7	0	743	734	10	1	19	0	236	239	15	1	9	1	948	931	8	1	1	2	508	520	4	9	9	2	700	705	8
0	8	0	2645	2643	17	3	19	0	71	76	71	3	9	1	196	197	9	3	1	2	681	695	6	11	9	2	1593	1580	12
2	8	0	113	135	11	1	1	1	160	155	4	5	9	1	471	503	7	5	1	2	1147	1164	9	13	9	2	78	83	30
4	8	0	441	438	6	3	1	1	550	545	5	7	9	1	289	301	8	7	1	2	203	194	7	15	9	2	344	335	11

Observed and calculated structure factors for K42

h	k	l	10Fo	10Fc	10s
17	9	2	623	632	10
19	9	2	294	291	14
0	10	2	4241	4453	21
2	10	2	612	605	7
4	10	2	745	741	8
6	10	2	65	51	30
8	10	2	363	353	9
10	10	2	1926	1917	15
12	10	2	313	323	11
14	10	2	365	356	11
16	10	2	183	194	16
18	10	2	343	327	12
1	11	2	278	302	9
3	11	2	717	730	8
5	11	2	92	113	21
7	11	2	50	28	49
9	11	2	685	686	9
11	11	2	1736	1745	13
13	11	2	39	43	39
15	11	2	269	267	13
17	11	2	116	125	27
0	12	2	1374	1398	12
2	12	2	46	7	46
4	12	2	42	50	41
6	12	2	863	875	9
8	12	2	191	186	13
10	12	2	835	824	9
12	12	2	251	246	12
14	12	2	544	535	10
16	12	2	371	365	12
1	13	2	175	169	13
3	13	2	0	36	1
5	13	2	1825	1857	14
7	13	2	87	83	28
9	13	2	102	128	23
11	13	2	76	91	43
13	13	2	143	126	20
15	13	2	539	551	11
0	14	2	509	485	9
2	14	2	333	321	10
4	14	2	738	742	9
6	14	2	457	428	10
8	14	2	227	228	14
10	14	2	200	192	15
12	14	2	92	82	13
14	14	2	198	197	12
1	15	2	592	573	9
3	15	2	295	300	12
5	15	2	1492	1505	12
7	15	2	518	530	10
9	15	2	113	93	26
11	15	2	390	379	12
13	15	2	169	165	20
0	16	2	989	981	10
2	16	2	176	147	16
4	16	2	85	96	18
6	16	2	468	467	11
8	16	2	55	54	55
10	16	2	725	713	11
1	17	2	241	221	14
3	17	2	411	412	12
5	17	2	158	186	20
7	17	2	0	21	1
9	17	2	385	373	13
0	18	2	793	781	11
2	18	2	51	13	51
4	18	2	249	244	16
6	18	2	381	402	13
1	1	3	258	254	6
3	1	3	717	718	6
5	1	3	292	293	6
7	1	3	228	228	7
9	1	3	396	405	7
11	1	3	1403	1395	11
13	1	3	393	404	9
15	1	3	66	58	14
17	1	3	365	360	10
19	1	3	475	491	11
21	1	3	886	879	11
0	2	3	2405	2376	15
2	2	3	496	480	5
4	2	3	27	34	26
6	2	3	1126	1103	9
8	2	3	832	831	8
10	2	3	423	434	8
12	2	3	746	736	8
14	2	3	340	341	10
16	2	3	1119	1123	10
18	2	3	170	152	16
20	2	3	66	69	66
1	3	3	500	512	5
3	3	3	284	290	6
5	3	3	1123	1107	9
7	3	3	760	754	7
9	3	3	221	212	9
11	3	3	1334	1329	11
13	3	3	112	108	17
15	3	3	63	88	45
17	3	3	209	224	14
19	3	3	170	131	18
21	3	3	424	422	12
0	4	3	2122	2040	16
2	4	3	75	80	14
4	4	3	394	390	6
6	4	3	217	206	8
8	4	3	294	310	8
10	4	3	325	331	9
12	4	3	791	786	8
14	4	3	148	122	14
16	4	3	229	247	13
18	4	3	138	142	20
20	4	3	73	53	56
1	5	3	50	67	28
3	5	3	435	447	6
5	5	3	1001	999	8
7	5	3	851	845	8
9	5	3	428	429	8
11	5	3	163	157	12
13	5	3	540	542	9
15	5	3	105	85	23
17	5	3	318	307	12
19	5	3	101	73	29
0	6	3	620	622	6
2	6	3	79	62	15
4	6	3	480	466	7
6	6	3	1184	1186	9
8	6	3	342	340	8
10	6	3	100	104	17
12	6	3	291	296	10
14	6	3	84	89	27
16	6	3	1128	1128	10
18	6	3	401	382	11
20	6	3	362	379	13
1	7	3	120	122	11
3	7	3	305	319	7
5	7	3	1171	1154	9
7	7	3	221	210	9
9	7	3	506	522	8
11	7	3	798	793	8
13	7	3	164	137	14
15	7	3	185	162	14
17	7	3	611	609	10
19	7	3	164	133	19
0	8	3	819	810	8
2	8	3	173	175	10
4	8	3	147	160	8
6	8	3	569	561	7
8	8	3	62	14	32
10	8	3	69	42	33
12	8	3	573	569	9
14	8	3	159	166	11
16	8	3	272	236	12
18	8	3	158	144	20
1	9	3	585	571	7
3	9	3	75	60	24
5	9	3	210	209	10
7	9	3	214	210	11
9	9	3	117	108	17
11	9	3	900	894	9
13	9	3	38	31	37
15	9	3	92	61	29
17	9	3	525	530	11
0	10	3	874	871	8
2	10	3	793	804	8
4	10	3	439	441	8
6	10	3	186	172	11
8	10	3	210	213	12
10	10	3	70	60	38
12	10	3	127	136	19
14	10	3	661	663	10
16	10	3	73	71	50
1	11	3	380	370	8
3	11	3	254	240	10
5	11	3	719	712	8
7	11	3	170	178	14
9	11	3	451	445	10
11	11	3	109	119	24
13	11	3	93	89	28
15	11	3	104	80	27
17	11	3	532	520	12
0	12	3	298	302	10
2	12	3	270	253	10
4	12	3	327	332	10
6	12	3	152	121	15
8	12	3	113	128	21
10	12	3	228	222	13
12	12	3	264	279	13
14	12	3	143	149	23
16	12	3	417	423	12
1	13	3	234	228	12
3	13	3	445	462	10
5	13	3	377	384	10
7	13	3	132	131	17
9	13	3	316	302	12
11	13	3	374	377	11
13	13	3	0	22	1
15	13	3	165	173	20
0	14	3	43	6	42
2	14	3	273	266	12
4	14	3	430	420	10
6	14	3	213	212	13
8	14	3	359	380	11
10	14	3	27	17	26
12	14	3	0	21	1
1	15	3	192	188	15
3	15	3	176	172	16
5	15	3	501	485	10
7	15	3	174	153	17
9	15	3	127	136	25
11	15	3	350	354	13
0	16	3	136	130	22
2	16	3	76	82	45
4	16	3	182	181	17
6	16	3	1105	1091	11
8	16	3	244	246	15
10	16	3	112	107	32
1	17	3	138	106	21
3	17	3	317	307	13
5	17	3	486	456	12
7	17	3	20	5	19
0	18	3	223	232	16
2	18	3	143	150	23
0	0	4	6641	6688	19
2	0	4	334	344	6
4	0	4	718	742	7
6	0	4	400	399	7
8	0	4	344	349	8
10	0	4	2679	2717	22
12	0	4	923	925	9
14	0	4	388	391	9
16	0	4	156	132	16
18	0	4	668	651	10
20	0	4	165	139	19
1	1	4	242	210	7
3	1	4	93	75	13
5	1	4	246	220	8
7	1	4	77	51	19
9	1	4	1306	1322	11
11	1	4	1624	1614	13
13	1	4	155	148	13
15	1	4	166	177	15
17	1	4	43	49	43
19	1	4	586	561	11
0	2	4	317	342	7
2	2	4	191	185	8
4	2	4	443	438	7
6	2	4	454	482	7
8	2	4	110	95	14
10	2	4	465	461	8
12	2	4	292	302	10
14	2	4	629	643	9
16	2	4	719	734	10
18	2	4	34	40	33
20	2	4	141	136	22
1	3	4	242	250	7
3	3	4	395	401	7
5	3	4	3393	3421	19
7	3	4	140	144	11
9	3	4	793	812	8
11	3	4	87	71	23
13	3	4	379	390	9
15	3	4	760	767	9
17	3	4	716	719	10
19	3	4	198	209	17
0	4	4	580	605	6
2	4	4	422	414	7
4	4	4	693	718	7
6	4	4	1793	1803	14
8	4	4	256	260	9
10	4	4	370	370	9
12	4	4	120	156	17
14	4	4	866	894	9
16	4	4	1444	1428	12
18	4	4	175	186	17
1	5	4	1031	999	8
3	5	4	147	140	10
5	5	4	1559	1583	12
7	5	4	420	404	8
9	5	4	162	147	12
11	5	4	897	912	9
13	5	4	165	157	14
15	5	4	273	280	12
17	5	4	63	79	62
19	5	4	127	137	23
0	6	4	2221	2213	15
2	6	4	138	132	11
4	6	4	376	382	8
6	6	4	184	172	10
8	6	4	309	303	9
10	6	4	1271	1294	11
12	6	4	401	405	10
14	6	4	227	247	12
16	6	4	198	194	15
18	6	4	306	307	13
1	7	4	304	303	8
3	7	4	263	250	9
5	7	4	1365	1348	10
7	7	4	372	353	8
9	7	4	987	1000	9
11	7	4	730	710	9
13	7	4	380	378	10
15	7	4	246	247	13
17	7	4	313	317	13
0	8	4	1920	1945	14
2	8	4	20	6	19
4	8	4	192	194	10
6	8	4	556	527	8
8	8	4	411	412	9
10	8	4	1175	1210	11
12	8	4	154	135	16
14	8	4	140	125	18
16	8	4	226	206	14
18	8	4	105	67	29
1	9	4	62	61	34
3	9	4	248	257	10
5	9	4	1737	1771	14
7	9	4	509	513	9
9	9	4	0	6	1
11	9	4	187	179	14
13	9	4	151	142	16
15	9	4	356	378	12
17	9	4	602	590	11
0	10	4	879	893	9
2	10	4	31	28	30
4	10	4	494	514	9
6	10	4	206	220	12
8	10	4	358	381	10
10	10	4	511	501	10
12	10	4	164	172	16
14	10	4	906	920	10
16	10	4	374	393	13
1	11	4	192	186	13
3	11	4	409	389	9
5	11	4	1170	1180	10
7	11	4	82	73	27
9	11	4	37	44	37
11	11	4	0	21	1
13	11	4	135	123	21
15	11	4	814	800	11
0	12	4	919	927	9
2	12	4	267	248	11
4	12	4	154	167	16
6	12	4	315	314	11
8	12	4	209	233	14
10	12	4	413	403	11
12	12	4	362	361	12
14	12	4	68	33	67
1	13	4	260	245	11
3	13	4	144	130	17
5	13	4	273	258	11
7	13	4	290	294	12
9	13	4	484	479	11
11	13	4	730	728	11
13	13	4	215	182	16
0	14	4	1476	1482	12
2	14	4	261	266	12
4	14	4	293	310	12
6	14	4	476	499	11
8	14	4	174	147	17
10	14	4	1095	1106	11
12	14	4	69	41	69
1	15	4	228	234	14
3	15	4	419	408	11
5	15	4	255	223	13
7	15	4	154	153	20
9	15	4	144	153	23
0	16	4	146	135	19
2	16	4	156	164	20
4	16	4	163	142	19
6	16	4	454	461	12
8	16	4	62	3	61
1	17	4	128	133	13
3	17	4	240	230	16
1	1	5	72	66	20
3	1	5	284	284	8
5	1	5	593	593	7
7	1	5	49	57	49
9	1	5	364	372	9
11	1	5	267	261	11
13	1	5	151	164	16
15	1	5	75	25	36
17	1	5	747	749	10
19	1	5	414	401	12
0	2	5	627	615	7
2	2	5	37	25	37
4	2	5	445	458	8
6	2	5	448	455	8
8	2	5	415	410	8
10	2	5	164	158	13
12	2	5	770	769	9
14	2	5	64	58	63
16	2	5	315	288	12
18	2	5	132	137	22
1	3	5	98	112	16
3	3	5	201	193	9
5	3	5	488	497	8
7	3	5	103	120	18
9	3	5	132	124	15
11	3	5	270	275	11
13	3	5	327	323	10
15	3	5	42	29	42
17	3	5	534	539	11
0	4	5	0	54	1
2	4	5	77	22	21
4	4	5	151	149	12
6	4	5	670	669	8
8	4	5	173	194	9
10	4	5	92	97	23
12	4	5	521	505	9
14	4	5	270	280	12
16	4	5	692	679	10
18	4	5	268	263	13
1	5	5	163	149	12
3	5	5	176	177	8
5	5	5	794	804	8
7	5	5	591	580	8
9	5	5	410	409	9
11	5	5	290	278	11
13	5	5	468	480	10
15	5	5	129	120	23
17	5	5	161	185	20
0	6	5	101	335	9
2	6	5	133	132	14
4	6	5	55	32	44
6	6	5	419	415	8
8	6	5	105	109	10
10	6	5	35	25	35
12	6	5	257	246	12
14	6	5	0	4	1
16	6	5	726	719	10
1	7	5	44	38	43
3	7	5	494	503	8
5	7	5	39	18	38
7	7	5	282	293	10
9	7	5	169	163	10
11	7	5	409	187	10
13	7	5	190	172	15
15	7	5	50	28	50
17	7	5	62	69	62
0	8	5	824	834	9
2	8	5	74	79	28
4	8	5	29	3	29
6	8	5	567	552	9
8	8	5	156	153	16
10	8	5	93	70	23
12	8	5	342	347	11
14	8	5	522	503	11
16	8	5	793	784	11
1	9	5	671	675	8
3	9	5	100	101	21

Observed and calculated structure factors for K42

h	k	l	10Fo	10Fc	10s
5	9	5	562	562	9
7	9	5	310	320	11
9	9	5	56	58	56
11	9	5	1521	1528	12
13	9	5	76	70	42
15	9	5	79	61	48
0	10	5	1015	1009	10
2	10	5	514	517	9
4	10	5	176	180	14
6	10	5	446	424	10
8	10	5	99	92	27
10	10	5	246	265	14
12	10	5	0	28	1
14	10	5	497	506	12
1	11	5	144	135	17
3	11	5	256	231	11
5	11	5	439	441	10
7	11	5	483	490	10
9	11	5	257	256	13
11	11	5	404	427	12
13	11	5	165	168	19
0	12	5	1164	1151	10
2	12	5	470	474	10
4	12	5	84	80	31
6	12	5	661	680	10
8	12	5	130	131	22
10	12	5	147	123	20
12	12	5	235	235	15
1	13	5	271	287	13
3	13	5	235	255	14
5	13	5	941	965	10
7	13	5	198	181	16
9	13	5	311	322	13
11	13	5	1192	1188	11
0	14	5	868	855	10
2	14	5	259	252	14
4	14	5	383	390	12
6	14	5	374	385	12
8	14	5	211	214	16
1	15	5	97	80	30
3	15	5	228	226	16
5	15	5	117	109	27
7	15	5	293	276	14
0	16	5	267	252	14
2	16	5	278	279	14
4	16	5	177	151	18
0	0	6	2608	2618	18
2	0	6	120	115	15
4	0	6	670	676	8
6	0	6	676	684	8
8	0	6	438	434	9
10	0	6	900	905	9
12	0	6	701	714	10
14	0	6	794	797	10
16	0	6	862	848	10
1	1	6	142	144	14
3	1	6	129	116	15
5	1	6	1732	1747	13
7	1	6	83	55	24
9	1	6	351	360	10
11	1	6	246	231	12
13	1	6	0	22	1
15	1	6	466	460	11
17	1	6	317	313	13
0	2	6	1718	1712	14
2	2	6	197	192	10
4	2	6	184	184	11
6	2	6	494	480	9
8	2	6	224	235	12
10	2	6	784	797	9
12	2	6	289	301	12
14	2	6	56	27	55
16	2	6	351	380	12
1	3	6	188	169	11
3	3	6	96	78	20
5	3	6	836	830	8
7	3	6	64	54	43
9	3	6	1123	1134	10
11	3	6	1092	1085	10
13	3	6	289	283	12
15	3	6	66	85	66
0	4	6	2459	2488	18
2	4	6	100	97	19
4	4	6	361	354	9
6	4	6	486	497	9
8	4	6	173	168	15
10	4	6	1428	1428	12
12	4	6	249	266	13
14	4	6	70	70	51
16	4	6	202	214	17
1	5	6	285	282	10
3	5	6	309	314	10
5	5	6	453	452	9
7	5	6	106	99	19
9	5	6	245	232	11
11	5	6	346	347	11
13	5	6	81	74	38
15	5	6	223	227	15
0	6	6	158	154	14
2	6	6	0	9	1
4	6	6	548	543	9
6	6	6	834	825	9
8	6	6	306	286	11
10	6	6	106	102	24
12	6	6	161	175	17
14	6	6	859	862	10
1	7	6	607	603	9
3	7	6	127	126	17
5	7	6	2554	2511	17
7	7	6	94	108	28
9	7	6	424	408	10
11	7	6	459	457	11
13	7	6	235	264	15
15	7	6	635	637	11
0	8	6	296	286	11
2	8	6	204	191	12
4	8	6	321	325	11
6	8	6	263	265	12
8	8	6	380	374	11
10	8	6	104	93	27
12	8	6	224	215	15
14	8	6	410	411	12
1	9	6	336	336	11
3	9	6	127	116	19
5	9	6	58	49	57
7	9	6	477	482	10
9	9	6	484	480	11
11	9	6	713	714	10
13	9	6	69	64	68
0	10	6	2231	2186	16
2	10	6	295	288	11
4	10	6	343	326	11
6	10	6	554	544	10
8	10	6	138	131	20
10	10	6	1293	1301	11
12	10	6	190	174	18
1	11	6	36	53	36
3	11	6	349	343	11
5	11	6	415	422	11
7	11	6	95	86	30
9	11	6	510	503	11
11	11	6	689	703	11
0	12	6	533	549	10
2	12	6	49	50	49
4	12	6	26	82	25
6	12	6	901	921	10
8	12	6	0	41	1
10	12	6	432	439	12
1	13	6	72	10	61
3	13	6	0	15	1
5	13	6	1382	1383	13
7	13	6	215	202	16
0	14	6	0	13	1
2	14	6	373	373	12
4	14	6	341	330	13
1	1	7	67	74	38
3	1	7	271	269	11
5	1	7	25	13	24
7	1	7	267	239	11
9	1	7	218	223	13
11	1	7	714	742	10
13	1	7	286	317	13
15	1	7	90	98	40
0	2	7	727	727	9
2	2	7	292	283	10
4	2	7	32	11	11
6	2	7	459	456	10
8	2	7	337	336	11
10	2	7	133	143	20
12	2	7	545	535	11
14	2	7	150	168	21
1	3	7	181	182	13
3	3	7	0	25	1
5	3	7	416	411	10
7	3	7	461	455	10
9	3	7	174	189	16
11	3	7	768	754	10
13	3	7	0	16	1
0	4	7	987	948	9
2	4	7	118	113	20
4	4	7	282	278	11
6	4	7	39	78	39
8	4	7	250	234	12
10	4	7	238	214	13
12	4	7	459	478	12
14	4	7	136	141	24
1	5	7	37	13	36
3	5	7	238	234	12
5	5	7	370	381	11
7	5	7	501	502	10
9	5	7	304	306	12
11	5	7	70	57	69
13	5	7	317	331	14
0	6	7	253	266	12
2	6	7	94	101	28
4	6	7	212	209	14
6	6	7	678	666	10
8	6	7	214	243	15
10	6	7	130	113	21
12	6	7	176	201	19
1	7	7	29	49	29
3	7	7	280	287	12
5	7	7	701	681	10
7	7	7	117	138	25
9	7	7	386	387	12
11	7	7	483	484	12
0	8	7	478	483	10
2	8	7	147	137	19
4	8	7	287	281	12
6	8	7	318	315	12
8	8	7	76	63	49
10	8	7	48	40	47
1	9	7	392	375	11
3	9	7	0	19	1
5	9	7	171	174	17
7	9	7	103	110	28
9	9	7	22	11	21
0	10	7	586	583	10
2	10	7	448	442	11
4	10	7	224	206	14
6	10	7	183	174	17
8	10	7	107	101	30
1	11	7	204	202	16
3	11	7	161	149	19
5	11	7	534	511	11
7	11	7	131	140	25
0	12	7	133	108	23
2	12	7	140	159	25
4	12	7	221	230	17
0	0	8	2497	2533	19
2	0	8	131	128	20
4	0	8	280	277	12
6	0	8	688	705	10
8	0	8	79	35	42
10	0	8	1485	1465	13
1	1	8	74	77	43
3	1	8	100	122	28
5	1	8	492	481	10
7	1	8	179	173	17
9	1	8	711	716	10
11	1	8	478	477	12
0	2	8	31	1	30
2	2	8	81	72	12
4	2	8	267	262	13
6	2	8	511	497	10
8	2	8	0	36	1
10	2	8	235	247	16
1	3	8	158	134	17
3	3	8	301	286	11
5	3	8	1810	1799	14
7	3	8	0	29	1
9	3	8	458	450	11
11	3	8	149	139	22
0	4	8	202	211	15
2	4	8	282	276	12
4	4	8	295	280	12
6	4	8	566	581	10
8	4	8	75	61	54
10	4	8	166	165	20
1	5	8	524	539	11
3	5	8	116	141	26
5	5	8	456	448	11
7	5	8	18	20	18
9	5	8	146	154	23
0	6	8	1910	1876	14
2	6	8	156	168	20
4	6	8	322	327	12
6	6	8	459	463	11
8	6	8	126	133	25
1	7	8	75	85	54
3	7	8	181	169	17
5	7	8	921	927	10
7	7	8	186	205	18
0	8	8	971	958	10
2	8	8	69	57	68
4	8	8	31	13	30
6	8	8	347	376	13
1	9	8	0	9	1
3	9	8	129	145	26
5	9	8	1243	1237	11
0	10	8	1033	1044	11
2	10	8	141	111	24
1	1	9	74	52	53
3	1	9	216	212	17
5	1	9	237	243	15
0	2	9	0	31	1
2	2	9	0	18	1
4	2	9	218	217	16
6	2	9	49	6	49
1	3	9	138	150	23
3	3	9	0	17	1
5	3	9	0	43	1
0	4	9	413	408	12
2	4	9	29	51	28
4	4	9	85	81	46
1	5	9	0	2	1
3	5	9	129	129	25

Observed and calculated structure factors for K43

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	772	788	7	4	8	0	485	479	5	3	1	1	382	369	4	7	9	1	299	298	5	7	1	2	95	103	5
4	0	0	1247	1263	11	6	8	0	641	634	6	5	1	1	936	948	9	9	9	1	39	41	20	9	1	2	677	678	7
6	0	0	492	501	4	8	8	0	400	394	5	7	1	1	129	106	4	11	9	1	1636	1661	18	11	1	2	689	697	7
8	0	0	819	816	8	10	8	0	1231	1238	13	9	1	1	420	414	4	13	9	1	103	95	10	13	1	2	23	3	23
10	0	0	3614	3636	21	12	8	0	188	196	7	11	1	1	746	772	8	15	9	1	122	113	9	15	1	2	647	652	6
12	0	0	1326	1380	15	14	8	0	115	119	9	13	1	1	354	361	5	17	9	1	138	140	9	17	1	2	110	105	9
14	0	0	281	273	5	16	8	0	319	322	7	15	1	1	106	105	8	19	9	1	182	195	9	19	1	2	37	17	16
16	0	0	198	200	7	18	8	0	50	65	26	17	1	1	705	712	7	0	10	1	1264	1292	12	21	1	2	360	336	7
18	0	0	521	506	6	20	8	0	313	313	8	19	1	1	487	488	7	2	10	1	791	781	8	0	2	2	4039	4001	16
20	0	0	317	316	7	1	9	0	0	10	1	21	1	1	791	773	7	4	10	1	243	249	5	2	2	2	421	411	4
22	0	0	1666	1696	16	3	9	0	441	442	4	0	2	1	143	166	3	6	10	1	451	446	5	4	2	2	568	551	5
3	1	0	259	259	2	5	9	0	1784	1814	21	2	2	1	528	541	5	8	10	1	165	165	7	6	2	2	507	510	5
5	1	0	480	491	5	7	9	0	837	822	9	4	2	1	490	482	4	10	10	1	288	280	6	8	2	2	303	300	4
7	1	0	385	380	3	9	9	0	0	9	1	6	2	1	308	286	3	12	10	1	33	16	32	10	2	2	1282	1274	14
9	1	0	1540	1553	18	11	9	0	712	697	7	8	2	1	535	543	5	14	10	1	647	636	6	12	2	2	513	518	5
11	1	0	2876	2907	22	13	9	0	218	226	7	10	2	1	159	175	5	16	10	1	316	326	7	14	2	2	52	46	14
13	1	0	337	349	5	15	9	0	583	598	6	12	2	1	912	916	9	18	10	1	247	252	9	16	2	2	363	360	6
15	1	0	257	250	6	17	9	0	467	462	7	14	2	1	127	121	7	1	11	1	165	179	6	18	2	2	47	3	20
17	1	0	352	360	6	19	9	0	195	201	9	16	2	1	598	612	6	3	11	1	164	171	6	20	2	2	0	18	1
19	1	0	572	571	7	0	10	0	286	297	5	18	2	1	34	24	33	5	11	1	727	748	7	1	3	2	484	478	4
21	1	0	764	769	7	2	10	0	71	76	10	20	2	1	206	211	8	7	11	1	520	522	6	3	3	2	226	221	3
0	2	0	1185	1255	9	4	10	0	332	343	5	22	2	1	230	247	9	9	11	1	310	313	6	5	3	2	1074	1043	11
2	2	0	340	359	3	6	10	0	279	274	5	1	3	1	358	360	3	11	11	1	290	299	7	7	3	2	230	229	4
4	2	0	584	598	6	8	10	0	329	333	5	3	3	1	277	270	3	13	11	1	126	145	9	9	3	2	1469	1484	14
6	2	0	95	98	4	10	10	0	562	552	6	5	3	1	367	356	3	15	11	1	183	171	8	11	3	2	1387	1398	15
8	2	0	235	230	4	12	10	0	213	211	7	7	3	1	467	454	4	17	11	1	441	447	7	13	3	2	431	428	5
10	2	0	594	608	6	14	10	0	1117	1137	12	9	3	1	242	245	4	0	12	1	1047	1066	12	15	3	2	209	201	6
12	2	0	386	385	5	16	10	0	235	231	8	11	3	1	252	271	5	2	12	1	530	531	5	17	3	2	354	361	7
14	2	0	845	845	8	18	10	0	521	508	7	13	3	1	241	251	6	4	12	1	127	123	7	19	3	2	816	822	8
16	2	0	731	747	8	1	11	0	331	321	5	15	3	1	58	53	15	6	12	1	650	653	7	21	3	2	579	564	7
18	2	0	43	4	27	3	11	0	212	215	6	17	3	1	309	309	7	8	12	1	133	114	8	0	4	2	1772	1709	15
20	2	0	143	134	9	5	11	0	790	774	8	19	3	1	211	204	8	10	12	1	130	130	9	2	4	2	589	577	6
22	2	0	314	297	8	7	11	0	95	101	8	21	3	1	331	334	8	12	12	1	252	249	7	4	4	2	21	5	21
1	3	0	393	395	4	9	11	0	97	102	9	0	4	1	1136	1137	13	14	12	1	75	75	14	6	4	2	228	212	4
3	3	0	662	661	7	11	11	0	509	510	6	2	4	1	110	116	4	16	12	1	710	697	7	8	4	2	21	33	21
5	3	0	4710	4660	18	13	11	0	132	137	8	4	4	1	234	228	3	1	13	1	413	403	6	10	4	2	1948	1989	22
7	3	0	566	543	5	15	11	0	836	832	8	6	4	1	743	710	7	3	13	1	371	368	6	12	4	2	205	209	6
9	3	0	968	993	10	17	11	0	457	478	8	8	4	1	438	435	4	5	13	1	978	974	10	14	4	2	258	251	6
11	3	0	283	275	5	0	12	0	1447	1466	17	10	4	1	167	147	5	7	13	1	43	61	23	16	4	2	52	52	16
13	3	0	256	264	6	2	12	0	245	251	6	12	4	1	691	705	7	9	13	1	315	319	7	18	4	2	473	468	7
15	3	0	846	846	8	4	12	0	228	221	6	14	4	1	264	265	6	11	13	1	1126	1129	11	20	4	2	311	300	8
17	3	0	942	944	9	6	12	0	543	554	6	16	4	1	576	583	6	13	13	1	162	166	9	1	5	2	926	893	9
19	3	0	276	290	7	8	12	0	199	203	7	18	4	1	254	254	7	15	13	1	227	227	8	3	5	2	31	28	18
21	3	0	426	413	7	10	12	0	659	647	6	20	4	1	52	61	24	0	14	1	734	752	7	5	5	2	1786	1764	18
0	4	0	2026	2086	13	12	12	0	477	482	7	1	5	1	136	143	4	2	14	1	233	235	7	7	5	2	261	255	4
2	4	0	662	658	6	14	12	0	86	81	12	3	5	1	464	463	5	4	14	1	420	420	6	9	5	2	375	379	5
4	4	0	971	965	10	16	12	0	123	97	10	5	5	1	1381	1361	16	6	14	1	257	263	7	11	5	2	622	623	6
6	4	0	1754	1712	19	1	13	0	499	500	6	7	5	1	855	850	9	8	14	1	307	291	7	13	5	2	77	83	10
8	4	0	466	461	5	3	13	0	217	227	7	9	5	1	530	528	5	10	14	1	262	266	7	15	5	2	250	248	7
10	4	0	465	467	4	5	13	0	354	364	6	11	5	1	244	270	5	12	14	1	163	172	9	17	5	2	703	715	7
12	4	0	299	308	5	7	13	0	513	515	6	13	5	1	577	581	6	14	14	1	353	355	8	19	5	2	382	384	7
14	4	0	787	785	8	9	13	0	429	419	6	15	5	1	58	47	14	1	15	1	27	7	27	21	5	2	457	441	8
16	4	0	1996	2000	19	11	13	0	865	883	9	17	5	1	214	217	7	3	15	1	346	351	7	0	6	2	1131	1091	12
18	4	0	70	87	15	13	13	0	294	313	8	19	5	1	54	40	17	5	15	1	202	194	7	2	6	2	48	61	10
20	4	0	232	233	8	15	13	0	277	275	8	21	5	1	702	678	7	7	15	1	337	339	7	4	6	2	920	925	9
22	4	0	474	467	8	0	14	0	1323	1363	15	0	6	1	579	546	5	9	15	1	48	38	23	6	6	2	2427	2377	21
1	5	0	1483	1477	14	2	14	0	371	373	6	2	6	1	166	146	4	11	15	1	123	116	10	8	6	2	261	247	5
3	5	0	41	6	10	4	14	0	216	218	7	4	6	1	225	228	4	13	15	1	180	177	9	10	6	2	47	57	16
5	5	0	3077	3066	18	6	14	0	781	778	8	6	6	1	902	894	9	0	16	1	305	294	7	12	6	2	418	407	5
7	5	0	900	896	8	8	14	0	107	107	10	8	6	1	578	570	6	2	16	1	217	227	8	14	6	2	893	906	9
9	5	0	70	89	9	10	14	0	1316	1292	13	10	6	1	127	129	7	4	16	1	30	4	29	16	6	2	1448	1466	16
11	5	0	378	393	5	12	14	0	53	62	26	12	6	1	140	324	5	6	16	1	1281	1283	13	18	6	2	55	34	18
13	5	0	333	338	5	14	14	0	0	16	1	14	6	1	39	0	21	8	16	1	348	356	7	20	6	2	72	70	16
15	5	0	247	248	6	1	15	0	244	236	7	16	6	1	993	994	10	10	16	1	20	34	20	1	7	2	768	753	8
17	5	0	475	482	6	3	15	0	408	403	7	18	6	1	292	287	7	12	16	1	53	49	26	3	7	2	43	33	13
19	5	0	185	189	8	5	15	0	514	513	6	20	6	1	444	444	7	1	17	1	80	88	13	5	7	2	4363	4368	24
21	5	0	361	367	8	7	15	0	35	54	34	1	7	1	150	133	4	3	17	1	270	276	8	7	7	2	161	153	6
0	6	0	761	771	7	9	15	0	129	114	9	3	7	1	566	552	5	5	17	1	781	771	7	9	7	2	493	503	5
2	6	0	236	232	4	11	15	0	401	397	7	5	7	1	554	555	6	7	17	1	231	237	8	11	7	2	169	187	7
4	6	0	408	417	4	13	15	0	432	423	7	7	7	1	213	211	5	9	17	1	372	364	8	13	7	2	319	307	6
6	6	0	599	597	6	0	16	0	611	606	6	9	7	1	432	434	5	0	18	1	307	316	7	15	7	2	916	951	9
8	6	0	722	722	7	2	16	0	224	215	7	11	7	1	36	35	26	2	18	1	94	95	13	17	7	2	945	947	10
10	6	0	1326	1354	15	4	16	0	197	187	8	13	7	1	69	64	10	4	18	1	324	330	8	19	7	2	111	113	10
12	6	0	206	210	6	6	16	0	784	794	8	15	7	1	27	13	26	6	18	1	339	326	8	0	8	2	477	474	5
14	6	0	484	487	6	8	16	0	112	104	10	17	7	1	247	236	7	1	19	1	358	359	8	2	8	2	520	516	5
16	6	0	579	572	6	10	16	0	108	84	10	19	7	1	145	143	9	3	19	1	426	429	8	4	8	2	136	141	6
18	6	0	361	356	7	12	16	0	449	453	8	0	8	1	542	531	5	0	0	2	3374	3311	15	6	8	2	413	415	5
20	6	0	108	29	12	1	17	0	325	324	7	2	8	1	90	28	6	2	0	2	660	669	6	8	8	2	591	602	6
1	7	0	636	617	6	3	17	0	284	276	7	4	8	1	69	77	9	4	0	2	257	255	3	10	8	2	0	14	1
3	7	0	192	194	4	5	17	0	1771	1771	18	6	8	1	286	292	5	6	0	2	744	720	7	12	8	2	122	111	8
5	7	0	1374	1395	13	7	17	0	55	37	18	8	8	1	51	73	14	8	0	2	594	593	6	14	8	2	529	514	6
7	7	0	519	509	5	9	17	0	61	52	17	10	8	1	12	17	11	10	0	2	1430	1406	14	16	8	2	894	887	9
9	7	0	1140	1155	12	0	18	0	345	362	7	12	8	1	484	479	6	12	0	2	978	999	11	18	8	2	53	53	26
11	7	0	564	537	6	2	18	0	337	333	8	14	8	1	548	544	6	14	0	2	1308	1326	14	1	9	2	489	475	5
13	7	0	383	362	6	4	18	0	26	16	25	16	8	1	633	616	6	16	0	2	714	723	7	3	9	2	112	101	7
15	7	0	280	282	6	6	18	0	284	289	8	18	8	1	335	330	7	18	0	2	764	758	7	5	9	2	523	513	5
17	7	0	303	301	7	8	18	0	342	328	8	20	8	1	270	274	8	20	0	2	108	117	11	7	9	2	465	458	5
19	7	0	694	707	7	1	19	0	223	213	8	1	9	1	959	941	10	1	1	2	573	580	5	9	9	2	665	662	6
0	8	0	2474	2486	19	3	19	0	144	138	10	3	9	1	78	71	8	3	1	2	884	858	9	11	9	2	1576	1574	18
2	8	0	222	225	4	1	1	1	171	171	2	5	9	1	366	387	5	5	1	2	977	963	10	13	9	2	122	115	8

Observed and calculated structure factors for K43

h	k	l	10Fo	10Fc	10s
15	9	2	237	244	8
17	9	2	683	684	7
19	9	2	293	303	8
0	10	2	4319	4298	25
2	10	2	681	671	7
4	10	2	746	746	7
6	10	2	157	139	6
8	10	2	226	231	6
10	10	2	1810	1820	19
12	10	2	336	328	7
14	10	2	366	365	7
16	10	2	253	251	8
18	10	2	218	224	9
1	11	2	415	426	5
3	11	2	728	728	7
5	11	2	27	30	26
7	11	2	33	35	33
9	11	2	573	575	6
11	11	2	1788	1784	20
13	11	2	85	49	10
15	11	2	202	202	8
17	11	2	61	68	20
0	12	2	1277	1295	14
2	12	2	81	78	9
4	12	2	83	83	10
6	12	2	859	865	9
8	12	2	117	138	9
10	12	2	741	734	7
12	12	2	261	266	7
14	12	2	518	502	7
16	12	2	431	434	7
1	13	2	225	228	6
3	13	2	114	106	8
5	13	2	1743	1751	19
7	13	2	64	14	13
9	13	2	163	156	8
11	13	2	166	166	9
13	13	2	79	79	14
15	13	2	518	521	7
0	14	2	418	421	6
2	14	2	349	356	6
4	14	2	667	671	6
6	14	2	473	474	7
8	14	2	201	220	8
10	14	2	151	152	9
12	14	2	19	17	19
14	14	2	342	348	8
1	15	2	603	593	6
3	15	2	226	219	7
5	15	2	1434	1431	14
7	15	2	522	519	7
9	15	2	86	73	12
11	15	2	417	418	7
13	15	2	105	104	13
0	16	2	919	944	9
2	16	2	121	115	10
4	16	2	17	25	17
6	16	2	586	575	7
8	16	2	63	71	19
10	16	2	733	723	7
1	17	2	219	232	8
3	17	2	409	410	7
5	17	2	149	137	9
7	17	2	88	76	13
9	17	2	338	342	8
0	18	2	684	683	7
2	18	2	62	63	19
4	18	2	239	248	8
6	18	2	401	389	8
1	1	3	260	251	3
3	1	3	590	574	6
5	1	3	158	118	4
7	1	3	279	281	4
9	1	3	350	362	5
11	1	3	1273	1312	13
13	1	3	440	443	6
15	1	3	171	170	7
17	1	3	330	332	7
19	1	3	471	479	7
21	1	3	756	742	7
0	2	3	2163	2123	16
2	2	3	615	595	6
4	2	3	56	50	8
6	2	3	1081	1062	10
8	2	3	664	652	6
10	2	3	216	223	5
12	2	3	678	689	7
14	2	3	332	333	6
16	2	3	989	1009	10
18	2	3	213	213	8
20	2	3	138	133	10
1	3	3	547	535	5
3	3	3	237	229	6
5	3	3	1030	1016	10
7	3	3	729	720	8
9	3	3	192	187	5
11	3	3	1323	1342	13
13	3	3	0	40	1
15	3	3	118	131	8
17	3	3	264	259	7
19	3	3	131	124	9
21	3	3	396	392	8
0	4	3	2248	2148	18
2	4	3	13	26	12
4	4	3	361	352	6
6	4	3	281	258	6
8	4	3	207	219	5
10	4	3	468	457	5
12	4	3	768	765	7
14	4	3	100	103	9
16	4	3	173	174	7
18	4	3	172	157	8
20	4	3	38	2	38
1	5	3	39	45	14
3	5	3	287	287	4
5	5	3	779	774	8
7	5	3	831	843	8
9	5	3	412	410	5
11	5	3	109	107	7
13	5	3	430	434	6
15	5	3	61	33	15
17	5	3	284	275	7
19	5	3	72	79	15
0	6	3	472	488	4
2	6	3	141	129	5
4	6	3	461	447	4
6	6	3	1204	1219	12
8	6	3	423	419	5
10	6	3	172	172	6
12	6	3	286	283	6
14	6	3	87	86	11
16	6	3	1077	1072	10
18	6	3	417	417	7
20	6	3	396	401	8
1	7	3	173	172	5
3	7	3	258	262	5
5	7	3	1254	1268	15
7	7	3	166	173	6
9	7	3	438	443	5
11	7	3	836	846	9
13	7	3	131	137	8
15	7	3	98	107	10
17	7	3	673	662	7
19	7	3	118	106	11
0	8	3	952	955	10
2	8	3	85	89	8
4	8	3	315	321	5
6	8	3	594	585	6
8	8	3	100	89	8
10	8	3	141	151	8
12	8	3	562	572	6
14	8	3	327	327	7
16	8	3	118	111	11
18	8	3	159	155	9
1	9	3	572	589	5
3	9	3	152	153	6
5	9	3	294	290	6
7	9	3	210	204	6
9	9	3	81	74	10
11	9	3	856	873	9
13	9	3	78	60	11
15	9	3	145	125	9
17	9	3	495	482	7
0	10	3	891	893	9
2	10	3	785	785	8
4	10	3	350	354	6
6	10	3	230	221	6
8	10	3	230	235	6
10	10	3	89	82	11
12	10	3	87	86	11
14	10	3	621	625	7
16	10	3	102	122	12
1	11	3	277	279	6
3	11	3	136	126	7
5	11	3	815	816	8
7	11	3	209	216	7
9	11	3	377	378	6
11	11	3	0	15	1
13	11	3	49	34	24
15	11	3	28	17	28
17	11	3	556	561	8
0	12	3	186	184	7
2	12	3	309	311	6
4	12	3	364	375	6
6	12	3	143	139	8
8	12	3	34	42	13
10	12	3	131	130	8
12	12	3	248	247	7
14	12	3	165	166	9
16	12	3	402	391	8
1	13	3	281	289	6
3	13	3	465	471	6
5	13	3	361	365	6
7	13	3	124	140	9
9	13	3	253	257	7
11	13	3	428	407	7
13	13	3	21	30	21
15	13	3	160	137	9
0	14	3	107	96	9
2	14	3	200	201	7
4	14	3	355	359	7
6	14	3	176	168	8
8	14	3	356	349	7
10	14	3	94	98	12
12	14	3	44	54	16
1	15	3	176	170	8
3	15	3	261	265	7
5	15	3	384	385	7
7	15	3	206	198	8
9	15	3	100	99	11
11	15	3	320	301	8
0	16	3	99	119	12
2	16	3	62	60	19
4	16	3	217	225	8
6	16	3	1092	1114	11
8	16	3	299	298	8
10	16	3	121	118	11
1	17	3	154	151	9
3	17	3	296	288	8
5	17	3	469	477	8
7	17	3	26	19	26
0	18	3	204	199	8
2	18	3	200	199	9
0	0	4	6526	6470	25
2	0	4	453	453	5
4	0	4	696	705	7
6	0	4	451	447	5
8	0	4	207	209	5
10	0	4	2619	2632	25
12	0	4	923	940	10
14	0	4	415	426	6
16	0	4	186	187	8
18	0	4	498	505	7
20	0	4	211	197	9
1	1	4	356	336	4
3	1	4	45	39	12
5	1	4	238	217	5
7	1	4	0	32	1
9	1	4	1160	1179	13
11	1	4	1645	1666	17
13	1	4	193	189	6
15	1	4	163	166	8
17	1	4	32	30	32
19	1	4	531	527	7
0	2	4	284	309	4
2	2	4	237	242	4
4	2	4	162	161	5
6	2	4	482	503	5
8	2	4	60	63	11
10	2	4	409	409	5
12	2	4	371	373	6
14	2	4	639	627	6
16	2	4	741	749	7
18	2	4	23	13	22
20	2	4	95	86	13
1	3	4	267	273	4
3	3	4	540	524	5
5	3	4	3279	3269	23
7	3	4	206	208	5
9	3	4	759	772	8
11	3	4	73	25	10
13	3	4	237	249	7
15	3	4	739	733	7
17	3	4	733	724	7
19	3	4	252	252	8
0	4	4	501	523	5
2	4	4	467	450	4
4	4	4	545	563	5
6	4	4	1931	1902	22
8	4	4	201	206	6
10	4	4	322	335	6
12	4	4	216	208	6
14	4	4	770	779	8
16	4	4	1442	1435	14
18	4	4	159	151	9
1	5	4	1024	1012	10
3	5	4	205	195	5
5	5	4	1463	1500	15
7	5	4	437	440	5
9	5	4	102	96	8
11	5	4	943	941	9
13	5	4	176	177	7
15	5	4	258	257	7
17	5	4	80	94	14
19	5	4	140	116	9
0	6	4	2017	2043	22
2	6	4	230	233	5
4	6	4	408	416	5
6	6	4	94	98	8
8	6	4	413	407	6
10	6	4	1234	1244	12
12	6	4	312	308	6
14	6	4	278	279	7
16	6	4	234	237	8
18	6	4	270	251	8
1	7	4	221	206	5
3	7	4	251	255	5
5	7	4	1271	1284	13
7	7	4	418	415	5
9	7	4	880	897	9
11	7	4	705	731	7
13	7	4	306	307	7
15	7	4	259	265	8
17	7	4	421	404	7
0	8	4	1761	1811	16
2	8	4	61	72	12
4	8	4	229	237	6
6	8	4	581	584	6
8	8	4	312	312	6
10	8	4	1070	1083	11
12	8	4	116	124	9
14	8	4	99	102	11
16	8	4	255	271	8
18	8	4	0	1	1
1	9	4	0	39	1
3	9	4	296	306	6
5	9	4	1740	1725	18
7	9	4	464	451	6
9	9	4	48	62	22
11	9	4	273	264	7
13	9	4	67	77	15
15	9	4	408	423	7
17	9	4	562	562	8
0	10	4	839	847	8
2	10	4	23	16	23
4	10	4	418	425	6
6	10	4	241	208	6
8	10	4	328	341	6
10	10	4	486	476	6
12	10	4	240	239	8
14	10	4	877	858	9
16	10	4	367	377	8
1	11	4	189	196	7
3	11	4	302	297	6
5	11	4	1004	1015	10
7	11	4	0	16	1
9	11	4	47	52	20
11	11	4	69	58	15
13	11	4	82	77	14
15	11	4	693	700	7
0	12	4	930	934	9
2	12	4	262	255	7
4	12	4	129	124	8
6	12	4	235	245	7
8	12	4	244	245	7
10	12	4	447	436	7
12	12	4	334	326	8
14	12	4	0	1	1
1	13	4	269	281	7
3	13	4	155	148	8
5	13	4	239	237	7
7	13	4	311	305	7
9	13	4	409	418	7
11	13	4	712	708	7
13	13	4	191	178	8
0	14	4	1339	1340	14
2	14	4	222	219	7
4	14	4	318	325	7
6	14	4	528	532	7
8	14	4	87	91	12
10	14	4	1034	1019	10
12	14	4	30	30	29
1	15	4	191	201	8
3	15	4	390	400	7
5	15	4	245	239	8
7	15	4	87	80	11
9	15	4	117	114	11
0	16	4	174	176	8
2	16	4	216	215	8
4	16	4	133	124	10
6	16	4	453	434	7
8	16	4	42	31	42
1	17	4	172	184	8
3	17	4	195	174	9
1	1	5	74	65	8
3	1	5	174	182	6
5	1	5	723	722	7
7	1	5	0	26	1
9	1	5	328	339	6
11	1	5	196	188	7
13	1	5	174	194	8
15	1	5	74	56	14
17	1	5	719	734	7
19	1	5	370	384	8
0	2	5	808	792	8
2	2	5	105	107	7
4	2	5	455	454	5
6	2	5	494	487	5
8	2	5	273	273	6
10	2	5	12	6	11
12	2	5	735	732	8
14	2	5	36	45	36
16	2	5	194	190	8
18	2	5	93	92	13
1	3	5	130	135	6
3	3	5	236	232	5
5	3	5	543	551	5
7	3	5	85	92	9
9	3	5	107	104	8
11	3	5	267	274	6
13	3	5	276	269	7
15	3	5	22	8	22
17	3	5	519	524	7
0	4	5	155	142	6
2	4	5	76	60	9
4	4	5	114	110	7
6	4	5	631	628	6
8	4	5	305	128	6
10	4	5	210	206	7
12	4	5	489	483	6
14	4	5	273	266	7
16	4	5	615	614	7
18	4	5	261	274	8
1	5	5	158	159	6
3	5	5	258	251	6
5	5	5	636	625	6
7	5	5	581	579	6
9	5	5	195	194	6
11	5	5	224	227	7
13	5	5	399	396	7
15	5	5	0	21	1
17	5	5	163	159	9
0	6	5	411	439	5
2	6	5	83	89	9
4	6	5	59	49	11
6	6	5	430	432	6
8	6	5	377	376	6
10	6	5	63	74	15
12	6	5	232	231	7
14	6	5	25	16	24
16	6	5	673	664	7
1	7	5	82	77	9
3	7	5	458	467	6
5	7	5	117	100	8
7	7	5	319	317	6
9	7	5	298	296	6
11	7	5	352	359	7
13	7	5	180	167	8
15	7	5	90	82	12
17	7	5	25	40	24
0	8	5	702	718	7
2	8	5	154	149	7
4	8	5	46	37	17
6	8	5	540	534	6
8	8	5	85	78	10
10	8	5	51	29	18
12	8	5	344	345	7
14	8	5	476	478	7
16	8	5	712	677	7
1	9	5	691	690	7

Observed and calculated structure factors for K43

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
1	9	5	35	25	35	9	1	6	383	378	6	8	8	6	157	162	7	0	4	7	1005	1019	11	7	1	8	229	224	8
5	9	5	493	489	6	11	1	6	176	186	7	10	8	6	117	128	10	2	4	7	76	79	12	9	1	8	643	640	7
7	9	5	112	306	6	13	1	6	106	95	10	12	8	6	140	133	10	4	4	7	234	239	7	11	1	8	502	498	8
9	9	5	27	14	26	15	1	6	430	417	7	14	8	6	157	157	8	6	4	7	123	124	9	0	2	8	29	29	29
11	9	5	1506	1508	14	17	1	6	302	299	8	1	9	6	152	152	6	8	4	7	174	180	8	2	2	8	95	109	12
13	9	5	136	141	10	0	2	6	1664	1657	17	3	9	6	74	70	12	10	4	7	294	295	7	4	2	8	226	222	8
15	9	5	138	118	9	2	2	6	233	240	6	5	9	6	27	3	27	12	4	7	461	475	7	6	2	8	525	512	7
0	10	5	1024	1012	10	4	2	6	217	220	6	7	9	6	517	524	7	14	4	7	141	118	9	8	2	8	39	14	38
2	10	5	512	507	6	6	2	6	527	532	6	9	9	6	447	444	7	1	5	7	5	17	5	10	2	8	202	212	9
4	10	5	113	109	9	8	2	6	276	270	6	11	9	6	717	707	7	3	5	7	156	146	8	1	3	8	157	141	8
6	10	5	467	452	6	10	2	6	772	784	8	13	9	6	20	39	20	5	5	7	237	252	7	3	3	8	337	343	7
8	10	5	112	120	9	12	2	6	294	289	7	0	10	6	2105	2095	20	7	5	7	516	508	7	5	3	8	1723	1722	17
10	10	5	283	279	7	14	2	6	47	36	23	2	10	6	331	325	7	9	5	7	306	294	7	7	3	8	0	2	1
12	10	5	55	73	25	16	2	6	406	404	8	4	10	6	326	318	7	11	5	7	44	22	29	9	3	8	431	422	7
14	10	5	496	479	7	1	3	6	260	253	6	6	10	6	595	594	7	13	5	7	270	265	8	11	3	8	173	166	9
1	11	5	67	67	13	3	3	6	69	69	12	8	10	6	55	52	21	0	6	7	230	215	7	0	4	8	250	250	7
3	11	5	153	147	8	5	3	6	805	813	8	10	10	6	1242	1240	12	2	6	7	121	126	10	2	4	8	294	303	7
5	11	5	523	507	6	7	3	6	110	104	8	12	10	6	192	184	9	4	6	7	196	200	7	4	4	8	193	192	8
7	11	5	528	522	7	9	3	6	986	1005	10	1	11	6	144	137	8	6	6	7	713	691	7	6	4	8	618	629	7
9	11	5	213	204	8	11	3	6	1100	1110	11	3	11	6	162	156	7	8	6	7	272	283	7	8	4	8	50	30	22
11	11	5	164	157	7	13	3	6	221	215	7	5	11	6	463	466	7	10	6	7	131	146	10	10	4	8	173	153	9
13	11	5	209	208	9	15	3	6	105	90	11	7	11	6	135	135	9	12	6	7	174	184	9	1	5	8	540	551	7
0	12	5	1061	1064	10	17	3	6	372	379	8	9	11	6	427	418	7	1	7	7	82	88	12	3	5	8	175	178	8
2	12	5	514	516	7	0	4	6	2289	2315	25	11	11	6	742	735	7	3	7	7	259	250	7	5	5	8	399	396	7
4	12	5	55	43	18	2	4	6	0	19	1	0	12	6	487	487	7	5	7	7	754	752	7	7	5	8	56	40	21
6	12	5	700	705	7	4	4	6	359	360	6	2	12	6	107	105	10	7	7	7	129	117	9	9	5	8	120	122	11
8	12	5	68	67	15	6	4	6	454	464	6	4	12	6	107	100	11	9	7	7	337	328	7	0	6	8	1778	1797	17
10	12	5	78	46	15	8	4	6	65	64	13	6	12	6	895	908	9	11	7	7	537	528	7	2	6	8	210	211	8
12	12	5	206	203	8	10	4	6	1302	1310	14	8	12	6	0	15	1	0	8	7	598	589	7	4	6	8	340	344	8
1	13	5	150	142	7	12	4	6	216	210	7	10	12	6	182	178	8	2	8	7	69	78	16	6	6	8	419	429	7
3	13	5	267	266	7	14	4	6	73	66	16	1	13	6	62	53	18	4	8	7	253	248	7	8	6	8	168	183	10
5	13	5	935	956	9	16	4	6	181	174	9	3	13	6	69	68	15	6	8	7	354	347	7	1	7	8	16	28	15
7	13	5	147	166	10	1	5	6	232	228	6	5	13	6	1289	1297	12	8	8	7	0	2	1	3	7	8	179	175	9
9	13	5	285	284	8	3	5	6	350	340	6	7	13	6	120	131	11	10	8	7	114	121	11	5	7	8	884	890	9
11	13	5	1247	1215	12	5	5	6	466	454	6	0	14	6	45	53	28	1	9	7	368	373	7	7	7	8	235	241	8
0	14	5	933	915	9	7	5	6	75	52	11	2	14	6	408	396	7	3	9	7	72	80	15	0	8	8	882	877	9
2	14	5	194	198	8	9	5	6	198	204	7	4	14	6	294	283	8	5	9	7	226	231	8	2	8	8	14	19	13
4	14	5	336	335	7	11	5	6	349	358	7	1	1	7	75	78	11	7	9	7	139	112	9	4	8	8	50	39	24
6	14	5	416	420	7	13	5	6	60	56	19	3	1	7	214	211	7	9	9	7	0	1	1	6	8	8	417	418	7
8	14	5	191	196	9	15	5	6	218	235	9	5	1	7	91	92	10	0	10	7	587	591	7	1	9	8	55	63	20
1	15	5	81	90	13	0	6	6	160	146	7	7	1	7	269	254	7	2	10	7	441	439	7	3	9	8	164	160	9
3	15	5	298	293	8	2	6	6	46	39	17	9	1	7	207	205	8	4	10	7	163	162	9	5	9	8	1210	1227	12
5	15	5	37	36	37	4	6	6	443	441	6	11	1	7	719	701	7	6	10	7	193	196	9	0	10	8	1028	1023	10
7	15	5	104	118	8	6	6	6	885	880	9	13	1	7	144	136	7	8	10	7	127	122	10	2	10	8	98	85	12
0	16	5	254	264	8	8	6	6	294	289	7	15	1	7	147	159	11	1	11	7	153	152	9	1	1	9	59	40	20
2	16	5	278	256	8	10	6	6	52	56	20	0	2	7	630	628	6	3	11	7	84	85	13	3	1	9	150	159	9
4	16	5	105	113	14	12	6	6	199	202	8	2	2	7	326	328	6	5	11	7	574	572	7	5	1	9	322	316	8
0	0	6	2495	2540	25	14	6	6	807	795	8	4	2	7	0	14	1	7	11	7	159	153	9	0	2	9	142	132	10
2	0	6	122	126	7	1	7	6	595	597	6	6	2	7	460	459	6	0	12	7	48	22	23	2	2	9	48	64	27
4	0	6	561	565	5	3	7	6	191	185	7	8	2	7	259	256	7	2	12	7	196	198	9	4	2	9	200	207	9
6	0	6	688	702	7	5	7	6	2398	2401	28	10	2	7	41	29	13	4	12	7	237	258	9	6	2	9	0	26	1
8	0	6	196	192	6	7	7	6	56	83	18	12	2	7	471	488	7	0	0	8	2392	2427	30	1	3	9	135	139	9
10	0	6	899	890	9	9	7	6	387	395	7	14	2	7	182	181	9	2	0	8	180	179	8	3	3	9	31	7	30
12	0	6	768	776	7	11	7	6	487	496	7	1	3	7	200	207	7	4	0	8	237	245	8	5	3	9	94	84	13
14	0	6	750	755	8	13	7	6	198	182	8	3	3	7	22	34	22	6	0	8	735	729	7	0	4	9	435	435	7
16	0	6	824	836	8	15	7	6	628	634	8	5	3	7	386	389	6	8	0	8	27	41	27	2	4	9	59	55	21
1	1	6	187	187	6	0	8	6	295	297	6	7	3	7	428	426	7	10	0	8	1436	1427	14	4	4	9	65	68	19
3	1	6	202	194	6	2	8	6	237	233	7	9	3	7	160	163	8	1	1	8	138	140	8	1	5	9	23	19	23
5	1	6	1614	1639	17	4	8	6	267	263	7	11	3	7	798	775	8	3	1	8	91	100	11	3	5	9	76	72	15
7	1	6	104	109	8	6	8	6	289	294	7	13	3	7	57	53	20	5	1	8	473	471	7						

Observed and calculated structure factors for K45

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	614	649	7	6	8	0	551	566	6	5	1	1	868	872	8	9	9	1	18	48	18	9	1	2	646	645	6
4	0	0	1256	1248	10	8	8	0	467	465	5	7	1	1	143	128	3	11	9	1	1681	1673	16	11	1	2	655	653	6
6	0	0	580	581	5	10	8	0	1337	1335	15	9	1	1	471	458	4	13	9	1	74	50	9	13	1	2	85	59	8
8	0	0	926	885	8	12	8	0	184	194	6	11	1	1	839	839	8	15	9	1	75	70	11	15	1	2	668	669	7
10	0	0	3868	3699	18	14	8	0	152	162	7	13	1	1	372	368	5	17	9	1	172	176	7	17	1	2	75	77	11
12	0	0	1380	1391	14	16	8	0	277	280	6	15	1	1	43	34	14	19	9	1	180	189	8	19	1	2	89	28	11
14	0	0	199	198	5	18	8	0	35	23	35	17	1	1	721	731	7	0	10	1	1224	1240	13	21	1	2	324	333	7
16	0	0	220	215	6	20	8	0	339	333	7	19	1	1	478	487	6	2	10	1	758	761	7	0	2	2	4119	4100	13
18	0	0	621	602	6	1	9	0	86	75	6	21	1	1	898	878	9	4	10	1	280	292	5	2	2	2	329	326	3
20	0	0	236	240	7	3	9	0	387	395	4	0	2	1	37	66	6	6	10	1	418	432	5	4	2	2	503	494	4
22	0	0	1652	1653	17	5	9	0	1801	1864	19	2	2	1	450	472	4	8	10	1	143	158	6	6	2	2	439	431	4
3	1	0	201	195	2	7	9	0	878	877	8	4	2	1	504	507	5	10	10	1	253	255	5	8	2	2	264	263	4
5	1	0	452	451	4	9	9	0	52	30	11	6	2	1	273	256	3	12	10	1	8	7	8	10	2	2	1286	1300	13
7	1	0	476	468	4	11	9	0	621	610	6	8	2	1	631	642	6	14	10	1	617	631	6	12	2	2	541	545	5
9	1	0	1715	1699	16	13	9	0	270	273	6	10	2	1	293	310	4	16	10	1	252	267	7	14	2	2	127	124	6
11	1	0	2913	2850	19	15	9	0	527	547	6	12	2	1	951	959	10	18	10	1	285	289	7	16	2	2	349	346	6
13	1	0	308	316	5	17	9	0	487	481	6	14	2	1	155	149	6	1	11	1	224	232	5	18	2	2	62	45	14
15	1	0	276	289	5	19	9	0	267	272	7	16	2	1	682	686	6	3	11	1	251	256	5	20	2	2	39	31	18
17	1	0	278	293	6	0	10	0	277	294	4	18	2	1	26	18	26	5	11	1	663	686	7	1	3	2	190	372	4
19	1	0	629	624	6	2	10	0	31	32	26	20	2	1	131	149	9	7	11	1	513	516	5	3	3	2	282	277	3
21	1	0	766	763	7	4	10	0	430	450	4	22	2	1	230	219	8	9	11	1	340	344	5	5	3	2	1028	1007	10
0	2	0	1328	1341	7	6	10	0	304	288	5	1	3	1	323	327	3	11	11	1	366	381	6	7	3	2	141	138	4
2	2	0	246	262	2	8	10	0	312	318	5	3	3	1	236	231	3	13	11	1	105	122	9	9	3	2	1642	1638	18
4	2	0	710	704	7	10	10	0	498	514	5	5	3	1	331	319	3	15	11	1	68	77	13	11	3	2	1323	1355	14
6	2	0	148	148	3	12	10	0	128	132	7	7	3	1	500	491	5	17	11	1	449	451	7	13	3	2	477	476	5
8	2	0	285	287	3	14	10	0	1201	1204	12	9	3	1	241	253	4	0	12	1	1097	1108	12	15	3	2	148	150	7
10	2	0	683	685	7	16	10	0	208	207	7	11	3	1	230	238	5	2	12	1	476	485	5	17	3	2	294	304	6
12	2	0	306	306	5	18	10	0	563	552	7	13	3	1	276	286	5	4	12	1	93	97	7	19	3	2	849	854	8
14	2	0	860	877	8	1	11	0	298	294	5	15	3	1	28	28	27	6	12	1	620	616	6	21	3	2	519	527	7
16	2	0	720	712	7	3	11	0	286	291	5	17	3	1	331	318	6	8	12	1	146	151	7	0	4	2	1932	1902	13
18	2	0	49	43	16	5	11	0	870	899	9	19	3	1	208	210	7	10	12	1	198	193	6	2	4	2	684	676	6
20	2	0	173	180	8	7	11	0	152	162	6	21	3	1	316	326	7	12	12	1	275	274	6	4	4	2	48	30	7
22	2	0	352	339	7	9	11	0	67	66	10	0	4	1	1073	1058	11	14	12	1	52	52	15	6	4	2	277	265	3
1	3	0	339	336	3	11	11	0	459	483	6	2	4	1	62	65	4	16	12	1	698	694	7	8	4	2	128	135	5
3	3	0	582	568	5	13	11	0	141	162	7	4	4	1	274	267	3	1	13	1	370	364	5	10	4	2	2071	2053	20
5	3	0	5217	4766	15	15	11	0	901	899	9	6	4	1	804	772	8	3	13	1	369	367	5	12	4	2	288	295	5
7	3	0	500	480	5	17	11	0	433	432	7	8	4	1	505	501	5	5	13	1	943	955	9	14	4	2	240	235	6
9	3	0	1031	1008	9	0	12	0	1521	1531	15	10	4	1	255	231	4	7	13	1	52	62	14	16	4	2	22	28	21
11	3	0	319	308	4	2	12	0	254	249	5	12	4	1	722	734	7	9	13	1	316	327	6	18	4	2	487	492	6
13	3	0	361	361	5	4	12	0	247	248	5	14	4	1	268	266	5	11	13	1	1061	1076	11	20	4	2	341	332	7
15	3	0	865	847	9	6	12	0	612	620	6	16	4	1	645	651	6	13	13	1	137	132	9	1	5	2	991	969	10
17	3	0	950	940	10	8	12	0	166	166	6	18	4	1	248	253	7	15	13	1	268	263	7	3	5	2	91	92	5
19	3	0	220	231	7	10	12	0	629	633	6	20	4	1	118	110	9	0	14	1	662	676	7	5	5	2	1843	1817	16
21	3	0	442	425	7	12	12	0	504	510	6	1	5	1	108	116	4	2	14	1	274	275	6	7	5	2	200	193	4
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4	4	0	1117	1106	12	1	13	0	442	439	5	7	5	1	885	872	9	8	14	1	324	304	6	13	5	2	51	36	13
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10	4	0	442	449	4	7	13	0	471	486	5	13	5	1	597	613	6	14	14	1	411	390	7	19	5	2	429	425	7
12	4	0	276	271	5	9	13	0	516	511	6	15	5	1	136	144	7	1	15	1	27	11	27	21	5	2	467	465	7
14	4	0	967	903	9	11	13	0	893	891	9	17	5	1	228	229	6	3	15	1	295	294	6	0	6	2	1087	1073	10
16	4	0	2029	1987	24	13	13	0	304	304	6	19	5	1	27	38	27	5	15	1	235	248	6	2	6	2	128	133	4
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3	5	0	60	53	5	4	14	0	199	209	6	4	6	1	209	207	3	13	15	1	138	138	8	10	6	2	0	18	1
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7	5	0	841	817	9	8	14	0	118	121	8	8	6	1	516	505	5	2	16	1	236	249	6	14	6	2	970	1004	10
9	5	0	162	169	5	10	14	0	1321	1332	13	10	6	1	122	109	6	4	16	1	31	17	30	16	6	2	1413	1442	14
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15	5	0	274	282	6	1	15	0	253	240	6	16	6	1	1020	1031	10	10	16	1	69	72	14	1	7	2	724	720	7
17	5	0	480	480	6	3	15	0	414	411	6	18	6	1	275	279	7	12	16	1	94	83	10	3	7	2	18	19	18
19	5	0	233	230	7	5	15	0	523	529	6	20	6	1	425	424	7	1	17	1	56	67	15	5	7	2	4705	4470	19
21	5	0	133	311	7	7	15	0	5	3	4	1	7	1	123	115	4	3	17	1	291	296	6	7	7	2	198	208	5
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2	6	0	150	147	3	11	15	0	177	177	7	5	7	1	415	417	4	7	17	1	223	222	7	11	7	2	133	132	6
4	6	0	410	421	4	13	15	0	439	432	7	7	7	1	186	198	5	9	17	1	408	403	7	13	7	2	149	156	5
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8	6	0	657	658	6	2	16	0	199	185	6	11	7	1	0	7	1	2	18	1	78	68	11	17	7	2	927	935	9
10	6	0	1147	1362	13	4	16	0	229	244	7	13	7	1	49	62	13	4	18	1	336	343	7	19	7	2	64	53	14
12	6	0	284	289	5	6	16	0	814	825	8	15	7	1	95	48	8	6	18	1	358	350	7	0	8	2	497	494	5
14	6	0	463	459	5	8	16	0	41	63	25	17	7	1	197	202	7	1	19	1	325	319	7	2	8	2	458	447	4
16	6	0	565	560	6	10	16	0	43	44	25	19	7	1	123	137	9	3	19	1	397	405	7	4	8	2	182	193	5
18	6	0	182	174	6	12	16	0	404	416	7	0	8	1	647	638	6	0	0	2	2941	3323	12	6	8	2	403	396	4
20	6	0	35	26	35	1	17	0	275	263	6	2	8	1	30	22	15	2	0	2	585	606	5	8	8	2	591	598	6
1	7	0	754	718	7	3	17	0	307	298	7	4	8	1	121	128	5	4	0	2	410	399	4	10	8	2	41	22	17
3	7	0	123	131	4	5	17	0	1878	1838	19	6	8	1	286	301	4	6	0	2	796	747	7	12	8	2	177	188	6
5	7	0	1372	1375	16	7	17	0	57	43	15	8	8	1	135	135	6	8	0	2	601	566	6	14	8	2	563	569	6
7	7	0	455	441	4	9	17	0	32	38	31	10	8	1	82	72	8	10	0	2	1401	1351	13	16	8	2	889	890	8
9	7	0	1258	1245	14	0	18	0	325	318	7	12	8	1	492	496	5	12	0	2	912	927	9	18	8	2	79	83	12
11	7	0	533	511	5	2	18	0	305	302	7	14	8	1	563	571	6	14	0	2	1371	1355	12	1	9	2	433	431	4
13	7	0	175	177	5	4	18	0	70	61	13	16	8	1	723	719	7	16	0	2	690	684	6	3	9	2	63	39	8
15	7	0	239	235	6	6	18	0	224	232	7	18	8	1	348	343	6	18	0	2	849	837	8	5	9	2	458	451	4
17	7	0	242	233	6	8	18	0	338	328	7	20	8	1	240	236	8	20	0	2	43	64	28	7	9	2	414	403	5
19	7	0	709	722	7	1	19	0	210	198	7	1	9	1	961	939	10	1	1	2	509	503	5	9	9	2	716	737	7
0	8	0	2657	2558	16	3	19	0	94	62	11	3	9	1	140	138	5	3	1	2	774	760	7	11	9	2	1562	1567	16
2	8	0	156	155	4	1	1	1	165	158	2	5	9	1	366	395	4	5	1	2	1068	1066	9	13	9	2	87	92	9
4	8	0	389	384	4	3	1	1	481	471	5	7	9	1	302	307	5	7	1	2	181	179	4	15	9	2	324	321	6

Observed and calculated structure factors for K45

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
17	9	2	635	621	6	1	3	3	532	535	5	0	12	3	232	232	6	12	4	4	168	172	6	12	14	4	54	44	18
19	9	2	305	306	7	3	3	3	253	256	3	2	12	3	265	273	5	14	4	4	862	868	8	1	15	4	207	198	7
0	10	2	4585	4377	21	5	3	3	1078	1058	11	4	12	3	348	346	5	16	4	4	1390	1417	15	3	15	4	199	403	6
2	10	2	661	657	7	7	3	3	742	728	8	6	12	3	117	116	7	18	4	4	152	157	8	5	15	4	245	251	7
4	10	2	740	737	7	9	3	3	185	194	5	8	12	3	85	82	8	1	5	4	997	982	10	7	15	4	121	117	9
6	10	2	75	81	9	11	3	3	1336	1317	14	10	12	3	178	177	7	3	5	4	149	144	5	9	15	4	142	117	8
8	10	2	279	278	5	13	3	3	78	81	9	12	12	3	277	269	6	5	5	4	1504	1547	19	0	16	4	134	153	9
10	10	2	1849	1856	23	15	3	3	85	104	10	14	12	3	119	133	10	7	5	4	398	395	5	2	16	4	170	169	8
12	10	2	325	314	6	17	3	3	244	242	6	16	12	3	397	387	7	9	5	4	153	158	6	4	16	4	182	178	8
14	10	2	350	357	6	19	3	3	120	132	9	1	13	3	239	247	6	11	5	4	905	909	10	6	16	4	460	455	7
16	10	2	239	233	7	21	3	3	401	397	7	3	13	3	455	463	6	13	5	4	188	183	6	8	16	4	28	3	27
18	10	2	279	277	7	0	4	3	2179	2094	15	5	13	3	348	343	6	15	5	4	276	277	6	1	17	4	351	340	7
1	11	2	345	343	5	2	4	3	55	60	7	7	13	3	136	135	7	17	5	4	87	92	10	3	17	4	208	190	7
3	11	2	704	705	7	4	4	3	378	378	4	9	13	3	262	264	6	19	5	4	159	155	8	1	1	5	74	74	7
5	11	2	113	69	6	6	4	3	220	214	4	11	13	3	363	362	6	0	6	4	2107	2146	19	3	1	5	244	247	5
7	11	2	11	7	10	8	4	3	273	273	4	13	13	3	25	4	24	2	6	4	160	167	5	5	1	5	663	661	6
9	11	2	626	651	6	10	4	3	370	366	5	15	13	3	189	174	8	4	6	4	391	401	4	7	1	5	38	37	17
11	11	2	1761	1744	17	12	4	3	762	794	8	0	14	3	85	18	9	6	6	4	151	150	5	9	1	5	375	382	5
13	11	2	64	46	12	14	4	3	126	114	7	2	14	3	246	243	6	8	6	4	367	356	5	11	1	5	254	240	6
15	11	2	225	227	7	16	4	3	229	231	6	4	14	3	366	369	6	10	6	4	1245	1260	13	13	1	5	191	196	6
17	11	2	77	87	12	18	4	3	164	161	8	6	14	3	179	183	7	12	6	4	385	381	6	15	1	5	22	1	22
0	12	2	1333	1331	15	20	4	3	67	55	14	8	14	3	354	362	6	14	6	4	269	259	6	17	1	5	733	738	7
2	12	2	21	13	20	1	5	3	73	68	5	10	14	3	33	17	32	16	6	4	224	220	6	19	1	5	370	386	7
4	12	2	31	24	30	3	5	3	356	363	4	12	14	3	52	50	19	18	6	4	287	275	7	0	2	5	717	718	7
6	12	2	827	838	9	5	5	3	899	890	8	1	15	3	172	172	7	1	7	4	276	273	5	2	2	5	68	61	7
8	12	2	118	158	7	7	5	3	870	860	9	3	15	3	207	209	6	3	7	4	210	208	5	4	2	5	477	481	5
10	12	2	805	797	7	9	5	3	440	448	5	5	15	3	433	445	6	5	7	4	1244	1275	15	6	2	5	471	463	5
12	12	2	223	228	7	11	5	3	127	113	6	7	15	3	193	194	7	7	7	4	175	168	5	8	2	5	340	338	5
14	12	2	564	552	6	13	5	3	450	460	5	9	15	3	129	131	9	9	7	4	951	971	10	10	2	5	94	97	8
16	12	2	394	381	7	15	5	3	77	59	9	11	15	3	335	320	7	11	7	4	693	696	6	12	2	5	761	755	8
1	13	2	193	196	6	17	5	3	298	291	6	0	16	3	141	101	8	13	7	4	326	324	6	14	2	5	71	75	12
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5	13	2	1846	1835	17	0	6	3	527	532	5	4	16	3	199	199	7	17	7	4	144	151	7	18	2	5	110	96	10
7	13	2	56	49	12	2	6	3	98	91	5	6	16	3	1091	1093	11	0	8	4	1876	1880	20	1	3	5	132	128	5
9	13	2	154	151	7	4	6	3	432	418	4	8	16	3	261	256	7	2	8	4	0	8	1	3	3	5	206	200	5
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2	14	2	315	310	6	14	6	3	92	99	9	7	17	3	5	27	4	12	8	4	116	117	8	13	3	5	293	291	6
4	14	2	731	734	7	16	6	3	1130	1108	11	0	18	3	209	212	8	14	8	4	153	144	7	15	3	5	14	32	34
6	14	2	435	425	6	18	6	3	404	406	7	2	18	3	176	174	8	16	8	4	227	230	7	17	3	5	521	517	7
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14	14	2	384	401	7	5	7	3	1173	1158	13	6	0	4	426	407	4	5	9	4	1733	1757	15	6	4	5	660	657	7
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3	15	2	284	289	6	9	7	3	493	489	5	10	0	4	2634	2651	21	9	9	4	41	35	18	10	4	5	135	125	7
5	15	2	1472	1460	14	11	7	3	821	811	8	12	0	4	953	940	10	11	9	4	196	199	6	12	4	5	517	506	6
7	15	2	493	494	6	13	7	3	131	131	7	14	0	4	362	364	6	13	9	4	123	116	8	14	4	5	271	263	6
9	15	2	143	134	8	15	7	3	162	155	7	16	0	4	179	188	7	15	9	4	376	385	7	16	4	5	668	669	7
11	15	2	368	363	7	17	7	3	627	620	6	18	0	4	582	576	6	17	9	4	577	571	7	18	4	5	267	275	7
13	15	2	155	143	9	19	7	3	124	106	9	20	0	4	130	133	9	0	10	4	850	846	9	1	5	5	160	151	5
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6	16	2	477	475	6	6	8	3	579	578	6	7	1	4	52	49	10	8	10	4	322	324	6	9	5	5	423	425	5
8	16	2	66	70	15	8	8	3	45	31	13	9	1	4	1288	1293	14	10	10	4	460	456	6	11	5	5	253	242	6
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2	18	2	0	26	1	5	9	3	305	297	5	4	2	4	430	434	5	9	11	4	38	20	25	8	6	5	331	332	5
4	18	2	221	217	7	7	9	3	225	222	5	6	2	4	449	472	4	11	11	4	24	10	24	10	6	5	81	67	9
6	18	2	393	405	7	9	9	3	72	73	9	8	2	4	100	101	6	13	11	4	108	103	9	12	6	5	234	225	6
1	1	3	263	262	3	11	9	3	852	876	9	10	2	4	446	464	5	15	11	4	760	762	7	14	6	5	19	1	19
3	1	3	660	650	7	13	9	3	35	25	34	12	2	4	320	317	5	0	12	4	968	964	10	16	6	5	700	693	6
5	1	3	191	196	4	15	9	3	84	87	11	14	2	4	641	655	6	2	12	4	268	262	5	1	7	5	69	68	9
7	1	3	257	256	4	17	9	3	518	516	7	16	2	4	718	726	7	4	12	4	135	135	7	3	7	5	484	489	5
9	1	3	387	403	4	0	10	3	801	824	9	18	2	4	41	23	25	6	12	4	281	286	6	5	7	5	84	21	8
11	1	3	1353	1368	14	2	10	3	761	767	7	20	2	4	122	126	10	8	12	4	226	225	6	7	7	5	315	309	5
13	1	3	435	441	5	4	10	3	382	393	5	1	3	4	237	243	4	10	12	4	425	413	6	9	7	5	332	323	6
15	1	3	97	100	8	6	10	3	191	193	5	3	3	4	465	462	5	12	12	4	343	340	6	11	7	5	365	373	6
17	1	3	351	355	6	8	10	3	224	233	6	5	3	4	3337	3340	19	14	12	4	35	10	34	13	7	5	166	168	7
19	1	3	446	476	6	10	10	3	73	57	10	7	3	4	162	162	5	1	13	4	210	226	6	15	7	5	33	36	32
21	1	3	862	848	9	12	10	3	94	98	8	9	3	4	770	783	7	3	13	4	115	103	7	17	7	5	37	54	36
0	2	3	2266	2213	14	14	10	3	618	621	6	11	3	4	22	48	22	5	13	4	331	255	6	0	8	5	769	784	7
2	2	3	552	528	5	16	10	3	45	62	26	13	3	4	124	125	6	7	13	4	276	278	6	2	8	5	112	114	7
4	2	3	16	8	16	1	11	3	328	324	5	15	3	4	716	727	7	9	13	4	495	497	6	4	8	5	49	3	12
6	2	3	1087	1081	12	3	11	3	209	210	5	17	3	4	718	723	7	11	13	4	697	703	7	6	8	5	535	533	5
8	2	3	733	731	8	5	11	3	740	749	8	19	3	4	198	201	8	13	13	4	162	168	8	8	8	5	113	126	8
10	2	3	352	357	5	7	11	3	214	211	6	0	4	4	477	523	5	0	14	4	1427	1404	15	10	8	5	39	41	21
12	2	3	715	726	7	9	11	3	392	405	6	2	4	4	408	393	4	2	14	4	252	242	6	12	8	5	375	365	6
14	2	3	354	346	5	11	11	3	203	105	6	4	4	4	650	680	7	4	14	4	313	313	6	14	8	5	489	494	6
16	2	3	1105	1083	11	13	11	3	54	53	15	6	4	4	1815	1818	19	6	14	4	490	498	6	16	8	5	769	757	7
18	2	3	209	201	7	15	11	3	70	63	13	8	4	4	221	221	5	8	14	4	105	97	10	1	9	5	677	680	7
20	2	3	79	87	13	17	11	3	533	549	7	10	4	4	296	302	5	10	14	4	1050	1054	10	3	9	5	62	68	10

Observed and calculated structure factors for K45

h	k	l	10Fo	10Fc	10s
5	9	5	493	489	5
7	9	5	116	114	6
9	9	5	54	45	15
11	9	5	1472	1510	15
13	9	5	92	108	10
15	9	5	94	93	10
0	10	5	971	975	10
2	10	5	491	498	5
4	10	5	147	147	7
6	10	5	456	444	6
8	10	5	116	116	8
10	10	5	254	254	6
12	10	5	64	64	14
14	10	5	479	477	7
1	11	5	108	106	8
3	11	5	218	209	6
5	11	5	467	462	6
7	11	5	516	515	6
9	11	5	226	234	7
11	11	5	409	413	6
13	11	5	200	186	7
0	12	5	1078	1082	11
2	12	5	470	475	6
4	12	5	57	60	14
6	12	5	668	667	7
8	12	5	112	96	9
10	12	5	142	98	8
12	12	5	227	225	8
1	13	5	115	113	6
3	13	5	256	268	7
5	13	5	907	934	9
7	13	5	180	169	7
9	13	5	298	294	7
11	13	5	1194	1169	11
0	14	5	879	858	8
2	14	5	237	233	7
4	14	5	160	150	6
6	14	5	193	206	7
8	14	5	200	208	8
1	15	5	82	93	11
3	15	5	248	246	7
5	15	5	75	76	12
7	15	5	111	108	7
0	16	5	234	224	7
2	16	5	272	270	7
4	16	5	121	118	9
0	0	6	2416	2534	22
2	0	6	105	91	7
4	0	6	637	640	6
6	0	6	659	678	7
8	0	6	367	374	5
10	0	6	871	867	8
12	0	6	716	736	7
14	0	6	800	788	8
16	0	6	805	812	8
1	1	6	142	138	6
3	1	6	160	152	6
5	1	6	1663	1695	16
7	1	6	49	51	14
9	1	6	358	359	6
11	1	6	210	214	6
13	1	6	63	50	12
15	1	6	435	432	6
17	1	6	118	113	7
0	2	6	1662	1690	15
2	2	6	196	197	5
4	2	6	209	196	5
6	2	6	498	488	5
8	2	6	249	249	6
10	2	6	770	788	7
12	2	6	320	302	6
14	2	6	17	18	17
16	2	6	400	397	7
1	3	6	188	187	5
3	3	6	110	114	6
5	3	6	772	784	8
7	3	6	67	55	10
9	3	6	1095	1104	12
11	3	6	1056	1071	11
13	3	6	255	250	6
15	3	6	49	55	19
0	4	6	2393	2405	22
2	4	6	72	73	9
4	4	6	325	334	5
6	4	6	481	491	5
8	4	6	115	115	7
10	4	6	1364	1374	14
12	4	6	271	269	6
14	4	6	64	64	13
16	4	6	197	194	8
1	5	6	255	255	5
3	5	6	298	301	5
5	5	6	478	472	5
7	5	6	65	76	11
9	5	6	224	227	6
11	5	6	355	346	6
13	5	6	88	79	10
15	5	6	238	226	7
0	6	6	175	170	6
2	6	6	15	18	20
4	6	6	541	546	5
6	6	6	818	823	8
8	6	6	300	298	6
10	6	6	118	122	8
12	6	6	170	172	8
14	6	6	856	854	8
1	7	6	576	588	6
3	7	6	154	161	6
5	7	6	2452	2444	25
7	7	6	118	108	8
9	7	6	185	190	6
11	7	6	452	471	6
13	7	6	216	210	7
15	7	6	611	616	7
0	8	6	332	322	6
2	8	6	193	195	6
4	8	6	296	292	6
6	8	6	275	274	6
8	8	6	356	355	6
10	8	6	114	118	9
12	8	6	185	187	8
14	8	6	402	398	7
1	9	6	320	317	6
3	9	6	116	105	8
5	9	6	41	42	23
7	9	6	467	480	6
9	9	6	510	498	6
11	9	6	698	713	7
13	9	6	50	53	22
0	10	6	2150	2146	25
2	10	6	327	319	6
4	10	6	320	326	6
6	10	6	564	556	6
8	10	6	100	88	9
10	10	6	1244	1250	12
12	10	6	176	170	8
1	11	6	70	72	12
3	11	6	339	342	6
5	11	6	448	448	6
7	11	6	96	96	11
9	11	6	483	470	6
11	11	6	699	701	7
0	12	6	502	505	6
2	12	6	37	46	36
4	12	6	49	60	19
6	12	6	908	897	9
8	12	6	39	30	39
10	12	6	418	421	7
1	13	6	0	29	1
3	13	6	42	40	24
5	13	6	1347	1365	14
7	13	6	174	175	8
0	14	6	54	40	16
2	14	6	374	366	7
4	14	6	323	332	7
1	1	7	80	80	9
3	1	7	249	255	6
5	1	7	60	55	12
7	1	7	255	251	6
9	1	7	228	232	6
11	1	7	738	729	7
13	1	7	140	132	7
15	1	7	123	120	10
0	2	7	669	656	6
2	2	7	295	299	6
4	2	7	25	24	25
6	2	7	447	447	6
8	2	7	299	299	6
10	2	7	100	95	8
12	2	7	530	528	6
14	2	7	185	187	8
1	3	7	198	189	6
3	3	7	40	20	18
5	3	7	186	189	6
7	3	7	443	439	6
9	3	7	183	174	7
11	3	7	744	753	7
13	3	7	0	32	1
0	4	7	992	976	11
2	4	7	118	111	7
4	4	7	263	273	6
6	4	7	96	84	9
8	4	7	216	214	7
10	4	7	218	227	7
12	4	7	463	478	7
14	4	7	142	133	9
1	5	7	21	15	20
3	5	7	205	202	6
5	5	7	322	323	6
7	5	7	494	506	6
9	5	7	316	326	7
11	5	7	43	31	31
13	5	7	271	286	7
0	6	7	227	222	6
2	6	7	96	107	8
4	6	7	190	186	6
6	6	7	675	666	7
8	6	7	241	248	7
10	6	7	144	139	8
12	6	7	193	193	8
1	7	7	65	69	12
3	7	7	263	270	6
5	7	7	705	685	6
7	7	7	130	122	8
9	7	7	358	360	7
11	7	7	493	497	7
0	8	7	540	522	6
2	8	7	119	113	8
4	8	7	291	288	6
6	8	7	334	328	6
8	8	7	29	42	28
10	8	7	59	62	15
1	9	7	371	382	6
3	9	7	24	38	24
5	9	7	226	224	7
7	9	7	125	112	8
9	9	7	0	13	1
0	10	7	570	555	6
2	10	7	421	418	6
4	10	7	192	183	7
6	10	7	204	185	7
8	10	7	133	115	9
1	11	7	162	176	8
3	11	7	131	131	8
5	11	7	526	534	7
7	11	7	155	152	8
0	12	7	53	58	18
2	12	7	166	171	8
4	12	7	251	246	7
0	0	8	2301	2477	26
2	0	8	156	148	7
4	0	8	257	261	6
6	0	8	709	702	7
8	0	8	0	9	1
10	0	8	1447	1426	14
1	1	8	91	89	9
3	1	8	120	119	8
5	1	8	510	502	6
7	1	8	186	182	7
9	1	8	702	696	7
11	1	8	486	480	7
0	2	8	29	9	29
2	2	8	80	78	10
4	2	8	274	264	6
6	2	8	505	497	6
8	2	8	0	17	1
10	2	8	249	245	7
1	3	8	135	133	7
3	3	8	313	316	6
5	3	8	1749	1755	19
7	3	8	0	20	1
9	3	8	434	432	7
11	3	8	159	157	8
0	4	8	238	242	7
2	4	8	268	270	6
4	4	8	262	258	7
6	4	8	587	590	6
8	4	8	37	44	37
10	4	8	135	127	9
1	5	8	538	531	6
3	5	8	139	140	8
5	5	8	423	425	6
7	5	8	34	19	34
9	5	8	167	163	8
0	6	8	1884	1839	19
2	6	8	177	183	7
4	6	8	333	338	7
6	6	8	445	447	7
8	6	8	166	161	8
1	7	8	61	68	15
3	7	8	156	144	8
5	7	8	889	882	9
7	7	8	199	213	8
0	8	8	915	918	9
2	8	8	53	54	17
4	8	8	23	6	22
6	8	8	369	372	7
1	9	8	0	24	1
3	9	8	171	154	8
5	9	8	1216	1228	12
0	10	8	1031	1016	10
2	10	8	146	128	8
1	1	9	82	61	11
3	1	9	211	195	7
5	1	9	278	277	7
0	2	9	84	88	11
2	2	9	44	33	21
4	2	9	247	237	7
6	2	9	26	8	25
1	3	9	162	157	8
3	3	9	42	26	24
5	3	9	77	63	12
0	4	9	438	424	7
2	4	9	44	40	21
4	4	9	68	70	13
1	5	9	35	10	34
3	5	9	117	106	9

Observed and calculated structure factors for K46

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	704	738	5	2	8	0	188	185	3	1	1	1	145	143	1	3	9	1	95	30	4	1	1	2	550	538	5
4	0	0	1127	1118	8	4	8	0	549	553	5	3	1	1	116	111	3	5	9	1	180	405	4	3	1	2	786	782	6
6	0	0	551	576	5	6	8	0	687	691	7	5	1	1	1007	1010	9	7	9	1	330	330	4	5	1	2	995	1007	11
8	0	0	1011	988	12	8	8	0	459	460	5	7	1	1	28	12	7	9	9	1	56	35	7	7	1	2	96	84	3
10	0	0	1905	1784	15	10	8	0	1161	1145	12	9	1	1	266	254	3	11	9	1	1685	1687	18	9	1	2	610	605	6
12	0	0	1418	1444	15	12	8	0	112	120	5	11	1	1	681	697	7	13	9	1	133	128	5	11	1	2	628	616	7
14	0	0	303	294	4	14	8	0	97	86	6	13	1	1	267	261	4	15	9	1	218	206	5	13	1	2	26	6	26
16	0	0	348	348	4	16	8	0	350	351	5	15	1	1	266	262	4	17	9	1	95	117	8	15	1	2	663	667	7
18	0	0	381	386	5	18	8	0	59	49	10	17	1	1	690	696	7	19	9	1	209	212	6	17	1	2	70	60	8
20	0	0	433	427	5	20	8	0	285	278	6	19	1	1	498	500	5	0	10	1	1376	1399	15	19	1	2	53	37	11
22	0	0	1868	1866	16	1	9	0	78	65	4	21	1	1	589	592	5	2	10	1	728	741	7	21	1	2	107	302	5
1	1	0	277	267	2	3	9	0	338	340	3	0	2	1	189	201	2	4	10	1	158	171	4	0	2	2	4142	4078	11
5	1	0	531	548	5	5	9	0	1892	1896	15	2	2	1	563	581	5	6	10	1	505	503	5	2	2	2	384	380	4
7	1	0	375	369	3	7	9	0	842	851	9	4	2	1	376	363	3	8	10	1	166	136	4	4	2	2	489	473	4
9	1	0	1456	1445	13	9	9	0	81	75	6	6	2	1	278	264	2	10	10	1	353	355	4	6	2	2	525	497	5
11	1	0	1062	1013	16	11	9	0	671	663	7	8	2	1	502	500	5	12	10	1	49	24	10	8	2	2	202	191	3
13	1	0	438	442	4	13	9	0	198	189	5	10	2	1	81	72	5	14	10	1	587	594	6	10	2	2	1346	1363	15
15	1	0	242	255	4	15	9	0	747	770	8	12	2	1	868	865	9	16	10	1	503	489	5	12	2	2	571	580	6
17	1	0	391	405	4	17	9	0	568	559	5	14	2	1	123	114	5	18	10	1	172	175	6	14	2	2	34	20	13
19	1	0	507	498	5	19	9	0	126	135	7	16	2	1	539	543	5	1	11	1	83	84	5	16	2	2	316	313	4
21	1	0	873	855	9	0	10	0	291	305	3	18	2	1	35	8	18	3	11	1	51	50	8	18	2	2	77	64	8
0	2	0	1260	1244	6	2	10	0	135	138	4	20	2	1	143	335	5	5	11	1	813	833	8	20	2	2	120	126	7
2	2	0	355	371	3	4	10	0	265	277	4	22	2	1	276	272	6	7	11	1	504	516	5	22	2	2	569	566	6
4	2	0	526	533	5	6	10	0	280	270	4	1	3	1	172	186	3	9	11	1	254	250	4	1	3	2	539	525	5
6	2	0	131	133	2	8	10	0	261	274	4	3	3	1	262	263	2	11	11	1	187	188	5	3	3	2	178	186	2
8	2	0	238	223	3	10	10	0	505	512	5	5	3	1	414	404	4	13	11	1	159	160	5	5	3	2	1161	1139	11
10	2	0	549	558	5	12	10	0	311	317	4	7	3	1	182	375	4	15	11	1	325	318	5	7	3	2	253	247	3
12	2	0	479	488	5	14	10	0	1004	1030	10	9	3	1	217	219	3	17	11	1	432	450	5	9	3	2	1268	1288	14
14	2	0	837	844	8	16	10	0	301	306	5	11	3	1	145	365	3	0	12	1	940	972	10	11	3	2	1521	1547	16
16	2	0	811	808	8	18	10	0	376	375	5	13	3	1	198	199	4	2	12	1	554	563	6	13	3	2	300	294	4
18	2	0	153	154	6	1	11	0	271	265	4	15	3	1	114	122	5	4	12	1	142	153	5	15	3	2	240	235	4
20	2	0	55	56	12	3	11	0	228	228	4	17	3	1	265	280	5	6	12	1	702	719	7	17	3	2	436	438	5
22	2	0	218	215	6	5	11	0	711	719	7	19	3	1	182	173	6	8	12	1	81	78	7	19	3	2	754	752	7
1	3	0	315	315	3	7	11	0	67	82	7	21	3	1	172	171	5	10	12	1	13	24	13	21	3	2	703	696	7
3	3	0	555	559	5	9	11	0	86	89	6	0	4	1	1249	1225	9	12	12	1	232	228	5	0	4	2	1775	1730	11
5	3	0	4615	4795	13	11	11	0	463	475	4	2	4	1	152	149	2	14	12	1	69	72	9	2	4	2	600	599	6
7	3	0	552	549	5	13	11	0	233	233	5	4	4	1	132	124	2	16	12	1	769	748	7	4	4	2	89	84	1
9	3	0	838	822	9	15	11	0	683	700	7	6	4	1	663	631	6	1	13	1	454	453	4	6	4	2	379	374	1
11	3	0	515	422	5	17	11	0	464	463	5	8	4	1	149	352	3	3	13	1	289	300	4	8	4	2	67	73	5
13	3	0	250	243	4	0	12	0	1494	1525	17	10	4	1	592	587	6	5	13	1	1013	1026	11	10	4	2	1961	2001	16
15	3	0	909	912	10	2	12	0	187	181	4	12	4	1	641	651	6	7	13	1	98	99	6	12	4	2	138	145	4
17	3	0	1008	999	9	4	12	0	332	333	4	14	4	1	256	258	4	9	13	1	277	285	5	14	4	2	152	153	5
19	3	0	301	299	5	6	12	0	530	537	5	16	4	1	474	485	5	11	13	1	1214	1215	12	16	4	2	19	24	19
21	3	0	106	296	5	8	12	0	199	192	5	18	4	1	238	237	5	13	13	1	176	177	6	18	4	2	515	514	5
0	4	0	2148	2074	9	10	12	0	734	743	8	20	4	1	37	47	23	15	13	1	153	150	6	20	4	2	243	249	5
2	4	0	711	699	6	12	12	0	497	505	5	22	4	1	294	297	6	0	14	1	879	890	9	1	5	2	998	954	11
4	4	0	851	858	10	14	12	0	112	115	7	1	5	1	104	104	3	2	14	1	164	160	5	3	5	2	44	52	6
6	4	0	3826	3867	13	16	12	0	28	10	27	3	5	1	162	160	3	4	14	1	387	377	4	5	5	2	1878	1839	13
8	4	0	423	416	4	1	13	0	587	580	6	5	5	1	1136	1117	12	6	14	1	282	285	5	7	5	2	252	246	3
10	4	0	468	482	5	3	13	0	239	240	4	7	5	1	867	845	9	8	14	1	244	232	5	9	5	2	477	483	5
12	4	0	276	256	4	5	13	0	330	330	4	9	5	1	410	411	4	10	14	1	411	405	5	11	5	2	661	662	7
14	4	0	608	612	6	7	13	0	491	497	5	11	5	1	261	286	4	12	14	1	153	144	6	13	5	2	91	73	5
16	4	0	2158	2121	19	9	13	0	301	296	5	13	5	1	550	554	5	14	14	1	288	287	5	15	5	2	331	313	4
18	4	0	57	51	9	11	13	0	932	930	10	15	5	1	177	184	5	1	15	1	15	20	14	17	5	2	703	678	6
20	4	0	147	139	6	13	13	0	283	284	5	17	5	1	215	206	5	3	15	1	375	386	5	19	5	2	343	339	5
22	4	0	537	536	5	15	13	0	277	277	6	19	5	1	23	4	23	5	15	1	112	122	7	21	5	2	355	346	6
1	5	0	1536	1506	10	0	14	0	1313	1304	13	21	5	1	570	563	5	7	15	1	146	156	5	0	6	2	1103	1116	12
3	5	0	51	37	4	2	14	0	353	354	4	0	6	1	551	519	5	9	15	1	15	14	14	2	6	2	28	30	9
5	5	0	3175	3041	13	4	14	0	227	224	5	2	6	1	101	94	3	11	15	1	143	134	6	4	6	2	761	771	7
7	5	0	932	932	9	6	14	0	693	709	7	4	6	1	278	266	3	13	15	1	211	209	6	6	6	2	2530	2498	15
9	5	0	61	63	5	8	14	0	143	138	6	6	6	1	977	996	9	0	16	1	190	184	5	8	6	2	286	281	3
11	5	0	419	434	4	10	14	0	1189	1204	12	8	6	1	545	521	5	2	16	1	186	189	5	10	6	2	171	172	4
13	5	0	215	227	4	12	14	0	78	85	11	10	6	1	129	124	4	4	16	1	53	60	12	12	6	2	158	166	4
15	5	0	210	219	4	14	14	0	21	18	21	12	6	1	363	355	4	6	16	1	1322	1292	12	14	6	2	752	764	7
17	5	0	487	485	5	1	15	0	309	310	5	14	6	1	44	20	10	8	16	1	346	350	5	16	6	2	1585	1587	14
19	5	0	169	162	5	3	15	0	355	351	5	16	6	1	976	987	10	10	16	1	48	46	14	18	6	2	55	28	12
21	5	0	476	468	5	5	15	0	518	526	5	18	6	1	265	266	5	12	16	1	22	47	22	20	6	2	58	71	11
0	6	0	767	768	7	7	15	0	129	129	6	20	6	1	477	470	5	1	17	1	126	124	6	1	7	2	656	648	6
2	6	0	208	218	2	9	15	0	200	198	5	1	7	1	157	148	3	3	17	1	198	197	6	3	7	2	90	90	4
4	6	0	310	268	3	11	15	0	419	412	5	3	7	1	458	468	4	5	17	1	826	830	8	5	7	2	4501	4402	17
6	6	0	486	468	5	13	15	0	373	374	5	5	7	1	782	790	8	7	17	1	237	228	5	7	7	2	167	166	4
8	6	0	677	687	7	0	16	0	585	578	6	7	7	1	206	195	3	9	17	1	275	288	6	9	7	2	450	462	4
10	6	0	1455	1469	15	2	16	0	279	270	5	9	7	1	331	342	3	0	18	1	312	317	5	11	7	2	85	91	6
12	6	0	134	139	4	4	16	0	138	138	6	11	7	1	78	106	6	2	18	1	115	121	7	13	7	2	335	326	4
14	6	0	412	407	4	6	16	0	762	772	8	13	7	1	60	62	7	4	18	1	297	310	5	15	7	2	975	1011	10
16	6	0	491	488	5	8	16	0	105	101	7	15	7	1	140	146	5	6	18	1	291	286	6	17	7	2	1045	1049	10
18	6	0	379	373	5	10	16	0	121	128	7	17	7	1	268	259	5	1	19	1	424	423	5	19	7	2	123	114	6
20	6	0	12	3	11	12	16	0	466	472	5	19	7	1	159	162	6	3	19	1	407	412	5	0	8	2	397	402	4
1	7	0	561	533	5	1	17	0	341	329	5	0	8	1	434	414	4	0	0	2	3209	3155	10	2	8	2	526	538	5
3	7	0	260	269	3	3	17	0	288	289	5	2	8	1	149	135	3	2	0	2	674	672	6	4	8	2	209	216	3
5	7	0	1374	1380	13	5	17	0	1731	1710	16	4	8	1	71	69	5	4	0	2	165	172	2	6	8	2	386	383	3
7	7	0	556	554	5	7	17	0	49	52	15	6	8	1	265	279	3	6	0	2	710	678	6	8	8	2	578	580	6
9	7	0	1100	1081	11	9	17	0	48	48	16	8	8	1	57	48	7	8	0	2	640	624	6	10	8	2	101	97	5
11	7	0	635	625	7	0	18	0	389	386	5	10	8	1	149	162	4	10	0	2	1505	1475	15	12	8	2	24	1	23
13	7	0	289	289	4	2	18	0	266	275	6	12	8	1	491	498	5	12	0	2	1104	1098	11	14	8	2	475	482	5
15	7	0	320	314	4	4	18	0	68	64	12	14	8	1	482	478	5	14	0	2	1267	1272	12	16	8	2	869	879	9
17	7	0	419	414	5	6	18	0	322	311	5	16	8	1	451	455	5	16	0	2	864	858	9	18	8	2	15	9	15
19	7	0	630	627	6	8	18	0	284	285	6	18	8	1	261	271	5	18	0	2	556	548	5	20	8	2	187	180	6
21	7	0	614	588	6	1	19	0	178	168	6	20	8	1	157	351	5	20	0	2	205	199	5	1	9	2	522	524	5
0	8	0	2653	2547	14	3	19	0	173	159	6	1	9	1	925	906	10	22	0	2	464	448	5	3	9	2	163	158	4

Observed and calculated structure factors for K46

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
5	9	2	565	568	6	10	2	3	28	14	18	5	11	3	875	879	9	17	3	4	771	773	8	11	13	4	745	753	8
7	9	2	518	511	5	12	2	3	665	677	7	7	11	3	203	208	5	19	3	4	254	261	6	13	13	4	171	172	6
9	9	2	548	552	5	14	2	3	310	313	4	9	11	3	327	321	4	0	4	4	535	552	5	0	14	4	1286	1278	12
11	9	2	1599	1594	19	16	2	3	940	935	10	11	11	3	73	70	8	2	4	4	495	493	5	2	14	4	198	203	5
13	9	2	213	215	5	18	2	3	180	194	6	13	11	3	19	13	20	4	4	4	438	467	4	4	14	4	330	335	5
15	9	2	102	95	7	20	2	3	273	262	5	15	11	3	164	152	6	6	4	4	2015	2024	16	6	14	4	483	487	5
17	9	2	744	759	7	1	3	3	502	509	5	17	11	3	539	547	5	8	4	4	178	181	4	8	14	4	122	121	7
19	9	2	289	285	6	3	3	3	224	224	3	0	12	3	117	116	5	10	4	4	353	360	4	10	14	4	934	940	9
0	10	2	4623	4327	18	5	3	3	945	958	9	2	12	3	344	344	4	12	4	4	187	193	5	12	14	4	42	41	17
2	10	2	589	588	6	7	3	3	716	692	7	4	12	3	407	405	4	14	4	4	628	630	6	1	15	4	276	271	5
4	10	2	668	669	7	9	3	3	194	188	4	6	12	3	234	217	5	16	4	4	1483	1540	15	3	15	4	355	360	5
6	10	2	129	129	5	11	3	3	1366	1399	17	8	12	3	35	2	17	18	4	4	130	131	7	5	15	4	256	257	5
8	10	2	265	264	4	13	3	3	29	11	16	10	12	3	41	37	15	1	5	4	994	978	10	7	15	4	39	20	18
10	10	2	1853	1820	19	15	3	3	204	207	5	12	12	3	211	212	5	3	5	4	152	141	3	9	15	4	189	188	6
12	10	2	388	396	4	17	3	3	243	255	5	14	12	3	153	163	6	5	5	4	1482	1522	16	0	16	4	178	175	6
14	10	2	303	314	5	19	3	3	105	98	7	16	12	3	464	444	5	7	5	4	423	422	4	2	16	4	262	260	6
16	10	2	178	183	6	21	3	3	446	422	5	1	13	3	363	356	4	9	5	4	0	10	1	4	16	4	63	63	10
18	10	2	174	168	6	0	4	3	2259	2202	13	3	13	3	399	406	4	11	5	4	920	941	9	6	16	4	445	434	5
1	11	2	456	463	4	2	4	3	10	19	10	5	13	3	425	429	4	13	5	4	57	70	9	8	16	4	48	39	16
3	11	2	699	707	7	4	4	3	295	293	3	7	13	3	111	122	6	15	5	4	244	254	5	1	17	4	372	374	5
5	11	2	29	24	21	6	4	3	298	289	3	9	13	3	216	216	5	17	5	4	116	128	6	3	17	4	195	193	6
7	11	2	0	31	1	8	4	3	154	162	4	11	13	3	504	502	5	19	5	4	101	101	8	5	17	4	1301	1282	14
9	11	2	528	534	5	10	4	3	649	652	7	13	13	3	44	36	15	0	6	4	1994	2029	16	1	1	5	45	36	8
11	11	2	1803	1829	20	12	4	3	686	691	7	15	13	3	64	54	11	2	6	4	217	223	3	3	1	5	119	129	4
13	11	2	36	25	19	14	4	3	105	108	6	0	14	3	234	226	5	4	6	4	322	320	3	5	1	5	781	796	8
15	11	2	65	61	11	16	4	3	101	96	7	2	14	3	128	122	6	6	6	4	157	159	4	7	1	5	32	35	12
17	11	2	73	54	10	18	4	3	119	126	7	4	14	3	297	302	5	8	6	4	389	378	4	9	1	5	229	229	4
0	12	2	1312	1296	12	20	4	3	84	87	8	6	14	3	122	137	6	10	6	4	1271	1319	13	11	1	5	141	138	5
2	12	2	129	131	5	1	5	3	73	72	4	8	14	3	294	292	5	12	6	4	227	226	5	13	1	5	117	123	6
4	12	2	194	184	4	3	5	3	207	209	3	10	14	3	226	238	5	14	6	4	217	223	5	15	1	5	181	180	5
6	12	2	801	810	8	5	5	3	594	579	6	12	14	3	60	42	12	16	6	4	191	184	5	17	1	5	700	713	7
8	12	2	192	197	5	7	5	3	826	827	8	1	15	3	187	185	5	18	6	4	247	248	5	19	1	5	385	390	6
10	12	2	658	667	7	9	5	3	303	309	4	3	15	3	298	302	5	1	7	4	186	180	4	0	2	5	826	839	9
12	12	2	101	296	5	11	5	3	123	120	5	5	15	3	313	315	5	3	7	4	286	291	4	2	2	5	163	156	4
14	12	2	418	426	5	13	5	3	420	421	4	7	15	3	241	227	5	5	7	4	1234	1247	12	4	2	5	152	156	3
16	12	2	507	521	5	15	5	3	225	235	5	9	15	3	86	72	8	7	7	4	416	423	4	6	2	5	476	473	5
1	13	2	140	143	5	17	5	3	263	263	5	11	15	3	335	318	5	9	7	4	848	851	9	8	2	5	242	238	4
3	13	2	74	53	7	19	5	3	54	12	13	0	16	3	207	208	5	11	7	4	735	758	7	10	2	5	175	182	5
5	13	2	1720	1717	19	0	6	3	488	482	5	2	16	3	45	38	14	13	7	4	231	231	5	12	2	5	681	688	7
7	13	2	69	33	8	2	6	3	176	170	3	4	16	3	258	267	5	15	7	4	270	280	5	14	2	5	38	37	15
9	13	2	53	62	10	4	6	3	493	483	5	6	16	3	1132	1127	11	17	7	4	486	481	5	16	2	5	126	129	7
11	13	2	139	149	6	6	6	3	1253	1280	15	8	16	3	292	305	5	0	8	4	1838	1851	16	18	2	5	118	118	7
13	13	2	140	133	6	8	6	3	382	375	4	10	16	3	171	183	6	2	8	4	53	51	8	1	3	5	132	131	4
15	13	2	536	544	5	10	6	3	172	173	4	1	17	3	183	193	6	4	8	4	283	299	4	3	3	5	247	239	4
0	14	2	315	321	4	12	6	3	326	326	4	3	17	3	216	223	6	6	8	4	617	618	6	5	3	5	566	584	6
2	14	2	331	337	4	14	6	3	59	67	9	5	17	3	538	541	5	8	8	4	353	357	4	7	3	5	73	65	6
4	14	2	664	675	6	16	6	3	1054	1064	10	7	17	3	13	29	12	10	8	4	986	1002	11	9	3	5	112	98	5
6	14	2	501	500	5	18	6	3	397	397	5	0	18	3	190	190	6	12	8	4	59	61	9	11	3	5	216	217	4
8	14	2	202	204	5	20	6	3	440	431	5	2	18	3	214	219	6	14	8	4	64	69	9	13	3	5	223	221	5
10	14	2	61	55	10	1	7	3	206	169	3	4	18	3	129	130	7	16	8	4	315	303	5	15	3	5	45	49	14
12	14	2	16	1	16	3	7	3	173	183	3	0	0	4	6276	6619	18	18	8	4	16	14	27	17	3	5	505	497	5
14	14	2	296	304	6	5	7	3	1432	1452	15	2	0	4	346	365	4	1	9	4	32	7	15	0	4	5	197	202	4
1	15	2	683	655	7	7	7	3	215	199	4	4	0	4	536	552	5	3	9	4	223	219	4	2	4	5	93	86	4
3	15	2	219	216	5	9	7	3	371	368	4	6	0	4	339	331	3	5	9	4	1787	1777	18	4	4	5	45	40	8
5	15	2	1447	1430	15	11	7	3	883	889	9	8	0	4	347	350	3	7	9	4	469	463	4	6	4	5	600	591	6
7	15	2	454	451	5	13	7	3	136	137	5	10	0	4	2800	2779	18	9	9	4	51	5	9	8	4	5	279	282	4
9	15	2	51	24	13	15	7	3	0	8	1	12	0	4	1012	1018	10	11	9	4	251	250	5	10	4	5	165	166	4
11	15	2	448	444	5	17	7	3	652	655	7	14	0	4	419	422	4	13	9	4	58	49	10	12	4	5	432	437	4
13	15	2	130	129	7	19	7	3	121	122	7	16	0	4	63	50	10	15	9	4	564	565	5	14	4	5	266	263	5
0	16	2	929	921	9	0	8	3	1053	1020	10	18	0	4	419	423	5	17	9	4	631	627	6	16	4	5	541	547	5
2	16	2	160	153	6	2	8	3	23	22	23	20	0	4	315	317	6	0	10	4	822	828	9	18	4	5	239	252	6
4	16	2	64	72	10	4	8	3	231	228	4	1	1	4	410	408	4	2	10	4	50	61	10	1	5	5	142	139	4
6	16	2	587	590	6	6	8	3	564	557	5	3	1	4	23	0	17	4	10	4	382	387	4	3	5	5	190	192	4
8	16	2	26	16	26	8	8	3	111	101	5	5	1	4	158	144	3	6	10	4	184	186	5	5	5	5	492	488	5
10	16	2	769	774	8	10	8	3	268	263	4	7	1	4	81	78	5	8	10	4	288	294	4	7	5	5	579	567	6
1	17	2	261	252	5	12	8	3	553	553	5	9	1	4	1055	1065	11	10	10	4	437	432	5	9	5	5	312	312	4
3	17	2	389	384	5	14	8	3	278	278	5	11	1	4	1740	1770	18	12	10	4	309	303	5	11	5	5	254	247	5
5	17	2	59	53	11	16	8	3	23	24	23	13	1	4	253	249	4	14	10	4	771	773	8	13	5	5	384	385	5
7	17	2	172	171	6	18	8	3	92	84	8	15	1	4	171	148	5	16	10	4	420	425	5	15	5	5	153	146	6
9	17	2	321	325	6	1	9	3	588	581	6	17	1	4	84	91	8	1	11	4	182	190	5	17	5	5	158	142	6
0	18	2	639	636	6	3	9	3	185	186	4	19	1	4	463	456	5	3	11	4	279	289	4	0	6	5	405	426	4
2	18	2	95	105	8	5	9	3	270	269	4	0	2	4	305	323	3	5	11	4	930	939	9	2	6	5	53	50	7
4	18	2	290	291	6	7	9	3	212	215	4	2	2	4	234	237	3	7	11	4	7	26	6	4	6	5	16	21	15
6	18	2	396	389	5	9	9	3	55	57	8	4	2	4	332	332	3	9	11	4	58	63	9	6	6	5	507	497	5
1	1	3	203	198	2	11	9	3	894	907	9	6	2	4	446	474	4	11	11	4	57	57	11	8	6	5	338	350	4
3	1	3	520	515	5	13	9	3	84	80	6	8	2	4	76	77	5	13	11	4	136	143	7	10	6	5	72	81	7
5	1	3	27	30	9	15	9	3	205	200	5	10	2	4	369	379	4	15	11	4	571	568	5	12	6	5	251	250	5
7	1	3	380	382	4	17	9	3	429	445	5	12	2	4	421	430	4	0	12	4	982	989	9	14	6	5	36	31	21
9	1	3	210	214	3	0	10	3	968	994	9	14	2	4	619	628	6	2	12	4	178	185	5	16	6	5	653	654	6
11	1	3	1218	1234	11	2	10	3	716	720	7	16	2	4	784	790	8	4	12	4	235	230	5	1	7	5	105	95	5
13	1	3	147	154	4	4	10	3	257	261	4	18	2	4	147	155	6	6	12	4	242	241	5	3	7	5	397	405	4
15	1	3	319	320	4	6	10	3	283	278	4	20	2	4	9	25	9	8	12	4	229	226	5	5	7	5	252	251	4
17	1	3	329	334	5	8	10	3	192	191	4	1	3	4	196	190	3	10	12	4	536	533	5	7	7	5	298	300	4
19	1	3	480	490	5	10	10	3	177	169	5	3	3	4	425	426	4	12	12	4	356	357	5	9	7	5	231	224	5
21	1	3	574	573	5	12	10	3	65	69	9	5	3	4	3327	3376	16	14	12	4	41	38	20	11	7	5	301	306	5
0	2	3	2065	2027	12	14	10	3	579	576	6	7	3	4	197	202	4	1	13	4	170	162	4	13	7	5	153	154	6
2	2	3	672	667	6	16	10	3	287	280	5	9	3	4	624	628	6	3	13	4	180	180	5	15	7	5	178	181	6
4	2	3	205	196	3	18	10	3	99	108	8	11	3	4	132	142	5	5	13	4	227	224	5	17	7	5	43	16	16
6	2	3	1057	1029	9	1	11	3	246	206	4	13	3	4	234	233	4	7	13	4	302	308	5	0	8	5	628	653	6
8	2	3	615	607	6	3	11	3	5	17	5	15	3	4	787	798	9	9	13	4	111	300	5	2	8	5	202	203	4

Observed and calculated structure factors for K46

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
4	8	5	115	117	5	14	0	6	704	723	7	0	8	6	271	268	4	11	3	7	838	832	9	1	1	8	175	177	5
6	8	5	553	539	5	16	0	6	910	905	9	2	8	6	269	253	4	13	3	7	58	62	11	3	1	8	78	78	8
8	8	5	67	76	8	1	1	6	194	196	4	4	8	6	297	303	4	0	4	7	1111	1084	11	5	1	8	420	435	5
10	8	5	117	123	6	3	1	6	160	157	4	6	8	6	278	273	5	2	4	7	47	40	11	7	1	8	251	248	5
12	8	5	346	347	5	5	1	6	1579	1635	18	8	8	6	349	351	5	4	4	7	175	166	5	9	1	8	580	567	6
14	8	5	431	435	5	7	1	6	138	148	5	10	8	6	194	197	5	6	4	7	163	163	5	11	1	8	564	557	6
16	8	5	563	562	6	9	1	6	342	350	4	12	8	6	50	55	13	8	4	7	128	128	6	0	2	8	34	21	22
1	9	5	665	675	7	11	1	6	199	204	5	14	8	6	329	330	5	10	4	7	437	440	5	2	2	8	114	118	6
3	9	5	0	5	1	13	1	6	96	101	7	1	9	6	391	395	4	12	4	7	449	446	5	4	2	8	207	198	5
5	9	5	517	501	5	15	1	6	425	413	5	3	9	6	22	29	21	14	4	7	121	107	7	6	2	8	515	498	5
7	9	5	327	324	4	17	1	6	306	297	5	5	9	6	67	49	9	1	5	7	43	6	11	8	2	8	0	17	1
9	9	5	33	22	20	0	2	6	1674	1695	17	7	9	6	557	559	6	3	5	7	96	95	6	10	2	8	202	190	6
11	9	5	1520	1530	15	2	2	6	205	212	4	9	9	6	361	360	5	5	5	7	144	140	5	1	3	8	108	107	6
13	9	5	161	159	6	4	2	6	173	166	4	11	9	6	740	731	7	7	5	7	501	495	5	3	3	8	293	282	5
15	9	5	192	184	6	6	2	6	505	510	5	13	9	6	42	35	18	9	5	7	228	223	5	5	3	8	1785	1771	22
0	10	5	1095	1100	11	8	2	6	204	204	5	0	10	6	2125	2132	21	11	5	7	31	24	31	7	3	8	0	2	1
2	10	5	462	464	5	10	2	6	833	852	9	2	10	6	257	255	5	13	5	7	256	258	6	9	3	8	347	337	5
4	10	5	58	43	8	12	2	6	323	331	5	4	10	6	242	251	5	0	6	7	216	213	5	11	3	8	120	111	6
6	10	5	513	504	5	14	2	6	70	75	8	6	10	6	566	566	5	2	6	7	138	140	5	0	4	8	225	227	5
8	10	5	89	90	7	16	2	6	358	366	5	8	10	6	80	81	8	4	6	7	202	201	5	2	4	8	330	328	5
10	10	5	342	344	5	1	3	6	291	290	4	10	10	6	1247	1258	13	6	6	7	722	731	8	4	4	8	143	133	6
12	10	5	89	85	7	3	3	6	22	22	21	12	10	6	262	257	6	8	6	7	262	253	5	6	4	8	682	694	7
14	10	5	438	437	5	5	3	6	860	868	9	1	11	6	182	188	5	10	6	7	140	140	6	8	4	8	0	16	1
1	11	5	0	7	1	7	3	6	127	120	5	3	11	6	149	145	5	12	6	7	202	202	6	10	4	8	171	167	6
3	11	5	60	64	9	9	3	6	862	868	8	5	11	6	475	481	5	1	7	7	107	111	6	1	5	8	529	537	5
5	11	5	573	568	6	11	3	6	1184	1192	11	7	11	6	151	157	6	3	7	7	193	189	5	3	5	8	151	165	6
7	11	5	495	507	5	13	3	6	127	128	6	9	11	6	372	373	5	5	7	7	891	871	9	5	5	8	404	404	5
9	11	5	160	158	6	15	3	6	118	122	7	11	11	6	786	784	8	7	7	7	125	114	6	7	5	8	41	33	18
11	11	5	260	271	5	17	3	6	415	420	5	0	12	6	491	501	5	9	7	7	279	260	5	9	5	8	64	63	11
13	11	5	206	207	6	0	4	6	2320	2304	18	2	12	6	127	128	6	11	7	7	565	562	5	0	6	8	1791	1776	22
0	12	5	973	988	10	2	4	6	43	33	9	4	12	6	146	151	6	0	8	7	658	653	7	2	6	8	198	198	5
2	12	5	527	529	5	4	4	6	324	325	4	6	12	6	849	851	9	2	8	7	18	11	17	4	6	8	293	290	5
4	12	5	14	18	13	6	4	6	500	514	5	8	12	6	75	64	9	4	8	7	166	162	6	6	6	8	450	438	5
6	12	5	743	746	8	8	4	6	88	96	7	10	12	6	345	348	6	6	8	7	366	354	5	8	6	8	149	156	6
8	12	5	55	48	11	10	4	6	1315	1325	14	1	13	6	23	9	22	8	8	7	30	25	29	1	7	8	34	13	13
10	12	5	44	29	16	12	4	6	138	145	6	3	13	6	67	39	10	10	8	7	213	220	6	3	7	8	215	208	5
12	12	5	193	189	6	14	4	6	18	5	18	5	13	6	1273	1265	13	12	8	7	364	369	6	5	7	8	859	868	8
1	13	5	191	385	5	16	4	6	209	210	6	7	13	6	115	102	7	1	9	7	344	348	5	7	7	8	250	248	6
3	13	5	197	201	5	1	5	6	296	292	4	0	14	6	118	113	7	3	9	7	108	110	7	0	8	8	913	899	9
5	13	5	992	994	11	3	5	6	306	309	4	2	14	6	178	176	5	5	9	7	246	246	5	2	8	8	33	26	13
7	13	5	193	190	6	5	5	6	534	525	5	4	14	6	294	284	6	7	9	7	133	137	7	4	8	8	73	82	10
9	13	5	250	247	6	7	5	6	81	76	6	6	14	6	187	168	6	9	9	7	0	0	1	6	8	8	435	433	5
11	13	5	1277	1277	13	9	5	6	288	286	5	1	1	7	77	78	7	11	9	7	555	551	5	1	9	8	60	49	11
0	14	5	1043	1019	11	11	5	6	308	307	5	3	1	7	190	182	5	0	10	7	624	616	6	3	9	8	106	99	8
2	14	5	144	137	6	13	5	6	65	70	10	5	1	7	129	132	5	2	10	7	409	414	5	5	9	8	1233	1244	11
4	14	5	300	299	5	15	5	6	296	296	5	7	1	7	284	276	5	4	10	7	131	125	6	0	10	8	1013	998	10
6	14	5	440	434	5	0	6	6	112	103	5	9	1	7	137	135	6	6	10	7	203	199	5	2	10	8	50	47	15
8	14	5	138	146	7	2	6	6	86	89	6	11	1	7	667	671	6	8	10	7	109	111	8	1	1	9	0	15	1
10	14	5	427	411	5	4	6	6	300	309	4	13	1	7	263	258	5	1	11	7	111	113	7	3	1	9	126	122	7
1	15	5	70	71	10	6	6	6	984	971	11	15	1	7	246	241	6	3	11	7	18	22	18	5	1	9	374	371	5
3	15	5	321	319	5	8	6	6	298	294	5	0	2	7	622	615	6	5	11	7	598	599	6	0	2	9	183	186	6
5	15	5	50	24	15	10	6	6	69	45	8	2	2	7	329	332	4	7	11	7	149	142	6	2	2	9	109	107	7
7	15	5	134	128	6	12	6	6	200	200	5	4	2	7	27	26	27	0	12	7	17	26	21	4	2	9	116	128	7
0	16	5	123	115	5	14	6	6	679	678	7	6	2	7	488	485	5	2	12	7	225	218	6	6	2	9	54	46	13
2	16	5	236	225	6	16	6	6	803	803	8	8	2	7	254	255	5	4	12	7	272	271	6	1	3	9	97	99	8
4	16	5	50	65	15	1	7	6	509	518	5	10	2	7	69	75	9	1	13	7	228	228	6	3	3	9	0	10	1
0	0	6	2457	2542	18	3	7	6	88	90	7	12	2	7	446	439	5	0	0	8	2434	2487	22	5	3	9	145	136	6
2	0	6	157	147	4	5	7	6	2450	2434	20	14	2	7	190	186	6	2	0	8	133	131	6	0	4	9	442	427	5
4	0	6	505	517	5	7	7	6	111	114	6	1	3	7	245	234	4	4	0	8	171	170	5	2	4	9	40	44	18
6	0	6	688	702	7	9	7	6	353	350	5	3	3	7	18	15	18	6	0	8	675	672	7	4	4	9	57	61	12
8	0	6	409	408	4	11	7	6	422	426	5	5	3	7	399	396	4	8	0	8	34	30	23	1	5	9	28	26	28
10	0	6	926	928	9	13	7	6	219	209	5	7	3	7	374	378	5	10	0	8	1493	1510	16	3	5	9	53	51	13
12	0	6	780	799	7	15	7	6	705	698	7	9	3	7	140	138	6	12	0	8	547	546	5	0	6	9	152	146	6

Observed and calculated structure factors for K47

h	k	l	10Fo	10Fc	10s
2	0	0	705	740	8
4	0	0	1134	1133	12
6	0	0	549	563	5
8	0	0	1006	979	10
10	0	0	3753	3789	22
12	0	0	1417	1433	16
14	0	0	291	286	6
16	0	0	354	343	7
18	0	0	394	401	7
20	0	0	417	425	8
22	0	0	1857	1876	18
3	1	0	270	264	3
5	1	0	531	547	5
7	1	0	366	374	4
9	1	0	1507	1461	13
11	1	0	2997	3014	23
13	1	0	420	428	6
15	1	0	239	253	7
17	1	0	402	396	7
19	1	0	494	499	8
21	1	0	860	866	9
0	2	0	1225	1257	9
2	2	0	358	361	3
4	2	0	539	546	5
6	2	0	134	133	4
8	2	0	219	226	4
10	2	0	572	563	6
12	2	0	473	477	5
14	2	0	869	846	8
16	2	0	804	804	8
18	2	0	133	139	10
20	2	0	50	56	29
22	2	0	231	226	10
1	3	0	318	316	3
3	3	0	558	561	5
5	3	0	4780	4793	17
7	3	0	560	545	5
9	3	0	837	830	8
11	3	0	411	410	5
13	3	0	253	247	6
15	3	0	904	911	9
17	3	0	1038	999	10
19	3	0	286	288	8
21	3	0	314	300	9
0	4	0	2061	2062	13
2	4	0	683	682	6
4	4	0	863	871	9
6	4	0	3898	3844	18
8	4	0	427	421	4
10	4	0	473	481	5
12	4	0	238	254	6
14	4	0	628	625	6
16	4	0	2109	2137	21
18	4	0	82	53	14
20	4	0	160	148	10
22	4	0	540	532	9
1	5	0	1522	1491	15
3	5	0	17	19	12
5	5	0	3141	3053	18
7	5	0	925	924	9
9	5	0	86	53	8
11	5	0	405	428	6
13	5	0	215	233	7
15	5	0	238	227	7
17	5	0	475	481	7
19	5	0	168	165	9
21	5	0	461	461	8
0	6	0	761	767	7
2	6	0	208	215	4
4	6	0	278	276	4
6	6	0	493	475	5
8	6	0	718	690	7
10	6	0	1457	1454	13
12	6	0	136	150	8
14	6	0	405	410	7
16	6	0	490	498	7
18	6	0	371	366	8
20	6	0	36	2	35
1	7	0	555	537	5
3	7	0	261	262	4
5	7	0	1360	1377	14
7	7	0	547	547	5
9	7	0	1081	1080	12
11	7	0	646	624	6
13	7	0	295	296	7
15	7	0	312	318	7
17	7	0	410	405	8
19	7	0	619	632	8
21	7	0	626	603	9
0	8	0	2574	2532	20
2	8	0	182	185	5
4	8	0	548	544	5
6	8	0	686	689	7
8	8	0	453	451	5
10	8	0	1155	1163	11
12	8	0	140	134	8
14	8	0	96	86	10
16	8	0	359	352	8
18	8	0	59	52	21
20	8	0	300	288	9
1	9	0	79	56	8
3	9	0	342	348	5
5	9	0	1855	1883	23
7	9	0	854	846	8
9	9	0	72	62	11
11	9	0	679	662	7
13	9	0	202	192	7
15	9	0	734	756	7
17	9	0	574	560	8
19	9	0	124	142	12
0	10	0	309	312	5
2	10	0	128	134	6
4	10	0	275	281	6
6	10	0	257	262	6
8	10	0	261	275	6
10	10	0	505	518	6
12	10	0	305	311	7
14	10	0	1028	1028	9
16	10	0	291	301	8
18	10	0	395	388	9
1	11	0	261	269	6
3	11	0	226	230	6
5	11	0	693	720	7
7	11	0	79	80	11
9	11	0	89	86	10
11	11	0	471	478	7
13	11	0	220	226	8
15	11	0	706	716	8
17	11	0	447	463	8
0	12	0	1513	1524	15
2	12	0	194	190	7
4	12	0	322	313	6
6	12	0	543	543	6
8	12	0	179	191	8
10	12	0	739	734	7
12	12	0	505	506	7
14	12	0	115	110	11
16	12	0	0	17	1
1	13	0	570	572	6
3	13	0	232	238	7
5	13	0	349	344	7
7	13	0	496	500	7
9	13	0	318	304	7
11	13	0	927	935	9
13	13	0	272	285	9
15	13	0	257	271	9
0	14	0	1327	1305	14
2	14	0	348	351	7
4	14	0	228	222	8
6	14	0	714	709	7
8	14	0	153	143	9
10	14	0	1200	1201	12
12	14	0	102	85	12
14	14	0	55	11	26
1	15	0	299	302	7
3	15	0	355	359	7
5	15	0	521	525	7
7	15	0	114	124	11
9	15	0	184	184	9
11	15	0	413	410	8
13	15	0	368	371	8
0	16	0	583	593	7
2	16	0	267	269	8
4	16	0	141	142	10
6	16	0	766	780	8
8	16	0	108	101	12
10	16	0	133	129	11
12	16	0	475	479	8
1	17	0	341	325	8
3	17	0	287	287	8
5	17	0	1714	1707	16
7	17	0	0	38	1
9	17	0	42	52	42
0	18	0	371	378	8
2	18	0	283	283	8
4	18	0	52	66	27
6	18	0	296	308	9
8	18	0	289	287	9
1	19	0	173	175	10
3	19	0	149	154	11
1	1	1	149	147	3
3	1	1	324	323	3
5	1	1	1000	1006	10
7	1	1	21	4	20
9	1	1	288	273	5
11	1	1	711	713	7
13	1	1	277	272	6
15	1	1	261	253	7
17	1	1	700	702	7
19	1	1	508	502	7
21	1	1	638	620	8
0	2	1	185	203	3
2	2	1	557	579	6
4	2	1	383	377	3
6	2	1	280	265	4
8	2	1	515	505	5
10	2	1	76	52	8
12	2	1	860	877	9
14	2	1	111	115	9
16	2	1	548	557	7
18	2	1	33	2	32
20	2	1	348	330	8
22	2	1	281	273	9
1	3	1	375	385	4
3	3	1	264	260	3
5	3	1	411	401	4
7	3	1	191	385	4
9	3	1	216	221	5
11	3	1	149	155	5
13	3	1	187	203	7
15	3	1	107	108	10
17	3	1	288	287	7
19	3	1	179	181	9
21	3	1	389	367	8
0	4	1	1231	1215	14
2	4	1	142	146	4
4	4	1	138	129	4
6	4	1	675	640	6
8	4	1	359	368	5
10	4	1	586	566	6
12	4	1	658	661	6
14	4	1	252	253	7
16	4	1	497	502	7
18	4	1	223	238	9
20	4	1	38	39	38
22	4	1	282	294	10
1	5	1	98	110	5
3	5	1	379	377	4
5	5	1	1170	1143	12
7	5	1	855	850	9
9	5	1	424	426	5
11	5	1	261	290	6
13	5	1	542	560	6
15	5	1	172	163	8
17	5	1	199	211	9
19	5	1	0	2	1
21	5	1	584	578	8
0	6	1	552	530	5
2	6	1	95	94	5
4	6	1	281	268	4
6	6	1	970	980	10
8	6	1	527	524	5
10	6	1	133	127	7
12	6	1	365	361	6
14	6	1	18	18	17
16	6	1	988	992	10
18	6	1	278	273	8
20	6	1	477	471	8
1	7	1	167	152	5
3	7	1	471	474	4
5	7	1	769	768	7
7	7	1	209	203	6
9	7	1	340	338	6
11	7	1	84	99	10
13	7	1	64	56	13
15	7	1	118	136	10
17	7	1	267	260	8
19	7	1	145	151	12
0	8	1	458	432	4
2	8	1	129	114	6
4	8	1	64	55	10
6	8	1	266	283	5
8	8	1	67	56	10
10	8	1	131	146	8
12	8	1	485	500	6
14	8	1	478	492	7
16	8	1	469	475	8
18	8	1	280	279	8
20	8	1	355	356	9
1	9	1	906	901	9
1	9	1	61	36	10
3	9	1	374	395	5
5	9	1	130	134	6
7	9	1	40	37	21
9	9	1	1654	1686	16
11	9	1	131	120	9
13	9	1	209	203	8
15	9	1	104	125	13
17	9	1	207	212	10
19	9	1	1359	1380	13
0	10	1	739	742	7
2	10	1	176	174	6
4	10	1	492	499	6
6	10	1	141	143	7
8	10	1	342	350	6
10	10	1	32	20	31
12	10	1	585	592	7
14	10	1	475	475	8
16	10	1	167	176	11
18	10	1	111	88	8
1	11	1	71	66	11
3	11	1	814	829	8
5	11	1	510	515	6
7	11	1	237	251	7
9	11	1	194	199	8
11	11	1	162	161	8
13	11	1	308	311	8
15	11	1	440	456	8
17	11	1	956	973	9
0	12	1	554	559	6
2	12	1	158	154	7
4	12	1	706	712	7
6	12	1	96	92	10
8	12	1	0	30	1
10	12	1	242	236	8
12	12	1	67	73	18
14	12	1	750	750	8
16	12	1	448	445	6
1	13	1	304	308	7
3	13	1	1009	1018	10
5	13	1	90	97	11
7	13	1	292	286	7
9	13	1	1207	1203	12
11	13	1	191	181	9
13	13	1	151	152	11
15	13	1	868	884	9
0	14	1	165	169	8
2	14	1	370	374	7
4	14	1	279	281	7
6	14	1	234	241	8
8	14	1	404	396	8
10	14	1	148	150	9
12	14	1	290	287	9
14	14	1	6	12	5
1	15	1	380	380	7
3	15	1	121	126	10
5	15	1	377	358	8
7	15	1	12	17	11
9	15	1	136	124	10
11	15	1	214	204	9
13	15	1	389	377	7
0	16	1	190	188	8
2	16	1	38	56	38
4	16	1	1278	1285	13
6	16	1	342	346	8
8	16	1	40	42	39
10	16	1	51	45	30
12	16	1	138	126	10
1	17	1	210	210	9
3	17	1	828	820	8
5	17	1	236	229	9
7	17	1	296	289	9
9	17	1	304	316	9
0	18	1	114	118	12
2	18	1	304	304	9
4	18	1	274	280	9
6	18	1	423	415	8
1	19	1	406	410	9
3	19	1	3325	3355	14
0	0	2	673	670	7
2	0	2	175	180	4
4	0	2	702	673	7
6	0	2	633	617	6
8	0	2	1483	1474	16
10	0	2	1084	1091	11
12	0	2	1250	1266	13
14	0	2	844	853	8
16	0	2	568	567	7
18	0	2	207	200	9
20	0	2	451	443	9
1	1	2	554	545	5
3	1	2	804	787	8
5	1	2	1002	1000	9
7	1	2	85	79	6
9	1	2	624	614	6
11	1	2	629	625	6
13	1	2	28	3	28
15	1	2	664	669	7
17	1	2	61	62	16
19	1	2	34	42	33
21	1	2	318	306	9
0	2	2	4186	4071	16
2	2	2	388	387	4
4	2	2	497	486	5
6	2	2	521	502	5
8	2	2	212	195	5
10	2	2	1389	1359	16
12	2	2	555	571	6
14	2	2	26	21	25
16	2	2	327	322	7
18	2	2	74	56	14
20	2	2	117	124	13
1	3	2	526	519	5
3	3	2	194	190	4
5	3	2	1168	1136	12
7	3	2	251	245	5
9	3	2	1283	1298	12
11	3	2	1529	1545	17
13	3	2	298	302	6
15	3	2	244	233	7
17	3	2	428	435	7
19	3	2	746	746	8
21	3	2	722	699	8
0	4	2	1779	1735	16
2	4	2	597	590	6
4	4	2	92	77	6
6	4	2	378	364	4
8	4	2	75	74	8
10	4	2	1949	1997	23
12	4	2	166	152	7
14	4	2	166	162	7
16	4	2	26	26	25
18	4	2	518	510	8
20	4	2	264	258	9
1	5	2	962	947	10
3	5	2	51	52	9
5	5	2	1842	1835	19
7	5	2	244	245	5
9	5	2	471	472	5
11	5	2	677	654	6
13	5	2	57	65	15
15	5	2	310	305	7
17	5	2	698	685	7
19	5	2	340	347	9
21	5	2	365	353	9
0	6	2	1134	1111	10
2	6	2	27	36	26
4	6	2	794	790	8
6	6	2	2525	2485	21
8	6	2	285	281	5
10	6	2	154	161	7
12	6	2	361	368	6
14	6	2	769	770	8
16	6	2	1587	1594	15
18	6	2	20	27	19
20	6	2	85	77	13
1	7	2	663	647	6
3	7	2	85	84	7
5	7	2	4477	4407	23
7	7	2	161	163	7
9	7	2	449	465	6
11	7	2	82	88	11
13	7	2	340	332	7
15	7	2	993	1011	10
17	7	2	1052	1047	10
19	7	2	114	112	12
0	8	2	406	404	5
2	8	2	548	532	5
4	8	2	213	217	6
6	8	2	390	390	5
8	8	2	578	574	6
10	8	2	91	80	10
12	8	2	15	14	14
14	8	2	480	485	7
16	8	2	860	886	8
18	8	2	24	4	23
20	8	2	188	188	11
1	9	2	526	516	6
3	9	2	149	150	6
5	9	2	557	558	5

Observed and calculated structure factors for K47

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	9	2	519	509	6	12	2	3	683	687	7	9	11	3	327	320	7	0	4	4	518	544	5	0	14	4	1279	1290	13
9	9	2	569	564	6	14	2	3	310	316	7	11	11	3	82	65	13	2	4	4	491	489	5	2	14	4	207	203	8
11	9	2	1591	1595	16	16	2	3	958	957	10	13	11	3	21	12	20	4	4	4	455	471	5	4	14	4	334	327	8
13	9	2	199	205	8	18	2	3	185	198	9	15	11	3	166	149	10	6	4	4	2037	2013	24	6	14	4	468	478	8
15	9	2	123	103	10	20	2	3	256	259	9	17	11	3	547	553	9	8	4	4	171	185	7	8	14	4	128	126	11
17	9	2	760	752	8	1	3	3	516	508	5	0	12	3	105	114	10	10	4	4	348	358	6	10	14	4	931	945	10
19	9	2	278	278	9	3	3	3	233	224	4	2	12	3	143	138	7	12	4	4	199	192	7	12	14	4	57	45	24
0	10	2	4402	4321	25	5	3	3	974	965	10	4	12	3	416	404	7	14	4	4	627	640	7	1	15	4	267	265	8
2	10	2	598	595	6	7	3	3	713	698	7	6	12	3	207	212	8	16	4	4	1548	1551	16	3	15	4	366	362	8
4	10	2	664	674	6	9	3	3	205	194	6	8	12	3	31	15	30	18	4	4	131	132	11	5	15	4	255	256	9
6	10	2	133	128	8	11	3	3	1380	1398	14	10	12	3	56	37	21	1	5	4	994	978	10	7	15	4	45	26	39
8	10	2	252	261	7	13	3	3	8	1	8	12	12	3	237	218	8	3	5	4	155	148	6	9	15	4	168	180	10
10	10	2	1833	1826	20	15	3	3	183	196	8	14	12	3	158	163	11	5	5	4	1484	1520	17	0	16	4	175	181	10
12	10	2	376	387	7	17	3	3	251	251	8	16	12	3	463	443	9	7	5	4	424	425	6	2	16	4	264	256	9
14	10	2	305	314	8	19	3	3	96	99	13	1	13	3	150	147	7	9	5	4	0	16	1	4	16	4	54	68	30
16	10	2	170	186	10	21	3	3	427	424	9	3	13	3	405	413	7	11	5	4	927	946	9	6	16	4	437	439	8
18	10	2	173	175	10	0	4	3	2286	2200	19	5	13	3	420	421	7	13	5	4	79	81	12	8	16	4	0	14	1
1	11	2	464	460	6	2	4	3	152	18	5	7	13	3	125	123	10	15	5	4	254	261	8	1	17	4	176	168	9
3	11	2	701	709	7	4	4	3	302	297	5	9	13	3	212	214	8	17	5	4	114	121	12	3	17	4	190	189	10
5	11	2	6	10	5	6	4	3	291	283	5	11	13	3	500	486	8	19	5	4	82	99	17	1	1	5	37	41	22
7	11	2	29	32	29	8	4	3	172	169	6	13	13	3	53	44	26	0	6	4	2013	2030	23	3	1	5	133	116	7
9	11	2	527	537	7	10	4	3	650	637	6	15	13	3	46	54	46	2	6	4	212	225	6	5	1	5	803	789	8
11	11	2	1844	1831	17	12	4	3	706	700	7	0	14	3	206	214	8	4	6	4	334	331	6	7	1	5	32	12	31
13	11	2	42	23	27	14	4	3	101	101	11	2	14	3	137	132	9	6	6	4	139	154	7	9	1	5	235	241	7
15	11	2	73	77	16	16	4	3	134	105	9	4	14	3	297	299	8	8	6	4	386	380	6	11	1	5	151	150	8
17	11	2	71	56	16	18	4	3	140	130	10	6	14	3	128	140	11	10	6	4	1289	1309	13	13	1	5	142	133	9
0	12	2	1308	1290	13	20	4	3	84	78	17	8	14	3	319	303	8	12	6	4	238	235	7	15	1	5	190	174	8
2	12	2	122	132	9	1	5	3	67	67	8	10	14	3	223	226	9	14	6	4	220	223	8	17	1	5	714	717	8
4	12	2	174	175	8	3	5	3	208	218	5	12	14	3	50	48	29	16	6	4	176	187	9	19	1	5	400	388	9
6	12	2	799	815	8	5	5	3	611	601	6	1	15	3	188	174	9	18	6	4	257	245	9	0	2	5	843	834	8
8	12	2	177	191	8	7	5	3	829	832	9	3	15	3	282	296	8	1	7	4	189	178	6	2	2	5	150	156	7
10	12	2	671	668	7	9	5	3	314	323	6	5	15	3	315	314	8	3	7	4	285	292	6	4	2	5	160	164	6
12	12	2	305	300	8	11	5	3	134	121	8	7	15	3	226	231	9	5	7	4	1223	1250	12	6	2	5	479	472	6
14	12	2	418	427	8	13	5	3	422	424	7	9	15	3	84	70	15	7	7	4	428	422	6	8	2	5	243	238	7
16	12	2	520	511	8	15	5	3	207	215	8	11	15	3	332	311	9	9	7	4	854	850	9	10	2	5	156	169	8
1	13	2	130	150	9	17	5	3	272	268	8	0	16	3	211	206	9	11	7	4	750	763	7	12	2	5	700	696	7
3	13	2	62	60	15	19	5	3	0	36	1	2	16	3	18	35	17	13	7	4	251	241	7	14	2	5	60	36	17
5	13	2	1678	1715	17	0	6	3	482	479	5	4	16	3	263	262	8	15	7	4	288	283	8	16	2	5	152	137	10
7	13	2	54	30	19	2	6	3	178	166	5	6	16	3	1125	1121	11	17	7	4	482	475	8	18	2	5	96	109	15
9	13	2	68	66	18	4	6	3	492	478	5	8	16	3	314	297	9	0	8	4	1795	1840	18	1	3	5	122	133	7
11	13	2	133	152	11	6	6	3	1246	1272	13	10	16	3	167	180	11	2	8	4	42	52	21	3	3	5	240	235	6
13	13	2	130	127	12	8	6	3	384	376	6	1	17	3	165	190	11	4	8	4	279	294	6	5	3	5	569	580	6
15	13	2	533	540	8	10	6	3	167	171	7	3	17	3	226	233	9	6	8	4	607	619	6	7	3	5	70	68	11
0	14	2	340	328	7	12	6	3	332	329	6	5	17	3	534	525	8	8	8	4	339	351	7	9	3	5	124	96	8
2	14	2	349	339	7	14	6	3	52	68	18	7	17	3	16	26	15	10	8	4	1002	1016	10	11	3	5	224	222	7
4	14	2	647	667	7	16	6	3	1042	1074	11	0	18	3	179	189	10	12	8	4	53	73	20	13	3	5	231	222	8
6	14	2	489	496	7	18	6	3	410	404	8	2	18	3	238	218	9	14	8	4	74	70	14	15	3	5	59	37	17
8	14	2	217	212	8	20	6	3	427	431	9	4	18	3	124	124	12	16	8	4	307	305	9	17	3	5	492	500	8
10	14	2	68	65	16	1	7	3	190	169	6	0	0	4	6442	6605	23	18	8	4	36	12	35	0	4	5	174	189	6
12	14	2	22	0	22	3	7	3	183	196	6	2	0	4	369	375	5	1	9	4	86	6	10	2	4	5	94	80	8
14	14	2	308	310	9	5	7	3	1432	1436	16	4	0	4	543	562	5	3	9	4	217	225	7	4	4	5	52	46	17
1	15	2	660	646	7	7	7	3	191	195	6	6	0	4	354	344	5	5	9	4	1734	1775	19	6	4	5	609	598	6
3	15	2	210	215	9	9	7	3	369	370	6	8	0	4	333	337	5	7	9	4	469	462	6	8	4	5	294	292	6
5	15	2	1411	1420	15	11	7	3	896	884	9	10	0	4	2747	2779	26	9	9	4	0	5	1	10	4	5	145	148	7
7	15	2	468	458	8	13	7	3	155	140	8	12	0	4	1020	1009	10	11	9	4	245	243	8	12	4	5	455	443	7
9	15	2	10	15	10	15	7	3	36	1	35	14	0	4	418	418	7	13	9	4	60	52	18	14	4	5	259	258	8
11	15	2	459	443	8	17	7	3	668	657	8	16	0	4	49	61	25	15	9	4	552	556	8	16	4	5	572	562	8
13	15	2	128	123	11	19	7	3	126	108	12	18	0	4	422	433	8	17	9	4	635	631	8	18	4	5	261	253	9
0	16	2	913	922	9	0	8	3	1031	1015	11	20	0	4	309	315	9	0	10	4	817	836	9	1	5	5	144	139	7
2	16	2	140	153	9	2	8	3	19	29	18	1	1	4	408	403	5	2	10	4	51	55	16	3	5	5	181	196	7
4	16	2	54	71	24	4	8	3	232	233	6	3	1	4	0	4	1	4	10	4	385	392	7	5	5	5	503	500	6
6	16	2	589	578	8	6	8	3	571	562	6	5	1	4	172	151	6	6	10	4	197	195	8	7	5	5	572	574	6
8	16	2	25	39	25	8	8	3	104	103	8	7	1	4	74	74	9	8	10	4	290	294	7	9	5	5	320	318	7
10	16	2	782	765	8	10	8	3	264	255	7	9	1	4	1074	1074	11	10	10	4	447	439	7	11	5	5	254	250	7
1	17	2	268	247	8	12	8	3	559	558	7	11	1	4	1773	1769	18	12	10	4	301	299	8	13	5	5	384	385	7
3	17	2	404	388	8	14	8	3	280	289	8	13	1	4	250	243	7	14	10	4	783	772	8	15	5	5	129	134	11
5	17	2	86	57	14	16	8	3	36	17	35	15	1	4	145	145	9	16	10	4	433	428	9	17	5	5	160	145	10
7	17	2	156	163	10	18	8	3	86	95	15	17	1	4	88	82	12	1	11	4	184	185	8	0	6	5	395	423	6
9	17	2	320	321	9	1	9	3	574	583	6	19	1	4	456	461	8	3	11	4	288	296	7	2	6	5	69	54	11
0	18	2	653	626	8	3	9	3	171	176	6	0	2	4	313	326	5	5	11	4	933	951	9	4	6	5	0	24	1
2	18	2	88	94	14	5	9	3	281	277	6	2	2	4	241	238	5	7	11	4	31	21	31	6	6	5	492	494	6
4	18	2	276	285	9	7	9	3	200	214	7	4	2	4	348	338	5	9	11	4	55	58	20	8	6	5	334	351	7
6	18	2	392	391	9	9	9	3	49	53	18	6	2	4	464	478	5	11	11	4	68	52	15	10	6	5	79	80	12
1	1	3	203	203	4	11	9	3	899	906	9	8	2	4	77	73	10	13	11	4	131	142	11	12	6	5	249	251	8
3	1	3	527	522	5	13	9	3	77	78	12	10	2	4	380	382	6	15	11	4	602	583	8	14	6	5	32	28	31
5	1	3	19	39	18	15	9	3	188	194	9	12	2	4	429	424	6	0	12	4	1008	995	10	16	6	5	673	658	8
7	1	3	370	377	5	17	9	3	438	453	8	14	2	4	629	629	7	2	12	4	186	188	8	1	7	5	100	93	8
9	1	3	238	226	5	0	10	3	951	974	10	16	2	4	791	791	8	4	12	4	220	221	8	3	7	5	392	412	6
11	1	3	1238	1251	12	2	10	3	723	729	7	18	2	4	143	141	10	6	12	4	234	251	8	5	7	5	237	232	7
13	1	3	344	361	7	4	10	3	266	265	6	20	2	4	32	24	31	8	12	4	244	224	8	7	7	5	305	302	7
15	1	3	316	312	7	6	10	3	277	269	6	1	3	4	191	198	5	10	12	4	536	530	8	9	7	5	238	223	7
17	1	3	336	339	8	8	10	3	202	205	7	3	3	4	431	434	5	12	12	4	357	361	8	11	7	5	302	311	7
19	1	3	483	494	8	10	10	3	166	164	8	5	3	4	3225	3370	24	14	12	4	56	35	26	13	7	5	151	148	10
21	1	3	606	603	8	12	10	3	65	74	17	7	3	4	192	203	6	1	13	4	152	154	7	15	7	5	176	172	10
0	2	3	2078	2042	17	14	10	3	571	577	8	9	3	4	636	636	6	3	13	4	186	170	8	17	7	5	0	14	1
2	2	3	666	658	6	16	10	3	253	263	9	11	3	4	115	130	9	5	13	4	229	233	8	0	8	5	640	656	6
4	2	3	178	179	5	1	11	3	192	202	7	13	3	4	241	235	7	7	13	4	311	307	8	2	8	5	199	196	7
6	2	3	1069	1034	11	3	11	3	29	30	29	15	3	4	786	797	8	9	13	4	311	310	9	4	8	5	98	113	11
8	2	3	621	618	6	5	11	3	875	879	9	17	3	4	760	773	8	11	13	4	764	758	8	6	8	5	538	538	7
10	2	3	13	13	13	7	11	3	219	212	7	19	3	4	249	251	9	13	13	4	160	167	10	8	8	5	84	76	11

Observed and calculated structure factors for K47

h	k	l	10Fo	10Fc	10s
10	8	5	121	114	10
12	8	5	347	353	8
14	8	5	443	441	8
16	8	5	604	580	8
1	9	5	663	674	7
3	9	5	14	9	34
5	9	5	493	502	7
7	9	5	325	325	7
9	9	5	30	24	30
11	9	5	1520	1531	16
13	9	5	144	153	11
15	9	5	205	182	9
0	10	5	1103	1086	11
2	10	5	479	468	7
4	10	5	61	50	16
6	10	5	503	502	7
8	10	5	95	97	12
10	10	5	342	338	8
12	10	5	80	82	15
14	10	5	432	437	8
1	11	5	18	9	17
3	11	5	65	72	15
5	11	5	580	569	7
7	11	5	490	507	7
9	11	5	160	157	9
11	11	5	277	278	8
13	11	5	209	210	10
0	12	5	988	991	9
2	12	5	518	527	7
4	12	5	33	16	32
6	12	5	744	738	7
8	12	5	61	56	19
10	12	5	25	20	25
12	12	5	200	197	10
1	13	5	185	379	8
3	13	5	208	209	9
5	13	5	982	988	10
7	13	5	183	187	10
9	13	5	239	251	9
11	13	5	1292	1271	12
0	14	5	1048	1019	11
2	14	5	142	145	11
4	14	5	299	297	8
6	14	5	427	432	8
8	14	5	161	152	10
10	14	5	409	405	9
1	15	5	78	77	15
3	15	5	109	117	9
5	15	5	0	21	1
7	15	5	129	131	9
0	16	5	120	107	9
2	16	5	235	222	10
4	16	5	72	66	20
0	0	6	2476	2540	26
2	0	6	139	139	8
4	0	6	518	526	6
6	0	6	686	705	7
8	0	6	196	403	7
10	0	6	925	927	9
12	0	6	784	794	8
14	0	6	735	721	8
16	0	6	906	912	9
1	1	6	192	190	7
3	1	6	160	154	7
5	1	6	1611	1647	15
7	1	6	161	143	8
9	1	6	150	151	7
11	1	6	219	208	8
13	1	6	81	95	13
15	1	6	418	419	8
17	1	6	100	102	9
0	2	6	1688	1698	18
2	2	6	223	213	7
4	2	6	169	167	7
6	2	6	501	510	6
8	2	6	195	206	8
10	2	6	853	853	8
12	2	6	329	328	8
14	2	6	65	74	16
16	2	6	387	374	8
1	3	6	293	288	6
3	3	6	37	29	37
5	3	6	856	866	9
7	3	6	106	119	9
9	3	6	863	876	9
11	3	6	1173	1196	12
13	3	6	128	133	10
15	3	6	126	120	11
17	3	6	416	421	9
0	4	6	2283	2317	27
2	4	6	31	28	30
4	4	6	335	325	7
6	4	6	497	514	7
8	4	6	80	95	14
10	4	6	1359	1330	13
12	4	6	150	152	9
14	4	6	6	11	5
16	4	6	208	219	10
1	5	6	285	283	7
3	5	6	114	111	7
5	5	6	521	516	7
7	5	6	75	74	11
9	5	6	282	281	7
11	5	6	326	322	8
13	5	6	53	70	24
15	5	6	291	290	8
0	6	6	110	108	9
2	6	6	92	86	10
4	6	6	310	317	7
6	6	6	978	968	9
8	6	6	292	297	8
10	6	6	24	37	24
12	6	6	198	204	9
14	6	6	702	683	8
16	6	6	817	806	8
1	7	6	505	516	7
3	7	6	94	100	12
5	7	6	2396	2438	30
7	7	6	116	109	10
9	7	6	139	152	8
11	7	6	425	425	8
13	7	6	210	209	9
15	7	6	681	700	8
0	8	6	276	266	7
2	8	6	239	249	7
4	8	6	310	302	7
6	8	6	280	282	8
8	8	6	148	146	8
10	8	6	174	184	9
12	8	6	71	63	16
14	8	6	325	335	9
1	9	6	401	389	7
3	9	6	0	30	1
5	9	6	50	37	23
7	9	6	568	559	7
9	9	6	145	367	8
11	9	6	740	732	8
13	9	6	39	28	38
0	10	6	2107	2131	22
2	10	6	249	260	8
4	10	6	262	251	8
6	10	6	554	565	8
8	10	6	83	77	14
10	10	6	1282	1262	12
12	10	6	260	252	9
1	11	6	183	185	9
3	11	6	350	343	8
5	11	6	479	477	8
7	11	6	162	155	10
9	11	6	382	377	8
11	11	6	789	785	8
0	12	6	499	499	8
2	12	6	140	131	10
4	12	6	146	142	11
6	12	6	860	854	8
8	12	6	50	55	33
10	12	6	352	350	9
1	13	6	0	13	1
3	13	6	19	39	18
5	13	6	1278	1267	13
7	13	6	84	106	17
0	14	6	115	113	13
2	14	6	178	178	8
4	14	6	284	281	9
6	14	6	174	164	11
1	1	7	73	81	12
3	1	7	185	184	8
5	1	7	132	128	9
7	1	7	283	275	7
9	1	7	142	140	9
11	1	7	688	680	8
13	1	7	264	266	9
15	1	7	233	236	10
0	2	7	616	615	7
2	2	7	341	334	7
4	2	7	15	21	14
6	2	7	470	480	7
8	2	7	248	252	8
10	2	7	77	63	15
12	2	7	451	449	8
14	2	7	177	183	10
1	3	7	236	233	7
3	3	7	0	16	1
5	3	7	396	397	7
7	3	7	374	379	7
9	3	7	134	141	10
11	3	7	832	829	8
13	3	7	44	58	44
0	4	7	1092	1077	11
2	4	7	45	44	22
4	4	7	175	170	8
6	4	7	151	156	9
8	4	7	138	134	9
10	4	7	423	429	8
12	4	7	448	449	8
14	4	7	103	103	14
1	5	7	28	5	27
3	5	7	100	97	11
5	5	7	174	151	9
7	5	7	497	501	7
9	5	7	235	230	8
11	5	7	31	21	30
13	5	7	257	256	9
0	6	7	204	203	8
2	6	7	153	138	9
4	6	7	199	200	8
6	6	7	718	725	7
8	6	7	240	256	8
10	6	7	141	140	10
12	6	7	216	206	9
1	7	7	110	112	10
3	7	7	201	195	8
5	7	7	865	861	9
7	7	7	118	110	11
9	7	7	250	258	9
11	7	7	562	554	8
0	8	7	665	640	7
2	8	7	8	18	8
4	8	7	172	169	9
6	8	7	163	150	8
8	8	7	48	23	31
10	8	7	207	211	9
12	8	7	175	169	9
1	9	7	351	347	8
3	9	7	93	107	13
5	9	7	257	254	9
7	9	7	149	139	10
9	9	7	129	0	10
11	9	7	546	552	8
0	10	7	611	611	8
2	10	7	420	413	8
4	10	7	132	122	12
6	10	7	201	195	9
8	10	7	126	114	11
1	11	7	157	114	10
3	11	7	24	29	23
5	11	7	587	590	8
7	11	7	137	145	11
0	12	7	13	22	13
2	12	7	220	217	9
4	12	7	281	269	9
1	13	7	252	226	9
0	0	8	2464	2489	22
2	0	8	153	138	9
4	0	8	182	171	9
6	0	8	664	675	8
8	0	8	27	22	27
10	0	8	1509	1511	15
12	0	8	537	543	8
1	1	8	173	176	9
3	1	8	81	80	14
5	1	8	443	442	8
7	1	8	240	247	9
9	1	8	584	572	8
11	1	8	570	559	8
0	2	8	0	15	1
2	2	8	126	118	10
4	2	8	214	203	9
6	2	8	515	502	8
8	2	8	31	14	31
10	2	8	193	191	10
1	3	8	101	105	13
3	3	8	271	284	8
5	3	8	1766	1777	19
7	3	8	0	1	1
9	3	8	350	336	8
11	3	8	96	115	15
0	4	8	230	235	8
2	4	8	122	122	8
4	4	8	141	138	11
6	4	8	685	691	8
8	4	8	0	14	1
10	4	8	201	161	9
1	5	8	527	533	8
3	5	8	174	164	9
5	5	8	419	408	8
7	5	8	25	33	25
9	5	8	65	72	20
0	6	8	1843	1787	19
2	6	8	196	194	9
4	6	8	289	290	8
6	6	8	442	441	8
8	6	8	149	153	11
1	7	8	26	12	25
3	7	8	198	205	9
5	7	8	870	869	9
7	7	8	244	246	9
0	8	8	895	900	9
2	8	8	68	25	18
4	8	8	78	79	17
6	8	8	427	431	9
1	9	8	45	46	44
3	9	8	99	104	14
5	9	8	1225	1248	12
0	10	8	1017	1006	9
2	10	8	51	49	28
1	1	9	27	19	26
3	1	9	123	123	11
5	1	9	368	364	9
0	2	9	169	175	10
2	2	9	115	108	12
4	2	9	135	132	12
6	2	9	49	41	32
1	3	9	105	102	12
3	3	9	21	7	21
5	3	9	176	127	11
0	4	9	415	424	8
2	4	9	31	45	31
4	4	9	72	61	17
1	5	9	44	27	36
3	5	9	53	48	28
0	6	9	117	139	14

Observed and calculated structure factors for K49

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	605	630	6	4	8	0	360	367	3	3	1	1	440	440	4	7	9	1	344	345	4	7	1	2	179	175	3
4	0	0	1206	1180	9	6	8	0	551	552	5	5	1	1	906	902	10	9	9	1	43	43	12	9	1	2	623	603	6
6	0	0	630	634	6	8	8	0	477	477	5	7	1	1	88	71	3	11	9	1	1682	1701	20	11	1	2	618	610	6
8	0	0	921	896	9	10	8	0	1307	1296	13	9	1	1	413	416	4	13	9	1	94	67	7	13	1	2	74	69	6
10	0	0	1970	1715	17	12	8	0	141	146	5	11	1	1	821	854	8	15	9	1	116	117	7	15	1	2	636	641	6
12	0	0	1377	1395	17	14	8	0	172	175	6	13	1	1	358	358	4	17	9	1	171	175	6	17	1	2	51	43	11
14	0	0	172	162	5	16	8	0	285	290	5	15	1	1	116	106	6	19	9	1	178	193	7	19	1	2	23	16	23
16	0	0	274	271	5	18	8	0	36	27	25	17	1	1	718	716	7	0	10	1	1236	1249	12	21	1	2	319	317	6
18	0	0	549	535	5	20	8	0	320	299	6	19	1	1	471	481	5	2	10	1	763	762	7	0	2	2	4105	4140	12
20	0	0	247	249	6	1	9	0	102	85	4	21	1	1	826	820	8	4	10	1	234	240	4	2	2	2	311	309	3
22	0	0	1677	1705	18	3	9	0	357	358	3	0	2	1	69	94	3	6	10	1	453	461	4	4	2	2	477	462	4
3	1	0	161	154	2	5	9	0	1898	1912	17	2	2	1	503	517	5	8	10	1	166	173	5	6	2	2	437	423	4
5	1	0	426	440	4	7	9	0	898	873	8	4	2	1	477	486	5	10	10	1	253	254	5	8	2	2	226	215	3
7	1	0	498	498	5	9	9	0	39	16	13	6	2	1	227	209	2	12	10	1	16	18	16	10	2	2	1319	1312	16
9	1	0	1724	1684	14	11	9	0	622	592	6	8	2	1	581	593	6	14	10	1	595	587	6	12	2	2	548	556	6
11	1	0	1036	2876	17	13	9	0	284	282	5	10	2	1	203	216	4	16	10	1	292	307	6	14	2	2	118	111	5
13	1	0	348	353	4	15	9	0	571	571	5	12	2	1	920	950	10	18	10	1	224	243	6	16	2	2	328	318	5
15	1	0	295	306	4	17	9	0	495	502	6	14	2	1	174	165	4	1	11	1	179	177	4	18	2	2	55	34	10
17	1	0	305	302	5	19	9	0	240	235	6	16	2	1	670	675	7	3	11	1	247	244	4	20	2	2	40	16	23
19	1	0	565	584	6	0	10	0	289	307	4	18	2	1	42	45	14	5	11	1	689	701	7	1	3	2	371	373	3
21	1	0	777	783	8	2	10	0	56	51	7	20	2	1	207	205	6	7	11	1	547	540	5	3	3	2	312	311	3
0	2	0	1423	1386	7	4	10	0	457	475	4	22	2	1	198	208	7	9	11	1	303	310	5	5	3	2	1047	1012	9
2	2	0	225	236	2	6	10	0	271	268	4	1	3	1	351	351	3	11	11	1	354	348	5	7	3	2	111	107	4
4	2	0	713	720	6	8	10	0	261	266	4	3	3	1	238	236	2	13	11	1	111	118	7	9	3	2	1616	1594	16
6	2	0	176	180	3	10	10	0	483	495	5	5	3	1	359	349	3	15	11	1	119	126	7	11	3	2	1406	1397	17
8	2	0	320	308	3	12	10	0	149	148	6	7	3	1	479	476	4	17	11	1	464	461	6	13	3	2	401	399	4
10	2	0	687	700	7	14	10	0	1173	1163	13	9	3	1	208	218	3	0	12	1	1077	1085	11	15	3	2	160	147	5
12	2	0	305	311	4	16	10	0	212	209	6	11	3	1	254	263	4	2	12	1	472	485	5	17	3	2	324	320	5
14	2	0	857	865	9	18	10	0	488	491	6	13	3	1	249	257	4	4	12	1	111	108	5	19	3	2	782	795	8
16	2	0	706	708	7	1	11	0	247	244	4	15	3	1	76	66	7	6	12	1	644	642	6	21	3	2	530	534	6
18	2	0	33	10	19	3	11	0	304	310	4	17	3	1	293	293	5	8	12	1	161	161	5	0	4	2	1940	1920	12
20	2	0	168	163	7	5	11	0	861	898	9	19	3	1	182	193	6	10	12	1	156	156	5	2	4	2	685	664	6
22	2	0	315	317	6	7	11	0	170	175	5	21	3	1	321	328	6	12	12	1	282	290	5	4	4	2	83	71	3
1	3	0	291	285	3	9	11	0	56	43	9	0	4	1	1070	1052	10	14	12	1	31	30	31	6	4	2	361	354	3
3	3	0	531	527	5	11	11	0	429	442	5	2	4	1	90	95	3	16	12	1	746	728	7	8	4	2	129	150	4
5	3	0	5184	4807	14	13	11	0	193	196	5	4	4	1	238	235	2	1	13	1	387	376	4	10	4	2	2007	2015	17
7	3	0	501	480	5	15	11	0	833	843	8	6	4	1	792	763	7	3	13	1	356	361	4	12	4	2	290	292	4
9	3	0	957	945	10	17	11	0	181	394	6	8	4	1	495	490	4	5	13	1	941	956	9	14	4	2	200	204	5
11	3	0	369	366	4	0	12	0	1614	1596	19	10	4	1	318	293	4	7	13	1	75	79	8	16	4	2	22	7	21
13	3	0	353	353	4	2	12	0	240	228	4	12	4	1	715	721	7	9	13	1	297	307	5	18	4	2	486	486	5
15	3	0	842	841	9	4	12	0	255	246	4	14	4	1	242	251	5	11	13	1	1088	1096	11	20	4	2	306	307	6
17	3	0	960	956	9	6	12	0	604	619	6	16	4	1	657	644	6	13	13	1	152	149	7	1	5	2	992	976	8
19	3	0	205	207	6	8	12	0	126	137	6	18	4	1	255	252	5	15	13	1	271	258	6	3	5	2	144	144	3
21	3	0	408	392	6	10	12	0	667	682	7	20	4	1	68	58	11	0	14	1	696	699	8	5	5	2	1921	1859	14
0	4	0	2152	2061	10	12	12	0	503	500	5	1	5	1	112	111	3	2	14	1	268	266	5	7	5	2	203	188	3
2	4	0	562	563	5	14	12	0	61	81	11	3	5	1	500	497	4	4	14	1	394	392	5	9	5	2	419	424	4
4	4	0	1118	1098	11	16	12	0	83	69	9	5	5	1	1480	1460	13	6	14	1	286	290	5	11	5	2	649	650	6
6	4	0	1905	1644	14	1	13	0	430	436	4	7	5	1	901	897	10	8	14	1	306	308	5	13	5	2	13	8	13
8	4	0	456	449	4	3	13	0	156	156	5	9	5	1	547	550	5	10	14	1	209	216	6	15	5	2	279	280	5
10	4	0	404	416	4	5	13	0	416	423	5	11	5	1	290	318	4	12	14	1	172	183	7	17	5	2	713	714	7
12	4	0	234	240	4	7	13	0	435	454	5	13	5	1	551	561	5	14	14	1	359	362	6	19	5	2	410	395	6
14	4	0	845	854	8	9	13	0	528	520	5	15	5	1	61	61	9	1	15	1	50	33	11	21	5	2	418	410	6
16	4	0	2047	2017	21	11	13	0	912	925	9	17	5	1	232	221	5	3	15	1	288	282	5	0	6	2	1075	1075	9
18	4	0	72	65	8	13	13	0	289	285	6	19	5	1	0	3	1	5	15	1	235	237	5	2	6	2	174	172	3
20	4	0	206	209	6	15	13	0	230	233	6	21	5	1	709	699	7	7	15	1	366	358	5	4	6	2	1081	1090	10
22	4	0	427	436	6	0	14	0	1500	1485	14	0	6	1	517	480	5	9	15	1	56	63	12	6	6	2	2365	2303	16
1	5	0	1411	1383	11	2	14	0	392	392	5	2	6	1	173	163	3	11	15	1	136	119	7	8	6	2	293	284	4
3	5	0	57	57	4	4	14	0	215	206	5	4	6	1	211	203	3	13	15	1	143	144	7	10	6	2	6	9	6
5	5	0	3341	3158	14	6	14	0	675	677	6	6	6	1	884	902	10	0	16	1	263	275	5	12	6	2	319	326	4
7	5	0	831	799	8	8	14	0	132	138	6	8	6	1	510	499	5	2	16	1	238	233	5	14	6	2	976	973	10
9	5	0	154	166	4	10	14	0	1289	1301	13	10	6	1	152	140	4	4	16	1	0	1	1	16	6	2	1456	1472	16
11	5	0	320	336	4	12	14	0	100	100	9	12	6	1	332	334	4	6	16	1	1272	1263	13	18	6	2	0	8	1
13	5	0	299	307	4	14	14	0	65	21	11	14	6	1	22	29	22	8	16	1	282	293	6	20	6	2	104	102	9
15	5	0	257	262	5	1	15	0	258	240	5	16	6	1	1038	1036	11	10	16	1	70	61	10	1	7	2	666	654	6
17	5	0	501	501	5	3	15	0	391	390	5	18	6	1	281	285	6	12	16	1	100	86	9	3	7	2	42	42	8
19	5	0	219	229	6	5	15	0	543	542	5	20	6	1	438	438	6	1	17	1	93	97	8	5	7	2	4589	4499	18
21	5	0	313	319	6	7	15	0	39	28	18	1	7	1	159	155	3	3	17	1	304	305	6	7	7	2	212	211	4
0	6	0	940	921	8	9	15	0	110	109	7	3	7	1	576	574	5	5	17	1	710	709	7	9	7	2	444	458	4
2	6	0	146	152	3	11	15	0	376	379	6	5	7	1	452	450	4	7	17	1	223	225	6	11	7	2	57	59	8
4	6	0	381	390	3	13	15	0	385	388	6	7	7	1	203	206	4	9	17	1	383	371	6	13	7	2	353	352	5
6	6	0	522	509	5	0	16	0	612	621	6	9	7	1	418	428	4	0	18	1	274	288	6	15	7	2	896	919	9
8	6	0	623	621	6	2	16	0	180	172	5	11	7	1	25	24	25	2	18	1	69	78	10	17	7	2	960	973	9
10	6	0	1383	1357	17	4	16	0	272	266	5	13	7	1	48	48	10	4	18	1	316	322	6	19	7	2	34	37	33
12	6	0	264	270	4	6	16	0	805	821	9	15	7	1	22	6	22	6	18	1	314	316	6	0	8	2	480	488	5
14	6	0	440	438	5	8	16	0	56	65	12	17	7	1	225	213	6	1	19	1	330	334	6	2	8	2	414	415	4
16	6	0	541	537	5	10	16	0	67	62	10	19	7	1	121	126	8	3	19	1	376	388	6	4	8	2	209	215	4
18	6	0	383	375	5	12	16	0	401	412	6	0	8	1	663	644	6	0	0	2	2907	3294	11	6	8	2	412	408	4
20	6	0	33	23	33	1	17	0	259	260	6	2	8	1	32	6	10	2	0	2	538	561	5	8	8	2	539	540	5
1	7	0	711	689	7	3	17	0	300	303	6	4	8	1	74	79	5	4	0	2	400	396	4	10	8	2	31	20	17
3	7	0	121	121	3	5	17	0	1910	1865	17	6	8	1	287	305	4	6	0	2	761	716	7	12	8	2	151	150	5
5	7	0	1350	1341	15	7	17	0	13	32	12	8	8	1	128	132	5	8	0	2	509	494	5	14	8	2	545	546	5
7	7	0	452	439	4	9	17	0	65	57	11	10	8	1	107	46	5	10	0	2	1338	1320	16	16	8	2	881	876	9
9	7	0	1220	1220	12	0	18	0	311	316	6	12	8	1	519	520	5	12	0	2	920	932	10	18	8	2	56	36	11
11	7	0	587	554	6	2	18	0	289	286	6	14	8	1	570	561	5	14	0	2	1275	1290	14	1	9	2	428	402	4
13	7	0	328	326	5	4	18	0	77	81	9	16	8	1	707	690	7	16	0	2	684	692	7	3	9	2	59	46	7
15	7	0	216	217	5	6	18	0	239	243	6	18	8	1	346	338	6	18	0	2	736	725	7	5	9	2	452	457	4
17	7	0	262	267	6	8	18	0	305	301	6	20	8	1	270	269	6	20	0	2	84	79	9	7	9	2	398	393	4
19	7	0	664	663	6	1	19	0	159	167	7	1	9	1	972	942	11	1	1	2	447	458	4	9	9	2	748	742	7
0	8	0	2698	2576	15	3	19	0	62	61	13	3	9	1	135	129	4	3	1	2	728	725	7	11	9	2	1559	1557	14
2	8	0	132	136	4	1	1	1	169	162	1	5	9	1	340	367	4	5	1	2	1064	1069	12	13	9	2	109	108	6

Observed and calculated structure factors for K49

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
15	9	2	290	294	5	20	2	3	142	144	7	17	11	3	542	547	6	8	4	4	178	185	4	8	14	4	121	115	7
17	9	2	619	619	6	1	3	3	542	539	5	0	12	3	213	215	5	10	4	4	267	272	4	10	14	4	1038	1023	10
19	9	2	288	296	6	3	3	3	242	241	3	2	12	3	282	280	5	12	4	4	150	158	5	12	14	4	65	54	12
0	10	2	4539	4429	20	5	3	3	1036	1039	10	4	12	3	351	354	5	14	4	4	822	827	8	1	15	4	209	203	6
2	10	2	646	645	7	7	3	3	710	710	7	6	12	3	149	148	5	16	4	4	1426	1436	13	3	15	4	388	386	6
4	10	2	717	732	7	9	3	3	180	179	4	8	12	3	81	76	7	18	4	4	135	126	7	5	15	4	266	263	6
6	10	2	59	54	7	11	3	3	1311	1332	13	10	12	3	152	141	6	1	5	4	931	940	9	7	15	4	105	98	8
8	10	2	277	285	4	13	3	3	71	60	7	12	12	3	293	273	5	3	5	4	148	135	4	9	15	4	102	113	8
10	10	2	1845	1860	21	15	3	3	138	137	5	14	12	3	116	118	8	5	5	4	1501	1559	17	0	16	4	182	182	6
12	10	2	337	324	5	17	3	3	251	247	5	16	12	3	415	415	6	7	5	4	377	370	4	2	16	4	167	166	6
14	10	2	336	335	5	19	3	3	115	115	7	1	13	3	274	267	5	9	5	4	166	165	5	4	16	4	179	189	7
16	10	2	202	207	6	21	3	3	407	414	6	3	13	3	451	455	5	11	5	4	877	891	9	6	16	4	463	456	6
18	10	2	263	252	6	0	4	3	2200	2098	14	5	13	3	346	343	5	13	5	4	160	161	5	8	16	4	16	3	16
1	11	2	363	363	4	2	4	3	56	43	5	7	13	3	123	126	6	15	5	4	265	261	5	1	17	4	339	336	6
3	11	2	671	683	7	4	4	3	357	355	3	9	13	3	229	235	6	17	5	4	133	125	7	3	17	4	207	198	7
5	11	2	60	59	8	6	4	3	219	216	4	11	13	3	186	379	5	19	5	4	161	152	7	1	1	5	66	65	6
7	11	2	14	14	14	8	4	3	257	267	4	13	13	3	35	21	26	0	6	4	2118	2166	17	3	1	5	209	214	4
9	11	2	649	649	6	10	4	3	436	431	4	15	13	3	173	167	7	2	6	4	169	170	4	5	1	5	683	688	7
11	11	2	1827	1785	22	12	4	3	764	770	8	0	14	3	15	25	14	4	6	4	374	379	4	7	1	5	0	5	1
13	11	2	62	51	10	14	4	3	99	105	6	2	14	3	216	223	5	6	6	4	169	169	4	9	1	5	357	346	4
15	11	2	189	179	6	16	4	3	222	211	6	4	14	3	317	331	5	8	6	4	334	329	4	11	1	5	250	245	5
17	11	2	63	66	12	18	4	3	159	156	6	6	14	3	142	152	6	10	6	4	1237	1261	14	13	1	5	188	199	5
0	12	2	1378	1340	13	20	4	3	15	11	15	8	14	3	363	358	5	12	6	4	351	352	5	15	1	5	59	58	11
2	12	2	0	3	1	1	5	3	88	76	4	10	14	3	57	38	11	14	6	4	249	246	5	17	1	5	731	721	7
4	12	2	38	6	12	3	5	3	321	326	3	12	14	3	61	68	12	16	6	4	187	194	6	19	1	5	362	373	6
6	12	2	804	809	8	5	5	3	847	830	9	1	15	3	160	151	6	18	6	4	272	269	6	0	2	5	731	735	7
8	12	2	143	159	6	7	5	3	883	877	9	3	15	3	211	214	6	1	7	4	263	259	4	2	2	5	95	93	5
10	12	2	761	775	7	9	5	3	429	434	4	5	15	3	439	446	5	3	7	4	179	185	4	4	2	5	446	462	4
12	12	2	228	218	5	11	5	3	133	131	5	7	15	3	219	225	6	5	7	4	1246	1250	13	6	2	5	434	427	4
14	12	2	551	546	5	13	5	3	416	420	5	9	15	3	121	110	7	7	7	4	356	358	4	8	2	5	301	302	4
16	12	2	383	391	6	15	5	3	0	18	1	11	15	3	334	328	6	9	7	4	944	957	10	10	2	5	27	27	27
1	13	2	182	183	5	17	5	3	278	285	6	0	16	3	159	135	6	11	7	4	729	731	7	12	2	5	735	738	7
3	13	2	59	53	9	19	5	3	21	40	21	2	16	3	97	77	8	13	7	4	281	274	5	14	2	5	81	84	8
5	13	2	1880	1863	21	0	6	3	496	503	5	4	16	3	213	213	6	15	7	4	212	213	6	16	2	5	238	229	6
7	13	2	38	39	16	2	6	3	113	102	4	6	16	3	1111	1119	11	17	7	4	385	376	6	18	2	5	66	74	12
9	13	2	143	143	6	4	6	3	427	415	4	8	16	3	248	249	6	0	8	4	1862	1904	18	1	3	5	120	134	5
11	13	2	106	107	7	6	6	3	1177	1198	12	10	16	3	105	94	8	2	8	4	15	8	15	3	3	5	216	211	4
13	13	2	126	134	7	8	6	3	350	353	4	1	17	3	161	166	6	4	8	4	153	151	5	5	3	5	538	559	6
15	13	2	510	519	6	10	6	3	164	174	5	3	17	3	331	317	6	6	8	4	505	499	5	7	3	5	107	105	5
0	14	2	390	392	5	12	6	3	298	304	5	5	17	3	438	433	6	8	8	4	367	371	4	9	3	5	84	77	6
2	14	2	299	296	5	14	6	3	112	108	7	7	17	3	0	25	1	10	8	4	1131	1131	12	11	3	5	268	273	5
4	14	2	733	750	7	16	6	3	1120	1111	11	0	18	3	219	218	6	12	8	4	90	77	7	13	3	5	260	264	5
6	14	2	455	448	5	18	6	3	419	408	6	2	18	3	189	184	6	14	8	4	145	146	7	15	3	5	19	2	19
8	14	2	192	187	6	20	6	3	399	403	6	4	18	3	151	146	7	16	8	4	240	238	6	17	3	5	502	494	6
10	14	2	104	112	8	1	7	3	197	186	4	0	0	4	5703	6598	19	18	8	4	54	35	13	0	4	5	95	91	5
12	14	2	68	62	10	3	7	3	276	284	4	2	0	4	357	367	3	1	9	4	43	30	9	2	4	5	101	59	5
14	14	2	379	398	6	5	7	3	1210	1181	12	4	0	4	631	662	7	3	9	4	239	242	4	4	4	5	110	105	5
1	15	2	518	514	5	7	7	3	166	169	4	6	0	4	363	352	4	5	9	4	1774	1788	20	6	4	5	650	651	7
3	15	2	300	299	5	9	7	3	442	446	4	8	0	4	269	273	4	7	9	4	488	494	5	8	4	5	344	354	4
5	15	2	1463	1475	16	11	7	3	815	818	8	10	0	4	2674	2653	19	9	9	4	23	26	23	10	4	5	171	165	5
7	15	2	461	464	5	13	7	3	137	135	6	12	0	4	939	955	9	11	9	4	195	195	5	12	4	5	508	500	5
9	15	2	164	148	6	15	7	3	121	116	7	14	0	4	311	325	5	13	9	4	136	130	6	14	4	5	251	243	6
11	15	2	361	365	6	17	7	3	616	611	6	16	0	4	142	150	6	15	9	4	394	403	6	16	4	5	669	665	6
13	15	2	139	143	7	19	7	3	89	88	9	18	0	4	542	520	6	17	9	4	588	578	6	18	4	5	268	272	6
0	16	2	1042	1027	10	0	8	3	874	866	9	20	0	4	147	149	7	0	10	4	849	842	8	1	5	5	151	146	4
2	16	2	145	142	6	2	8	3	109	108	5	1	1	4	244	237	3	2	10	4	78	80	6	3	5	5	274	273	4
4	16	2	46	48	13	4	8	3	318	318	4	3	1	4	110	108	4	4	10	4	513	525	5	5	5	5	683	686	7
6	16	2	472	474	6	6	8	3	562	566	6	5	1	4	295	286	4	6	10	4	205	204	5	7	5	5	612	610	6
8	16	2	42	42	18	8	8	3	57	17	8	7	1	4	67	62	6	8	10	4	282	283	5	9	5	5	401	402	5
10	16	2	727	736	7	10	8	3	144	116	5	9	1	4	1257	1268	13	10	10	4	435	438	5	11	5	5	296	267	5
1	17	2	254	247	6	12	8	3	586	593	6	11	1	4	1635	1634	19	12	10	4	173	180	6	13	5	5	380	375	5
3	17	2	375	375	6	14	8	3	361	358	5	13	1	4	205	201	5	14	10	4	881	888	9	15	5	5	25	30	24
5	17	2	137	134	7	16	8	3	163	159	6	15	1	4	224	220	5	16	10	4	366	364	6	17	5	5	162	158	7
7	17	2	7	34	7	18	8	3	162	167	7	17	1	4	27	8	27	1	11	4	141	128	5	0	6	5	385	403	4
9	17	2	395	390	6	1	9	3	586	581	6	19	1	4	541	537	6	3	11	4	353	360	5	2	6	5	91	94	5
0	18	2	762	744	8	3	9	3	97	92	5	0	2	4	360	384	3	5	11	4	1097	1125	12	4	6	5	49	61	9
2	18	2	0	17	1	5	9	3	338	336	4	2	2	4	154	158	4	7	11	4	74	76	8	6	6	5	446	443	4
4	18	2	214	216	6	7	9	3	240	244	5	4	2	4	436	449	4	9	11	4	12	10	11	8	6	5	330	334	5
6	18	2	406	407	6	9	9	3	60	61	8	6	2	4	414	444	4	11	11	4	40	2	17	10	6	5	76	88	8
1	1	3	259	251	3	11	9	3	864	892	9	8	2	4	126	122	4	13	11	4	134	128	7	12	6	5	239	232	5
3	1	3	619	617	6	13	9	3	38	37	17	10	2	4	463	471	4	15	11	4	725	712	7	14	6	5	26	7	26
5	1	3	173	168	3	15	9	3	154	131	6	12	2	4	312	313	5	0	12	4	1012	1009	10	16	6	5	709	692	7
7	1	3	300	304	3	17	9	3	511	508	6	14	2	4	653	647	6	2	12	4	241	234	5	1	7	5	91	90	6
9	1	3	357	358	4	0	10	3	818	816	8	16	2	4	728	724	7	4	12	4	135	143	6	3	7	5	467	477	4
11	1	3	1343	1374	13	2	10	3	743	751	8	18	2	4	0	23	1	6	12	4	290	282	5	5	7	5	51	32	10
13	1	3	426	429	4	4	10	3	322	337	4	20	2	4	122	115	8	8	12	4	184	187	6	7	7	5	317	311	5
15	1	3	163	165	6	6	10	3	214	211	5	1	3	4	201	198	3	10	12	4	449	452	5	9	7	5	294	284	5
17	1	3	354	352	5	8	10	3	228	230	5	3	3	4	429	432	4	12	12	4	334	335	6	11	7	5	361	360	5
19	1	3	453	472	5	10	10	3	55	52	10	5	3	4	3249	3365	18	14	12	4	24	8	23	13	7	5	154	147	6
21	1	3	821	801	8	12	10	3	94	86	7	7	3	4	165	163	4	1	13	4	224	222	5	15	7	5	67	67	11
0	2	3	2227	2181	13	14	10	3	565	570	5	9	3	4	719	729	7	3	13	4	97	92	7	17	7	5	47	43	18
2	2	3	579	570	5	16	10	3	78	88	10	11	3	4	90	95	6	5	13	4	268	263	5	0	8	5	758	783	8
4	2	3	45	34	6	1	11	3	285	286	4	13	3	4	304	314	5	7	13	4	253	257	6	2	8	5	148	135	5
6	2	3	1122	1101	10	3	11	3	185	186	5	15	3	4	726	725	7	9	13	4	493	499	5	4	8	5	49	38	10
8	2	3	697	694	7	5	11	3	752	749	7	17	3	4	742	737	8	11	13	4	714	722	7	6	8	5	539	530	5
10	2	3	279	286	4	7	11	3	240	236	5	19	3	4	169	183	7	13	13	4	150	158	7	8	8	5	115	116	6
12	2	3	715	734	7	9	11	3	375	372	5	0	4	4	460	493	5	0	14	4	1408	1418	13	10	8	5	32	23	31
14	2	3	358	352	5	11	11	3	89	87	7	2	4	4	381	363	3	2	14	4	243	235	5	12	8	5	383	383	5
16	2	3	1087	1083	11	13	11	3	61	45	10	4	4	4	629	671	6	4	14	4	315	312	5	14	8	5	477	477	6
18	2	3	227	225	6	15	11	3	14	20	14	6	4	4	1833	1855	17	6	14	4	466	464	5	16	8	5	750	738	7

Observed and calculated structure factors for K49

h	k	l	10Fo	10Fc	10s
1	9	5	675	680	6
3	9	5	83	59	6
5	9	5	480	475	5
7	9	5	350	344	5
9	9	5	44	44	14
11	9	5	1547	1531	16
13	9	5	114	121	7
15	9	5	137	124	7
0	10	5	990	985	10
2	10	5	480	498	5
4	10	5	117	108	6
6	10	5	467	467	5
8	10	5	124	127	7
10	10	5	257	258	6
12	10	5	68	71	10
14	10	5	458	464	6
1	11	5	75	69	8
3	11	5	199	203	5
5	11	5	485	476	5
7	11	5	531	524	5
9	11	5	206	207	6
11	11	5	382	383	6
13	11	5	177	176	6
0	12	5	1053	1054	11
2	12	5	469	478	5
4	12	5	62	55	9
6	12	5	682	676	7
8	12	5	101	102	7
10	12	5	77	68	9
12	12	5	245	243	6
1	13	5	322	320	5
3	13	5	264	258	5
5	13	5	923	938	9
7	13	5	179	180	6
9	13	5	284	277	6
11	13	5	1188	1181	13
0	14	5	903	878	9
2	14	5	220	228	6
4	14	5	325	324	6
6	14	5	439	436	6
8	14	5	215	211	6
1	15	5	111	111	8
3	15	5	235	234	6
5	15	5	58	59	13
7	15	5	327	322	6
0	16	5	228	228	6
2	16	5	256	253	6
4	16	5	110	106	8
0	0	6	2326	2499	20
2	0	6	75	71	6
4	0	6	618	637	6
6	0	6	663	678	7
8	0	6	331	333	5
10	0	6	847	851	8
12	0	6	711	719	7
14	0	6	758	745	8
16	0	6	824	826	8
1	1	6	128	120	5
3	1	6	146	139	5
5	1	6	1644	1696	20
7	1	6	66	65	8
9	1	6	343	337	5
11	1	6	235	230	5
13	1	6	45	41	16
15	1	6	411	413	6
17	1	6	326	322	6
0	2	6	1695	1710	19
2	2	6	177	184	5
4	2	6	172	172	5
6	2	6	482	487	5
8	2	6	223	217	5
10	2	6	791	791	8
12	2	6	300	312	5
14	2	6	33	16	32
16	2	6	391	386	6
1	3	6	189	188	5
3	3	6	121	120	5
5	3	6	765	769	8
7	3	6	39	38	14
9	3	6	1071	1068	10
11	3	6	1078	1091	11
13	3	6	190	200	6
15	3	6	55	57	14
17	3	6	325	336	6
0	4	6	2420	2399	20
2	4	6	78	68	6
4	4	6	301	310	5
6	4	6	513	523	5
8	4	6	133	128	6
10	4	6	1328	1350	13
12	4	6	254	250	6
14	4	6	48	46	15
16	4	6	222	218	6
1	5	6	275	268	5
3	5	6	270	264	5
5	5	6	498	495	5
7	5	6	72	83	8
9	5	6	238	243	5
11	5	6	339	339	5
13	5	6	116	106	7
15	5	6	254	246	6
0	6	6	175	182	5
2	6	6	27	26	27
4	6	6	533	540	5
6	6	6	818	829	8
8	6	6	310	307	5
10	6	6	130	123	6
12	6	6	148	153	6
14	6	6	830	822	8
1	7	6	548	546	5
3	7	6	137	135	6
5	7	6	2391	2447	22
7	7	6	114	120	6
9	7	6	355	357	5
11	7	6	429	430	5
13	7	6	211	210	6
15	7	6	615	608	6
0	8	6	342	335	5
2	8	6	182	177	5
4	8	6	308	306	5
6	8	6	269	272	5
8	8	6	311	323	5
10	8	6	143	153	6
12	8	6	166	164	7
14	8	6	393	381	6
1	9	6	309	302	5
3	9	6	102	106	7
5	9	6	41	36	16
7	9	6	464	471	5
9	9	6	503	494	5
11	9	6	713	706	7
13	9	6	30	30	29
0	10	6	2180	2172	21
2	10	6	301	310	5
4	10	6	306	311	5
6	10	6	515	526	5
8	10	6	95	87	7
10	10	6	1260	1246	12
12	10	6	197	188	6
1	11	6	93	93	8
3	11	6	340	329	5
5	11	6	453	460	5
7	11	6	122	101	7
9	11	6	458	460	6
11	11	6	739	730	7
0	12	6	489	501	6
2	12	6	61	48	11
4	12	6	56	47	12
6	12	6	868	878	8
8	12	6	40	34	23
10	12	6	394	398	6
1	13	6	24	19	23
3	13	6	48	45	14
5	13	6	1373	1384	14
7	13	6	159	158	7
0	14	6	31	49	31
2	14	6	347	346	6
4	14	6	345	341	6
6	14	6	142	142	7
1	1	7	72	71	8
3	1	7	227	226	5
5	1	7	78	70	7
7	1	7	278	269	5
9	1	7	199	198	6
11	1	7	721	728	8
13	1	7	316	329	6
15	1	7	141	161	8
0	2	7	658	649	7
2	2	7	316	314	5
4	2	7	21	17	21
6	2	7	469	472	5
8	2	7	273	278	5
10	2	7	61	60	11
12	2	7	525	515	6
14	2	7	195	189	6
1	3	7	183	193	5
3	3	7	46	29	11
5	3	7	385	377	5
7	3	7	438	441	5
9	3	7	168	164	6
11	3	7	751	756	7
13	3	7	30	42	29
0	4	7	1010	981	10
2	4	7	87	82	7
4	4	7	249	245	5
6	4	7	92	93	8
8	4	7	197	197	6
10	4	7	276	272	5
12	4	7	469	469	6
14	4	7	122	114	7
1	5	7	12	12	11
3	5	7	163	169	6
5	5	7	286	287	5
7	5	7	522	515	5
9	5	7	309	307	6
11	5	7	65	41	9
13	5	7	259	254	6
0	6	7	212	212	5
2	6	7	108	111	6
4	6	7	179	181	5
6	6	7	666	672	7
8	6	7	246	243	6
10	6	7	136	149	7
12	6	7	202	197	6
1	7	7	67	84	10
3	7	7	256	255	5
5	7	7	690	692	7
7	7	7	117	118	7
9	7	7	332	329	6
11	7	7	499	500	6
0	8	7	542	530	5
2	8	7	92	88	7
4	8	7	247	250	6
6	8	7	330	331	6
8	8	7	27	21	26
10	8	7	99	90	8
1	9	7	378	377	5
3	9	7	60	43	9
5	9	7	252	250	6
7	9	7	122	128	8
9	9	7	30	14	30
0	10	7	549	540	6
2	10	7	417	413	5
4	10	7	151	147	7
6	10	7	198	190	6
8	10	7	116	117	8
1	11	7	157	153	6
3	11	7	124	116	7
5	11	7	529	530	6
7	11	7	172	168	7
0	12	7	37	36	21
2	12	7	182	181	6
4	12	7	256	244	6
0	0	8	2318	2473	24
2	0	8	126	136	7
4	0	8	231	221	6
6	0	8	671	673	6
8	0	8	0	7	1
10	0	8	1421	1416	14
1	1	8	96	92	7
3	1	8	127	128	6
5	1	8	510	515	5
7	1	8	188	174	6
9	1	8	679	674	6
11	1	8	492	485	6
0	2	8	68	19	9
2	2	8	82	66	6
4	2	8	261	269	6
6	2	8	482	474	5
8	2	8	59	48	11
10	2	8	253	247	6
1	3	8	112	107	7
3	3	8	307	298	5
5	3	8	1733	1755	17
7	3	8	8	15	8
9	3	8	399	394	6
11	3	8	115	129	8
0	4	8	288	264	5
2	4	8	248	253	6
4	4	8	254	249	6
6	4	8	604	611	6
8	4	8	0	18	1
10	4	8	105	104	9
1	5	8	505	508	5
3	5	8	137	142	7
5	5	8	427	432	6
7	5	8	20	5	20
9	5	8	180	168	7
0	6	8	1832	1838	17
2	6	8	180	186	6
4	6	8	331	325	6
6	6	8	452	446	6
8	6	8	143	147	7
1	7	8	62	58	10
3	7	8	130	128	7
5	7	8	862	867	8
7	7	8	209	207	6
0	8	8	954	938	9
2	8	8	53	38	14
4	8	8	0	3	1
6	8	8	352	357	6
1	9	8	36	32	27
3	9	8	121	127	8
5	9	8	1202	1239	13
0	10	8	1036	996	10
2	10	8	141	135	7
1	1	9	62	45	10
3	1	9	182	164	6
5	1	9	281	290	6
0	2	9	95	100	9
2	2	9	66	56	11
4	2	9	216	219	6
6	2	9	0	7	1
1	3	9	161	146	7
3	3	9	0	8	1
5	3	9	84	83	9
0	4	9	433	412	6
2	4	9	50	58	13
4	4	9	57	59	13
1	5	9	0	10	1
3	5	9	82	82	10

Observed and calculated structure factors for K50

h	k	l	10Fo	10Fc	10s
2	0	0	675	713	6
4	0	0	1127	1113	11
6	0	0	588	597	5
8	0	0	1055	1025	11
10	0	0	1963	1782	24
12	0	0	1474	1466	14
14	0	0	319	305	7
16	0	0	378	151	7
18	0	0	402	199	8
20	0	0	445	444	8
22	0	0	1839	1848	19
1	1	0	256	250	1
5	1	0	519	534	5
7	1	0	390	192	4
9	1	0	1472	1461	15
11	1	0	1068	2992	25
13	1	0	446	452	6
15	1	0	243	251	7
17	1	0	395	399	8
19	1	0	517	507	8
21	1	0	826	838	9
0	2	0	1224	1274	10
2	2	0	327	338	3
4	2	0	541	564	5
6	2	0	153	149	4
8	2	0	252	244	5
10	2	0	547	566	5
12	2	0	446	459	6
14	2	0	844	847	8
16	2	0	810	798	8
18	2	0	159	153	9
20	2	0	45	58	29
22	2	0	222	221	10
1	3	0	289	291	3
3	3	0	508	511	5
5	3	0	5157	4828	19
7	3	0	544	524	5
9	3	0	821	806	8
11	3	0	431	438	6
13	3	0	258	260	7
15	3	0	918	922	9
17	3	0	989	1011	10
19	3	0	298	303	8
21	3	0	291	289	10
0	4	0	2085	2057	14
2	4	0	669	660	6
4	4	0	916	911	9
6	4	0	4101	3838	20
8	4	0	408	396	5
10	4	0	466	468	5
12	4	0	229	239	7
14	4	0	631	631	7
16	4	0	2063	2092	22
18	4	0	66	50	16
20	4	0	158	143	10
22	4	0	536	526	9
1	5	0	1485	1482	16
3	5	0	78	84	6
5	5	0	3198	3069	20
7	5	0	912	902	9
9	5	0	49	49	12
11	5	0	394	418	6
13	5	0	205	212	7
15	5	0	262	233	7
17	5	0	504	501	8
19	5	0	158	151	10
21	5	0	459	460	9
0	6	0	775	791	7
2	6	0	181	185	5
4	6	0	228	231	5
6	6	0	459	442	5
8	6	0	670	659	7
10	6	0	1507	1484	14
12	6	0	142	152	8
14	6	0	396	388	7
16	6	0	463	474	8
18	6	0	379	372	8
20	6	0	0	10	1
1	7	0	573	571	6
3	7	0	249	256	5
5	7	0	1354	1364	15
7	7	0	531	521	5
9	7	0	1086	1107	11
11	7	0	640	613	6
13	7	0	271	285	7
15	7	0	304	311	7
17	7	0	392	394	8
19	7	0	636	638	8
21	7	0	588	586	9
0	8	0	2613	2585	22
2	8	0	154	158	6
4	8	0	559	559	5
6	8	0	678	681	7
8	8	0	472	479	6
10	8	0	1188	1166	12
12	8	0	112	116	9
14	8	0	87	88	12
16	8	0	363	349	8
18	8	0	40	38	40
20	8	0	293	278	10
1	9	0	101	97	7
3	9	0	322	330	6
5	9	0	1869	1892	17
7	9	0	888	872	9
9	9	0	106	102	9
11	9	0	665	650	7
13	9	0	198	194	8
15	9	0	751	768	8
17	9	0	563	560	8
19	9	0	145	151	11
0	10	0	269	285	6
2	10	0	127	130	7
4	10	0	286	285	6
6	10	0	277	285	6
8	10	0	255	272	7
10	10	0	498	505	7
12	10	0	299	297	8
14	10	0	1020	1030	10
16	10	0	298	307	9
18	10	0	359	372	9
1	11	0	263	266	6
3	11	0	251	247	6
5	11	0	714	735	7
7	11	0	77	84	12
9	11	0	90	86	11
11	11	0	459	476	8
13	11	0	236	247	9
15	11	0	706	706	8
17	11	0	461	465	9
0	12	0	1497	1513	16
2	12	0	181	170	7
4	12	0	363	360	7
6	12	0	559	562	7
8	12	0	199	198	8
10	12	0	749	742	7
12	12	0	521	517	8
14	12	0	139	138	10
16	12	0	28	14	28
1	13	0	590	586	7
3	13	0	216	228	8
5	13	0	296	305	7
7	13	0	479	489	7
9	13	0	295	290	8
11	13	0	935	920	9
13	13	0	265	278	9
15	13	0	284	273	9
0	14	0	1329	1300	13
2	14	0	368	367	7
4	14	0	194	209	8
6	14	0	698	712	7
8	14	0	159	150	9
10	14	0	1169	1205	13
12	14	0	78	91	18
14	14	0	29	27	28
1	15	0	324	331	8
3	15	0	352	350	8
5	15	0	521	529	8
7	15	0	115	123	11
9	15	0	207	214	10
11	15	0	419	423	9
13	15	0	374	373	9
0	16	0	547	558	8
2	16	0	267	259	9
4	16	0	117	127	11
6	16	0	757	777	8
8	16	0	88	82	16
10	16	0	164	109	11
12	16	0	481	481	9
1	17	0	311	316	9
3	17	0	294	291	9
5	17	0	1696	1703	18
7	17	0	32	60	32
9	17	0	0	31	1
0	18	0	398	407	9
2	18	0	241	272	10
4	18	0	46	70	37
6	18	0	290	306	10
8	18	0	280	278	10
1	19	0	166	175	10
3	19	0	137	147	11
1	1	1	143	142	3
3	1	1	319	320	3
5	1	1	1003	988	9
7	1	1	26	4	26
9	1	1	277	266	5
11	1	1	688	699	7
13	1	1	266	267	7
15	1	1	253	258	7
17	1	1	685	687	7
19	1	1	514	507	8
21	1	1	591	595	9
0	2	1	146	172	3
2	2	1	547	569	5
4	2	1	353	358	3
6	2	1	293	276	4
8	2	1	516	518	4
10	2	1	73	56	8
12	2	1	873	862	9
14	2	1	111	107	9
16	2	1	546	554	7
18	2	1	0	2	1
20	2	1	324	329	9
22	2	1	267	268	10
1	3	1	379	382	3
3	3	1	257	252	3
5	3	1	397	383	4
7	3	1	377	382	4
9	3	1	229	232	5
11	3	1	356	366	6
13	3	1	199	213	7
15	3	1	109	111	9
17	3	1	272	288	8
19	3	1	169	174	9
21	3	1	383	369	9
0	4	1	1262	1223	10
2	4	1	132	142	4
4	4	1	141	132	4
6	4	1	658	635	6
8	4	1	338	346	5
10	4	1	592	581	6
12	4	1	634	642	6
14	4	1	257	270	7
16	4	1	463	479	7
18	4	1	229	241	9
20	4	1	60	44	21
22	4	1	287	283	9
1	5	1	116	116	5
3	5	1	392	387	4
5	5	1	1139	1128	11
7	5	1	846	840	8
9	5	1	411	412	5
11	5	1	283	297	6
13	5	1	558	560	6
15	5	1	184	172	8
17	5	1	204	200	8
19	5	1	50	7	29
21	5	1	571	568	9
0	6	1	538	511	5
2	6	1	100	100	6
4	6	1	282	280	4
6	6	1	986	989	9
8	6	1	531	520	5
10	6	1	114	108	8
12	6	1	362	364	7
14	6	1	19	14	18
16	6	1	977	982	9
18	6	1	258	257	9
20	6	1	486	475	9
1	7	1	149	136	5
3	7	1	470	454	5
5	7	1	802	809	8
7	7	1	215	207	6
9	7	1	349	354	6
11	7	1	92	104	9
13	7	1	66	75	13
15	7	1	151	144	9
17	7	1	260	253	9
19	7	1	163	161	9
0	8	1	446	425	5
2	8	1	126	117	6
4	8	1	54	46	11
6	8	1	276	296	6
8	8	1	31	46	10
10	8	1	152	160	7
12	8	1	472	477	7
14	8	1	488	493	7
16	8	1	454	460	8
18	8	1	289	281	9
20	8	1	361	345	9
1	9	1	920	893	9
3	9	1	41	31	19
5	9	1	384	414	6
7	9	1	324	323	6
9	9	1	34	31	34
11	9	1	1689	1678	17
13	9	1	151	135	8
15	9	1	195	204	9
17	9	1	94	108	12
19	9	1	217	216	10
0	10	1	1374	1407	14
2	10	1	714	730	7
4	10	1	179	177	7
6	10	1	492	504	6
8	10	1	108	114	10
10	10	1	370	361	7
12	10	1	0	23	1
14	10	1	614	605	8
16	10	1	492	495	8
18	10	1	177	186	11
1	11	1	91	98	10
3	11	1	17	49	37
5	11	1	831	834	8
7	11	1	513	500	7
9	11	1	281	270	7
11	11	1	189	195	9
13	11	1	173	184	9
15	11	1	337	317	9
17	11	1	403	426	9
0	12	1	946	972	9
2	12	1	563	566	6
4	12	1	173	163	8
6	12	1	759	729	7
8	12	1	76	81	11
10	12	1	0	22	1
12	12	1	234	220	8
14	12	1	62	70	23
16	12	1	751	746	9
1	13	1	471	455	7
3	13	1	272	292	8
5	13	1	1004	1024	10
7	13	1	105	99	10
9	13	1	307	285	8
11	13	1	1244	1219	13
13	13	1	175	171	9
15	13	1	154	148	10
0	14	1	905	908	9
2	14	1	145	157	9
4	14	1	389	392	7
6	14	1	273	265	8
8	14	1	215	220	9
10	14	1	393	410	8
12	14	1	135	143	11
14	14	1	283	293	9
1	15	1	45	32	27
3	15	1	379	390	8
5	15	1	123	123	10
7	15	1	374	354	8
9	15	1	0	31	1
11	15	1	150	139	11
13	15	1	214	215	10
0	16	1	390	387	8
2	16	1	183	181	9
4	16	1	53	62	26
6	16	1	1313	1292	13
8	16	1	357	354	9
10	16	1	37	45	36
12	16	1	41	39	41
1	17	1	134	116	10
3	17	1	171	189	10
5	17	1	816	832	8
7	17	1	230	230	10
9	17	1	291	296	9
0	18	1	327	309	9
2	18	1	109	119	12
4	18	1	334	323	9
6	18	1	281	282	10
1	19	1	432	434	9
3	19	1	399	410	9
0	0	2	3194	3362	15
2	0	2	647	665	6
4	0	2	205	203	4
6	0	2	743	702	7
8	0	2	658	641	6
10	0	2	1488	1470	17
12	0	2	1057	1070	10
14	0	2	1292	1296	13
16	0	2	859	861	9
18	0	2	541	546	8
20	0	2	214	208	9
22	0	2	430	424	9
1	1	2	530	539	5
3	1	2	774	761	7
5	1	2	1049	1038	10
7	1	2	96	92	6
9	1	2	587	598	6
11	1	2	607	610	6
13	1	2	30	27	29
15	1	2	671	676	7
17	1	2	74	58	14
19	1	2	43	27	43
21	1	2	294	298	9
0	2	2	3950	4088	17
2	2	2	370	368	3
4	2	2	476	456	4
6	2	2	492	479	5
8	2	2	185	182	5
10	2	2	1386	1370	14
12	2	2	591	590	6
14	2	2	33	7	32
16	2	2	317	312	8
18	2	2	64	51	17
20	2	2	122	128	11
1	3	2	511	503	5
3	3	2	192	186	4
5	3	2	1146	1134	11
7	3	2	244	235	5
9	3	2	1316	1307	13
11	3	2	1527	1537	15
13	3	2	307	293	7
15	3	2	251	236	7
17	3	2	425	425	8
19	3	2	742	757	8
21	3	2	697	692	9
0	4	2	1781	1757	17
2	4	2	634	620	6
4	4	2	85	84	7
6	4	2	185	371	5
8	4	2	95	102	7
10	4	2	2034	2020	25
12	4	2	165	144	7
14	4	2	152	149	8
16	4	2	37	24	36
18	4	2	525	521	8
20	4	2	244	251	10
1	5	2	1000	986	10
3	5	2	56	54	9
5	5	2	1853	1840	21
7	5	2	238	229	5
9	5	2	504	511	6
11	5	2	672	670	6
13	5	2	92	77	10
15	5	2	300	311	8
17	5	2	698	696	8
19	5	2	325	340	9
21	5	2	355	349	9
0	6	2	1110	1086	11
2	6	2	33	48	16
4	6	2	779	779	8
6	6	2	2589	2494	23
8	6	2	298	302	6
10	6	2	139	156	8
12	6	2	352	364	7
14	6	2	760	767	8
16	6	2	1556	1571	16
18	6	2	47	33	23
20	6	2	66	65	17
1	7	2	659	634	6
3	7	2	102	118	7
5	7	2	4469	4416	25
7	7	2	186	183	6
9	7	2	445	452	6
11	7	2	75	82	12
13	7	2	356	343	7
15	7	2	1015	1018	10
17	7	2	1039	1053	11
19	7	2	109	123	13
0	8	2	409	414	5
2	8	2	525	530	5
4	8	2	252	254	6
6	8	2	362	354	6
8	8	2	557	570	6
10	8	2	96	94	10
12	8	2	0	25	1
14	8	2	480	496	8
16	8	2	866	866	8
18	8	2	0	5	1
20	8	2	204	176	10
1	9	2	553	522	6
3	9	2	139	130	7
5	9	2	534	536	6

Observed and calculated structure factors for K50

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
7	9	2	502	497	6	12	2	3	643	659	7	9	11	3	342	335	7	0	4	4	519	550	5	0	14	4	1256	1286	14
9	9	2	548	551	7	14	2	3	297	310	7	11	11	3	88	75	13	2	4	4	496	483	5	2	14	4	219	216	9
11	9	2	1574	1591	17	16	2	3	920	933	9	13	11	3	12	4	12	4	4	4	484	494	5	4	14	4	315	320	9
13	9	2	223	239	8	18	2	3	181	195	9	15	11	3	163	151	11	6	4	4	2019	2005	18	6	14	4	487	478	8
15	9	2	115	103	11	20	2	3	272	250	9	17	11	3	523	531	9	8	4	4	171	172	7	8	14	4	156	133	10
17	9	2	760	754	8	1	3	3	512	503	5	0	12	3	120	112	9	10	4	4	362	364	7	10	14	4	956	942	10
19	9	2	298	285	10	3	3	3	241	234	5	2	12	3	329	338	7	12	4	4	176	177	8	12	14	4	98	51	13
0	10	2	4348	4339	28	5	3	3	961	958	9	4	12	3	421	421	7	14	4	4	650	646	7	1	15	4	100	297	8
2	10	2	585	571	6	7	3	3	702	696	7	6	12	3	225	226	8	16	4	4	1507	1525	15	3	15	4	369	354	8
4	10	2	646	648	7	9	3	3	191	192	7	8	12	3	14	12	13	18	4	4	140	130	11	5	15	4	276	265	9
6	10	2	114	110	8	11	3	3	1372	1396	16	10	12	3	26	40	26	1	5	4	994	972	10	7	15	4	27	31	26
8	10	2	260	275	7	13	3	3	0	6	1	12	12	3	217	211	9	3	5	4	133	127	7	9	15	4	207	205	10
10	10	2	1846	1822	17	15	3	3	182	197	8	14	12	3	165	161	10	5	5	4	1493	1539	14	0	16	4	159	155	11
12	10	2	418	414	8	17	3	3	244	259	9	16	12	3	474	453	9	7	5	4	426	410	6	2	16	4	243	248	10
14	10	2	310	307	8	19	3	3	106	108	12	1	13	3	360	352	7	9	5	4	15	10	15	4	16	4	60	59	21
16	10	2	186	178	9	21	3	3	417	414	9	3	13	3	389	402	8	11	5	4	924	932	10	6	16	4	431	432	9
18	10	2	180	174	11	0	4	3	2272	2201	20	5	13	3	430	434	8	13	5	4	52	55	21	8	16	4	55	21	26
1	11	2	448	443	6	2	4	3	0	16	1	7	13	3	127	117	10	15	5	4	248	262	9	1	17	4	371	360	9
3	11	2	697	694	7	4	4	3	299	292	5	9	13	3	216	220	9	17	5	4	138	132	11	3	17	4	215	197	10
5	11	2	39	34	27	6	4	3	286	291	6	11	13	3	511	501	8	19	5	4	114	97	13	1	1	5	39	32	20
7	11	2	0	14	1	8	4	3	149	156	7	13	13	3	28	26	28	0	6	4	1987	2032	25	3	1	5	123	134	8
9	11	2	557	550	7	10	4	3	642	643	7	15	13	3	66	54	23	2	6	4	189	210	6	5	1	5	764	779	8
11	11	2	1863	1811	18	12	4	3	688	694	7	0	14	3	241	242	8	4	6	4	294	301	6	7	1	5	0	29	1
13	11	2	76	34	15	14	4	3	121	114	9	2	14	3	128	119	10	6	6	4	177	179	7	9	1	5	215	232	8
15	11	2	48	65	35	16	4	3	99	99	12	4	14	3	313	318	8	8	6	4	353	364	7	11	1	5	149	142	8
17	11	2	65	60	20	18	4	3	127	135	11	6	14	3	147	152	10	10	6	4	1299	1319	13	13	1	5	117	129	10
0	12	2	1313	1320	14	20	4	3	82	88	16	8	14	3	284	277	9	12	6	4	252	239	8	15	1	5	186	177	9
2	12	2	121	118	9	1	5	3	80	66	7	10	14	3	234	242	9	14	6	4	211	206	9	17	1	5	704	708	9
4	12	2	200	183	8	3	5	3	219	226	5	12	14	3	22	35	22	16	6	4	193	180	10	19	1	5	395	399	9
6	12	2	810	817	8	5	5	3	614	595	6	1	15	3	195	200	9	18	6	4	243	251	10	0	2	5	828	824	8
8	12	2	219	218	8	7	5	3	838	829	8	3	15	3	299	304	8	1	7	4	200	197	7	2	2	5	177	157	6
10	12	2	672	677	8	9	5	3	313	310	6	5	15	3	298	308	9	3	7	4	286	290	6	4	2	5	336	347	6
12	12	2	293	282	8	11	5	3	141	131	8	7	15	3	214	219	10	5	7	4	1217	1243	12	6	2	5	481	481	6
14	12	2	415	412	8	13	5	3	435	425	7	9	15	3	97	88	12	7	7	4	408	411	7	8	2	5	259	245	7
16	12	2	506	512	9	15	5	3	211	226	8	11	15	3	339	321	9	9	7	4	856	864	8	10	2	5	164	174	8
1	13	2	139	121	8	17	5	3	251	257	8	0	16	3	217	211	9	11	7	4	741	750	7	12	2	5	696	694	7
3	13	2	45	46	26	19	5	3	16	42	16	2	16	3	29	24	28	13	7	4	237	230	8	14	2	5	34	30	33
5	13	2	1714	1713	18	0	6	3	493	497	5	4	16	3	260	274	9	15	7	4	259	281	9	16	2	5	142	142	10
7	13	2	48	28	20	2	6	3	180	164	6	6	16	3	1142	1121	11	17	7	4	469	469	9	18	2	5	123	107	11
9	13	2	11	43	30	4	6	3	506	495	5	8	16	3	289	304	10	0	8	4	1832	1868	19	1	3	5	122	129	8
11	13	2	134	140	10	6	6	3	1278	1286	14	10	16	3	173	191	11	2	8	4	23	36	23	3	3	5	238	229	6
13	13	2	144	133	10	8	6	3	384	376	6	1	17	3	167	185	11	4	8	4	300	302	7	5	3	5	555	562	6
15	13	2	544	544	9	10	6	3	165	165	7	3	17	3	220	214	10	6	8	4	615	618	7	7	3	5	78	71	12
0	14	2	316	310	8	12	6	3	329	326	7	5	17	3	561	535	9	8	8	4	369	370	7	9	3	5	113	105	9
2	14	2	325	321	8	14	6	3	51	73	21	7	17	3	0	30	1	10	8	4	1033	1017	10	11	3	5	214	212	8
4	14	2	679	682	7	16	6	3	1027	1057	10	0	18	3	198	192	10	12	8	4	76	62	12	13	3	5	231	234	8
6	14	2	499	493	8	18	6	3	384	389	9	2	18	3	210	222	10	14	8	4	70	69	18	15	3	5	71	42	15
8	14	2	198	191	9	20	6	3	419	432	9	4	18	3	144	139	12	16	8	4	304	300	9	17	3	5	528	504	8
10	14	2	78	45	14	1	7	3	161	153	6	0	0	4	6204	6641	26	18	8	4	41	24	41	0	4	5	186	195	7
12	14	2	0	3	1	3	7	3	167	176	6	2	0	4	354	358	5	1	9	4	43	28	20	2	4	5	93	76	9
14	14	2	297	307	10	5	7	3	1457	1459	14	4	0	4	523	544	5	3	9	4	219	212	7	4	4	5	49	54	17
1	15	2	655	656	8	7	7	3	186	194	7	6	0	4	330	325	6	5	9	4	1737	1771	17	6	4	5	609	597	6
3	15	2	230	225	8	9	7	3	374	375	6	8	0	4	371	372	6	7	9	4	461	473	7	8	4	5	284	279	7
5	15	2	1412	1441	15	11	7	3	888	883	9	10	0	4	2776	2784	28	9	9	4	39	28	32	10	4	5	359	357	7
7	15	2	445	440	8	13	7	3	134	135	9	12	0	4	1022	1022	10	11	9	4	233	237	9	12	4	5	438	423	8
9	15	2	35	27	34	15	7	3	6	7	6	14	0	4	432	435	7	13	9	4	69	47	16	14	4	5	274	272	9
11	15	2	449	439	9	17	7	3	667	659	8	16	0	4	49	16	23	15	9	4	540	561	9	16	4	5	534	539	9
13	15	2	135	127	11	19	7	3	140	129	11	18	0	4	427	430	9	17	9	4	636	633	9	18	4	5	247	251	10
0	16	2	914	915	9	0	8	3	1007	1013	11	20	0	4	335	323	9	0	10	4	802	817	8	1	5	5	144	141	7
2	16	2	158	164	10	2	8	3	87	25	8	1	1	4	388	389	5	2	10	4	57	52	16	3	5	5	189	196	7
4	16	2	84	95	15	4	8	3	242	237	6	3	1	4	6	13	6	4	10	4	398	395	7	5	5	5	482	486	6
6	16	2	575	579	8	6	8	3	560	558	6	5	1	4	161	139	6	6	10	4	197	179	8	7	5	5	575	569	7
8	16	2	40	31	40	8	8	3	120	107	8	7	1	4	62	67	10	8	10	4	294	291	8	9	5	5	312	310	7
10	16	2	774	765	9	10	8	3	232	256	8	9	1	4	1072	1083	11	10	10	4	425	421	8	11	5	5	257	252	8
1	17	2	269	258	9	12	8	3	561	550	7	11	1	4	1748	1757	16	12	10	4	292	295	9	13	5	5	385	386	8
3	17	2	383	373	8	14	8	3	287	289	8	13	1	4	257	252	7	14	10	4	771	771	8	15	5	5	135	141	11
5	17	2	52	35	27	16	8	3	0	13	1	15	1	4	138	141	10	16	10	4	436	421	9	17	5	5	144	139	12
7	17	2	156	157	12	18	8	3	75	99	17	17	1	4	72	82	16	1	11	4	203	184	8	0	6	5	381	406	6
9	17	2	310	323	9	1	9	3	581	577	6	19	1	4	450	458	9	3	11	4	319	308	7	2	6	5	52	61	17
0	18	2	650	638	9	3	9	3	175	178	7	0	2	4	102	330	5	5	11	4	944	950	9	4	6	5	0	17	1
2	18	2	105	96	13	5	9	3	263	251	7	2	2	4	221	226	5	7	11	4	140	21	9	6	6	5	490	496	7
4	18	2	283	290	9	7	9	3	209	208	7	4	2	4	357	346	5	9	11	4	63	56	17	8	6	5	337	346	7
6	18	2	358	378	9	9	9	3	93	55	10	6	2	4	428	465	6	11	11	4	53	56	22	10	6	5	78	62	12
1	1	3	194	193	4	11	9	3	905	909	9	8	2	4	85	87	9	13	11	4	143	153	11	12	6	5	249	255	9
3	1	3	536	524	5	13	9	3	101	83	10	10	2	4	385	383	7	15	11	4	598	575	9	14	6	5	54	22	23
5	1	3	36	38	16	15	9	3	202	198	9	12	2	4	420	417	7	0	12	4	989	989	10	16	6	5	653	651	9
7	1	3	375	373	5	17	9	3	431	441	9	14	2	4	633	629	7	2	12	4	188	174	8	1	7	5	85	80	10
9	1	3	226	226	6	0	10	3	982	1006	11	16	2	4	767	779	8	4	12	4	255	255	8	3	7	5	389	401	7
11	1	3	1238	1234	12	2	10	3	723	726	7	18	2	4	145	152	11	6	12	4	282	268	8	5	7	5	260	254	7
13	1	3	369	365	7	4	10	3	281	278	7	20	2	4	0	23	1	8	12	4	217	226	9	7	7	5	297	301	7
15	1	3	327	315	7	6	10	3	277	273	7	1	3	4	172	177	6	10	12	4	534	536	8	9	7	5	249	238	8
17	1	3	324	320	8	8	10	3	193	178	8	3	3	4	418	407	5	12	12	4	362	365	9	11	7	5	298	305	8
19	1	3	493	491	8	10	10	3	161	172	9	5	3	4	3309	3391	25	14	12	4	97	59	13	13	7	5	166	163	10
21	1	3	562	571	9	12	10	3	78	76	12	7	3	4	189	190	6	1	13	4	366	358	8	15	7	5	173	175	10
0	2	3	2062	2056	18	14	10	3	590	588	8	9	3	4	614	620	6	3	13	4	156	165	9	17	7	5	0	25	1
2	2	3	673	652	6	16	10	3	286	284	9	11	3	4	153	154	8	5	13	4	198	202	9	0	8	5	642	646	7
4	2	3	196	192	5	1	11	3	214	211	7	13	3	4	243	248	8	7	13	4	292	293	9	2	8	5	205	197	7
6	2	3	1039	1034	11	3	11	3	26	8	26	15	3	4	801	804	8	9	13	4	298	301	9	4	8	5	92	107	11
8	2	3	619	620	6	5	11	3	888	883	9	17	3	4	783	778	8	11	13	4	744	746	9	6	8	5	562	549	7
10	2	3	0	8	1	7	11	3	194	195	8	19	3	4	253	262	9	13	13	4	153	160	11	8	8	5	73	64	14

Observed and calculated structure factors for K50

h	k	l	10Fo	10Fc	10s
10	8	5	114	127	11
12	8	5	329	329	8
14	8	5	445	441	8
16	8	5	564	563	9
1	9	5	673	675	7
3	9	5	34	8	33
5	9	5	520	516	7
7	9	5	318	312	8
9	9	5	40	15	40
11	9	5	1507	1522	15
13	9	5	179	164	10
15	9	5	174	178	11
0	10	5	1093	1096	11
2	10	5	449	460	7
4	10	5	38	48	38
6	10	5	529	504	8
8	10	5	83	75	14
10	10	5	351	343	8
12	10	5	85	85	15
14	10	5	455	447	9
1	11	5	39	13	39
3	11	5	81	56	14
5	11	5	584	577	8
7	11	5	507	499	8
9	11	5	155	167	11
11	11	5	289	277	9
13	11	5	227	231	10
0	12	5	1005	999	10
2	12	5	536	532	8
4	12	5	0	5	1
6	12	5	759	757	8
8	12	5	41	49	40
10	12	5	56	25	24
12	12	5	195	179	10
1	13	5	190	187	8
3	13	5	199	200	9
5	13	5	989	987	10
7	13	5	191	188	10
9	13	5	254	249	10
11	13	5	1281	1281	12
0	14	5	1043	1039	10
2	14	5	123	131	12
4	14	5	308	304	9
6	14	5	425	423	9
8	14	5	139	136	12
10	14	5	431	421	9
1	15	5	63	65	17
3	15	5	317	123	9
5	15	5	0	17	1
7	15	5	317	130	9
0	16	5	313	315	10
2	16	5	216	219	10
4	16	5	76	67	18
0	0	6	2480	2537	28
2	0	6	137	129	8
4	0	6	530	544	7
6	0	6	680	682	7
8	0	6	406	404	7
10	0	6	883	912	9
12	0	6	787	792	8
14	0	6	764	741	8
16	0	6	901	891	9
1	1	6	182	174	7
3	1	6	138	128	8
5	1	6	1646	1656	16
7	1	6	143	131	8
9	1	6	334	329	7
11	1	6	213	216	8
13	1	6	81	84	15
15	1	6	425	426	9
17	1	6	310	309	10
0	2	6	1677	1715	16
2	2	6	187	200	8
4	2	6	145	144	8
6	2	6	482	492	7
8	2	6	187	191	8
10	2	6	846	862	8
12	2	6	342	336	8
14	2	6	55	63	22
16	2	6	370	357	9
1	3	6	273	273	7
3	3	6	40	28	24
5	3	6	871	864	8
7	3	6	116	111	9
9	3	6	873	882	8
11	3	6	1175	1187	11
13	3	6	114	123	11
15	3	6	125	125	12
17	3	6	408	416	9
0	4	6	2298	2319	29
2	4	6	66	44	13
4	4	6	323	321	7
6	4	6	523	527	7
8	4	6	107	109	11
10	4	6	1318	1330	13
12	4	6	138	150	11
14	4	6	40	3	39
16	4	6	195	205	10
1	5	6	306	310	7
3	5	6	313	314	7
5	5	6	526	525	7
7	5	6	79	78	12
9	5	6	294	295	8
11	5	6	302	299	8
13	5	6	74	71	17
15	5	6	284	289	9
0	6	6	107	109	11
2	6	6	86	83	12
4	6	6	324	317	8
6	6	6	966	970	10
8	6	6	289	303	8
10	6	6	59	49	20
12	6	6	200	194	9
14	6	6	686	681	9
16	6	6	824	804	9
1	7	6	502	510	7
3	7	6	99	83	10
5	7	6	2394	2443	23
7	7	6	111	113	11
9	7	6	340	347	8
11	7	6	405	416	8
13	7	6	224	219	10
15	7	6	715	697	9
0	8	6	283	263	8
2	8	6	242	246	8
4	8	6	330	330	8
6	8	6	258	258	8
8	8	6	339	346	8
10	8	6	215	194	9
12	8	6	69	67	18
14	8	6	318	341	10
1	9	6	391	392	8
3	9	6	33	44	33
5	9	6	46	38	27
7	9	6	562	556	8
9	9	6	165	163	9
11	9	6	741	727	9
13	9	6	41	45	40
0	10	6	2136	2140	23
2	10	6	257	249	8
4	10	6	236	232	9
6	10	6	556	554	8
8	10	6	105	92	13
10	10	6	1277	1264	13
12	10	6	269	259	10
1	11	6	164	169	10
3	11	6	330	334	8
5	11	6	481	482	8
7	11	6	143	142	10
9	11	6	412	394	9
11	11	6	773	773	9
0	12	6	511	519	8
2	12	6	128	125	10
4	12	6	160	153	10
6	12	6	846	852	9
8	12	6	87	76	15
10	12	6	338	353	10
1	13	6	9	12	8
3	13	6	57	32	22
5	13	6	1264	1260	13
7	13	6	102	111	14
0	14	6	128	121	11
2	14	6	159	373	9
4	14	6	297	288	9
6	14	6	170	157	11
1	1	7	85	79	12
3	1	7	178	184	8
5	1	7	118	124	10
7	1	7	269	266	8
9	1	7	152	138	9
11	1	7	694	672	8
13	1	7	269	266	9
15	1	7	235	235	10
0	2	7	619	619	7
2	2	7	327	335	7
4	2	7	24	26	23
6	2	7	476	479	8
8	2	7	258	251	8
10	2	7	64	71	20
12	2	7	430	435	9
14	2	7	184	176	10
1	3	7	257	242	8
3	3	7	20	10	19
5	3	7	408	405	8
7	3	7	377	371	8
9	3	7	140	137	10
11	3	7	850	834	8
13	3	7	60	51	22
0	4	7	1092	1077	12
2	4	7	51	44	20
4	4	7	155	169	10
6	4	7	151	157	10
8	4	7	127	130	12
10	4	7	436	435	8
12	4	7	448	443	9
14	4	7	119	114	13
1	5	7	11	6	10
3	5	7	90	93	13
5	5	7	142	145	10
7	5	7	494	504	8
9	5	7	212	221	9
11	5	7	0	25	1
13	5	7	251	258	10
0	6	7	210	218	8
2	6	7	139	132	10
4	6	7	201	206	9
6	6	7	719	734	8
8	6	7	250	256	9
10	6	7	147	129	10
12	6	7	204	201	10
1	7	7	121	110	10
3	7	7	185	187	9
5	7	7	888	880	9
7	7	7	114	104	12
9	7	7	281	263	9
11	7	7	574	558	9
0	8	7	638	640	8
2	8	7	15	15	15
4	8	7	179	166	9
6	8	7	358	350	9
8	8	7	24	26	23
10	8	7	219	216	10
12	8	7	362	364	10
1	9	7	351	339	8
3	9	7	96	110	13
5	9	7	230	245	10
7	9	7	116	138	13
9	9	7	15	5	15
11	9	7	553	551	9
0	10	7	628	632	8
2	10	7	410	413	8
4	10	7	127	124	11
6	10	7	221	200	10
8	10	7	104	96	17
1	11	7	126	116	11
3	11	7	48	21	31
5	11	7	609	595	9
7	11	7	136	136	12
0	12	7	34	30	33
2	12	7	234	220	9
4	12	7	280	276	10
0	0	8	2478	2502	24
2	0	8	130	140	10
4	0	8	166	167	9
6	0	8	675	668	8
8	0	8	42	40	41
10	0	8	1499	1507	15
12	0	8	525	535	9
1	1	8	170	163	10
3	1	8	96	82	12
5	1	8	411	421	8
7	1	8	249	243	9
9	1	8	588	582	9
11	1	8	552	555	9
0	2	8	6	24	6
2	2	8	111	117	10
4	2	8	221	204	8
6	2	8	503	489	8
8	2	8	35	20	35
10	2	8	198	187	10
1	3	8	92	89	13
3	3	8	263	271	8
5	3	8	1801	1781	17
7	3	8	39	3	39
9	3	8	131	128	9
11	3	8	105	95	13
0	4	8	217	228	9
2	4	8	322	319	8
4	4	8	161	160	10
6	4	8	675	680	8
8	4	8	25	7	24
10	4	8	177	172	11
1	5	8	535	528	8
3	5	8	139	155	11
5	5	8	418	420	9
7	5	8	24	31	23
9	5	8	52	66	29
0	6	8	1745	1779	17
2	6	8	189	180	10
4	6	8	256	264	9
6	6	8	478	464	9
8	6	8	149	143	11
1	7	8	47	25	29
3	7	8	207	204	10
5	7	8	862	866	9
7	7	8	238	246	10
0	8	8	895	909	9
2	8	8	42	34	41
4	8	8	108	77	12
6	8	8	431	430	9
1	9	8	44	32	43
3	9	8	98	96	14
5	9	8	1227	1241	12
0	10	8	1014	997	9
2	10	8	51	47	33
1	1	9	0	11	1
3	1	9	117	126	13
5	1	9	376	364	9
0	2	9	177	180	10
2	2	9	106	111	13
4	2	9	134	122	11
6	2	9	49	47	37
1	3	9	98	100	16
3	3	9	22	0	22
5	3	9	112	126	15
0	4	9	428	422	9
2	4	9	20	44	20
4	4	9	82	65	15
1	5	9	44	28	43
3	5	9	71	49	18
0	6	9	126	132	12

Observed and calculated structure factors for K52

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
2	0	0	716	730	6	2	8	0	201	200	4	1	1	1	170	159	2	5	9	1	295	320	4	3	1	2	826	809	8
4	0	0	1199	1210	9	4	8	0	447	442	4	3	1	1	411	405	4	7	9	1	336	342	4	5	1	2	951	956	9
6	0	0	533	545	5	6	8	0	634	643	6	5	1	1	994	991	11	9	9	1	52	32	11	7	1	2	116	108	4
8	0	0	862	827	8	8	8	0	419	412	4	7	1	1	58	42	5	11	9	1	1668	1677	15	9	1	2	636	631	6
10	0	0	3719	3630	17	10	8	0	1205	1201	11	9	1	1	384	387	4	13	9	1	102	92	8	11	1	2	664	665	7
12	0	0	1390	1382	13	12	8	0	147	161	6	11	1	1	775	794	8	15	9	1	166	163	7	13	1	2	18	9	18
14	0	0	207	197	5	14	8	0	149	138	6	13	1	1	340	339	5	17	9	1	151	154	8	15	1	2	593	607	6
16	0	0	223	223	6	16	8	0	344	345	6	15	1	1	172	160	6	19	9	1	202	199	7	17	1	2	73	59	10
18	0	0	448	442	6	18	8	0	67	68	13	17	1	1	703	701	7	0	10	1	1257	1255	13	19	1	2	0	12	1
20	0	0	255	262	7	20	8	0	276	275	7	19	1	1	465	476	6	2	10	1	733	746	7	21	1	2	344	334	7
22	0	0	1760	1738	16	1	9	0	24	17	24	21	1	1	756	744	7	4	10	1	207	210	5	0	2	2	3904	4050	12
1	1	0	247	236	2	1	9	0	395	406	4	0	2	1	195	224	2	6	10	1	476	483	5	2	2	2	401	387	4
5	1	0	463	475	4	5	9	0	1828	1845	18	2	2	1	521	541	4	8	10	1	177	172	5	4	2	2	537	523	5
7	1	0	406	406	4	7	9	0	824	818	7	4	2	1	467	476	4	10	10	1	261	260	5	6	2	2	517	502	5
9	1	0	1591	1563	15	9	9	0	32	8	32	6	2	1	258	239	3	12	10	1	30	27	29	8	2	2	272	264	4
11	1	0	3001	2939	18	11	9	0	674	655	6	8	2	1	538	539	5	14	10	1	559	565	6	10	2	2	1280	1273	13
13	1	0	336	346	5	13	9	0	212	216	6	10	2	1	129	99	5	16	10	1	331	345	6	12	2	2	520	531	5
15	1	0	277	285	5	15	9	0	585	595	6	12	2	1	917	922	9	18	10	1	210	217	7	14	2	2	55	50	10
17	1	0	152	158	6	17	9	0	489	489	6	14	2	1	183	170	5	1	11	1	130	133	6	16	2	2	358	356	5
19	1	0	535	533	6	19	9	0	196	191	7	16	2	1	611	618	6	3	11	1	176	181	5	18	2	2	45	22	17
21	1	0	790	790	8	0	10	0	306	317	4	18	2	1	64	44	12	5	11	1	726	757	8	20	2	2	19	6	18
0	2	0	1269	1306	7	2	10	0	26	30	25	20	2	1	242	238	7	7	11	1	526	540	5	1	3	2	488	472	5
2	2	0	106	326	3	4	10	0	365	379	4	22	2	1	210	216	7	9	11	1	277	275	5	3	3	2	240	238	3
4	2	0	607	615	6	6	10	0	264	248	5	1	3	1	368	373	3	11	11	1	279	296	6	5	3	2	1072	1044	10
6	2	0	116	123	3	8	10	0	265	282	5	3	3	1	247	245	2	13	11	1	129	139	7	7	3	2	198	200	4
8	2	0	264	254	3	10	10	0	498	505	5	5	3	1	414	391	3	15	11	1	171	179	7	9	3	2	1429	1448	18
10	2	0	611	621	6	12	10	0	229	228	6	7	3	1	446	439	4	17	11	1	462	470	6	11	3	2	1436	1455	13
12	2	0	195	199	4	14	10	0	1097	1087	11	9	3	1	192	195	4	0	12	1	996	1020	10	13	3	2	394	391	5
14	2	0	824	826	8	16	10	0	226	231	6	11	3	1	277	284	4	2	12	1	495	500	5	15	3	2	188	175	6
16	2	0	746	745	7	18	10	0	477	461	6	13	3	1	218	228	5	4	12	1	137	136	6	17	3	2	382	381	6
18	2	0	30	37	30	1	11	0	278	275	4	15	3	1	71	81	9	6	12	1	643	660	6	19	3	2	733	750	7
20	2	0	124	114	8	3	11	0	262	254	5	17	3	1	284	287	6	8	12	1	140	134	6	21	3	2	565	568	7
22	2	0	285	278	7	5	11	0	783	787	7	19	3	1	176	179	7	10	12	1	104	100	8	0	4	2	1738	1740	13
1	3	0	344	340	3	7	11	0	114	124	6	21	3	1	305	324	7	12	12	1	256	266	6	2	4	2	578	581	5
3	3	0	614	611	6	9	11	0	54	59	12	0	4	1	1127	1138	11	14	12	1	20	27	20	4	4	2	46	40	7
5	3	0	4920	4694	13	11	11	0	476	486	5	2	4	1	107	111	3	16	12	1	728	718	7	6	4	2	317	301	3
7	3	0	556	532	5	13	11	0	168	182	6	4	4	1	207	201	3	1	13	1	401	397	5	8	4	2	54	69	7
9	3	0	947	931	9	15	11	0	767	775	7	6	4	1	755	721	7	3	13	1	342	353	5	10	4	2	1876	1918	19
11	3	0	332	319	4	17	11	0	398	414	7	8	4	1	442	441	4	5	13	1	943	942	10	12	4	2	219	227	5
13	3	0	275	277	5	0	12	0	1533	1572	14	10	4	1	402	385	4	7	13	1	93	87	8	14	4	2	214	209	5
15	3	0	814	803	8	2	12	0	250	254	5	12	4	1	691	706	7	9	13	1	281	293	6	16	4	2	49	32	15
17	3	0	941	954	9	4	12	0	226	224	5	14	4	1	261	249	5	11	13	1	1085	1106	11	18	4	2	472	465	6
19	3	0	224	230	7	6	12	0	557	555	5	16	4	1	588	593	6	13	13	1	163	160	7	20	4	2	269	266	7
21	3	0	420	397	7	8	12	0	168	172	6	18	4	1	243	254	6	15	13	1	246	241	7	1	5	2	943	908	9
0	4	0	2026	2029	10	10	12	0	661	672	7	20	4	1	52	29	17	0	14	1	744	755	7	3	5	2	67	71	5
2	4	0	645	640	6	12	12	0	479	479	6	1	5	1	103	107	3	2	14	1	217	226	6	5	5	2	1875	1822	15
4	4	0	963	965	8	14	12	0	60	64	14	3	5	1	436	439	4	4	14	1	365	371	5	7	5	2	265	255	4
6	4	0	3913	3740	14	16	12	0	83	72	11	5	5	1	1344	1306	14	6	14	1	302	300	6	9	5	2	392	385	4
8	4	0	474	471	4	1	13	0	474	482	5	7	5	1	898	885	9	8	14	1	287	278	6	11	5	2	631	612	6
10	4	0	413	419	4	3	13	0	200	198	5	9	5	1	543	535	5	10	14	1	253	263	6	13	5	2	16	11	19
12	4	0	278	283	5	5	13	0	407	399	5	11	5	1	267	288	5	12	14	1	171	189	8	15	5	2	254	251	6
14	4	0	739	748	7	7	13	0	470	477	5	13	5	1	526	533	5	14	14	1	329	323	7	17	5	2	672	678	6
16	4	0	2051	2045	23	9	13	0	446	448	6	15	5	1	16	20	16	1	15	1	25	29	24	19	5	2	350	355	6
18	4	0	66	69	12	11	13	0	921	930	8	17	5	1	217	213	6	3	15	1	316	318	6	21	5	2	411	400	7
20	4	0	214	192	7	13	13	0	299	296	6	19	5	1	34	9	14	5	15	1	190	190	6	0	6	2	1113	1083	10
22	4	0	490	472	7	15	13	0	225	238	7	21	5	1	647	633	7	7	15	1	378	364	6	2	6	2	86	93	5
1	5	0	1457	1451	12	0	14	0	1365	1368	13	0	6	1	577	548	6	9	15	1	29	46	28	4	6	2	968	971	9
3	5	0	5	2	4	2	14	0	352	357	5	2	6	1	132	131	4	11	15	1	113	100	9	6	6	2	2417	2389	17
5	5	0	3168	3058	14	4	14	0	221	231	6	4	6	1	217	205	3	13	15	1	151	161	8	8	6	2	265	250	4
7	5	0	863	867	9	6	14	0	695	709	7	6	6	1	911	913	9	0	16	1	295	289	6	10	6	2	52	42	11
9	5	0	75	74	6	8	14	0	106	114	8	8	6	1	523	506	5	2	16	1	206	209	7	12	6	2	362	363	5
11	5	0	366	393	4	10	14	0	1207	1223	12	10	6	1	176	170	5	4	16	1	26	28	26	14	6	2	891	889	8
13	5	0	303	327	5	12	14	0	59	81	16	12	6	1	340	332	5	6	16	1	1248	1267	13	16	6	2	1508	1504	14
15	5	0	197	219	6	14	14	0	10	15	30	14	6	1	15	24	15	8	16	1	295	300	7	18	6	2	11	12	11
17	5	0	464	482	6	1	15	0	227	230	6	16	6	1	999	999	10	10	16	1	16	42	35	20	6	2	84	90	12
19	5	0	212	211	7	3	15	0	404	410	6	18	6	1	297	284	6	12	16	1	68	61	15	1	7	2	695	683	7
21	5	0	181	186	7	5	15	0	513	529	6	20	6	1	452	442	6	1	17	1	120	110	8	3	7	2	0	9	1
0	6	0	753	773	7	7	15	0	96	84	8	1	7	1	181	172	3	3	17	1	283	281	6	5	7	2	4459	4380	18
2	6	0	233	229	3	9	15	0	93	92	10	3	7	1	525	527	5	5	17	1	712	715	7	7	7	2	178	175	5
4	6	0	396	409	4	11	15	0	356	370	6	5	7	1	538	538	5	7	17	1	205	217	7	9	7	2	460	470	4
6	6	0	565	554	5	13	15	0	378	385	7	7	7	1	225	219	4	9	17	1	343	341	7	11	7	2	103	113	6
8	6	0	703	696	7	0	16	0	626	621	6	9	7	1	381	389	4	0	18	1	309	312	6	13	7	2	304	300	5
10	6	0	1313	1317	13	2	16	0	223	222	6	11	7	1	46	55	11	2	18	1	95	99	11	15	7	2	873	899	9
12	6	0	211	201	5	4	16	0	220	224	6	13	7	1	57	55	11	4	18	1	306	291	7	17	7	2	968	988	9
14	6	0	459	459	5	6	16	0	836	830	8	15	7	1	43	33	18	6	18	1	290	285	7	19	7	2	50	46	19
16	6	0	564	559	6	8	16	0	89	92	11	17	7	1	231	231	6	1	19	1	372	360	7	0	8	2	463	459	4
18	6	0	354	353	6	10	16	0	87	96	11	19	7	1	117	123	9	3	19	1	391	393	7	2	8	2	491	482	4
20	6	0	40	37	33	12	16	0	422	438	7	0	8	1	566	548	6	0	0	2	3220	3282	11	4	8	2	149	169	5
1	7	0	595	575	6	1	17	0	317	314	6	2	8	1	60	44	7	2	0	2	629	635	6	6	8	2	431	427	4
3	7	0	189	194	3	3	17	0	268	271	6	4	8	1	41	44	10	4	0	2	263	268	3	8	8	2	563	571	5
5	7	0	1376	1346	16	5	17	0	1775	1771	18	6	8	1	273	285	4	6	0	2	713	670	7	10	8	2	40	30	16
7	7	0	544	530	5	7	17	0	34	34	33	8	8	1	105	108	6	8	0	2	540	529	5	12	8	2	82	77	8
9	7	0	1107	1115	11	9	17	0	78	69	11	10	8	1	25	27	25	10	0	2	1370	1362	12	14	8	2	497	491	6
11	7	0	622	595	6	0	18	0	322	325	7	12	8	1	509	514	5	12	0	2	1029	1027	11	16	8	2	853	872	8
13	7	0	334	326	5	2	18	0	310	308	6	14	8	1	530	536	5	14	0	2	1210	1228	12	18	8	2	48	23	19
15	7	0	245	260	6	4	18	0	65	51	13	16	8	1	619	609	6	16	0	2	721	722	8	1	9	2	478	461	5
17	7	0	342	339	6	6	18	0	274	271	7	18	8	1	328	323	6	18	0	2	685	672	7	3	9	2	104	97	6
19	7	0	599	613	6	8	18	0	325	323	7	20	8	1	298	295	7	20	0	2	123	120	8	5	9	2	503	510	5
21	7	0	581	570	7	1	19	0	191	182	7	1	9	1	940	928	10	22	0	2	330	331	7	7	9	2	450	454	5
0	8	0	2535	2481	16	3	19	0	95	93	10	3	9	1	96	94	5	1	1	2	540	530	5	9	9	2	681	680	6

Observed and calculated structure factors for K52

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
11	9	2	1563	1582	16	16	2	3	1008	1021	10	13	11	3	39	24	26	4	4	4	560	568	6	4	14	4	333	330	6
13	9	2	111	121	7	18	2	3	238	230	6	15	11	3	40	32	35	6	4	4	1908	1932	19	6	14	4	504	488	6
15	9	2	223	224	7	20	2	3	184	182	8	17	11	3	564	560	7	8	4	4	204	213	5	8	14	4	111	96	9
17	9	2	664	660	6	1	3	3	548	540	5	0	12	3	158	156	6	10	4	4	292	289	5	10	14	4	969	964	9
19	9	2	269	278	7	3	3	3	227	228	3	2	12	3	303	294	5	12	4	4	196	199	6	12	14	4	44	43	27
0	10	2	4302	4333	20	5	3	3	1022	992	11	4	12	3	376	377	5	14	4	4	720	737	7	1	15	4	205	196	7
2	10	2	670	669	7	7	3	3	714	712	7	6	12	3	162	164	6	16	4	4	1446	1465	14	3	15	4	411	404	6
4	10	2	722	744	8	9	3	3	185	172	5	8	12	3	62	55	11	18	4	4	147	134	8	5	15	4	260	253	7
6	10	2	123	126	6	11	3	3	1338	1346	14	10	12	3	77	90	11	1	5	4	982	981	10	7	15	4	80	49	10
8	10	2	221	234	5	13	3	3	48	32	12	12	12	3	256	253	7	3	5	4	165	164	5	9	15	4	97	99	10
10	10	2	1820	1790	16	15	3	3	161	167	6	14	12	3	104	115	9	5	5	4	1460	1499	13	0	16	4	197	192	7
12	10	2	339	326	6	17	3	3	247	251	6	16	12	3	413	409	7	7	5	4	412	412	5	2	16	4	214	212	7
14	10	2	338	334	6	19	3	3	115	102	8	1	13	3	299	290	5	9	5	4	115	107	6	4	16	4	160	147	7
16	10	2	240	241	7	21	3	3	393	391	7	3	13	3	444	449	5	11	5	4	911	933	10	6	16	4	474	470	7
18	10	2	196	199	7	0	4	3	2232	2159	15	5	13	3	331	341	6	13	5	4	163	168	6	8	16	4	36	26	36
1	11	2	433	429	5	2	4	3	34	38	11	7	13	3	131	121	7	15	5	4	322	241	6	1	17	4	376	373	7
3	11	2	725	729	7	4	4	3	351	343	4	9	13	3	233	220	6	17	5	4	137	112	8	3	17	4	170	172	8
5	11	2	35	41	19	6	4	3	245	241	4	11	13	3	397	394	6	19	5	4	135	139	8	1	1	5	69	59	7
7	11	2	28	34	27	8	4	3	232	230	4	13	13	3	14	30	11	0	6	4	2040	2059	18	3	1	5	195	192	5
9	11	2	558	568	5	10	4	3	509	495	5	15	13	3	154	142	8	2	6	4	222	232	4	5	1	5	745	759	8
11	11	2	1799	1810	17	12	4	3	751	752	7	0	14	3	93	84	9	4	6	4	403	410	4	7	1	5	21	14	21
13	11	2	31	18	31	14	4	3	107	105	7	2	14	3	191	185	6	6	6	4	123	128	6	9	1	5	316	328	5
15	11	2	141	152	8	16	4	3	186	177	6	4	14	3	299	303	6	8	6	4	392	390	5	11	1	5	198	205	6
17	11	2	27	38	27	18	4	3	152	152	7	6	14	3	139	134	7	10	6	4	1234	1218	12	13	1	5	180	186	7
0	12	2	1276	1262	12	20	4	3	28	9	27	8	14	3	346	334	6	12	6	4	304	293	5	15	1	5	112	99	8
2	12	2	54	61	12	1	5	3	74	71	5	10	14	3	87	96	10	14	6	4	271	268	6	17	1	5	710	717	7
4	12	2	79	79	9	3	5	3	265	277	4	12	14	3	90	79	10	16	6	4	225	223	7	19	1	5	359	371	7
6	12	2	827	831	8	5	5	3	719	717	7	1	15	3	143	143	7	18	6	4	240	247	7	0	2	5	816	822	8
8	12	2	137	140	7	7	5	3	861	863	9	3	15	3	250	240	6	1	7	4	206	195	5	2	2	5	117	117	6
10	12	2	690	703	7	9	5	3	420	423	4	5	15	3	395	387	6	3	7	4	231	241	5	4	2	5	436	446	4
12	12	2	279	264	6	11	5	3	124	108	5	7	15	3	228	239	7	5	7	4	1245	1250	14	6	2	5	459	452	5
14	12	2	522	503	6	13	5	3	407	400	5	9	15	3	101	95	9	7	7	4	421	418	5	8	2	5	265	270	5
16	12	2	444	447	7	15	5	3	85	85	9	11	15	3	324	303	7	9	7	4	885	884	9	10	2	5	63	58	9
1	13	2	212	214	5	17	5	3	275	276	6	0	16	3	133	141	8	11	7	4	778	753	8	12	2	5	722	726	8
3	13	2	88	98	8	19	5	3	17	28	16	2	16	3	58	59	14	13	7	4	277	271	6	14	2	5	89	86	9
5	13	2	1777	1771	16	0	6	3	436	447	4	4	16	3	219	228	7	15	7	4	265	239	6	16	2	5	197	186	7
7	13	2	20	13	19	2	6	3	138	128	4	6	16	3	1125	1116	11	17	7	4	444	432	6	18	2	5	69	76	13
9	13	2	156	159	7	4	6	3	425	415	4	8	16	3	255	255	7	0	8	4	1731	1824	20	1	3	5	137	139	5
11	13	2	148	156	7	6	6	3	1188	1213	13	10	16	3	95	99	10	2	8	4	54	58	11	3	3	5	221	221	5
13	13	2	100	107	9	8	6	3	372	362	5	1	17	3	180	172	7	4	8	4	223	219	5	5	3	5	563	582	6
15	13	2	479	490	7	10	6	3	188	202	5	3	17	3	295	293	7	6	8	4	594	578	6	7	3	5	82	91	8
0	14	2	368	364	6	12	6	3	300	302	5	5	17	3	442	433	6	8	8	4	319	325	5	9	3	5	86	68	7
2	14	2	340	339	6	14	6	3	101	101	8	7	17	3	47	28	20	10	8	4	1037	1047	10	11	3	5	260	263	6
4	14	2	687	690	7	16	6	3	1076	1081	11	0	18	3	184	192	8	12	8	4	98	95	8	13	3	5	251	242	6
6	14	2	485	486	6	18	6	3	410	407	6	2	18	3	187	199	8	14	8	4	116	116	8	15	3	5	25	11	25
8	14	2	217	214	6	20	6	3	410	409	7	4	18	3	122	119	9	16	8	4	289	292	7	17	3	5	495	493	6
10	14	2	93	103	10	1	7	3	211	202	4	0	0	4	6231	6514	18	18	8	4	0	3	1	0	4	5	142	148	5
12	14	2	27	21	26	3	7	3	238	252	4	2	0	4	393	410	4	1	9	4	7	17	6	2	4	5	99	65	6
14	14	2	343	345	7	5	7	3	1293	1255	13	4	0	4	650	663	7	3	9	4	279	284	5	4	4	5	82	86	7
1	15	2	565	570	6	7	7	3	147	159	5	6	0	4	414	400	4	5	9	4	1763	1745	22	6	4	5	642	627	6
3	15	2	250	257	6	9	7	3	413	417	5	8	0	4	241	235	5	7	9	4	449	454	5	8	4	5	322	332	5
5	15	2	1390	1416	14	11	7	3	842	845	9	10	0	4	2615	2619	21	9	9	4	54	64	13	10	4	5	241	232	5
7	15	2	469	471	6	13	7	3	126	130	7	12	0	4	948	956	9	11	9	4	236	241	6	12	4	5	478	491	6
9	15	2	96	99	10	15	7	3	82	90	10	14	0	4	345	347	5	13	9	4	75	77	11	14	4	5	261	249	6
11	15	2	416	410	6	17	7	3	621	629	6	16	0	4	173	178	7	15	9	4	423	422	6	16	4	5	624	625	6
13	15	2	119	110	9	19	7	3	89	84	11	18	0	4	464	454	6	17	9	4	578	572	7	18	4	5	267	273	7
0	16	2	969	965	9	0	8	3	924	938	10	20	0	4	167	173	8	0	10	4	830	856	9	1	5	5	149	139	5
2	16	2	125	122	8	2	8	3	90	82	6	1	1	4	332	332	4	2	10	4	0	17	1	3	5	5	252	247	5
4	16	2	0	19	1	4	8	3	299	301	4	3	1	4	48	35	8	4	10	4	458	456	5	5	5	5	606	592	6
6	16	2	524	520	6	6	8	3	576	577	6	5	1	4	251	235	4	6	10	4	211	216	6	7	5	5	606	604	6
8	16	2	62	69	15	8	8	3	60	55	10	7	1	4	57	21	8	8	10	4	305	298	6	9	5	5	396	397	5
10	16	2	729	728	6	10	8	3	166	166	6	9	1	4	1168	1165	11	10	10	4	444	444	6	11	5	5	227	242	6
1	17	2	238	236	7	12	8	3	579	584	5	11	1	4	1721	1694	21	12	10	4	246	247	6	13	5	5	368	362	6
3	17	2	403	384	6	14	8	3	346	339	6	13	1	4	193	190	6	14	10	4	825	828	8	15	5	5	29	10	28
5	17	2	120	115	9	16	8	3	102	95	9	15	1	4	193	186	6	16	10	4	374	375	7	17	5	5	160	151	8
7	17	2	80	87	11	18	8	3	153	147	8	17	1	4	39	42	29	1	11	4	182	168	6	0	6	5	415	448	5
9	17	2	354	350	7	1	9	3	594	585	6	19	1	4	496	491	6	3	11	4	320	314	5	2	6	5	68	75	8
0	18	2	695	681	7	3	9	3	117	123	5	0	2	4	308	334	4	5	11	4	1009	1021	10	4	6	5	57	58	10
2	18	2	55	51	19	5	9	3	379	365	5	2	2	4	216	215	4	7	11	4	31	27	30	6	6	5	448	452	5
4	18	2	233	239	7	7	9	3	233	233	5	4	2	4	389	384	4	9	11	4	32	32	32	8	6	5	330	340	5
6	18	2	437	425	7	9	9	3	65	46	9	6	2	4	459	486	5	11	11	4	21	43	21	10	6	5	117	113	8
1	1	3	248	241	3	11	9	3	886	883	8	8	2	4	87	84	7	13	11	4	113	112	9	12	6	5	240	234	6
3	1	3	591	583	5	13	9	3	47	56	18	10	2	4	406	417	5	15	11	4	636	642	7	14	6	5	12	4	12
5	1	3	83	80	5	15	9	3	167	160	7	12	2	4	382	377	5	0	12	4	1003	1004	10	16	6	5	673	665	6
7	1	3	334	329	4	17	9	3	493	485	6	14	2	4	610	619	6	2	12	4	248	250	6	1	7	5	113	105	6
9	1	3	315	326	4	0	10	3	825	840	8	16	2	4	743	748	8	4	12	4	150	138	6	3	7	5	445	450	5
11	1	3	1297	1322	14	2	10	3	732	734	7	18	2	4	54	50	16	6	12	4	241	243	6	5	7	5	96	91	7
13	1	3	415	415	5	4	10	3	296	299	5	20	2	4	89	76	11	8	12	4	217	216	6	7	7	5	324	319	5
15	1	3	218	224	6	6	10	3	255	240	5	1	3	4	230	235	4	10	12	4	481	461	6	9	7	5	260	258	6
17	1	3	334	341	6	8	10	3	227	231	5	3	3	4	482	481	5	12	12	4	333	328	6	11	7	5	323	335	6
19	1	3	456	469	6	10	10	3	101	76	8	5	3	4	3276	3293	18	14	12	4	37	7	36	13	7	5	158	150	8
21	1	3	733	722	7	12	10	3	110	71	8	7	3	4	204	202	5	1	13	4	267	274	6	15	7	5	101	98	9
0	2	3	2092	2061	14	14	10	3	552	552	6	9	3	4	714	720	7	3	13	4	129	130	7	17	7	5	27	28	26
2	2	3	613	605	6	16	10	3	132	135	9	11	3	4	52	60	11	5	13	4	262	262	6	0	8	5	713	715	7
4	2	3	69	64	5	1	11	3	244	237	5	13	3	4	256	257	6	7	13	4	281	289	6	2	8	5	148	153	6
6	2	3	1084	1068	11	3	11	3	138	138	6	15	3	4	695	699	7	9	13	4	435	434	6	4	8	5	68	56	10
8	2	3	641	647	7	5	11	3	811	808	8	17	3	4	734	738	7	11	13	4	741	737	7	6	8	5	530	522	5
10	2	3	152	166	5	7	11	3	251	244	5	19	3	4	207	203	7	13	13	4	166	175	8	8	8	5	105	109	7
12	2	3	698	716	7	9	11	3	336	342	6	0	4	4	463	494	5	0	14	4	1317	1326	14	10	8	5	37	34	37
14	2	3	360	356	5	11	11	3	34	33	34	2	4	4	440	436	4	2	14	4	208	210	7	12	8	5	395	379	6

Observed and calculated structure factors for K52

h	k	l	10Fo	10Fc	10s
14	8	5	462	469	6
16	8	5	692	675	6
1	9	5	666	676	6
3	9	5	55	43	12
5	9	5	456	439	5
7	9	5	349	340	6
9	9	5	33	30	33
11	9	5	1519	1517	15
13	9	5	139	137	8
15	9	5	166	162	8
0	10	5	986	998	10
2	10	5	481	482	5
4	10	5	86	86	8
6	10	5	495	487	6
8	10	5	116	121	7
10	10	5	261	263	6
12	10	5	84	82	11
14	10	5	438	425	7
1	11	5	32	40	31
3	11	5	166	159	6
5	11	5	543	522	6
7	11	5	519	524	6
9	11	5	188	182	6
11	11	5	334	346	7
13	11	5	191	192	8
0	12	5	1004	1011	10
2	12	5	491	490	6
4	12	5	54	33	13
6	12	5	690	689	7
8	12	5	72	84	12
10	12	5	26	26	26
12	12	5	234	226	7
1	13	5	347	340	6
3	13	5	248	249	6
5	13	5	938	928	9
7	13	5	179	182	7
9	13	5	267	264	7
11	13	5	1204	1193	11
0	14	5	938	923	9
2	14	5	189	195	7
4	14	5	314	307	6
6	14	5	460	444	6
8	14	5	187	186	8
1	15	5	110	106	9
3	15	5	262	268	7
5	15	5	25	26	25
7	15	5	332	330	7
0	16	5	247	234	7
2	16	5	239	237	7
4	16	5	86	84	12
0	0	6	2486	2525	21
2	0	6	113	116	6
4	0	6	563	576	5
6	0	6	705	707	7
8	0	6	166	158	5
10	0	6	870	877	9
12	0	6	780	781	8
14	0	6	714	712	7
16	0	6	832	832	8
1	1	6	165	169	5
3	1	6	183	186	5
5	1	6	1598	1629	15
7	1	6	107	110	7
9	1	6	356	368	5
11	1	6	187	193	7
13	1	6	82	84	10
15	1	6	380	378	6
17	1	6	114	108	7
0	2	6	1671	1674	21
2	2	6	230	225	5
4	2	6	207	201	5
6	2	6	522	526	5
8	2	6	241	246	6
10	2	6	777	781	8
12	2	6	295	300	6
14	2	6	15	26	14
16	2	6	428	405	6
1	3	6	256	252	5
3	3	6	88	73	7
5	3	6	789	810	8
7	3	6	96	101	7
9	3	6	982	983	10
11	3	6	1144	1133	12
13	3	6	194	198	7
15	3	6	83	79	11
17	3	6	379	384	7
0	4	6	2273	2310	22
2	4	6	9	23	9
4	4	6	338	339	5
6	4	6	487	491	5
8	4	6	78	80	9
10	4	6	1300	1288	14
12	4	6	202	209	7
14	4	6	55	52	15
16	4	6	183	187	8
1	5	6	243	240	5
3	5	6	308	305	5
5	5	6	497	482	5
7	5	6	43	48	18
9	5	6	230	227	6
11	5	6	361	353	6
13	5	6	98	83	9
15	5	6	227	241	7
0	6	6	139	148	7
2	6	6	38	36	21
4	6	6	447	452	5
6	6	6	893	898	9
8	6	6	273	281	6
10	6	6	69	66	12
12	6	6	185	189	7
14	6	6	755	764	8
1	7	6	560	558	5
3	7	6	157	152	6
5	7	6	2347	2400	24
7	7	6	116	107	7
9	7	6	369	363	6
11	7	6	450	461	6
13	7	6	167	184	8
15	7	6	597	611	7
0	8	6	324	310	6
2	8	6	222	227	6
4	8	6	269	270	6
6	8	6	288	288	6
8	8	6	347	347	6
10	8	6	141	149	8
12	8	6	110	109	9
14	8	6	349	343	7
1	9	6	341	341	6
3	9	6	76	66	10
5	9	6	0	7	1
7	9	6	512	513	6
9	9	6	448	451	6
11	9	6	713	727	7
13	9	6	46	22	21
0	10	6	2081	2130	25
2	10	6	318	320	6
4	10	6	318	316	6
6	10	6	574	574	6
8	10	6	68	60	11
10	10	6	1219	1217	12
12	10	6	198	197	7
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3	11	6	364	365	6
5	11	6	462	464	6
7	11	6	145	142	8
9	11	6	411	400	6
11	11	6	760	754	7
0	12	6	452	454	6
2	12	6	93	83	9
4	12	6	95	84	10
6	12	6	893	889	9
8	12	6	20	22	19
10	12	6	366	364	7
1	13	6	72	52	12
3	13	6	81	69	12
5	13	6	1337	1316	14
7	13	6	111	115	10
0	14	6	60	75	15
2	14	6	394	378	7
4	14	6	307	307	7
6	14	6	167	160	8
1	1	7	78	74	9
3	1	7	223	221	6
5	1	7	180	124	6
7	1	7	278	276	6
9	1	7	198	193	6
11	1	7	705	705	7
13	1	7	304	314	7
15	1	7	186	194	8
0	2	7	622	594	6
2	2	7	328	320	6
4	2	7	20	15	20
6	2	7	470	461	6
8	2	7	274	270	6
10	2	7	0	2	1
12	2	7	506	502	6
14	2	7	199	207	7
1	3	7	210	209	6
3	3	7	0	20	1
5	3	7	366	370	6
7	3	7	424	419	6
9	3	7	144	146	8
11	3	7	785	775	8
13	3	7	55	49	17
0	4	7	1029	1037	10
2	4	7	78	70	9
4	4	7	226	223	6
6	4	7	113	119	8
8	4	7	167	174	7
10	4	7	325	328	6
12	4	7	468	471	6
14	4	7	121	110	10
1	5	7	0	1	1
3	5	7	128	144	8
5	5	7	225	218	6
7	5	7	520	519	6
9	5	7	306	300	6
11	5	7	24	15	24
13	5	7	232	243	7
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2	6	7	122	122	7
4	6	7	177	179	7
6	6	7	690	687	7
8	6	7	235	246	7
10	6	7	157	171	8
12	6	7	210	199	7
1	7	7	95	102	8
3	7	7	241	234	6
5	7	7	758	746	7
7	7	7	116	107	8
9	7	7	301	305	7
11	7	7	524	523	7
0	8	7	594	589	6
2	8	7	67	63	11
4	8	7	237	230	6
6	8	7	358	348	6
8	8	7	41	5	23
10	8	7	121	137	9
1	9	7	380	371	6
3	9	7	75	67	10
5	9	7	288	287	6
7	9	7	126	133	9
9	9	7	45	15	21
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2	10	7	414	415	6
4	10	7	147	137	8
6	10	7	213	197	7
8	10	7	131	125	8
1	11	7	143	130	8
3	11	7	100	90	10
5	11	7	562	567	6
7	11	7	166	169	8
0	12	7	19	1	18
2	12	7	193	190	8
4	12	7	265	261	7
0	0	8	2419	2458	25
2	0	8	158	161	7
4	0	8	216	229	7
6	0	8	697	704	7
8	0	8	22	27	22
10	0	8	1398	1416	14
12	0	8	513	521	7
1	1	8	136	141	8
3	1	8	94	89	9
5	1	8	487	482	6
7	1	8	225	222	7
9	1	8	625	622	6
11	1	8	527	521	7
0	2	8	10	18	10
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4	2	8	241	234	6
6	2	8	515	502	6
8	2	8	39	23	29
10	2	8	224	214	7
1	3	8	152	128	7
3	3	8	323	321	6
5	3	8	1693	1734	19
7	3	8	12	3	12
9	3	8	394	393	7
11	3	8	143	150	9
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3	5	8	161	160	7
5	5	8	389	397	6
7	5	8	38	32	37
9	5	8	133	134	9
0	6	8	1802	1795	19
2	6	8	210	213	7
4	6	8	346	343	7
6	6	8	434	431	6
8	6	8	174	176	8
1	7	8	13	28	13
3	7	8	172	169	7
5	7	8	890	878	8
7	7	8	256	245	7
0	8	8	903	892	9
2	8	8	46	16	19
4	8	8	56	42	20
6	8	8	411	410	7
1	9	8	35	54	35
3	9	8	153	152	8
5	9	8	1223	1227	11
0	10	8	1023	1020	10
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1	1	9	44	37	26
3	1	9	156	153	8
5	1	9	331	347	7
0	2	9	164	162	8
2	2	9	69	76	13
4	2	9	199	200	8
6	2	9	31	20	31
1	3	9	141	135	8
3	3	9	24	5	24
5	3	9	126	108	9
0	4	9	444	440	7
2	4	9	11	48	11
4	4	9	67	64	13
1	5	9	25	11	25
3	5	9	100	75	10