Crystal-Chemical Studies of Fine-Grained Materials Using Powder-Diffraction Methods and Computer Simulation

By

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CRYSTAL-CHEMICAL STUDIES OF FINE-GRAINED MATERIALS USING POWDER-DIFFRACTION METHODS AND COMPUTER SIMULATION

BY

JIAN-JIE LIANG

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

DOCTOR OF PHILOSOPHY

献给爸妈

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It is not always straight forward in dealing with X-ray instrumental problems. I was fortunate to have Neil Ball, Ron Chapman, and Surgil Mejia always ready to help whenever there was a demand.

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ABSTRACT

Many geologically and technologically important materials occur only as fine-grained powders. Comprehensive crystal-chemistry of these materials needs to be characterized by powder-diffraction methods. The reliability of the Rietveld method, one of the most important powder methods, was assessed by simultaneous Rietveld and single-crystal studies of a number of minerals representative of major (alumino-)silicate mineral groups. For moderately complex and anhydrous minerals, structure refinements comparable to those of single-crystal methods can be achieved, even when the mineral is in a powder mixture but the content is greater than 10 wt%. Preferred orientation in micaceous materials can be minimized during sample preparation, and residual preferred orientation can be corrected semi-empirically during data processing. Rietveld refinement of framework atomic positions in zeolites are comparable with single-crystal refinement, whereas those of the extraframework species were more difficult. Rietveld refinements of cation site-occupancies were reliable, independent of the complexities of the crystal structure.

Computer-based theoretical studies can supplement experimental observation and assist data interpretation. Static structure-energy minimization, in which electrostatic interactions, bond-bending and polarizations were considered explicitly, was used to calculate H positions in a number of phyllosilicates. Experimentally determined H-positions in well-studied phyllosilicates were reproduced. H-positions in muscovite and certain H-positions in dickite were calculated split, and confirmed by variable-temperature

neutron diffraction and FTIR experiments.

Coupling Rietveld refinement with theoretical calculations can greatly increase the capability and reliability of the Rietveld method. An algorithm of the Coupled Rietveld--Static Structure-Energy Minimization (CRSSEM) was developed, in which Rietveld refinement is dynamically regulated by the structure-energy calculation. The method had been successfully applied to a number of materials whose structures are so complex that false-convergence was reported in their unaided Rietveld refinements. The method had also been shown effective to refine layer structures when two very similar polytypes coexist.

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CRSSEM:	Coupled Rietveld--Static Structure-Energy Minimization
EPMA:	Electron Microprobe Analysis
FTIR:	Fourier-Transform InfraRed spectroscopy
FTIR PAS:	Photo-Acoustic Fourier-Transform InfraRed Spectroscopy
MD:	Molecular Dynamics
SREF:	Single-crystal site-scattering REFinement
SSEM:	Static-Structure Energy Minimization
XRD:	X-Ray Diffraction

CHAPTER 1.

INTRODUCTION

Powder-diffraction methods and computer simulation play important roles in the study of the crystal-chemistry of fine-grained materials. Many naturally occurring crystalline materials and most synthetic products occur, or can only be prepared, as fine-grained powders. Their characterization, which is essential to the understanding of their physical-chemical properties, cannot be done with conventional single-crystal diffraction methods. There is also a large number of technologically important materials, such as industrial ceramics and superconductors, which are deliberately prepared in sub-micrometer ranges of individual grain size. The physical-chemical properties of these materials are necessarily different from their coarse-grained counterparts due to the different histories of crystal growth. With the development of the Rietveld method, the powder-diffraction techniques have recently emerged as powerful tools in providing crystal-chemical information for powdered materials. However, powder-diffraction methods suffer from difficulties in resolving overlapping information, reducing the reliability of results derived from powder-diffraction studies. Systematic assessment of powder characterization is necessary to establish confidence in utilizing and further improving the methods.

Powder-diffraction studies of crystal chemistry of fine-grained materials can be assisted by computer simulation of the crystal structure of the same material in that difficult crystal structure refinement can be constrained by the simulation. Computer simulation of crystal structures has its roots in quantitative models of crystal chemistry obtained either directly through experimental observation or from quantum-mechanical calculations. Computer simulation models the behaviour of individual atoms in a given structural configuration, and relates such behaviour to material properties. Development of the method hinges not only on the development of computing power, but also on increased understanding of atomic interactions.

1.1. History of Rietveld Method and Its Current State of Development

The pioneering experiments on powder X-ray diffraction (Friedrick 1913; Keene 1913), neutron diffraction (Elsasser 1936; Mitchell & Power 1936) and synchrotron X-ray diffraction (Bathow *et al.* 1966) established the technique as an important tool for identification and characterization of crystalline materials. However, until recently most of our detailed understanding of crystalline materials resulted from *single-crystal* X-ray or neutron diffraction. Development of the Rietveld method (Rietveld 1967, 1969) allowed crystal structure refinement using powder-diffraction data. The method was initially proposed for neutron diffraction data, taking advantage of the relatively simple peak-profile in the diffractogram that can be modeled using simple Gaussian profile function. The accessibility of laboratory X-ray sources was the driving force to adapt the Rietveld method for use with X-ray data (Malmros & Thomas 1977; Young *et al.* 1977). Modelling the more complex peak-profiles in X-ray diffraction was, and still is, a major difficulty for the method. Despite this difficulty, a large number of successful Rietveld refinements of crystal structures has been reported (Jenkins & Hawthorne 1995; Bish & Post 1989, and references in these articles). With the advent of high-resolution laboratory X-ray sources that use $K\alpha_1$ radiation only, and super-high-resolution synchrotron X-ray radiation, the Rietveld technique has developed from a refinement method toward an *ab initio* crystal structure solution method (although pioneer work had also been done with instruments that use $K\alpha_2$ as well, see Cheetham & Wilkinson 1993 and references therein).

The Rietveld method is still under active development. In structure refinement, apart from profile shape, other effects such as absorption (especially micro-absorption) and extinction, also need to be better understood and modelled. Inadequate modelling of these effects, complicated by uncertainties in structural parameters, may cause convergence to false minima (Suitch & Young 1983; Young & Hewat 1988). Soft constraints in the form of prescribed bond-distances (Cartlidges & Meier 1984; McCusker *et al.* 1985; Bish & Von Dreele 1989) and angles (Marler *et al.* 1993) can be used to bring about convergence to reasonable bond lengths and angles in the refined structure.

1.2. The Nature of Computer Simulation of Crystal Structures

Computer simulation depends on an initial configuration, the starting model, of the system to be simulated. Such configuration can be constructed from understanding of similar materials, or from partial experimental observation (*e.g.*, crystal-structure obtained from diffraction experiments that lacks light-atom positions). The simulation process is governed by a set of rules, the interaction model, that dictates how individual units (atoms) in the system behave. Such behaviour is simulated using certain numerical technique, with a computer, such that an equilibrium of the interactions among the individual units (atoms) be achieved.

Computer simulation of crystal structures is a topic in between empirical and *ab initio* studies of crystal structures. Therefore we can find traces of computer simulation in the earliest empirical studies of crystal structures, which can best be summarized into the Pauling's rules (Pauling 1929, 1960). In Pauling's first rule, crystal structures are considered to consist of positively charged cations, surrounded by negatively charged anions, with the number of anions surrounding the cations and the cation-anion separation determined by the ionic radii and the ratio of the radii. Early computer simulations of mineral structures (Giese 1971) built almost entirely on this first rule. The second rule proposed the concept of bond-strength that relates the stability of a structure to the formal charges of the ions and their corresponding coordination numbers. The second rule became the basis of the powerful bond-valence theory (Brown & Shannon 1973; Brown 1981; Brown & Altermatt 1985; Brese & O'Keeffe 1991) that gives experimental crystallographic studies the ability of prediction. The other Pauling's rules are more phenomenal in nature. Hawthorne (1992) refined these rules into three new, more general rules that include (1) the electro-neutrality; (2) prediction of coordination number from ionic-radius ratio and (3) prediction of mean bond length from the sum of the ionic radii of the bonded atoms. These rules are used, consciously or unconsciously, in modern theoretical and experimental crystallographic studies.

Computer simulation also has its root in modern physics and chemistry. Crystal structures are believed to be a manifestation of a balance of the interatomic interactions that are represented by the first-order, electrostatic interaction model (ionic model, Born & Landé 1918; Born & Mayer 1932). Individual atoms are assigned formal charges, and are treated in the ionic model as point charges. Contemporary computer simulation adds to the first-order interaction certain higher-order terms to account for interatomic repulsion, polarization and covalency. Such addition basically recognizes the electron density distribution around individual atoms, and their distortion in the crystalline environment. While this improved interaction model had proven a very good approximation of total energy model in a structure, the additive nature of the interaction terms had never been theoretically justified. Correlation between individual energy terms are totally neglected. In the quantum-mechanical derivation of multi-body interaction (Hehre *et al.* 1985), individual interaction terms in computer simulation can be readily identified in the total Hamiltonian of the Schrödinger equation. It was clearly demonstrated that the Hamiltonian is not separatable in terms of these individual interaction terms. In another words, these interaction terms do correlate with each other. Therefore, until such correlation is adequately approximated, computer simulation will remain semi-quantitative in theoretical crystal structure study.

1.3. Overview of the Thesis

The thesis falls into three distinct parts:

(1) The reliability of Rietveld refinement of silicate minerals. Both Rietveld and single-crystal studies have been done on the same minerals, and the reliability of Rietveld determination of atomic positions and their corresponding standard deviations is assessed. Rietveld determination of cation-site occupancies is also evaluated with individual displacement factors fixed at reasonable values.

(2) Prediction of H-atom positions in micas and clay minerals using one of the two common computer simulation methods, the Static Structure-Energy Minimization (SSEM) method. Clay minerals usually occur in fine-grained state. Locating H-atom positions in clay minerals using powder diffraction method has been difficult. The micas are minerals that closely resemble clay minerals but are much better understood due to the fact that they usually occur in good, large crystals. Applicability of computer simulation in reproducing H-atom positions in micas will serve as a basis of predicting H-atom position in clay minerals.

Neutron-diffraction experiments or infrared (IR) spectroscopy were used to assess the computationally predicted H-positions.

(3) Development of the Coupled Rietveld--Static Structure Energy-Minimization (CRSSEM) method in which the Rietveld method and the SSEM method were dynamically coupled together. The Rietveld part represents the interpretation of the powder diffraction experiment data, and the SSEM part represents constraints from our theoretical understanding of crystal chemistry. Coupling Rietveld refinement with structure-energy calculation ensures the crystal-chemical validity of the final refined structure. The CRSSEM method had been successfully applied to the structure refinements of minor phases in binary mixtures, crystal structures of two polytypes of a new mica species, and the complex structure of a new synthetic zeolite.

Chapter 2.

Powder Diffraction and the Rietveld Method

Good Rietveld refinement depends on (1) accurate powder-diffraction intensity data; (2) a good model for the Bragg peak-shape; (3) a starting model which is reasonably close to the correct structure. In addition, certain corrections with regard to displacement of Bragg peak positions (due to poor instrument alignment, sample surface displacement from the focusing circle, *etc.*) and instrument-related intensity distortions (*e.g.* micro-absorption) are also essential.

2.1. Powder-Diffraction Intensity-Data Collection

The intensity data are normally collected on a diffractometer in the step-scan mode over a range of Bragg angles (2Θ angles). Data should be collected to as high a 2Θ angle as possible, because the high-angle data are critical to the refinement of accurate atomic positions and displacement factors (Post & Bish 1989). It has been shown (Hill & Madsen 1984, 1986) that it is necessary to collect the intensity data at individual step-widths of one-fifth to one-half (usually 0.0n °2Θ) of the half-width of the resolved peaks in the pattern with a counting time that accumulates no more than a few thousand counts for the strongest peak. Finer step-widths may improve the *apparent* precision of the data, but the assigned standard deviations are wrong due to serial correlation, which is the correlation between neighbouring step-intensity data that may be too closely sampled from each other to be independent observations. Bérar & Lelann (1991) explicitly showed the effects of serial correlation in the underestimation of the standard deviations in Rietveld analysis, and proposed a correction procedure to give true standard deviations.

Rietveld refinement requires a random powder mount in the data collection. Different methods have been described. With side- or back-loading methods (Klug & Alexander 1974), the powder sample is loaded into a volume of about 20×15×2 mm^3 in a sample holder from the side or back of the holder. The sample can also be prepared (Post & Bish 1989) by sieving the powder onto a Whatman glass micro-fibre filter. Other sample-preparation methods include dilution with a second phase, dusting the sample onto glass-fibre filters (Davis 1986), and spray drying (Smith *et al.* 1979). However, none of the existing methods produced randomly oriented powder, and some suffer from transparency effects (Klug & Alexander 1974).

2.2. Background Correction

The raw intensity data need to be corrected for background. The background arises from many sources (Klug & Alexander 1974), including fluorescence from the sample, detector noise, thermal-diffuse scattering from the sample, disordered or amorphous impurities, incoherent scattering, and scattering of X-rays from air, sample holder and diffractometer slits. With relatively simple patterns (in which Bragg peaks are well separated and the background intensities can be measured between these peaks), the background intensity can be removed by interpolating between the measured points. However, this is not possible for most complex diffraction patterns. In Rietveld work, the background is usually modelled by a polynomial function (Wiles & Young 1981):

$$Y_{ib}(c)=B_0+B_1TT_i+B_2TT_i^2+B_3TT_i^3+B_4TT_i^4+B_5TT_i^5 \qquad 2\text{-}1$$

in which TT_i = $2\Theta_i$ - 90°, $B_0 ... B_5$ are refinable parameters determined by least squares along with the structural parameters. The background can also be modelled by a cosine Fourier-series (Larson & Von Dreele 1988):

$$Y_{ib}(c)=B_1+\sum_{j=2}^{12}B_j\cos(2\theta_j-1) \qquad 2\text{-}2$$

The success in refining the background depends on how well the peak shape is known (Prince 1981; Albinati & Williams 1982). If the diffraction pattern is poorly resolved, the background parameters tend to correlate with the peak shape and structural parameters (especially the displacement factors).

2.3. Modelling the Peak Shape

The peak shape in an X-ray powder-diffraction pattern depends on the type of sample and the data-collection procedure (Klug & Alexander 1974). The sample-related properties, including crystallite-size distribution and crystal-structure distortions, determine the natural peak-shape (which is usually non-Gaussian). The natural peak-shape is modified by instrumental factors, including (1) the geometry of the X-ray source; (2) the displacement of the flat sample-surface from the focusing circle (flat-specimen error); (3) axial divergence of the X-ray beam; (4) specimen transparency; (5) effects of slits; (6) misalignment of the diffractometer. The resultant XRD peak-shape is therefore very complex (rather than a simple Gaussian as in neutron diffraction). The peak shape can be modelled by combined Gaussian and Lorentzian functions (Young & Wiles 1982) such as the widely used pseudo-Voigt function (Wertheim *et al.* 1974):

$$I_{ik}=\eta L_{ik}+(1-\eta)G_{ik} \qquad \text{2-3}$$

in which I_{ik} is the intensity of the i^{th} point in the pattern due to the k^{th} line; η is the mixing parameter (which can be refined); L_{ik} and G_{ik} are the Lorentzian and Gaussian components at the i^{th} point due to the k^{th} reflection:

$$L_{ik}=\frac{\sqrt{4}}{\pi H_k}[1+\frac{4(\sqrt{2}-1)}{H_k^2}(2\theta_i-2\theta_k)^2]^{-1} \qquad \text{2-4}$$

$$G_{ik} = \frac{2\sqrt{\ln 2}}{H_k} \exp[\frac{-4ln2}{H_K^2}(2\theta_i - 2\theta_k)^2] \qquad 2\text{-}5$$

where H_k is the Full-Width at Half-Maximum peak-height (FWHM) of the k^{th} reflection. The refinable constant can be interpreted as the degree of Lorentzian versus Gaussian character. The sample-related effects (*e.g.*, particle-size broadening) can be described by the Lorentzian part of equation 2-3, and the instrument-related effects can be described by the Gaussian part of the equation. The half-width function, H_k, can vary independently for the Lorentzian and Gaussian components (David 1986), and information on particle-size can be extracted (Keijser *et al.* 1983; David & Matthewman 1985; Larson & Von Dreele 1988; Madsen & Hill 1988). Further improvement in modelling peak-shape can be achieved by varying the mixing coefficient, η, in equation 2-3 as a function of diffraction angle, 2Θ (Hill 1984; Hill & Howard 1985; Toraya 1986). Other peak-shape functions in use are the Pearson VII (Brown & Edmonds 1980) and pure Voigt (Langford 1978), which are similar or analytically more complicated.

Peak-shapes in an XRD pattern are usually asymmetric (Klug & Alexander 1974) due to a variety of sample- and instrument-related effects (*e.g.*, axial divergence, disorder, etc.). It can be corrected using a refinable semi-empirical asymmetry factor by multiplying the terms in the profile function (equation 2-3) by

$$[1 - P(2\theta_i - 2\theta_k)^2 \frac{s}{\tan\theta_k}] \qquad 2\text{-}6$$

where P and s are refinable parameters.

The peak width (expressed as FWHM) can be modelled as a function of $\tan\Theta$ (Caglioti *et al.* 1958) by

$$H^2 = u\tan^2\theta + v\tan\theta + w \qquad \text{2-7}$$

in which u, v and w are refinable parameters. These parameters are specific to a given instrumental configuration and the peak-shape function used.

There had been many approaches (Howard 1982, Thompson *et al.* 1987, Howard & Snyder 1989, Yau & Howard 1989) to describing profile shape with respect to the analytical functions in modelling the profile shape and to the corresponding functions modelling the half-width of the diffraction peaks. In an attempt to approximate asymmetry, Howard (1982), in the study using high-resolution neutron diffraction instrumentation, proposed a profile function consisting sums of Gaussians in place of a simple Gaussian multiplied by Rietveld's semi-empirical asymmetry factor (equation 2-6). The profile function has the form

$$G_{ik}(\theta_i - \theta_k) = \frac{1}{6}[G(\theta_i - \theta_k) + 4G(\theta_i - \theta_k + \frac{1}{4}P\cot2\theta_k + G(\theta_i - \theta_k + P\cot2\theta_k)] \qquad \text{2-8}$$

in which P is related to FWHM and the volume of the sample. Other symbols are the same as above. Thompson *et al.* (1987) modified the pseudo-Voigt function (equation 2-3) such that, instead of refining the mixing parameter η and H (equations 2-3,7), the variation of the Gaussian and Lorentzian half widths (H_G and H_L) were refined directly. H_G and H_L can be approximated closely by the functions $V\tan\theta$ and $X/\cos\theta$, in which V and X are refinable parameters. The advantage of using this modification is that the refined values of V and X can be directly related to instrumental broadening and particle-size effects. Howard and Snyder's approach to the modelling of profile shape is similar to that of Thompson *et al.* (1987) in that the sample-related broadening and asymmetry was treated separately from the instrumental effects. The former were represented by a Lorentzian-type function, whereas the latter by a pair of split-Pearson VII functions in which profile parameters were refined for each of the two sides of a Bragg peak. Such a split-profile treatment was found to be effective in modelling instrument-related asymmetry over a wide two-theta range. Berar and Baldinozzi (1993) considered explicitly individual effects that produce asymmetry, including axial divergence, equatorial divergence and specimen transparency, in their derivation of an approximate function for the correction of asymmetry. The proposed functions have the form

$$g(d\theta) = g_0(d\theta)[1 + A(\theta)F_a(d\theta/H) + B(\theta)F_b(d\theta)/H)] \qquad 2\text{-}9$$

$$A(\theta) = A_0/\tan(\theta) + A_1/\tan(2\theta) \qquad 2\text{-}10$$

$$B(\theta) = B_0/\tan(\theta) + B_1/\tan(2\theta) \qquad 2\text{-}11$$

$$F_a(z) = 2\ z\ \exp(-z^2) \qquad 2\text{-}12$$

$$F_b(z) = (8z^3 - 12z)\ \exp(-z^2) \qquad 2\text{-}13$$

in which $d\theta = \theta_i - \theta_k$ and $z = d\theta/H$. Significant improvement was attained in the refinement of the standard $PbSO_4$ data recorded for the IUCr Commission on Powder Diffraction Round Robin on Rietveld Refinement; R_{wp} decreased from 10.2% to 7.9% and the Durbin-Watson d-value rose from 0.72 to 0.92.

A lot of attention has also been directed recently to the correction of diffraction intensity for extinction (Sabine 1988, Sabine *et al.* 1988) and absorption (Hermann & Ermrich 1987, Ottani *et al.* 1993, Pitschke *et al.* 1993, and Pitschke *et al.* 1993). Extinction (primary) is caused by multiple scattering of the diffracted beam (Stout and Jensen 1968) such that the intensity of the diffracted beam is proportional to $|F|$, rather than $|F|^2$. In powder diffraction, extinction can be corrected by the factor

$$E = E_L \cos^2\theta + E_B \sin^2\theta \qquad \text{2-14}$$

$$E_L = 1 - x/2 + X^2 - 5X^2/48 + 7x^4/192 \quad (x \leq 1) \qquad \text{2-15}$$

$$E_L = (2/\pi x)^{1/2} \, [1 - 1/8x - 3/128x^2 - 15/1024x^2] \quad (x > 1) \qquad \text{2-16}$$

$$F_a(z) = 2\, z \exp(-z^2) \qquad \text{2-13}$$

$$E_B = (1 + x)^{-1/2} \qquad \text{2-18}$$

$$x = (KN_c \lambda F D)^2 \qquad \text{2-19}$$

in which N_c is the number of unit cells per unit volume, and λ is the wavelength. K is the shape factor whose value is unity for a cube of edge D, 3/4 for a sphere of diameter D, and $8/3\pi$ for a cylinder of diameter D. In an actual refinement, x is the variable refined.

Both bulk porosity and surface roughness (intensity data collected in reflection geometry) of the sample can contribute to absorption of the diffracted beam (Hermann & Ermrich 1987). Absorption by the bulk porosity is referred to as "macro-absorption", whereas that by rough surface is "micro-absorption" (Ottani 1993). Pitschke *et al.* (1992) gave expressions that are rather easy to implement in a Rietveld program. However, the scope was limited to the modelling of micro-absorption of surface roughness in Bragg-Brentano geometry. Ottani *et al.* (1993) gave a complete set of factors for absorption correction in X-ray powder diffraction, covering both macro- and micro-absorption and intensity data collection in both reflection and transmission geometry. For reflection geometry, depending on different boundary conditions, the absorption-correction factor, ABS, can be expressed as

(i) $0 < T \leq R(\beta - \alpha)/2 \cos\theta$

$$(ABS)^{-1} = (1 - e^{-2\mu T/\sin\theta}) \qquad \text{2-20}$$

(ii) $R(\beta - \alpha)/2 \cos\theta < T \leq R(\beta + \alpha)/2 \cos\theta$

$$(ABS)^{-1} = [1 + (\frac{2T\cos\theta - R(\beta - \alpha)}{2R\alpha} + \frac{1}{A})e^{-2\mu T/\sin\theta} - \frac{1}{A}e^{-(B - A)/2}] \qquad \text{2-21}$$

(iii) $T \geq R(\beta - \alpha)/2 \cos\theta$

$$(ABS)^{-1} = [1 - \frac{1}{A}(e^{-(B - A)/2} - e^{-(B + A)/2})] \qquad 2\text{-}22$$

in which R is the radius of the diffraction circle, T is the specimen thickness, α is the equatorial angle on the specimen of the divergence slit, β is the equatorial angle on the specimen of the receiving slit, and μ is the sample linear absorption coefficient. The values of A and B are defined as

$$A = \frac{2\mu 2R\alpha}{\sin 2\theta}; \quad B = \frac{2\mu 2R\beta}{\sin 2\theta} \qquad 2\text{-}23$$

For transmission geometry, ABS is also dependent on the boundary conditions:

(i) $0 < T \leq R(\beta - \alpha)/2 \sin\theta$

$$(ABS)^{-1} = \frac{\sec\theta}{e^{-\mu T(1-\sec\theta)}} \qquad 2\text{-}24$$

(ii) $R(\beta - \alpha)/2 \sin\theta < T \leq R(\beta + \alpha)/2 \sin\theta$

$$(ABS)^{-1} = \frac{1}{e^{-\mu T(1-\sec\theta)}} (\sec\theta - \frac{(R\beta - R\alpha - 2T\sin\theta)^2}{2R\alpha 2T \sin 2\theta}) \qquad 2\text{-}25$$

(iii) $T \geq R(\beta - \alpha)/2 \sin\theta$

$$(ABS)^{-1} = \frac{R\beta}{T \sin 2\theta \; e^{-\mu T(1 - \sec\theta)}} \qquad 2\text{-}26$$

Implementation of an absorption correction had been shown to help to refine displacement factors to obtain results that makes physical sense (Pitschke 1993).

2.4. Preferred Orientation Correction

Preferred orientation of samples (especially those having good cleavage or strong non-spherical growth habit) can cause systematic distortions of intensity distribution in the diffraction patterns. Such distortion can be modelled with analytical functions. One of the most commonly used is the so called March-function (Dollase 1986):

$$P_K = (G_1^2 \cos^2\alpha + (1/G_1) \sin^2\alpha)^{-3/2}) \qquad \text{2-27}$$

in which, G_1 is a refinable parameter, and α is the angle between the diffraction vector and the presumed cylindrical-symmetry axis of the texture (e.g. the normal of a cleavage surface).

2.5. Structure Refinement

Establishing a good starting model is essential in Rietveld structure-refinement. The starting model can be obtained from the known structure of other members in a solid solution (McCusker *et al.* 1985; Post & Bish 1989). In a few cases, it can be derived from high-resolution transmission electron-microscopy (Post & Bish 1988). The structure parameters (cell dimensions, atomic positions, site occupancies and overall displacement factors) are usually refined along with the scale factor, the background parameters and parameters related to peak shape, width and asymmetry, using the least-squares method. The quantity to be minimized is

$$R=\sum_{i} w_i(Y_{io}-Y_{ic})^2 \qquad 2\text{-}28$$

in which Y_{io} and w_i are the observed step intensities and the weight assigned to it at step i; Y_{ic} is the corresponding calculated intensity

$$Y_{ic}=Y_{ib}+\sum_{k=k_1}^{k_n} PSF_{ik}\cdot F_k \qquad 2\text{-}29$$

in which Y_{ib} is the calculated background correction, PSF_{ik} is the value of the normalized peak-shape function of reflection k [*c.f.* equation 2-3], and F_k is the Bragg intensity of the k^{th} reflection contributing to the intensity at point i. *PSF* involves all profile-shape (including asymmetry) parameters, and F contains all structure parameters plus the scale factor. The configuration in F corresponding to the minimum of R in equation 2-8 is taken as the final refined structure.

2.6. Convergence and Least-squares Error Criteria

When the quantity R in equation 2-8 becomes smaller as the least-squares process proceeds, the system is said to be converging. The convergence criteria specify the point at which the least-squares process (the refinement) is stopped. The refinement will be halted if all the variables pass the test (Howard & Preston 1989)

$$\frac{\Delta\beta_i}{|\beta_i|+\tau} \leq \varepsilon \qquad 2\text{-}30$$

where $|\beta_i|$ and $\Delta\beta_i$ are the magnitude and adjustment of variable β_i during a single cycle of refinement, τ (on the order of 0.001) is a number to prevent division by zero, and ε determines the number of significant digits of the variable obtained from the refinement. An alternative convergence criterion is to compare the shift of the variable with its standard deviation, which can be estimated as

$$\sigma_i = \sqrt{\frac{M_{ii}^{-1}\sum_j (2\theta_j)\cdot[I(2\theta_j)^{obs} - I(2\theta_j)^{calc}]^2}{N-P}} \qquad 2\text{-}31$$

in which σ_i is the variance of the i^{th} variable, M_{ii}^{-1} is the corresponding diagonal element in the inverted normal-equations matrix, $I(2\Theta_j)^{obs}$ and $I(2\Theta_j)^{calc}$ are the observed and calculated intensities at the 2Θ step j, and N and P are the total number of observations and variables, respectively. The system is said to have reached convergence when the condition, $\Delta\beta_i < (\alpha \times \sigma_i)$, is satisfied for all variables in a given refinement cycle; α is a user defined parameter, usually on the order of 0.3 (Howard & Preston 1989).

The least-squares error-criteria usually used in Rietveld refinement are (Post & Bish 1989)

$$R_p = \frac{\sum |Y_{io} - Y_{ic}|}{\sum Y_{io}} \qquad 2\text{-}32$$

$$R_{wp} = \sqrt{\frac{\sum W_i(Y_{io}-Y_{ic})^2}{\sum W_i Y_{io}^2}} \qquad 2\text{-}33$$

$$R_B = \frac{\sum |I_{ko}-I_{kc}|}{\sum I_{ko}} \qquad 2\text{-}34$$

$$R_{\exp} = \sqrt{\frac{N-P}{\sum W_i Y_{io}^2}} \qquad 2\text{-}35$$

$$GofF = \frac{\sum W_i(Y_{io}-Y_{ic})^2}{N-P} = \left(\frac{R_{wp}}{R_{\exp}}\right)^2 \qquad 2\text{-}36$$

$$d = \sum_{i=2}^{N}\left[\frac{Y_{io}-Y_{ic}}{\sigma_i}-\frac{Y_{io-1}-Y_{ic-1}}{\sigma_{i-1}}\right]^2 / \sum_{i=1}^{N}\left(\frac{Y_{io}-Y_{ic}}{\sigma_i}\right)^2 \qquad 2\text{-}37$$

The symbols in the expressions have the same meaning as above. R_p and R_{wp} are essentially the same, except that the latter is weighted. Their values represent the percent difference between the observed and calculated diffraction patterns. R_{exp} is the lower limit of R_p and R_{wp} based on counting statistics. A value of GofF (Goodness of Fit) near 1.0 is therefore an indication of near-perfect match of the observed and the calculated pattern. The calculation of R_B is strongly dependant on the structure model used, because the "observed" Bragg intensity (usually unmeasurable due to overlap) can only be determined by assuming that the Bragg intensities are in the same proportion as their calculated counterparts, although this is optimistic (Barerlocher 1986). The Durbin-Watson (d-) statistic (Flack & Vincent 1980; Hill & Madsen 1986) is a measure of the serial correlation in the profile. Serial correlation is the correlation between values (observations) taken in succession. There is no serial correlation between independent observations. In Rietveld method, the observed intensity at each step is taken as an independent observation. According to equation 2-31, the standard deviations approach zero when the number of steps, N, in the powder pattern approaches infinity (the step-width becomes infinitely small). This is in contrast to reality. In the diffraction experiment, the independent observations consist of the possible reflections. There are only finite number of reflections in a given 2θ range, and hence there is a lower limit of precision in error estimation of the least-squares process. This also sets a limit for the step size in the powder intensity-data collection such that each step remains an independent observation. To assess weather a specific actual step-size is smaller than the limit, the d statistic (Hill & Flack 1987) can be used:

$$d = \sum_{i=2}^{N} \frac{(\Delta_i/\sigma_i - \Delta_{i-1}/\sigma_{i-1})^2}{\sum_{i=1}^{N} (\Delta_i/\sigma_i)^2} \qquad \text{2-38}$$

where Δ_i/σ_i is the weighted residual of the least squares corresponding to the *i*th element (variable). When d deviates significantly from 2, it signifies that there is serial correlation in the data set, and that the step width may be too small.

2.7. Examples of Rietveld Refinement

2.7.1. Single-phase Rietveld Study of Simple Mineral Structures using X-ray

Diffraction Data

When the Rietveld method was introduced to X-ray powder diffraction (Young *et al.* 1977), the method was tested with quartz (SiO_2) and synthetic fluorapatite ($Ca_5(PO_4)_3F$). Most of the atomic positional parameters were within 2σ (σ being the estimated standard deviation) of the corresponding values from single-crystal studies, despite the use of a simple Gaussian peak-shape function. Studies with more sophisticated peak-shape functions (Thompson & Wood 1983), in which quartz and berlinite ($AlPO_4$) were studied, showed that while the atomic positions were refined to a level of accuracy compatible with their precision, the displacement factors were too large. Similar study of more complex structures (of olivine (Mg_2SiO_4)-related $Ni_3(PO_4)_2$; Nord & Stefanidis 1983) showed deviation of atomic positions as large as 5σ, and negative displacement factors. However, more recent studies of olivine, corundum (Al_2O_3) and plattnerite (β-PbO_2) (Hill & Madsen 1984) reported good agreement between Rietveld and single-crystal results. Rietveld refinement of platy minerals (*e.g.*, muscovite ($KAl_2AlSi_3O_{10}(OH)_2$), Sato *et al.* 1981) was less satisfactory. Deviations in interatomic distances as large as 0.27 Å were reported, and preferred orientation of the sample was attributed as the cause of the error.

2.7.2. Characterizing mineral-synthesis products

The Rietveld method has proven effective in characterizing very fine-grained products of mineral synthesis. The method was advocated as such by Hawthorne *et al.* (1984) and Raudsepp *et al.* (1984). Cation ordering and the M-site occupancies in the synthetic amphiboles and pyroxenes were characterized. The same procedure was extended to more complex systems of other synthetic amphiboles (Raudsepp *et al.* 1987a,b). Subsequent work characterized two solid-solution series of clinopyroxene: the diopside ($CaMgSi_2O_6$)-hedenbergite ($CaFeSi_2O_6$) join and the diopside-$CaNiSi_2O_6$ join (Raudsepp *et al.* 1990a,b). In these studies, the cation-site occupancies and the bulk compositions were determined. It is interesting that the work showed, through half-normal probability analysis, that the esd's were still underestimated by a factor of ~ 1.6, even after the correction, C_{esd}, suggested by Bérar & Lelann (1991):

$$C_{esd}=R'/R \qquad 2\text{-}39$$

in which R is the difference that Rietveld method tries to minimize (see equation 2-28). R′ is a modified difference that takes into account of serial correlation in the refinement:

$$R' = [\sum (1 - z_i^2)\, a_i^2] + [\sum (\sum z_i\, a_i)^2]$$

$$a_i = w_i^{-1/2}(I_{calc.} - I_{obs.}) \qquad 2\text{-}40$$

$$z_i = \frac{[2(a_i^2 + a_{i-1}^2)]^{1/2}}{2+[2a_i^2 + a_{i-1}^2]^{1/2}} \quad or \quad z_i = 0$$

There are two explanations for such underestimation; (1) the step width was too small (see discussion in 2.6); (2) there may be systematic contribution of error to the profile difference ($I_{calc.}$ - $I_{obs.}$, see equation 2-31). Effect (2) may be subtle, but is quite common in difficult refinements. For instance, if the integrated intensity of a Bragg reflection is overestimated (where structure factors are off the correct values du to the badly adjusted structural parameters), $I_{calc.}$ will tend to exceed $I_{obs.}$ over a large angular range centred on that reflection, depending on the range one chooses to consider on either side of a step in the diffraction pattern in the calculation.

Characterizing synthetic zeolites is another very active field of Rietveld refinement. The refinement of zeolite ZK-14 ($Ca_2Al_4Si_8O_{24}$) at different temperatures (Cartlidge & Meier 1984) is an example. There were 57 structural parameters, and soft constraints on T-O distances and O-T-O angles were initially applied, and then successfully removed for the room-temperature data at the end of the refinement. Reasonable bond-distances were obtained, although the displacement factors were too large.

2.7.3. Natural Zeolite and Clay Minerals

McCusker *et al.* (1985) refined the structure of gobbinsite ($Na_4(Ca,Mg,K_2)\ Al_6Si_{10}O_{32}\bullet 12H_2O$) using 64 structure parameters and 50 soft constraints on bond distances and angles. The results were satisfactory if soft constraints were used, but unreasonable bond distances resulted when such constraints were not used.

Structure refinement of kaolinite ($Al_4Si_4O_{10}(OH)_8$) was considered to be either pressing the limits (Young 1988) or beyond the limits (Thompson *et al.* 1989) of the Rietveld method. Suitch & Young (1983) and Young & Hewat (1988) both obtained unreasonable bond-distances. Bish & Von Dreele (1989) did a Rietveld refinement on the same material using X-ray diffraction data. Soft distance constraints were applied to the bond distances initially, and were lifted successfully in the final cycles of refinement. Reasonable bond-distances resulted. The same procedure was applied to the neutron diffraction data of Young & Hewat (1988) and met similar success (Bish 1993). As a result, both non-H atom and H-atom positions were determined. It is apparent that false-minima problem can be important in such work.

2.8. Multi-phase Rietveld Refinement

The Rietveld method can include more than one phase in the refinement. It is typical to refine the structure of the major phase while keeping the structure of the minor phase fixed (*e.g.*, Bish & Von Dreele 1989; Raudsepp *et al.* 1990a). The other use of multi-phase Rietveld refinement is to determine the modal amount of individual phases in a mixture from the Rietveld scale-factors (*e.g.* Hill & Howard 1987).

2.8.1. Structure Refinement of Powder Mixtures

In the refinement of the kaolinite structure (Bish & Von Dreele 1989), a minor amount of dickite ($Al_4Si_4O_{10}(OH)_8$) was detected in the powder pattern by inspecting the residual after single-phase refinement of kaolinite. Dickite was then included in the refinement as a second phase, with variable cell-dimensions and fixed atomic positions. The overall fit of the calculated pattern to the observed was significantly improved.

The work of Raudsepp *et al.* (1990a) focuses on another problem in mineral synthesis, the problem of characterizing a synthetic product which cannot be made pure. In two of their synthetic samples, there was up to ~ 8% ferrobustamite ($FeSiO_3$) in addition to the host clinopyroxene ($(Ni,Ca,Mg,Fe)_2Si_2O_6$). Two-phase refinement was used, and the scale factor and site occupancies of ferrobustamite were allowed to vary (the atomic positions were fixed at single-crystal values); there was a significant drop in R_{wp} from 12.1% in the single-phase (clinopyroxene only) refinement to 8.0% in the two-phase refinement.

2.8.2. Determination of Modal Amounts of Phases in Mixtures

The modal amount of a phase in a mixture can be calculated (Hill & Howard 1987) as

$$W_p = \frac{S_p(ZMV)_p}{\sum_i S_i(ZMV)_i}, \qquad 2\text{-}38$$

in which W_p is the weight percent of phase *p*, *S*, *Z*, *M* and *V* are the scale factor, the number of unit formula in the unit cell, the mass of the unit formula, and the volume of the unit cell, respectively.

Bish & Post (1988) used the Rietveld method to calculate the modal amount of the component phases in artificial mixtures of minerals. The binary 1:1 mixtures include quartz(SiO_2) - corundum(Al_2O_3), clinoptiolite($(Na,K)_6[Al_6Si_{30}O_{72}]\cdot 24H_2O$) - corundum, hematite($Fe_2O_3$) - corundum and biotite($K_2(Mg,Fe^{2+})_{6-5}(Al,Fe^{3+})_{0-1}(Al,Si)_8O2_{20}(OH,F)_4$) - corundum. For the first two mixtures, good modal values (absolute error of 0.2 wt%) were determined, with reasonable R_{wp} values of 18.8% and 14.9% for the quartz-corundum & clinoptilolite-corundum mixtures, respectively (R_{EXP} for all four binary mixtures are under or close to 10%). The biotite-corundum mixture presented the problem of preferred orientation, which produced an error of 2.5% absolute in the calculated modal amount, and an R_{wp} of 32.2%. The mixture of hematite-corundum presents another problem for Rietveld analysis when analyzing mixtures with one component having a much higher linear X-ray absorption coefficient than the other phase(s): hematite has a greater linear absorption coefficient than corundum, and this caused an underestimation of its modal amount by 6%.

2.9. Summary

Rietveld technique is a powerful powder-diffraction method for extracting structural information from the powder-diffraction pattern through least-square refinement of step-scan intensity data. Proper modelling of profile shape is of vital importance in this process.

The Rietveld method has been successful in refining crystal structures of various levels of difficulty. However, further development needs to be done in the following areas: (1) evaluating the reliability of the Rietveld refinement, in determining both structural parameters and modal amounts; (2) devising methods to deal with micaceous materials that tend to show strong preferred orientation during sample preparation; (3) avoiding false minima.

Chapter 3

Reliability Study of the Rietveld Method

The Rietveld method had experienced a rapid growth in its applications, particularly after its development as a technique for crystal-structure-refinement using powder X-ray diffraction data (see Chapter 2). Given such scale of application, the percentage of work dedicated to the study of precision and accuracy of the Rietveld method (Raudsepp *et al.* 1990a) is surprisingly small. Such study is especially important in establishing the validity of crystal-chemical information derived from mineral synthesis. It is also very important in establishing correct perceptions of the Rietveld method in the mineralogical community.

3.1. Olivine, Pyroxene and Their Binary Mixtures

Olivine [$(Mg,Fe)_2(SiO_4)$] and pyroxene [$(M2)(M1)(Si,Al,Fe^{3+})_2O_6$], M2 = Mg^{2+}, Fe^{2+}, Mn^{2+}, Li^{+}, Ca^{2+}, Na^{+}, M1 = Mg^{2+}, Fe^{2+}, Mn^{2+}, Al^{3+}, Fe^{3+}, Ti^{4+}, Cr^{3+}, V^{3+}, Ti^{3+}, Zr^{4+}, Sc^{3+}, Zn^{2+}, are important rock-forming minerals that have crystal structure of moderate complexity. Olivine does not have cleavage, which offers the advantage of giving diffraction patterns without intensity distortion due to preferred orientation of the sample. Pyroxene shows good columnar cleavage, which, when other aspects of Rietveld refinement are in check, will provide a basis to assess the techniques (including sample preparation and diffraction-intensity correction) for minimizing the preferred orientation effect. Besides, both olivine and pyroxene represent solid solution series, *i.e.*, structures in which a cation site may be shared by more than one cation species (e.g. Mg and Fe in olivine). The natural samples selected in the study do show such solid solution phenomena, and testing the ability of correctly determining cation ratios of the same site using the Rietveld method is also one of the purposes of the study. The fact that olivine and pyroxenes are usually well crystallized makes parallel single-crystal study possible, which will provide a basis for comparison.

Accurate determination of model distribution of two or more coexisting crystalline phases are of interest to both observational and experimental mineralogy. Rietveld method has the intrinsic capability of determining such modal distribution. By artificially mixing the two pure phases of olivine and pyroxene in different proportion, the accuracy of determination of modal distribution can be assessed.

3.1.1. Experimental

An olivine separate was produced by magnetic separation and hand picking from a dunite (volcanic bomb) from Hawaii, U.S.A. The pyroxene sample is from Laurel, Argenteuil Co., Quebec. It is a diopside and occurs intimately mixed with calcite; euhedral pyroxene crystals were easily detached, crushed and washed in dilute HCl to remove calcite impurities. The samples were ground in alcohol to less than 10 μm using an automated grinder. Binary mixtures of olivine and pyroxene were prepared at 10 wt% intervals. The mixtures were mixed by griding in alcohol to ensure thorough mixing.

Electron-microprobe analysis

Crystals of olivine and pyroxene were analyzed by electron microprobe using a CAMECA SX-50 operating in the wavelength-dispersion mode. Back-scattered electron images showed no discernible zoning in either mineral. Quantitative analysis was done in wavelength-dispersion mode with a beam diameter of 5 μm and an accelerating potential of 15 kV. A sample current of 20 nA measured on a Faraday cup and a counting time of 20 s were used for Na, Ca, Mg, Al, Fe, Ti, and Si, and 50 s at 40 nA for Cr, Mn, and Ni. The following standards were used: albite (Na$K\alpha$), fayalite (Fe$K\alpha$), diopside (Ca$K\alpha$, Si$K\alpha$), kyanite (Al$K\alpha$), olivine (Mg$K\alpha$), spessartine (Mn$K\alpha$), titanite (Ti$K\alpha$), and Ni_2Si

($NiK\alpha$). The data were reduced using the PAP routine of Pouchou & Pichoir (1985).

Mean compositions and unit formulae are given in Table 3-1-1.

Collection of X-ray powder-diffraction intensity data

Powder sample was mounted in an aluminum sample holder with 20 × 15 × 1.6 mm rectangular cavity. With a 1° divergent slit, the irradiated area was confined to the sample at 2θ angles greater than 19°. Samples were loaded from the back of the sample holder against a frosted glass slide. Upon removing the frosted glass slide, the sample surfaces were finely serrated with a razor blade. This technique tends to minimize preferred orientation of the powder sample due to cleavage or anisotropic morphology of a mineral.

A Philips 1710 powder diffractometer was used in the collection of the X-ray intensity data. The instrument uses a PW1050 Bragg-Brentano goniometer equipped with incident- and diffracted-beam Soller slits, 1° divergence and anti-scatter slits, a 0.2-mm receiving slit and a curved graphite diffracted-beam monochromator. The normal-focus Cu X-ray tube was operated at 40 kV and 40 mA, using a take-off angle of 6°. The profiles were taken with step increment of 0.05° 2θ. For the 1:1 mixture, intensity data were also collected with a step width of 0.01° 2θ to examine the effect of step-width variation on the results of the refinement. The count time at each step was between 2–3 s, with a maximum intensity of 2,000–3,000 counts. Other experimental details are given in Table 3-1-2. The sample-related parameters (*e.g.* U, V, W, given the same instrumental set up) for the same phase in the mixture samples (*e.g.* olivine) vary substantially from sample

TABLE 3-1-1. CHEMICAL COMPOSITIONS (WT%) AND UNIT FORMULAE OF OLIVINE AND PYROXENE

	Olivine	Diopside
SiO_2	39.47	53.04
Al_2O_3	0.02	1.84
TiO2	0.01	0.10
Cr2O3	0.02	0.02
FeO	11.36	1.28
MnO	0.19	0.04
NiO	0.36	0.03
MgO	47.51	17.84
CaO	0.20	25.58
Na_2O		0.05
	-----	-----
Total	99.14	99.82
	-----	-----
Si	0.987	1.932
Al	0.001	0.079
Ti	-	0.003
Cr	-	0.001
Fe	0.237	0.039
Mn	0.004	0.001
Ni	0.007	0.001
Mg	1.770	0.969
Ca	0.005	0.999
Na	-	0.004
O	4	6

to sample. This is probable due to the high correlation among these parameters themselves and between these parameters and the background parameters.

Rietveld structure-refinement

Structures were refined using the program LHPM1 [originally written as DBW3.2 by Wiles & Young (1981) and modified by Hill & Howard (1986)]. A pseudo-Voigt peak-shape was used (with variable-percentage Lorentzian-character), the FWHM (Full peak-Width at Half-Maximum height) was varied as a function of 2θ using the expression of Caglioti *et al.* (1958), and the peak asymmetry was corrected using the function of Rietveld (1969). Structural variables included atomic coordinates, M-site occupancies, and an overall isotropic displacement factor; non-structural variables were scale factor(s) and parameters for background correction, peak shape and asymmetry, and a preferred-orientation correction. Single-phase refinements of olivine and pyroxene were done as a measure of the optimal agreement to be expected between the Rietveld and single-crystal refinements. Individual isotropic-displacement parameters were fixed at 'reasonable' values (*i.e.*, the relative sizes of the parameters were taken from single-crystal work on analogous crystals) and an overall displacement parameter was refined to scale the individual values. Those site occupancies taken as variable were refined without constraints of any sort. Refinement was terminated when the maximum parameter shift/error was less than 0.01.

For refinement of the mixtures, there were 58 variable parameters. Otherwise, refinement was similar to the single-phase refinements except for the presence of two structures and two scale factors. Again, refinement was terminated when the maximum

TABLE 3-1-2. DETAILS OF STRUCTURE REFINEMENT WITH POWDER X-RAY DATA

		Olivine	Pyroxene	P1	P2	P3	P4	P5	P6	P7	P8	P9
2Θ scan range(°2Θ)		16-136	18-138	16-136	16-136	19-139	19-139	19-139	16-136	16-136	19-139	19-139
* SF	olivine	13.71(25)		1.15(14)	2.37(16)	3.67(14)	7.56(21)	10.59(28)	11.45(25)	18.1(4)	22.0(4)	19.3(3)
	pyroxene		6.21(14)	5.21(7)	4.67(7)	3.60(6)	5.36(6)	4.88(9)	3.77(7)	3.74(11)	2.71(7)	1.21(7)
+ N-p		1111	2367	2343	2343	2343	2343	2343	2343	2343	2344	2344
R_p(%)		8.72	9.31	9.41	9.42	9.65	7.06	7.49	7.58	8.00	6.67	7.15
R_{wp}		11.87	12.91	12.45	12.44	13.00	9.63	10.25	10.10	13.75	8.79	9.78
R_B	olivine	3.74		4.05	3.59	3.80	2.45	2.83	2.85	2.97	3.12	2.62
	pyroxene		3.59	4.48	4.85	4.42	2.54	3.68	3.49	6.26	2.95	2.43
** D-W		1.259	1.189	0.855	1.078	1.245	1.383	1.321	1.202	2.038	1.040	1.212
u	olivine	-0.011		0.01	0.01	-0.003	0.011	0.007	0.006	0.028	0.023	0.003
	pyroxene		0.008	0.025	0.042	0.046	0.015	-0.012	0.012	0.004	0.06	0.003
v	olivine	0.022		-0.01	0.03	0.012	0.014	0.013	-0.001	-0.040	-0.037	-0.002
	pyroxene		0.002	-0.002	-0.042	-0.041	0.007	0.050	0.006	0.03	-0.07	0.16
w	olivine	0.060		0.086	0.059	0.060	0.076	0.052	0.063	0.083	0.116	0.090
	pyroxene		0.043	0.069	0.081	0.013	0.070	0.041	0.058	0.056	0.112	0.06
γ_1	olivine	0.32		-0.57	0.06	0.21	0.12	0.29	0.23	0.24	0.11	0.10
	pyroxene		0.047	0.26	0.19	0.31	0.22	0.33	0.27	0.27	0.21	0.27
γ_2	olivine	0.0068		0.021	0.009	0.010	0.0080	0.0077	0.0083	0.0080	0.0079	0.0092
	pyroxene		0.0062	0.0083	0.010	0.0084	0.0090	0.0090	0.0098	0.010	0.0098	0.012

*SF = scale factor ($\times 10^4$)

+N-p = number of observations - number of variables; R_p = R index for pattern, R_{wp} = weighted R index for pattern; R_b = R index for structure (i.e. for the Bragg peaks).

** D-W = Durbin-Watson statistic

shift/error was less than 0.01. Details of structure-refinements are given in Table 3-1-2.

Two additional phases of refinement were done to investigate the effect of two specific factors on the refinement results. The 1:1 mixture was refined at different step intervals from 0.02–0.10° 2θ in order to test whether the step interval has a significant effect on the accuracy of the results (it is known that it has a significant effect on the *precision via* serial correlation). In addition, the mixtures were also refined with all structural parameters for both olivine and pyroxene fixed at their single-crystal values in order to see if there was an interaction between the scale factor and the structural parameters, such that compensating errors in both could give a good fit to the pattern but inaccurate results.

Collection and refinement of single-crystal X-ray intensity data

Single crystals of olivine and pyroxene were ground to spheres and mounted on a Nicolet *R*3*m* automated four-circle diffractometer equipped with a molybdenum-target X-ray tube and a highly oriented graphite crystal monochromator mounted with equatorial geometry. Cell dimensions (Table 3-1-3) were refined from the setting angles of 25 automatically aligned intense reflections. Intensity data were collected according to the procedure of Hawthorne & Groat (1985): the data collection was in θ - 2θ scan mode, using 96 steps with a scan range from [2θ(Mo$K\alpha_1$) - 1]° to [2θ(Mo$K\alpha_2$) - 1]°and a variable scan rate between 4.0 and 29.3°/min depending on the intensity of an initial one second count at the centre of the scan range. Backgrounds were measured for half the scan time at the beginning and end of each scan. Two standard reflections were monitored

TABLE 3-1-3. SINGLE-CRYSTAL X-RAY DIFFRACTION DATA COLLECTION AND REFINEMENT INFORMATION FOR OLIVINE AND DIOPSIDE

	Olivine	Diopside
a(Å)	4.764(1)	9.743(2)
b	10.226(3)	8.916(2)
c	6.004(2)	5.256(1)
β(°)		105.88(1)
V(Å^3)	292.5(1)	439.1(1)
Space group	Pbnm	C2/c
Z	4	4
Crystal Size(mm^3)	0.28×0.31×0.32	0.32×0.26×0.22
Radiation	MoKα	MoKα
Monochromator	Graphite	Graphite
R(azimuthal)%	1.74	1.34
Total no. $\|F\|$	462	649
No. of $\|F\|_{obs}$	458	648
$R_{(observed)}$%	2.4	3.2
$wR_{(observed)}$%	2.8	3.6

$R = \sum(|F|-|F|)/\sum|F|$

$wR = [\sum w(|F|-|F|)^2/\sum wF^2]^{0.5}$, w=1 every 60 measurements to check for stability and consistency of crystal alignment and instrumental drifting. All reflections calculated possible over the asymmetric unit, based on the crystal orientation matrix and unit cell parameters, were examined out to a maximum 2θ of 60°. Eleven strong reflections uniformly distributed with regard to 2θ were measured at 10° intervals of Ψ (the azimuthal angle corresponding to rotation of the crystal about its diffraction vector) from 0 - 350°. The data were used to perform absorption corrections, modeling the crystal shape as triaxial ellipsoids of variable shape and orientation. Intensities were corrected for background, absorption, Lorentz and polarization effects, and reduced to structure factors. Details concerning these procedures are given in Table 3-1-3.

Crystal structures were refined using the SHELXTL-PC system of programs; R indices are of the form given in Table 3-1-3. Full-matrix least-squares refinement converged to R indices of 2–3% for an anisotropic displacement model in which the site occupancies were refined unconstrained.

3.1.2. Results

Cell dimensions are given in Table 3-1-4, positional parameters in Table 3-1-5, site populations in Table 3-1-6 and selected interatomic distances in Table 3-1-7. Structure-factor tables and powder-diffraction step-scan intensities are given in Appendix S-1, 2, and Appendix P-1 to P-21.

Single-crystal refinement

TABLE 3-1-4. REFINED CELL-DIMENSIONS FOR OLIVINE AND PYROXENE

Sample number	Olivine wt%	Olivine				Diopside				
		a(Å)	b(Å)	c(Å)	V(Å^3)	a(Å)	b(Å)	c(Å)	β	V(Å^3)
SC		4.7642(14)	10.2258(28)	6.0045(18)	292.53	9.7429(19)	8.9161(15)	5.2557(10)	105.880(14)	439.14
SPh	100	4.7649(3)	10.2376(6)	5.9986(4)	292.61	9.7476(5)	8.9174(4)	5.2573(3)	105.900(4)	439.49
P1	9.9	4.7673(21)	10.249(4)	5.9996(20)	293.04	9.7501(8)	8.9207(7)	5.2593(4)	105.897(5)	439.94
P2	19.9	4.7659(12)	10.2414(20)	5.9983(12)	292.75	9.7497(9)	8.9189(7)	5.2576(4)	105.903(5)	439.68
P3	30.6	4.7654(4)	10.2396(13)	5.9984(8)	292.66	9.7489(9)	8.9181(8)	5.2574(5)	105.888(6)	439.62
P4	39.7	4.7652(4)	10.2388(8)	5.9992(5)	292.68	9.7489(7)	8.9184(6)	5.2577(3)	105.896(5)	439.65
P5	49.9	4.7651(4)	10.2385(8)	5.9983(5)	292.61	9.7485(8)	8.9179(7)	5.2566(4)	105.894(6)	439.52
P6	59.9	4.7644(3)	10.2370(6)	5.9975(4)	292.52	9.7464(9)	8.9163(8)	5.2562(5)	105.897(7)	439.60
P7	70.0	4.7649(4)	10.2370(7)	5.9980(4)	292.58	9.7493(14)	8.9142(12)	5.2564(8)	105.893(11)	439.36
P8	79.9	4.7659(3)	10.2396(6)	5.9993(3)	292.91	9.7498(16)	8.9160(15)	5.2586(9)	105.872(13)	439.70
P9	89.6	4.7660(3)	10.2379(5)	5.9992(3)	292.82	9.747(4)	8.914(3)	5.2590(24)	105.90(3)	439.46

SC: Single Crystal; SPh: Single Phase.

TABLE 3-1-5. ATOMIC POSITIONS FOR OLIVINE AND DIOPSIDE

		SC	SPh	P1	P2	P3	P4	P5	P6	P7	P8	P9
						Olivine						
M(1)	x	0	0	0	0	0	0	0	0	0	0	0
	y	0	0	0	0	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0	0	0	0	0
	B(Å^2)	0.40(1)										
M(2)	x	0.98978(18)	0.9924(12)	0.998(10)	0.990(5)	0.990(10)	0.990(2)	0.988(2)	0.988(1)	0.990(1)	0.990(1)	0.990(1)
	y	0.27774(8)	0.2769(4)	0.273(3)	0.277(2)	0.278(3)	0.278(1)	0.277(1)	0.277(1)	0.277(1)	0.2774(3)	0.2778(4)
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
	B(Å^2)	0.41(2)										
T	x	0.42657(16)	0.4288(9)	0.428(7)	0.420(4)	0.427(6)	0.428(1)	0.427(1)	0.427(1)	0.427(1)	0.428(1)	0.428(1)
	y	0.09441(7)	0.0949(5)	0.107(3)	0.096(2)	0.095(3)	0.095(1)	0.095(1)	0.096(1)	0.095(1)	0.095(4)	0.095(4)
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
	B(Å^2)	0.39(2)										
O(1)	x	0.7666(4)	0.7655(18)	0.782(18)	0.766(8)	0.769(4)	0.768(3)	0.769(3)	0.763(2)	0.765(2)	0.767(2)	0.768(2)
	y	0.0917(19)	0.0896(12)	0.081(8)	0.093(4)	0.095(2)	0.092(2)	0.090(2)	0.091(1)	0.091(1)	0.090(1)	0.089(1)
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
	B(Å^2)	0.50(4)										
O(2)	x	0.2199(4)	0.2197(19)	0.195(16)	0.223(8)	0.207(4)	0.217(3)	0.220(3)	0.216(2)	0.218(2)	0.216(2)	0.217(2)
	y	0.44786(18)	0.4477(12)	0.439(8)	0.443(3)	0.445(3)	0.443(2)	0.445(2)	0.446(1)	0.446(1)	0.446(1)	0.446(1)
	z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
	B(Å^2)	0.48(4)										
O(3)	x	0.27883(28)	0.2784(14)	0.202(12)	0.264(6)	0.276(3)	0.273(3)	0.272(2)	0.275(2)	0.278(2)	0.279(1)	0.278(1)
	y	0.16332(12)	0.1639(8)	0.163(5)	0.167(3)	0.164(2)	0.163(1)	0.163(1)	0.162(1)	0.163(1)	0.162(1)	0.161(1)
	z	0.03370(22)	0.0318(13)	0.166(9)	0.023(5)	0.030(3)	0.032(2)	0.031(2)	0.031(1)	0.032(1)	0.030(1)	0.03291)
	B(Å^2)	0.52(3)										

TABLE 3-1-5 (continue).

	Diopside										
M(1) x	0	0	0	0	0	0	0	0	0	0	0
y	0.90818(14)	0.908(1)	0.906(1)	0.908(1)	0.908(1)	0.907(1)	0.907(1)	0.907(1)	0.907(2)	0.905(2)	0.898(5)
z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
B(Å^2)	0.38(3)										
M(2) x	0	0	0	0	0	0	0	0	0	0	0
y	0.30152(9)	0.301(1)	0.302(1)	0.301(1)	0.302(1)	0.302(1)	0.302(1)	0.300(1)	0.300(1)	0.302(2)	0.299(3)
z	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4	1/4
B(Å^2)	0.67(2)										
T x	0.28645(7)	0.288(5)	0.287(1)	0.288(1)	0.287(1)	0.287(1)	0.288(1)	0.287(1)	0.288(1)	0.287(1)	0.293(1)
y	0.09328(8)	0.094(1)	0.094(1)	0.094(1)	0.093(1)	0.093(1)	0.094(1)	0.092(1)	0.091(1)	0.092(2)	0.090(3)
z	0.22934(14)	0.230(1)	0.232(1)	0.233(1)	0.231(1)	0.231(1)	0.231(1)	0.234(1)	0.229(2)	0.230(2)	0.234(4)
B(Å^2)	0.42(1)										
O(1) x	0.11533(22)	0.115(1)	0.115(1)	0.113(1)	0.114(1)	0.116(1)	0.115(1)	0.113(1)	0.113(2)	0.111(2)	0.118(5)
y	0.08722(22)	0.088(1)	0.091(1)	0.089(1)	0.089(1)	0.090(1)	0.089(2)	0.090(2)	0.089(3)	0.089(3)	0.080(6)
z	0.14135(36)	0.143(2)	0.138(2)	0.140(2)	0.135(2)	0.140(2)	0.140(2)	0.137(3)	0.136(4)	0.137(5)	0.145(11)
B(Å^2)	0.56(4)										
O(2) x	0.36136(21)	0.363(1)	0.363(1)	0.365(1)	0.365(1)	0.364(1)	0.364(1)	0.366(1)	0.365(3)	0.368(3)	0.366(6)
y	0.25015(23)	0.252(3)	0.250(1)	0.250(1)	0.250(1)	0.250(1)	0.251(1)	0.253(2)	0.251(3)	0.250(3)	0.250(6)
z	0.31912(38)	0.320(2)	0.322(2)	0.321(2)	0.318(2)	0.319(2)	0.321(2)	0.325(3)	0.327(4)	0.327(4)	0.320(9)
B(Å^2)	0.70(4)										
O(3) x	0.35085(20)	0.353(1)	0.352(1)	0.349(1)	0.350(1)	0.352(1)	0.352(2)	0.353(2)	0.353(3)	0.358(3)	0.368(5)
y	0.01806(22)	0.019(1)	0.018(1)	0.020(1)	0.020(1)	0.021(1)	0.019(1)	0.023(2)	0.025(3)	0.021(2)	0.028(6)
z	0.99519(37)	0.999(2)	0.004(2)	0.003(2)	0.998(3)	0.000(2)	0.007(3)	0.005(3)	0.010(5)	0.010(5)	0.023(12)
B(Å^2)	0.62(4)										

TABLE 3-1-6. REFINED M-SITE POPULATIONS FOR OLIVINE AND PYROXENE

	SC	SPh	P1	P2	P3	P4	P5	P6	P7	P8	P9
						Olivine					
M1 Mg	0.904(3)	0.924(7)	0.82(6)	0.854(28)	0.872(14)	0.918(10)	0.902(11)	0.906(7)	0.902(8)	0.910(6)	0.902(6)
Fe	0.096(3)	0.076(7)	0.18(6)	0.146(28)	0.128(14)	0.082(10)	0.098(11)	0.094(7)	0.098(8)	0.090(6)	0.098(6)
M2 Mg	0.912(3)	0.898(6)	0.902(41)	0.900(21)	0.900(13)	0.898(10)	0.902(10)	0.894(7)	0.898(7)	0.900(6)	0.900(6)
Fe	0.088(3)	0.102(6)	0.098(41)	0.100(21)	0.100(13)	0.102(10)	0.098(10)	0.106(7)	0.102(7)	0.100(6)	0.100(6)
						Diopside					
M1 Mg	0.992(4)	0.992(7)	0.984(8)	0.970(8)	0.982(10)	0.948(8)	0.976(11)	0.990(11)	0.992(17)	0.998(20)	0.962(41)
Fe	0.008(4)	0.008(7)	0.016(8)	0.030(8)	0.018(10)	0.052(8)	0.024(11)	0.010(11)	0.008(17)	0.002(20)	0.038(41)
M2 Mg	0.000(38)	0.038(7)	0.016(10)	0.024(10)	0.020(13)	0.040(10)	0.008(13)	0.026(14)	0.022(21)	-0.016(26)	0.04(6)
Fe	0.029(38)	-0.008(7)	0.008(10)	0.006(10)	0.004(13)	-0.012(10)	0.020(13)	0.004(14)	0.008(21)	0.044(26)	0.00(6)

TABLE 3-1-7. SELECTED ATOMIC DISTANCES (Å) IN OLIVINE AND PYROXENE

Sample number	SC	SPh	P1	P2	P3	P4	P5	P6	P7	P8	P9
Olivine (Wt%)			9.9	19.9	30.6	39.9	49.9	59.9	70.0	79.9	89.6
					Olivine						
T-O1	1.620(2)	1.603(6)	1.71(9)	1.65(4)	1.63(3)	1.623(15)	1.626(15)	1.603(11)	1.608(11)	1.620(8)	1.622(7)
T-O2	1.653(2)	1.663(12)	1.82(3)	1.71(5)	1.66(4)	1.698(20)	1.692(20)	1.680(16)	1.677(16)	1.673(11)	1.673(12)
T-O3	1.637(2)	1.647(17)	1.86(4)	1.72(4)	1.659(27)	1.654(12)	1.660(12)	1.645(10)	1.647(10)	1.647(8)	1.638(7)
mean	1.637(1)	1.638(7)	1.80(3)	1.69(2)	1.65(2)	1.658(9)	1.659(9)	1.643(7)	1.644(7)	1.647(5)	1.644(5)
M1-O1	2.090(2)	2.084(14)	2.00(6)	2.10(3)	2.102(16)	2.086(10)	2.077(10)	2.095(8)	2.092(9)	2.081(6)	2.075(6)
M1-O2	2.078(2)	2.079(13)	1.93(5)	2.082(28)	2.124(16)	2.099(10)	2.087(10)	2.094(7)	2.089(9)	2.093(6)	2.089(6)
M1-O3	2.143(2)	2.147(12)	2.18(7)	2.126(18)	2.141(16)	2.126(12)	2.119(10)	2.127(8)	2.138(9)	2.134(6)	2.126(6)
mean	2.104(1)	2.103(8)	2.04(3)	2.103(15)	2.092(9)	2.104(6)	2.094(6)	2.105(4)	2.104(5)	2.103(3)	2.097(3)
M2-O1	2.179(2)	2.201(16)	2.22(8)	2.16(4)	2.14(4)	2.181(17)	2.179(16)	2.187(13)	2.183(14)	2.192(9)	2.200(9)
M2-O2	2.056(2)	2.058(14)	1.94(9)	2.03(4)	2.00(4)	2.007(17)	2.044(18)	2.039(14)	2.039(14)	2.037(10)	2.039(10)
M2-O3a	2.225(2)	2.217(13)	2.23(5)	2.197(27)	2.22(3)	2.217(10)	2.222(10)	2.231(8)	2.228(9)	2.244(6)	2.237(6)
M2-O3b	2.068(2)	2.067(12)	2.05(5)	2.04(4)	2.06(3)	2.073(12)	2.067(12)	2.062(10)	2.061(10)	2.055(8)	2.069(7)
mean	2.132(1)	2.136(7)	2.11(3)	2.107(18)	2.105(18)	2.120(7)	2.128(7)	2.130(6)	2.128(6)	2.132(4)	2.136(4)

TABLE 3-1-7. (continue)

Sample number	SC	SPh	P1	P2	P3	P4	P5	P6	P7	P8	P9
Olivine Wt%			9.9	19.9	30.6	39.9	49.9	59.9	70.0	79.9	89.6
					Pyroxene						
T-O1	1.604(2)	1.617(8)	1.617(9)	1.639(9)	1.623(9)	1.610(8)	1.625(11)	1.632(11)	1.635(18)	1.654(20)	1.64(4)
T-O2	1.588(2)	1.601(10)	1.586(9)	1.589(10)	1.600(11)	1.595(8)	1.595(12)	1.636(13)	1.629(20)	1.626(23)	1.60(5)
T-O3a	1.668(2)	1.659(11)	1.649(10)	1.630(12)	1.648(12)	1.644(11)	1.622(14)	1.626(16)	1.589(23)	1.622(26)	1.59(6)
T-O3b	1.689(2)	1.714(11)	1.715(14)	1.715(12)	1.699(14)	1.731(11)	1.735(15)	1.732(16)	1.776(24)	1.765(26)	1.83(6)
mean	1.637(1)	1.648(5)	1.642(5)	1.643(5)	1.642(6)	1.645(5)	1.644(6)	1.656(7)	1.657(11)	1.667(12)	1.66(26)
M1-O1	2.057(2)	2.064(11)	2.043(9)	2.045(9)	2.027(11)	2.050(8)	2.050(12)	2.033(13)	2.027(20)	2.029(22)	2.09(5)
M1-O2a	2.119(2)	2.118(8)	2.160(12)	2.123(12)	2.139(14)	2.151(12)	2.135(15)	2.141(17)	2.142(26)	2.14(3)	2.14(6)
M1-O2b	2.052(2)	2.031(8)	2.035(10)	2.032(12)	2.023(15)	2.030(12)	2.030(15)	2.009(17)	2.024(26)	2.010(24)	1.96(7)
mean	2.076(1)	2.071(5)	2.079(6)	2.067(6)	2.063(8)	2.077(6)	2.072(8)	2.061(9)	2.070(14)	2.060(15)	2.06(3)
M2-O1	2.364(2)	2.354(10)	2.345(10)	2.355(10)	2.361(12)	2.356(10)	2.360(14)	2.328(16)	2.337(24)	2.337(29)	2.41(6)
M2-O2	2.343(2)	2.338(8)	2.327(9)	2.321(9)	2.335(11)	2.338(8)	2.327(12)	2.306(11)	2.297(19)	2.290(21)	2.32(4)
M2-O3a	2.563(2)	2.557(10)	2.541(10)	2.573(10)	2.570(12)	2.566(9)	2.535(14)	2.580(14)	2.582(14)	2.525(22)	2.53(5)
M2-O3b	2.718(2)	2.712(13)	2.738(12)	2.750(13)	2.722(15)	2.710(12)	2.737(15)	2.723(17)	2.713(26)	2.702(29)	2.66(7)
mean	2.497(1)	2.490(5)	2.488(5)	2.500(5)	2.497(6)	2.492(5)	2.490(7)	2.484(7)	2.482(11)	2.463(13)	2.480(28)

The results of single-crystal structure-refinements agree closely with the results of previous refinements of olivine and calcic pyroxene structures. The refined site-populations (Table 3-1-6) agree almost exactly with the bulk compositions of the crystals as determined by EMPA (electron-microprobe analysis) and SREF (single-crystal site-scattering refinement): olivine: EMPA: $Mg_{1.77}$ $Fe^{*}_{0.25}$ SiO_4; SREF: $Mg_{1.82}$ $Fe_{0.18}$ SiO_4; pyroxene: EMPA: $Ca_{1.00}$ $Mg_{0.97}$ $Fe^{*}_{0.04}$ Si_2 O_6 ; SREF: $Ca_{0.99}$ $Mg_{0.99}$ $Fe_{0.03}$ Si_2 O_6 (Fe^{*} = Fe+Ni+Mn).

Single-phase Rietveld refinements

Figure 3-1-1 shows the observed, calculated and difference X-ray powder-diffraction patterns from each single-phase refinement. As shown in Table 3-1-6, the site populations from the single-phase Rietveld refinements are statistically identical with the values from the single-crystal refinement. The single-crystal and Rietveld positional parameters can be compared using half-normal probability analysis (Abrahams & Keve 1971). If the data sets contain random normal distributions of errors, a half-normal probability plot should be linear of unit slope with zero intercept, provided that the standard deviations are correct. It is known that serial correlation in the powder-diffraction data leads to incorrect standard deviations, a measure of which is the Durbin-Watson statistic (Hill & Flack 1987). This problem was corrected using the procedure of Bérar & Lelann (1991); the assigned standard deviations given in the Tables are the corrected values.

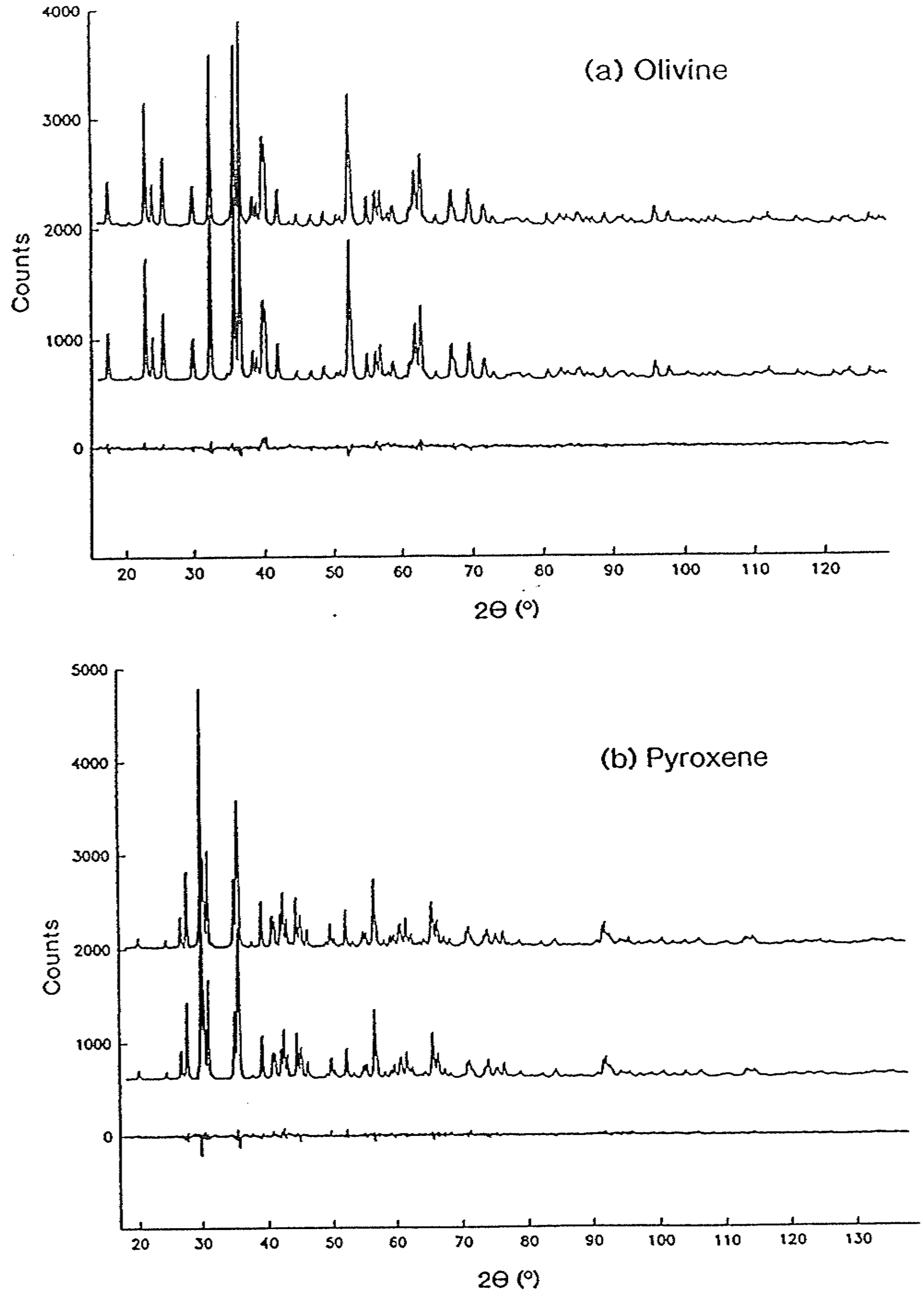

Figure 3-1-1. Observed (upper), calculated (middle) and difference (lower) X-ray powder-diffraction patterns from each single-phase refinement: (a) olivine; (b) pyroxene; the observed and calculated patterns are displaced vertically (by adding 2000 and 600 counts to every data point in each respective pattern) to avoid pattern overlap.

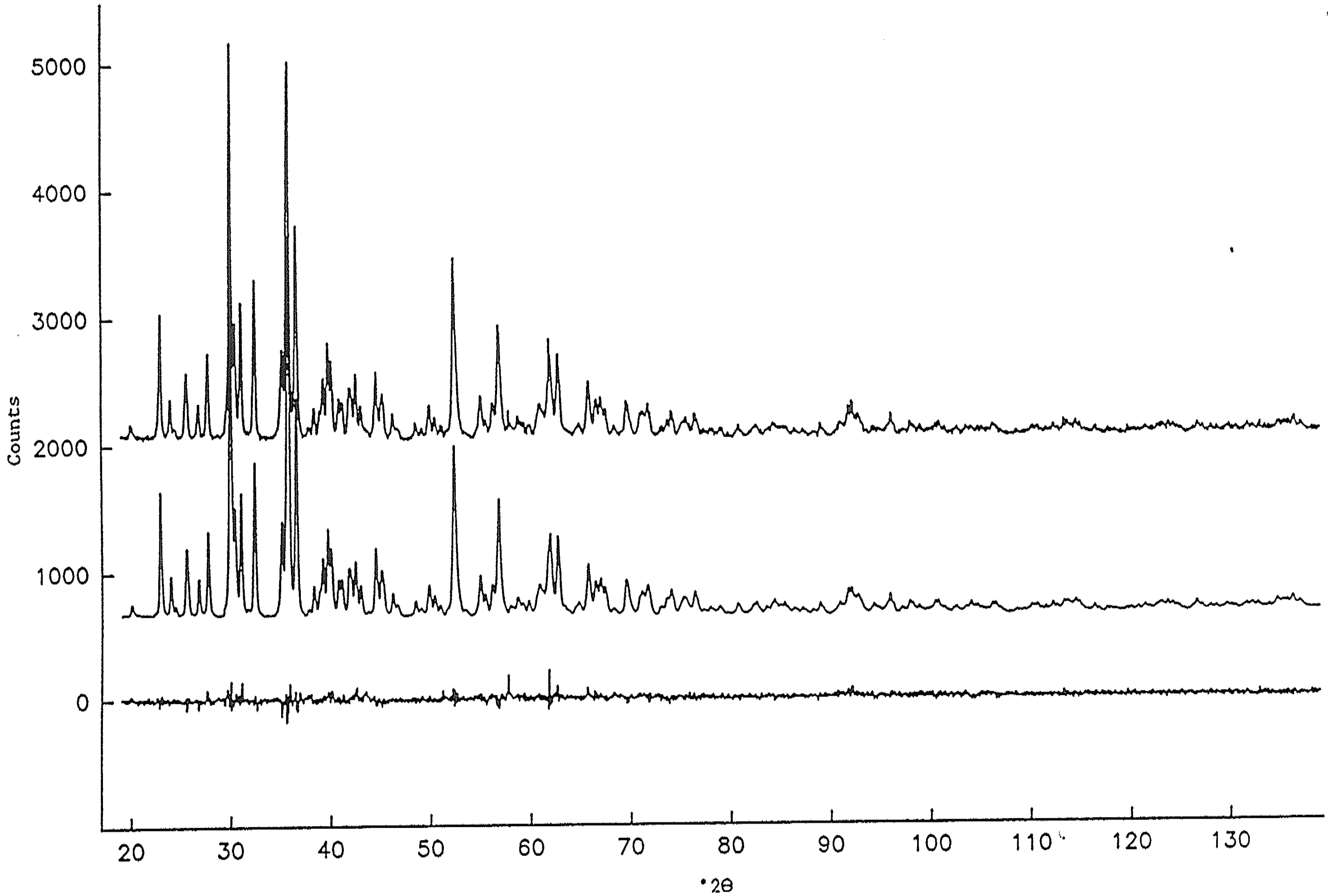

Figure 3.1-2. Typical observed (upper, plus 2000 counts), calculated (middle, plus 600 counts) and difference (lower) X-ray powder-diffraction patterns for a multi-phase refinement of the 50:50 olivine:pyroxene mixture.

Multi-phase Rietveld refinements

Figure 3-1-2 shows a typical observed, calculated and difference X-ray powder-diffraction pattern for a multi-phase refinement. The modal percentages of olivine and pyroxene were calculated from the following equation (Hill & Howard 1987, see also equation 2-18):

$$W_p = \frac{S_p(ZMV)_p}{S_p(ZMV)_p + S_q(ZMV)_q} \qquad 3\text{-}1$$

in which S is the refined scale factor, Z is the number of formula units per unit cell (Z = 4 for both olivine and *C2/m* pyroxene), M is the mass of the formula unit, and V is the unit-cell volume; p and q represent the phases in the mixture. The values for M and V were those determined from the multi-phase refinements, thus simulating the normal experimental situation in which M and V are determined from the refinement that also determines the values of S. The standard deviation of W_p was calculated by the equation:

$$\sigma_{W_p} = \sqrt{\left(\frac{\partial W_p}{\partial S_p} \cdot \sigma_{S_p}\right)^2 + \left(\frac{\partial W_p}{\partial V_p} \cdot \sigma_{V_p}\right)^2 + \left(\frac{\partial W_p}{\partial S_q} \cdot \sigma_{S_q}\right)^2 + \left(\frac{\partial W_p}{\partial V_q} \cdot \sigma_{V_q}\right)^2}$$

$$= \frac{(ZM)_p \cdot (ZM)_q}{[\,(SZMV)_p + (SZMV)_q\,]^2} \cdot \qquad 3\text{-}2$$

$$\sqrt{V_p^2 \cdot (SV)_q^2 \cdot \sigma_{S_p^2} + S_p^2 \cdot S_q^2 \cdot V_q^2 \cdot \sigma_{V_p^2} + S_p^2 \cdot V_p^2 \cdot V_q^2 \cdot \sigma_{S_q^2} + S_p^2 \cdot V_p^2 \cdot S_q^2 \cdot \sigma_{V_q^2}}$$

$$\approx \frac{(ZM)_p \cdot (ZM)_q}{[\,(SZMV)_p + (SZMV)_q]^2} \cdot \sqrt{V_p^2 \cdot (SV)_q^2 \cdot \sigma_{S_p^2} + S_p^2 \cdot V_p^2 \cdot V_q^2 \cdot \sigma_{S_q^2}}$$

Table 3-1-8 shows the calculated modal proportions.

3.1.3. Discussion

Modal proportions

A graphical comparison of the refined and known modal proportion of olivine is given in Figure 3-1-3; the refined modal proportions agree with the known values within the estimated standard deviations. The mean value of the absolute accuracy across all compositions is 0.9%; the relative value is 2.3% (omitting the sample lowest in olivine) and 3.0% for all mixtures. Thus the refined modal proportions are accurate to within their assigned level of precision.

The modal proportions were also derived by refinement with fixed structural and instrumental parameters (derived from the single-phase Rietveld refinements), and with fixed structural and variable instrumental parameters. The modal proportions calculated were very similar to the full-refinement results, with mean absolute deviations of 0.7 and 0.9%, respectively, compared to the full-refinement value of 0.9% absolute.

Effect of step width on modal values

Table 3-1-9 and Figure 3-1-3 show the variation in refined modal proportion of olivine for the 1:1 mixture as a function of step width from 0.02–0.10° 2θ. The refined values (by all three different methods) do not vary significantly with step width; accurate values are obtained up to a step width of 0.1° 2θ. Of course, the normally assigned standard deviations increase with increasing step-width (because of decreasing serial correlation); however, the variation disappears with correction *via* the method of Bérar & Lelann (1991).

TABLE 3-1-8 MODAL AMOUNT OF OLIVINE (WT%) IN THE OLIVINE-PYROXENE MIXTURES BY RIETVELD REFINEMENT

		P1	P2	P3	P4	P5	P6	P7	P8	P9
Refined	* (1)	9.3(3)	19.7(3)	33.8(4)	39.8(4)	50.5(5)	59.4(6)	69.6(9)	80.0(14)	90.3(15)
	(2)	8.8(3)	19.2(4)	33.8(5)	39.5(5)	49.8(7)	59.3(8)	69.2(9)	79.5(11)	88.3(13)
	(3)	9.1(6)	18.7(7)	31.7(10)	39.1(10)	49.7(15)	58.0(16)	68.8(25)	78.7(22)	89.9(28)
Actual		9.9	19.9	30.6	39.9	49.9	59.9	70.0	79.9	89.6

*(1) Background and scale factor only refined; structural parameters fixed at single-crystal values, instrumental parameters fixed at single-phase refinement values.
(2) Background, scale factor and instrumental parameters refined; structural parameters fixed at single-crystal values.
(3) Full multi-phase refinement with all possible variable parameters refined.

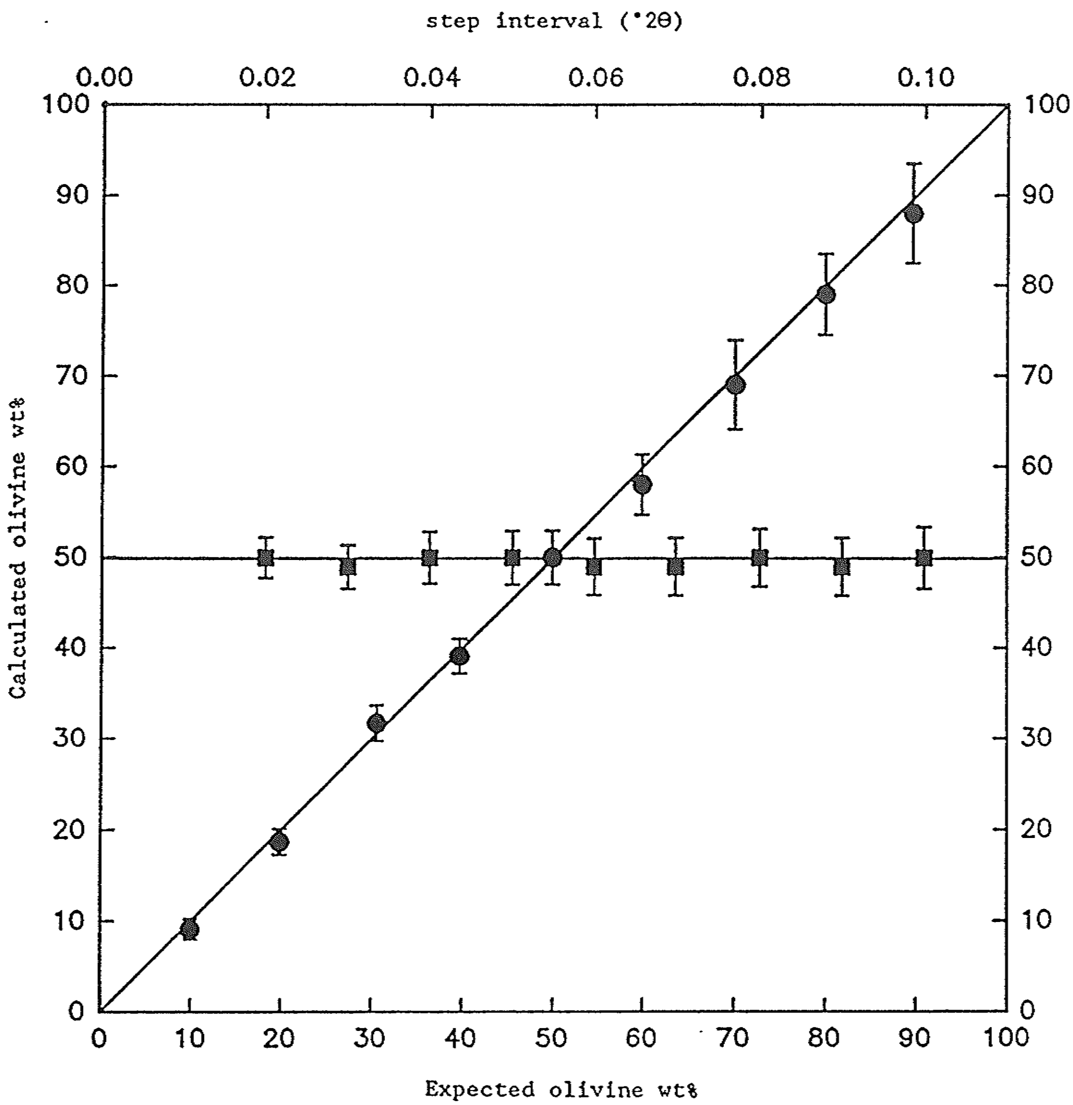

Figure 3-1-3. Modal proportion of olivine derived from Rietveld structure refinement compared with the known modal proportions (full circles), and values for the 1:1 mixture (full squares) as a function of step width; the diagonal line is drawn through zero with a slope of 1; the horizontal line is drawn through 50% olivine with a slope of 0.

TABLE 3-1-9. MODAL AMOUNT OF OLIVINE (WT%) IN THE 1:1 OLIVINE-PYROXENE MIXTURE BY THE RIETVELD REFINEMENT FOR DIFFERENT STEP WIDTHS.

		SW1	SW2	SW3	SW4	SW5	SW6	SW7	SW8	SW9
	*(1)	49.4(4)	50.5(5)	50.2(6)	50.0(5)	49.9(5)	49.9(6)	50.0(6)	49.7(6)	50.6(6)
Refined	(2)	49.6(6)	50.7(7)	50.0(7)	49.8(7)	49.9(7)	49.8(7)	49.6(7)	49.4(7)	49.9(8)
	(3)	49.8(11)	49.4(12)	49.6(14)	49.7(15)	49.4(15)	49.4(16)	49.9(16)	49.3(16)	50.1(17)
actual		49.9	49.9	49.9	49.9	49.9	49.9	49.9	49.9	49.9

* (1) Background and scale factor only refined; structural parameters fixed at single-crystal values, instrumental parameters fixed at single-phase refinement values.
(2) Background, scale factor and instrumental parameters refined; structural parameters fixed at single-crystal values.
(3) Full multi-phase refinement with all possible variable parameters refined.

Cell dimensions

The cell dimensions from the single-crystal refinements and the single- and multi-phase Rietveld refinements are shown in Table 3-1-4. The values obtained from the single- and multi-phase Rietveld refinements are fairly consistent. Where the phase is minor (*i.e.*, 10% of the mixture), the actual values can differ more from the mean value than the rest of the values (*e.g.*, *b* for olivine in sample P1, *a* for pyroxene in sample P9); however, the assigned standard deviations are also significantly larger in these cases, and these larger discrepancies are actually not significant (*i.e.*, $< 2.5\sigma$). There are significant differences between the powder- and single-crystal cell dimensions. In particular, *b* for olivine is ~ 0.012 Å longer for the Rietveld determinations, a difference of approximately four pooled standard deviations. It has been observed here and in previous work of this lab that single-crystal cell dimensions and bond-lengths do tend to be slightly shorter than corresponding powder-diffraction measurements. Given similar control over both sample- (*e.g.* sample-related asymmetry) and instrumental- (*e.g.* Lorentz-Polarization) related effects, Rietveld method gives more accurate cell dimensions because of the fact that, in powder diffraction, only one circle (θ - 2θ) is involved in the data-collection, whereas in single-crystal diffraction experiment, four-circles are involved. The potential for misalignment (hence the inaccuracy) is larger in single-crystal experiment. It is true that, in powder diffraction experiment that there are extra instrument-related effects (*e.g.* displacement of sample surface from the focusing circle, flat sample, and sample transparency) that may affect the accuracy in determining the cell-dimensions. However, these effects had been understood well (Klugg & Alexander 1971) and can be effectively corrected using analytical functions.

Cell dimensions for the 1:1 mixture (sample P5) were measured at a series of step widths from 0.02 to 0.10° 2θ. The values obtained were found to be independent of step width in this interval. Of course, as the step width approaches the peak width, information is rapidly lost, and the refinement degrades. However, when the step width is significantly narrower than the peak width, the refinement results are not sensitive to step width. This information is useful in optimizing data-collection efficiency.

Site populations and bulk compositions

Site populations are listed in Table 3-1-6. For the olivine, there are no significant differences between the values from the single-crystal and the single-phase Rietveld refinements. Where olivine is a minor phase (*i.e.*, 10% as in P1), there can be large differences between the actual value (as determined by all of the other refinements) and the refined value; the most notable case is for Mg at M1 in mixture P1 (Table 3-1-6), in which the relevant values are ~0.90(6) and 0.82(8). However, although the difference is large, so are the assigned standard deviations, and the value is accurate although very imprecise. With similar amounts of both phases, both accuracy and precision are good. The situation is similar for pyroxene, although the deviations at low amounts of the phase are actually less than for olivine. Because there are three scattering species (Ca,Fe,Mg) potentially occupying the M2 site in pyroxene, the site populations cannot be determined just from structure-refinement (Hawthorne 1983b). However, as the Ca content (of M2) is known from the electron-microprobe analysis, its value can be fixed while refining the Mg and Fe contents of M2. The agreement across the complete set of data is good (Table 3-1-6). Thus for both olivine and pyroxene, the site occupancies can be accurately determined, but attention must be paid to the variation in the magnitude of the standard deviations, which vary significantly with the modal proportion of each phase.

Atomic positions and interatomic distances

The half-normal probability analysis of the Rietveld and single-crystal results for the atomic positions in the olivine (Fig. 3-1-4a) shows a nearly linear distribution with zero intercept and a slope of 1.3 (as compared to the ideal value of 1.0). The linearity shows that there is no systematic difference between the Rietveld and the single-crystal refinements, but the slope of about 1.3 indicates that the standard deviations in the Rietveld refinement are still slightly underestimated (by a factor of 1.3) even after correction for serial correlation. For the pyroxene (Fig. 3-1-4b), the distribution is slightly nonlinear with a small non-zero intercept, indicative of some error. However, omission of the two largest deviations does result in a linear distribution with zero intercept, and a slope similar to that for the olivine, indicating that two of the refined parameters (x coordinates at the T and the O3 sites) are in error.

Different sets of refinement of the same phase can more easily be compared using the interatomic distances. For the olivine, there is very good agreement between the important bond-lengths determined by single-crystal refinement and by single-phase

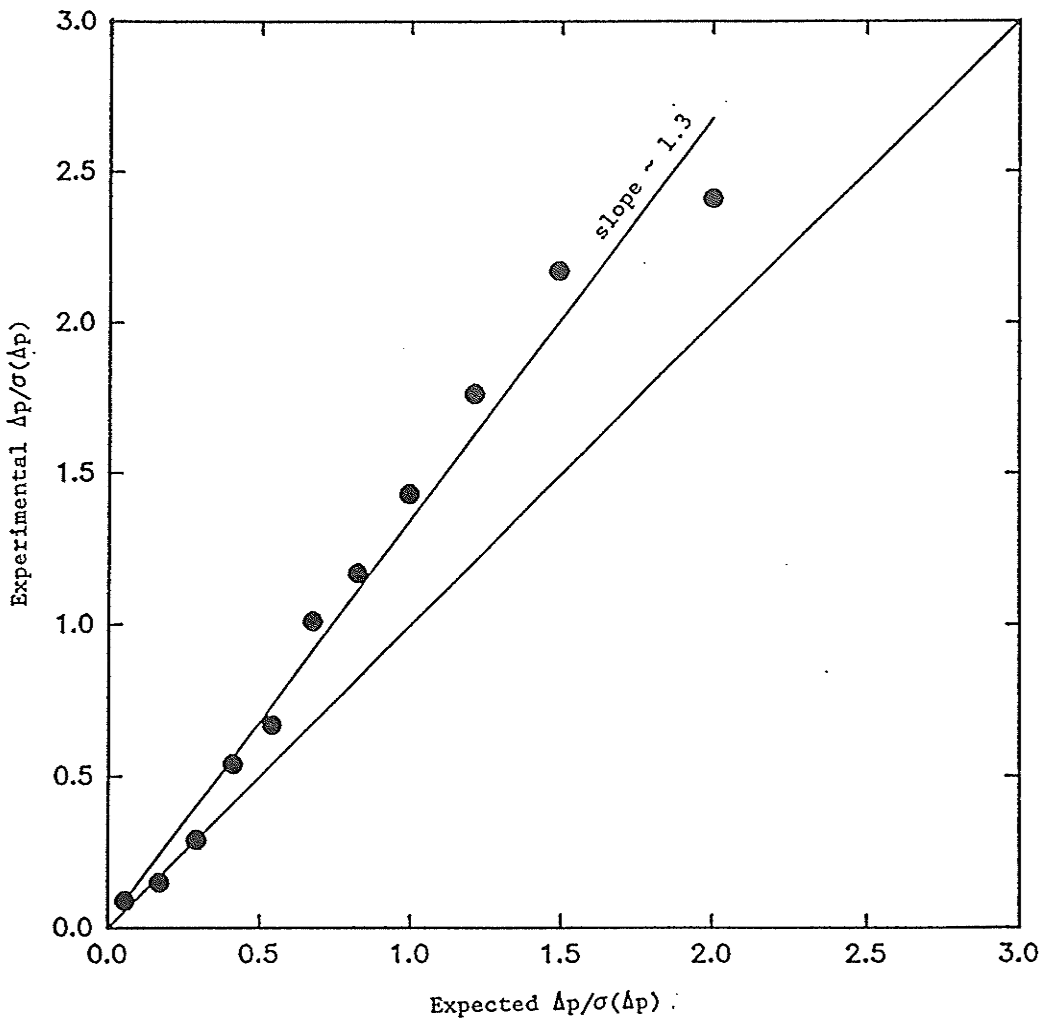

Figure 3-1-4. Half-normal probability plots for the atomic positions derived from single-crystal and single-phase Rietveld refinements: (a) olivine

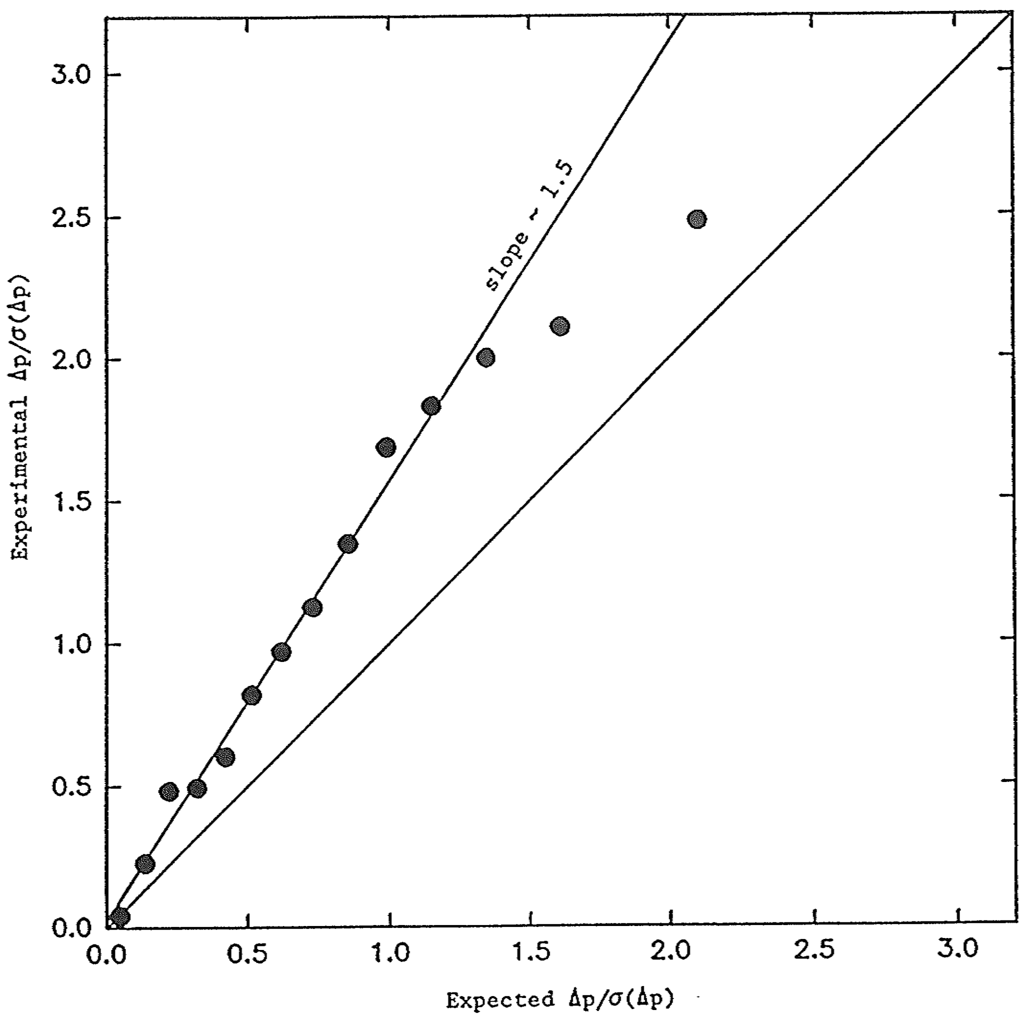

Figure 3-1-4 (continue) (b) pyroxene.

Rietveld refinement (Table 3-1-7). The maximum differences are 0.022(16) Å for M2–O1 and 0.017(6) Å for T–O1; these differences are not statistically significant. The situation is the same for the pyroxene refinements (Table 3-1-7); the maximum differences are 0.021(8) Å for M1–O2 and 0.025(11) Å for T–O3b; as with the olivine, these differences are not statistically significant.

The situation for the multiphase Rietveld refinements is less satisfactory, particularly where the modal proportion of the phase is small. For the olivine, there is a reasonable agreement between the single-crystal and single-phase refinement values and the results of the multiphase refinements when the modal proportion of olivine exceeds 30%. Below this value, the ordering of the bond lengths in terms of relative size is maintained, but large deviations occur, and these are significant where the modal proportion of olivine is 10%. Similar behaviour also occurs for the pyroxene results, although because of the slightly larger standard deviations, the differences are not statistically significant. To summarize, reasonably accurate interatomic distances can be obtained from Rietveld refinements of mixtures of olivine and pyroxene. However, where the modal proportion of either phase becomes small, the assigned standard deviations become so large that the interatomic distances are of no use for crystal-chemical purposes.

The interatomic distances for the refinement of the 1:1 mixture at a series of different step-widths from 0.02–0.10° 2θ are not significantly different from the single-crystal values with increasing step-width. This indicates that the larger step-widths (*i.e.*, up to 0.10° 2θ) do not lead to a loss of accuracy, at least in the 1:1 mixture.

3.2 The Muscovite Example

The effectiveness of the Rietveld method may be limited by preferred orientation during data collection, particularly where the material has a micaceous or fibrous habit. Intensities of basal reflections (00ℓ reflections) tend to be enhanced (reflection geometry) or diminished (transmission geometry) to a degree that prevents accurate refinement of the structure (Sato *et al.* 1981). There are comprehensive reviews (Bish & Reynolds 1989) on the numerous sample-loading methods. Whereas these methods are generally effective in preparing random mounts of non-micaceous materials, most of them are not totally effective for micaceous materials. However, it has been shown (Bish & Von Dreele 1989, Bish & Johnston 1993, Catti *et al.* 1994) that, with care and certain numerical corrections of the observed intensity data, good-quality Rietveld refinements can be done on naturally occurring fine-grained micaceous materials (*e.g.*, kaolinite and dickite). It is the purpose here to examine the accuracy of Rietveld refinement of micaceous materials by comparing the results of Rietveld and single-crystal structure-refinements, using muscovite-$2M_1$ as an example.

3.2.1. Experimental

The muscovite used in the present study is from Himalaya mine, Mesa Grande, California. Electron-microprobe analysis using a CAMECA SX-50 operating in wavelength dispersion mode (see section 3.1.1) shows that it has almost end-member composition of $KAl_2(Si_3Al)O_{10}(OH,F)_2$ (Table 3-2-1).

TABLE 3-2-1. CHEMICAL COMPOSITION AND UNIT FORMULA* OF MUSCOVITE

SiO_2	45.53	Si	3.068
Al_2O_3	36.34	$^{[4]}Al$	0.932
FeO	0.52	$^{[6]}Al$	1.954
MnO	0.22	Fe	0.029
MgO	–	Mn	0.013
CaO	–		
K_2O	10.18	K	0.876
Rb_2O	0.24	Na	0.096
Na_2O	0.74	Rb	0.010
F	1.20	OH	1.744
H_2O**	3.88	F	0.256
O=F	–0.50		
Total	98.35	O	10

* based on 12(O,OH,F) with OH+F=2.0
** estimated by stoichiometry

Single-crystal diffraction

A cleavage fragment of muscovite was mounted on a Nicolet *R3m* automated four-circle diffractometer. Details of intensity-data collection are similar to the corresponding section in 3.1.1. Parameters pertinent to the data collection are listed in Table 3-2-2.

Single-crystal structure-refinement

The structure was refined in the space group *C2/c* using the structural parameters of Richardson & Richardson (1982) as the starting model. Full-matrix least-squares refinement of positional and anisotropic-displacement parameters converged to an *R* index of 4.1%. Other details of the refinement can be found in relevant sections in 3.1.1.

Powder diffraction

The muscovite crystals were cut as finely as possible with a pair of scissors, and then ground in alcohol to less than 10 μm using an automated grinder. After drying, the powder was worked with a piece of weighing paper such that individual crystallites were dis-aggregated and randomized as much as possible.

Data collection in reflection geometry: Powders were front-loaded into Al holders, worked with a probe to remove any air pockets, and the surface was then chopped with a razor blade to minimize surface and near-surface preferred orientation of the crystallites. X-ray intensity data were collected on a Philips automated diffraction system PW1710 equipped with a graphite-crystal monochromator for Cu$K\alpha$ radiation. Intensities were measured at 0.02°2θ steps with counting times of 3 s per step and a scan range of 8–132°2θ.

TABLE 3-2-2. SINGLE-CRYSTAL X-RAY DIFFRACTION DATA-COLLECTION AND REFINEMENT INFORMATION FOR MUSCOVITE-2M_1

a (Å)	5.180(4)	Crystal size (mm)	0.60 x 0.20 x 0.01
b (Å)	8.993(6)	Radiation/Mono.	Mo$K\alpha$/Gr
c (Å)	20.069(13)	Total no. $\lvert F\rvert$	1376
β (°)	95.69(6)	No. of $\lvert F\rvert_{obs}$	981
V (Å^3)	930(1)	R(azimuthal) %	2.7
		R(observed) %	4.1
Space group	$C2/c$	wR(observed) %	4.5
Z	4		

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

$wR = [\Sigma(w|F_o|-|F_c|)^2/\Sigma wF_o^2]^{1/2}$, $w = 1$

Data collection in transmission geometry: A thin film of powder was spread (without solvent) on prolene over a circular area ~10 mm in diameter, whose boundary was confined by a thin-wire ring glued onto the prolene using hair spray. The thin film was finely serrated with a razor blade, and then carefully covered by prolene to fix the powder during data collection. Intensity data were collected on a Siemens D5000 X-ray diffractometer in the 2θ range 8–116° in steps of 0.02° 2θ with a step-counting time of 20 s. The instrument operates in transmission geometry and has a Ge curved crystal incident-beam monochromator that provides monochromatic Cu$K\alpha_1$ radiation. A Kevex Psi-II solid-state (energy-dispersive) detector was used to record the diffracted radiation. Details of the data collection are listed in Table 3-2-3.

Rietveld structure-refinement

Structure-refinement was done using the program LHPM3 (an upgrade of LHPM1 as used in 3.1.). The March model (Dollase 1986) was used in the preferred-orientation correction. Minor crystalline alumina (Al_2O_3) was introduced into the sample during grinding. This impurity phase was accounted for using simultaneous two-phase Rietveld refinement. Other details of the Rietveld refinement procedure can be found in relevant sections in 3.1.1.

3.2.2 Result and Discussion

Cell dimensions obtained from single-crystal and Rietveld refinements are given in Tables 3-2-2 and 3-2-3, respectively. Atomic positions are listed in Table 3-2-4 and

TABLE 3-2-3. DETAILS OF POWDER-DIFFRACTION INTENSITY-DATA COLLECTION AND RIETVELD REFINEMENT FOR MUSCOVITE-2M_1

	Trans.	Refl.		Trans.	Refl.
a (Å)	5.1765(4)	5.1805(7)	Unique reflections	718	718
b (Å)	8.9872(6)	8.994(1)	Structural parameters	37	37
c (Å)	20.072(1)	20.086(2)	Experimental parameters	20	20
β (°)	95.756(6)	95.740(7)	N–P	4888	
V ($Å^3$)	929.08	931.18	R_P	9.5	6.7
Space group	*C*2/*c*	*C*2/*c*	R_{WP}	12.4	8.7
2θ scan range (°)	8–116	8–116	R_{EXP}	8.1	5.9
step interval (°2θ)	0.02	0.02	R_{BRG}	2.3	2.5
integration time/step (s)	20	3	DW *d* statistic	1.42	0.97
maximum intensity (counts)	2496	3509	G1*	0.95(1)	0.96(2)

*: see equation 2-8

TABLE 3-2-4. FINAL ATOMIC COORDINATES OF MUSCOVITE-2M_1

	x	y	z	Occupancy	U_{iso}
			Rietveld refinement (transmission mode)		
Al	0.251(2)	0.080(1)	–0.0015(6)	0.97(1)	–
T1	0.449(2)	0.257(1)	0.1341(4)	0.98(1)	–
T2	0.033(2)	0.431(1)	0.3650(5)	0.95(1)	–
K	0	0.099(1)	1/4	0.86(2)	–
OH	0.037(3)	0.066(2)	0.4537(7)	1.00	–
O1	0.375(3)	0.245(2)	0.0537(10)	1.00	–
O2	0.042(3)	0.445(2)	0.4469(10)	1.00	–
O3	0.410(3)	0.088(2)	0.1678(10)	1.00	–
O4	0.244(3)	0.368(2)	0.1683(2)	1.00	–
O5	0.249(4)	0.307(2)	0.3440(3)	1.00	–
			Rietveld refinement (reflection mode)		
Al	0.249(2)	0.081(1)	–0.0012(5)	0.98(1)	–
T1	0.447(2)	0.256(1)	0.1346(4)	0.97(1)	–
T2	0.032(2)	0.428(1)	0.3642(4)	0.93(1)	–
K	0	0.104(1)	1/4	0.94(2)	–
OH	0.045(3)	0.068(2)	0.4526(6)	1.00	–
O1	0.379(3)	0.246(2)	0.0540(8)	1.00	–
O2	0.035(2)	0.442(2)	0.4483(8)	1.00	–
O3	0.413(3)	0.090(3)	0.1667(6)	1.00	–
O4	0.257(4)	0.372(2)	0.1691(6)	1.00	–
O5	0.248(4)	0.307(2)	0.3438(7)	1.00	–

TABLE 3-2-4. (continue)

	x	y	z	Occupancy	U_{iso}
			Single-crystal refinement		
Al	0.2510(2)	0.0838(1)	0.0000(1)	0.965(8)	71(3)
T1	0.4514(2)	0.2582(1)	0.1355(1)	0.944(8)	81(3)
T2	0.0345(2)	0.4295(1)	0.3646(1)	0.942(8)	78(3)
K	0	0.0986(2)	1/4	0.894(6)	226(5)
OH	0.0429(6)	0.0617(3)	0.4501(2)	1.00	135(8)
O1	0.3836(6)	0.2511(3)	0.0536(2)	1.00	136(8)
O2	0.0380(6)	0.4447(3)	0.4463(2)	1.00	134(8)
O3	0.4128(6)	0.0925(4)	0.1682(2)	1.00	189(9)
O4	0.2516(6)	0.3726(4)	0.1688(2)	1.00	189(9)
O5	0.2469(7)	0.3083(4)	0.3426(2)	1.00	208(10)

TABLE 3-2-5. INTERATOMIC DISTANCES (Å) AND ANGLES (°) FOR MUSCOVITE

	Single–crystal	Trans.	Refl.
T1–O1	1.646(3)	1.62(2)	1.62(2)
T1–O3	1.650(4)	1.68(2)	1.64(2)
T1–O4	1.649(4)	1.66(2)	1.64(2)
T1–O5a	1.643(4)	1.65(2)	1.66(2)
<T1–O>	1.647	1.65	1.64
O1–T1–O3	109.8(2)	108.4(12)	108.4(13)
O1–T1–O4	110.4(2)	110.9(9)	112.4(9)
O1–T1–O5a	112.3(2)	113.9(7)	112.5(8)
O3–T1–O4	107.3(2)	105.7(9)	108.6(9)
O3–T1–O5a	107.0(2)	106.7(10)	106.5(10)
O4–T1–O5a	109.8(2)	110.8(11)	108.2(11)
<O–T1–O>	109.4	109.4	109.4
T2–O2	1.643(3)	1.64(2)	1.69(2)
T2–O3b	1.642(4)	1.60(2)	1.62(2)
T2–O4c	1.646(3)	1.62(2)	1.65(2)
T2–O5	1.641(4)	1.66(2)	1.64(2)
<T2–O>	1.643	1.63	1.65
O2–T2–O3b	109.9(2)	110.6(11)	109.3(11)
O2–T2–O4c	110.6(2)	112.1(8)	110.2(9)
O2–T2–O5	112.5(2)	110.8(9)	111.1(9)
O3b–T2–O4c	107.1(2)	109.1(11)	107.8(10)
O3b–T2–O5	110.1(2)	109.3(10)	110.3(9)
O4c–T2–O5	106.5(2)	104.7(12)	108.1(11)
<O–T2–O>	109.4	109.4	109.5
Al–O1	1.936(3)	1.96(2)	1.93(2)
Al–O1f	1.924(3)	1.93(2)	1.97(2)
Al–O2g	1.920(3)	1.92(2)	1.93(2)
Al–O2h	1.939(3)	1.89(2)	1.89(2)
Al–OHc	1.913(3)	1.89(2)	1.89(2)
Al–OHi	1.913(3)	1.86(2)	1.89(2)
<Al–O>	1.924	1.91	1.92

TABLE 3-2-5. (continue)

		Single–crystal	Trans.	Refl.
K–O3	x2	2.824(3)	2.82(1)	2.85(1)
K–O4d	x2	2.833(4)	2.88(1)	2.86(2)
K–O5	x2	2.860(4)	2.87(1)	2.84(2)
<K–O_{inner}>		2.839	2.86	2.85
K–O3e	x2	3.308(3)	3.32(1)	3.32(1)
K–O4	x2	3.296(4)	3.25(1)	3.27(2)
K–O5d	x2	3.535(4)	3.55(2)	3.58(2)
<K–O_{outer}>		3.380	3.37	3.39

a: 1–x, y, ½–z; b: ½–x, ½+y, ½–z; c: –x, y, ½–z; d: –½+x, –½+y, z;
e: x–1, y, z; f: ½–x, ½–y, –z; g: ½–x, –½+y, ½–z; h: ½+x, ½–y, –½+z; i: x, –y, –½+z.

interatomic distances and angles are compared in Table 3-2-5. Structure-factors and powder-diffraction step-scan intensities are given in Appendix S-3 and Appendix P-22 and P-23.

The final calculated patterns from the Rietveld structure-refinement are compared to the observed patterns in Figure 3-2-1. The fit for the transmission-geometry data is very close (Fig. 3-2-1a), with no significant intensity in the difference pattern. The fit is not quite as close for the reflection-geometry data (Fig. 3-2-1b). There is some residual intensity associated with the 004, 006, $00\overline{10}$ and some *hkl* ($k = 3n$) peaks. These residuals are probably indications of partial stacking disorder. Notice the negative residual intensities that accompany the positive residual intensities. Such combination of residual intensities is characteristic of partial stacking disorder in phyllosilicates (Brindley 1980). The stacking disorder will preferentially suppress the intensities of the *hkl* ($k \neq 3n$) reflections, causing the intensities of the *hkl* ($k = 3n$) reflections to increase relative to the rest of the pattern. Such intensity distortion cannot be accounted for in a Rietveld refinement where stacking disorder is not modeled explicitly.

How significant is the preferred orientation in each sample? We can evaluate this by comparing the observed patterns with the ideal powder pattern calculated from the coordinates and site populations of the refined single-crystal structure (Fig. 3-2-2). Both powder patterns in Figure 3-2-2 show significant preferred-orientation effects, but they seem to be more severe in the transmission-geometry pattern as indicated by the intensity difference between the observed and ideal patterns (Fig. 3-2-2a). Nevertheless, the difference patterns in Figure 3-2-1 indicate that the preferred-orientation correction copes

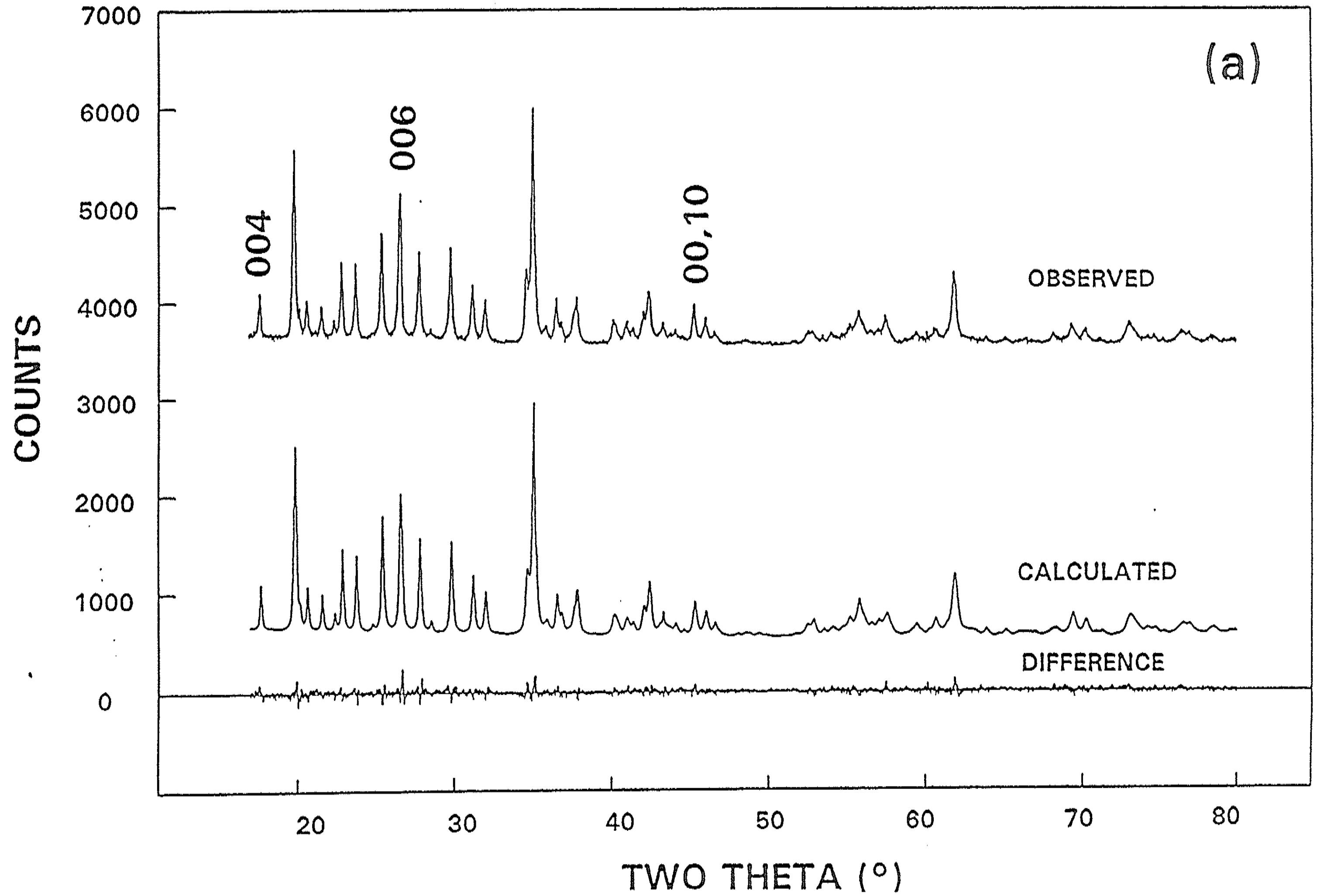

Figure 3-2-1. Observed (upper), Rietveld calculated (middle) and difference (lower) X-ray powder-diffraction patterns of muscovite-$2M_1$; constant counts have been added to each pattern to displace them vertically. (a) transmission mode;

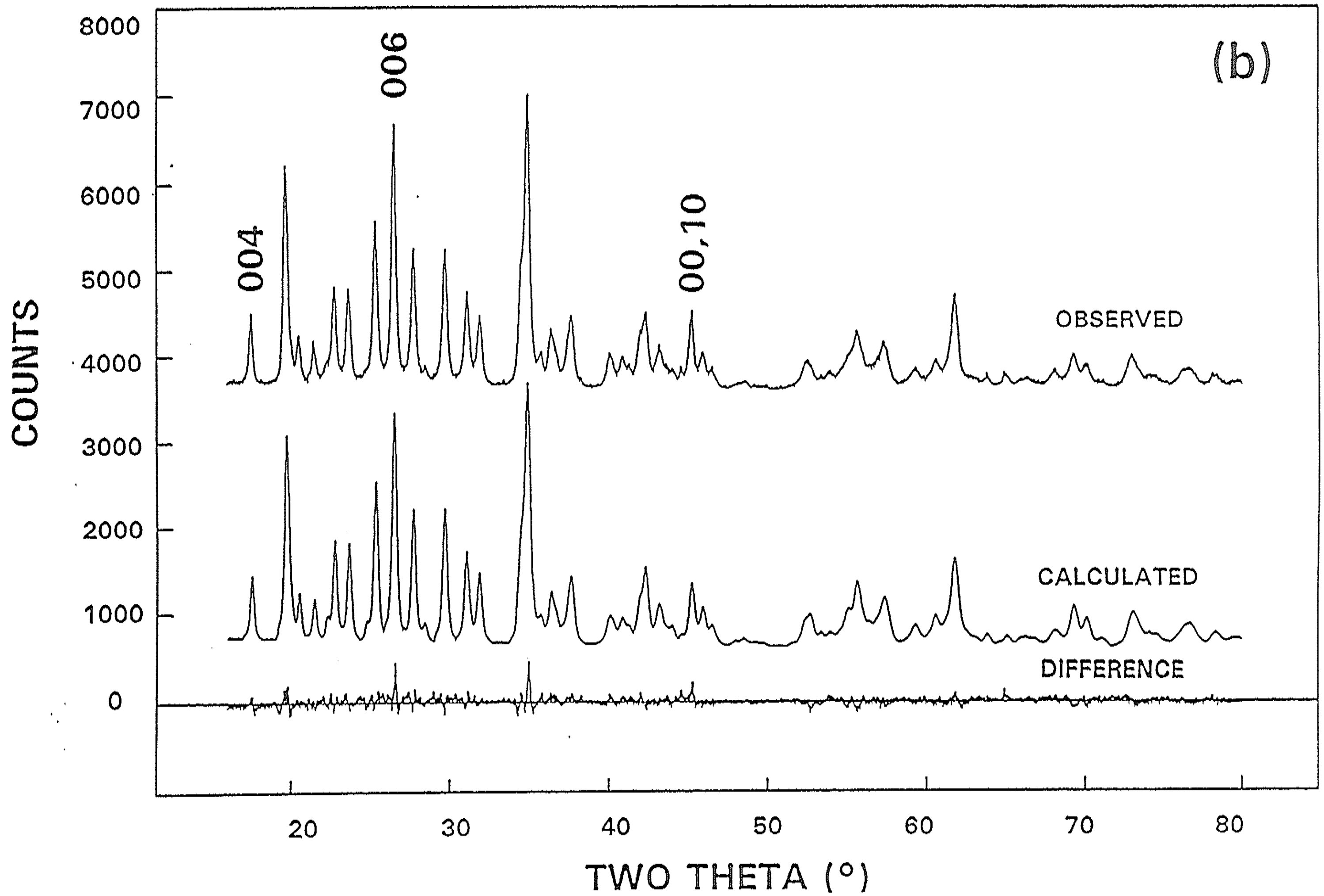

Figure 3-2-1. (continue) (b) reflection mode.

better with this effect in the transmission-geometry sample. Two other effects warrant comment here. First, note the increased resolution in the transmission-geometry pattern compared to that observed in the reflection-geometry pattern. Transmission geometry does not use parafocusing as in reflection geometry which is a cause for substantial line-broadening and asymmetry. Second, note the difficulty in modelling the shape of the basal reflection 002. This is primarily an instrumental effect. The Lorentz-Polarization term in the expression of diffraction intensity (Brindley 1980), and, accordingly, the diffraction intensity itself, increases rapidly to infinity towards 0° 2θ. However, the exact rate of the increase is a function of, in addition to the 2θ-angle, the degree of polarization of the radiation and the degree of randomness of the powder sample which are difficult to model closely. Therefor, the lowest-order reflection(s) is(are) usually omitted from the refinement (*e.g.*, Bish & Von Dreele 1989).

Accuracy of the refined structure

Agreement of the observed and calculated patterns is not an indication of accurate results; a model that produces good agreement can still incorporate systematic error and hence be inaccurate. However, in the present case, this possibility can be tested for each set of powder intensity-data, as both an electron-microprobe analysis and single-crystal structure-refinement results on the same material are available.

The unit formula calculated from the electron-microprobe analysis (Table 3-2-1) indicates the following site-occupancies: Al* = 1.02, T(1) = T(2) = 0.98 Si*, K* = 0.93; Al* = $^{[6]}$Al + 26 Fe/13 + 25 Mn/13, Si* = Si + 13 $^{[4]}$Al/14, K* = K + 11Na/19. These

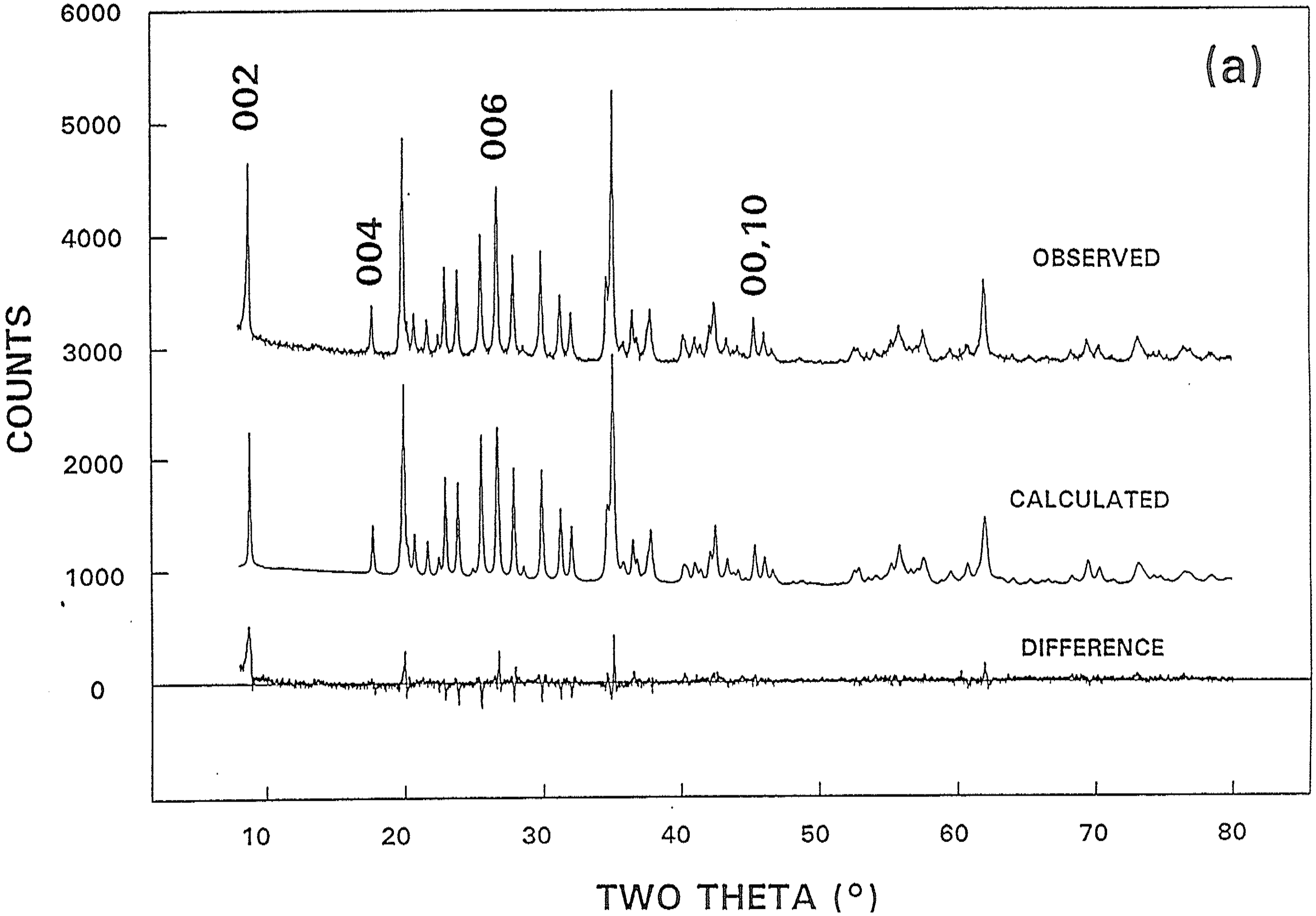

Figure 3-2-2. Observed (upper), calculated from refined single-crystal structure (middle) and difference (lower) X-ray powder-diffraction patterns of muscovite-$2M_1$; (a) transmission mode;

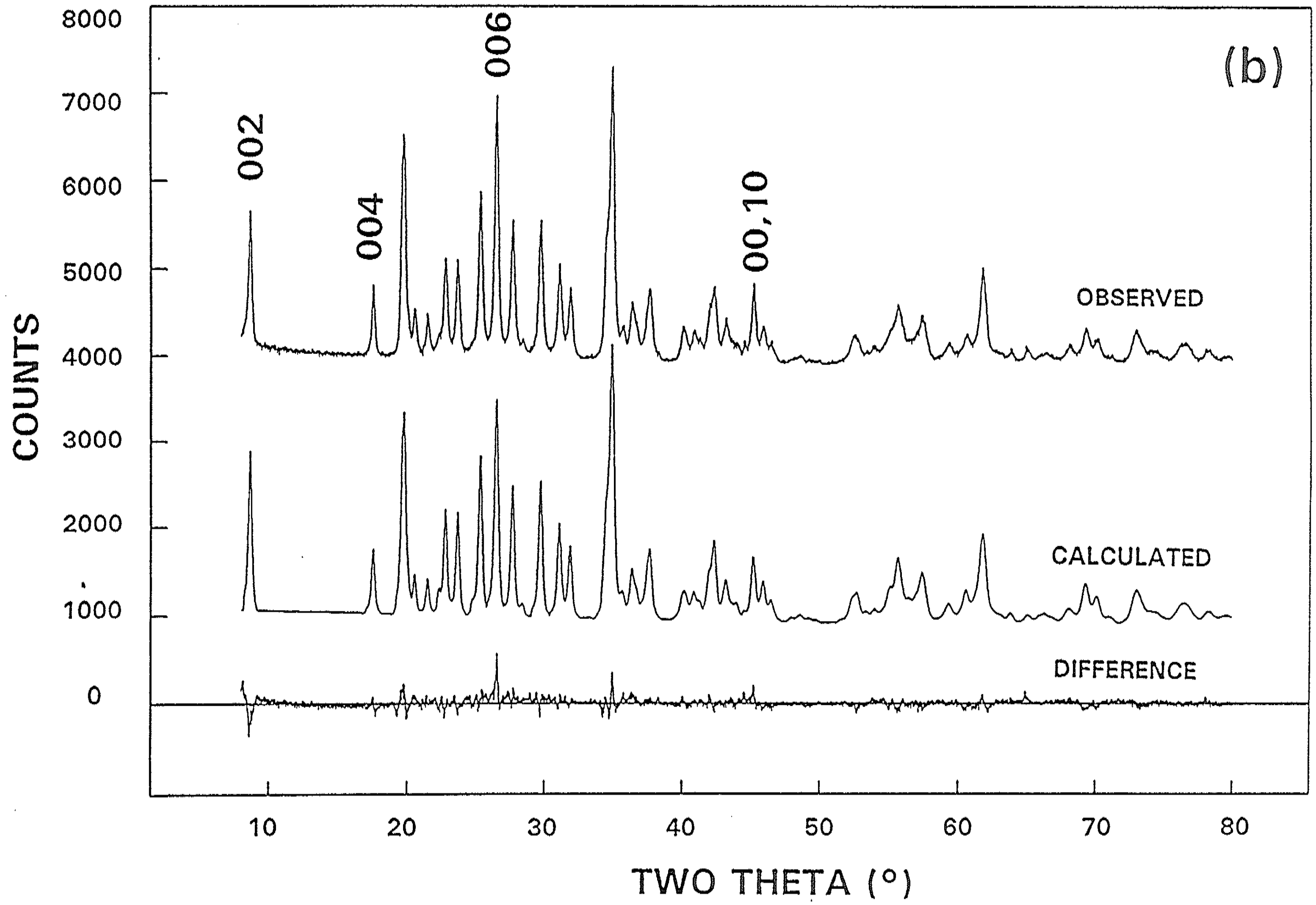

Figure 3-2-2. (continue) (b) reflection mode.

agree closely with the values derived from both single-crystal and Rietveld structure-refinement.

The half-normal probability plots are linear (Fig. 3-2-3), with r^2 values of 0.97 and 0.99, and slopes of 1.94(6) and 2.12(5) for the transmission and reflection data, respectively. In each case, the intercept passes though the origin (within the standard error of estimate) and hence there is no systematic error involved in the two sets of results. However, the slopes of the plots should be 1.0 if the assigned standard deviations are correct. For both sets of data, the slopes are 2.0 (within 2 standard deviations), indicating that the pooled standard deviations are wrong. The standard deviations from the Rietveld refinements (Table 3-2-3) are up to an order of magnitude larger than the standard deviations for the single-crystal refinement. The pooled standard deviations used in the half-normal probability-plot analysis are totally dominated by the standard deviations from the Rietveld refinement. Hence, any reasonable inaccuracy in the single-crystal standard deviations (*i.e.*, by a factor of 1 to 2) will have an insignificant effect on the pooled standard deviations; inaccuracy in the latter must result from inaccuracy in the Rietveld standard deviations.

It is well known (Hill & Flack 1987) that serial correlation in Rietveld structure-refinement results in significant underestimation in the calculated standard deviations, and Hill & Flack (1987) have shown that a weighted form of the Durbin-Watson statistic (Durbin & Watson 1971) is sensitive to the amount of serial correlation between least-squares residuals in Rietveld refinement of step-scan powder-diffraction data: a d statistic of ~2.0 indicates no serial correlation. The Durbin-Watson d statistic for the Rietveld

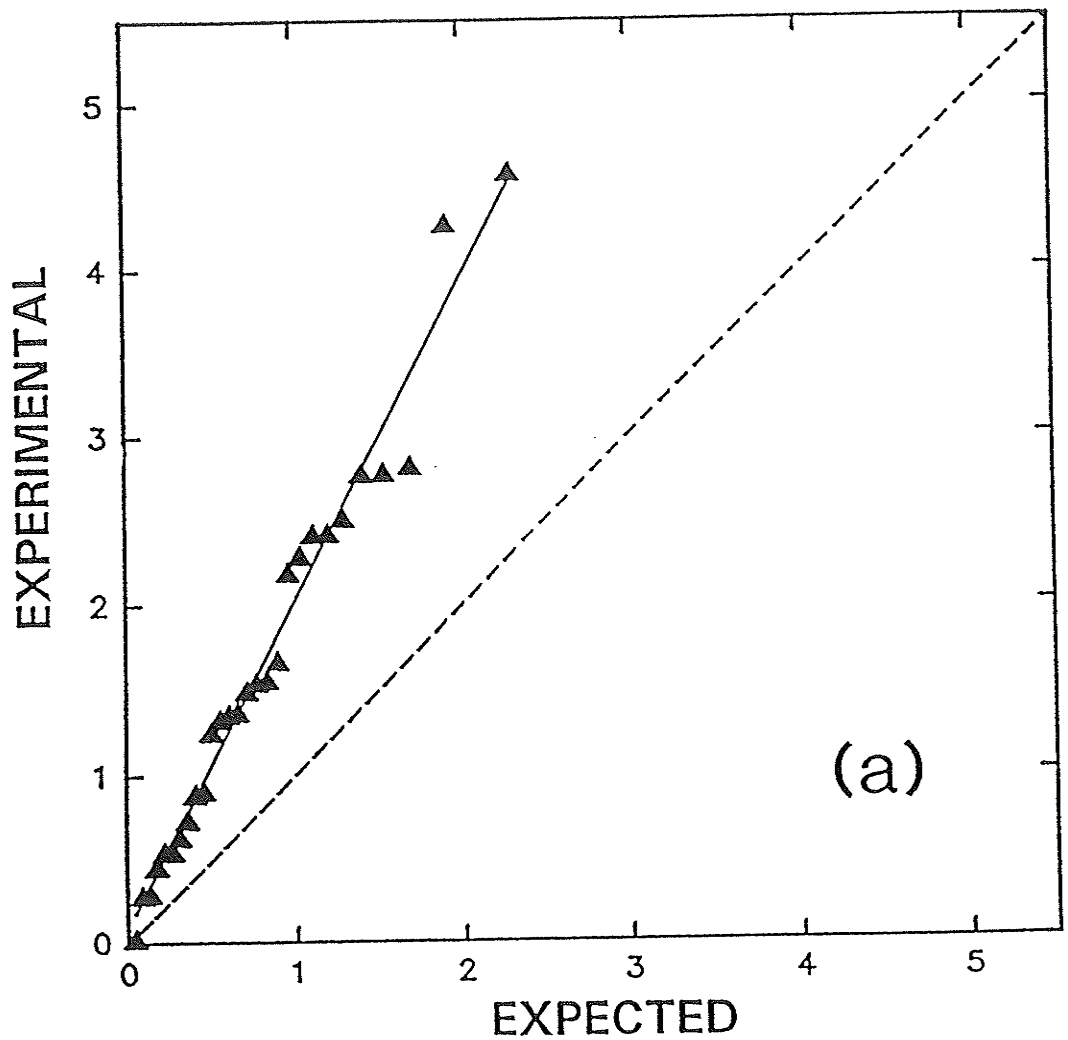

Figure 3-2-3. Half-normal probability plots for refined positional coordinates of muscovite-$2M_1$; (a) single-crystal and transmission-mode Rietveld refinements;

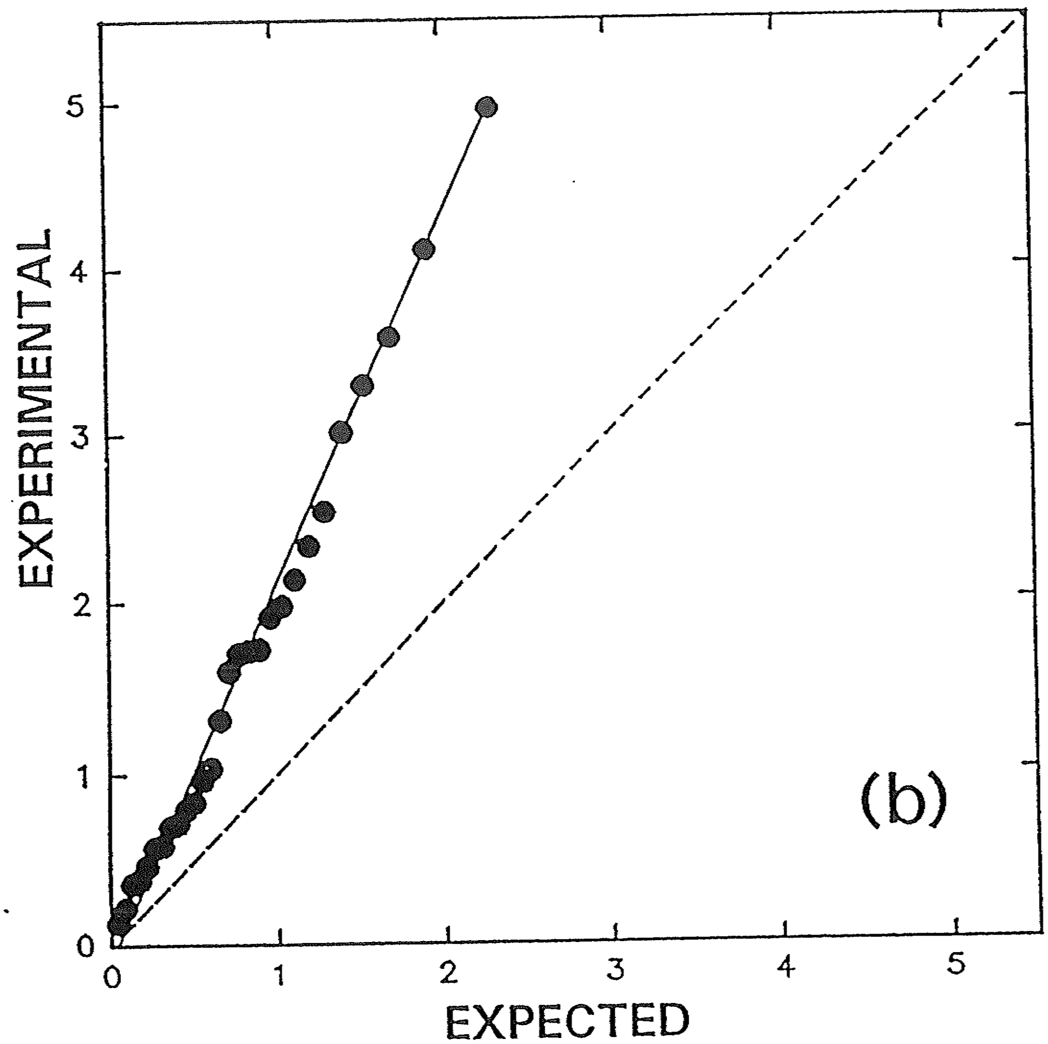

Figure 3-2-3. (continue) (b) single-crystal and reflection-mode Rietveld refinements.

refinements reported here do differ significantly from 2.0 (Table 3-2-3). Bérar & Lelann (1991) have introduced a method to correct standard deviations for serial correlation, and the standard deviations quoted in Table 3-2-4 have been corrected with this algorithm. Nevertheless, the slopes in Figure 3-2-3 show that both sets of standard deviations are still underestimated. The single-crystal standard deviations are up to an order of magnitude less than the standard deviations from the Rietveld refinements, and hence do not contribute significantly to the pooled standard deviations. Thus the slope of the half-normal probability plot is the factor by which the Rietveld standard deviations are incorrect (*i.e.*, 2.0). Nevertheless, there is good agreement between the refined parameters, indicating that a platy habit and the presence of preferred orientation in the sample does not preclude accurate structure-refinement by the Rietveld method.

3.3. Phlogopite

One important aspect of mica synthesis, the crystal structural characterization of the run-products, had been difficult due to the usually fine grain sizes and the micaceous habit. Partial structural information can be obtained through solid state NMR (Circone et al. 1991, Sanz & Rober 1992), vibrational spectroscopy (Robert & Kodama 1988, Robert et al. 1995) and calorimetric techniques (Circone & Navrotsky 1992). There had been a number of crystal structural studies of natural micaceous materials using powder diffraction techniques and Rietveld method (Adams 1983, Young & Hewat 1988, Bish & Von Dreele 1989, Walker & Bish 1992, Bish & Johnston 1993, Bish 1993, Liang et al.

1995, Liang & Hawthorne 1996). However, the present work represents the first in applying the Rietveld method to the crystal structural characterization of synthetic mica.

3.3.1. Experimental

Material

The synthetic mica, fluorophlogopite (NBS standard SRM675), was used unmodified. Grain sizes of the sample ranges from 0.5 mm to less than 10 μm. The sample was emerged in double distilled water, and the finer-grained portion (< 10 - 200 μm, average 40 μm) that suspends in the distilled water was separated from the coarse-grained portion (50 - 500 μm, average 300 μm) that does not suspend. Ethanel was added to the suspension to accelerate precipitation and to promote porosity in the natural-dried precipitate such that minimum effort is needed to disaggregate the dried precipitate.

Powder diffraction and Rietveld structure-refinement

Both the fine- and the coarse-grained portions were used in the experiment. Powders were front-loaded into Al holders. X-ray intensity data were collected on a Philips automated diffraction system PW1710. Intensities were measured at 0.05°2θ steps with counting times of 2.5 s per step and a scan range of 7 – 127° 2θ (to the higher angle limit of the diffractometer). Details of sample preparation and experimental procedures can be found in Liang & Hawthorne (1996) and Raudsepp *et al.* (1990). Parameters pertinent to the data collections are listed in Table 3-3-1.

Structure refinement was done using the program LHPM3 (originally written as

TABLE 3-3-1. DETAILS OF POWDER-DIFFRACTION INTENSITY-DATA COLLECTION AND RIETVELD REFINEMENT FOR FLUOROPHLOGOPITE

	$1M$	$2M_1$		$1M$	$2M_1$
a (Å)	5.312(3)	5.32(2)	Unique reflections	464	874
b (Å)	9.196(4)	9.17(4)	Structural parameters	23	5
c (Å)	10.148(2)	20.09(3)	Experimental parameters	15	
β (°)	100.09(3)	95.2(2)	N–P	2181	
V (Å^3)	488.07	976.3	R_P	13.1	
Space group	$C2/m$	$C2/c$	R_{WP}	17.3	
2θ scan range (°)		7–127	R_{EXP}	6.1	
step interval (°2θ)		0.05	R_{BRG}	7.2	8.7
integration time/step (s)		2.5	DW d statistic	0.32	
maximum intensity (counts)		8582	G1*	0.64(1)	

*: see equation 2-8

DBW3.2 by Wiles & Young 1981 and modified by Hill & Howard 1986). A pseudo-Voigt peak-shape was used, and the peak asymmetry was corrected using the function of Rietveld (1969). Simultaneous 2-phase refinement was used to accommodate the fact that there is minor $2M_1$ polymorph coexisting with the major $1M$ polymorph. Full structural refinement, with the starting model of McCauley *et al.* (1973), was done for the $1M$ polymorph. Only unit cell parameters and the scale factor were refined for the $2M_1$ polymorph, with atomic coordinates fixed at the values of a $2M_1$ biotite (Takeda & Ross 1975). Other details of the Rietveld refinement were similar to those as in Liang & Hawthorne (1996).

Electron microprobe analysis

Electron microprobe analysis of the fluorophlogopite sample was done using a CAMECA SX-50 operating in the wavelength-dispersion mode, with a beam diameter of 5 μm and an accelerating potential of 15 kV. A sample current of 20 nA measured on a Faraday cup and a counting time of 20 s were used for K, Mg, Al, Si and F. The following standards were used: diopside (Si$K\alpha$), kyanite (Al$K\alpha$), orthoclase (K$K\alpha$), zinnwaldite (F$K\alpha$), and olivine (Mg$K\alpha$). The data were reduced using the PAP routine of Pouchou & Pichoir (1985). Experimental details are as described by Hawthorne *et al.* (1993). The mean composition and unit formula are given in Table 3-3-2.

Fourier-Transform Infrared Photo-Acoustic Spectroscopy (FT-IR PAS)

The spectra were collected with a Bio-Rad FTS-60A (Bio-Rad, Cambridge, MA)

TABLE 3-3-2. CHEMICAL COMPOSITION AND UNIT FORMULA* OF PHLOGOPITE

SiO_2	wt%	42.96	Si	3.031
Al_2O_3		11.68	$^{[IV]}Al$	0.971
MgO		28.33	Mg	2.979
K_2O		11.18	K	1.006
H_2O**		0.92	OH	0.434
F		7.02	F	1.565
O=F		-2.96	O	10
Total		99.14		

* based on 12(O,OH,F) with OH+F=2.0
** estimated by stoichiometry

spectrometer. An MTEC Model 200 photoacoustic cell (MTEC, Ames, IA) with its accompanying preamplifier and power supply was used to acquire all the spectra. The sample tray was filled with the powder sample without attempting to compact the powder. The photoacoustic cell (with the sample) was purged with dry helium. A high-surface-area carbon-black sample (MTEC) was used as the reference material for all spectra. Different interferometer mirror speeds, corresponding to average modulation frequencies of 10, 5 and 2.5 KHz, respectively, were used in the collection of the spectra. Other experimental details can be found in Sowa & Mantsch (1994).

Single-crystal diffraction and structure refinement

A crystal of 0.4 x 0.3 x 0.03 mm was mounted on a Nicolet *R*3*m* automated four-circle diffractometer. Cell dimensions (Table 3-3-3) were refined from the setting angles of 25 automatically aligned intense reflections. The cell dimensions conform to those of the 1*M* polymorph of phlogopite. Intensity data were collected according to the procedure of Hawthorne & Groat (1985). Absorption corrections were done with the psi-scan method, modelling the crystal shape as a thin plate. Intensities were corrected for background, absorption, Lorentz and polarization effects, and reduced to structure factors. Details concerning these procedures are given in Table 3-3-3.

Crystal structures were refined using the SHELXTL-PC system of programs; R indices are of the form given in Table 3-3-3. The structure was refined in the space group *C*2/*m* (1*M* polytype) using the structural parameters of McCauley *et al.* (1973) as the starting model. Full-matrix least-squares refinement of positional and anisotropic-

TABLE 3-3-3. SINGLE-CRYSTAL X-RAY DIFFRACTION DATA-COLLECTION AND REFINEMENT INFORMATION FOR PHLOGOPITE 1M

a (Å)	5.313(2)	Crystal size (mm)	0.60 x 0.20 x 0.01
b (Å)	9.198(3)	Radiation/Mono.	Mo$K\alpha$/Gr
c (Å)	10.147(2)	Total no. $\|F\|$	736
β (°)	100.17(2)	No. of $\|F\|_{obs}$	671
V (Å^3)	488.6	R(azimuthal) %	2.0
		R(observed) %	3.7
Space group	$C2/m$	wR(observed) %	4.0
Z	4		

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

$wR = [\Sigma(w|F_o|-|F_c|)^2/\Sigma wF_o^2]^{1/2}$, $w = 1$

displacement parameters converged to an R index of 3.7%.

3.3.2. Result and Discussion

As substantial stacking disorder (see later discussion) was observed in the fine-grained portion of the fluorophlogopite sample, all result reported with respect to the Rietveld refinement are those using the coarse-grained portion of the material. The use of the fine-grained portion is to show different degrees of stacking disorder with respect to different grain sizes.

Cell dimensions obtained from single-crystal and Rietveld refinements are given in Tables 1 and 3, respectively. Atomic positions are listed in Table 3-3-4 and interatomic distances and angles are compared in Table 3-3-5. Structure-factors and powder-diffraction step-scan intensities may be obtained from The Depository of Unpublished Data, CISTI, National Research Council of Canada, Ottawa, Ontario, K1A 0S2.

Phase identification

Apart from the major $1M$ polymorph, there also exists minor $2M_1$ polymorph in the fluorophlogopite sample. Based on the refined scale factors of the $1M$ and the $2M_1$ polymorphs of 0.00123(8) and 0.000028(2), respectively, the 1M to $2M_1$ ratio can be calculated (Hill & Howard 1987) to be 92:8.

Accuracy of the Rietveld refined structure

The half-normal probability plot comparing the two sets of structural parameters

TABLE 3-3-4. FINAL ATOMIC COORDINATES OF FLUOROPHLOGOPITE-1M

	x	y	z	Occupancy	U_{iso}
			Single-crystal		
K	0	0	0	0.25	0.0333
Si	0.5753(1)	0.1666(1)	0.2250(1)	0.973(7)	0.0056
Mg1	0	1/2	1/2	0.242(3)	0.0048
Mg2	0	0.8311(2)	1/2	0.487(4)	0.0043
O1	0.8212(4)	0.2344(3)	0.1667(2)	1.000	0.0202
O2	0.5244(7)	0	0.1660(3)	0.500	0.0128
O3	0.6301(4)	0.1664(2)	0.3900(2)	1.000	0.00622
F	0.1334(5)	0	0.4021(3)	0.486(6)	0.0077
			Rietveld refinement		
K	0	0	0	0.25	-
Si	0.580(3)	0.164(1)	0.227(1)	0.96(4)	-
Mg1	0	1/2	1/2	0.24(2)	-
Mg2	0	0.831(1)	1/2	0.49(2)	-
O1	0.826(4)	0.234(2)	0.167(1)	1.000	-
O2	0.509(3)	0	0.168(2)	0.500	-
O3	0.644(6)	0.162(2)	0.389(1)	1.000	-
F	0.165(5)	0	0.402(1)	0.48(3)	-

TABLE 3-3-5. INTERATOMIC DISTANCES (Å) AND ANGLES (°) IN FLUOROPHLOGOPITE

	Single-crystal	Rietveld
T–O1	1.650(3)	1.67(2)
T–O1a	1.650(2)	1.67(2)
T–O2	1.651(1)	1.64(1)
T–O3	1.648(2)	1.62(1)
<T–O>	1.650	1.65
O1–O1a	2.674(1)	2.67(1)
O1–O2	2.671(3)	2.74(2)
O1–O3	2.716(3)	2.68(3)
O1a–O2	2.672(3)	2.63(2)
O1a–O3	2.711(3)	2.74(2)
O2–O3	2.716(3)	2.69(2)
<O–O>T	2.693	2.69
O1–T–O1a	108.3(1)	107(1)
O1–T–O2	108.1(2)	105(1)
O1–T–O3	110.9(1)	113(1)
O1a–T–O2	108.1(1)	112(1)
O1a–T–O3	110.6(1)	109(1)
O2–T–O3	110.8(1)	111(1)
<O–T–O>	109.5	
Mg1-O3b x4	2.083(2)	2.10(2)
Mg1-Fc x2	2.025(2)	1.88(2)
<Mg1-O/F>	2.054	1.99
Mg2-O3d x2	2.073(2)	2.14(2)
Mg2-O3e x2	2.083(2)	2.03(3)
Mg2-Ff x2	2.038(2)	2.12(1)
<Mg1-O/F>	2.065	2.10

TABLE 3-3-5. (continue)

		Single-crystal	Rietveld
K-O1g	x4	2.998(3)	2.99(1)
K–O1h	x4	3.275(2)	3.29(1)
K–O2	x2	2.992(3)	2.93(2)
K–O2i	x2	3.277(4)	3.36(2)
<K–O>		3.136	3.14

a: -1/2+x, 1/2–y, z; b: -1/2+x, 1/2+y, z; c:-1/2+x, 1/2+y, z; d: -1/2+x, 1/2+y, z; e: 1-x, 1-y, 1-z; f: x, 1+y, z; g: -1+x, y, z; h: -1/2+x, -1/2+y, z; i: -1+x, y, z.

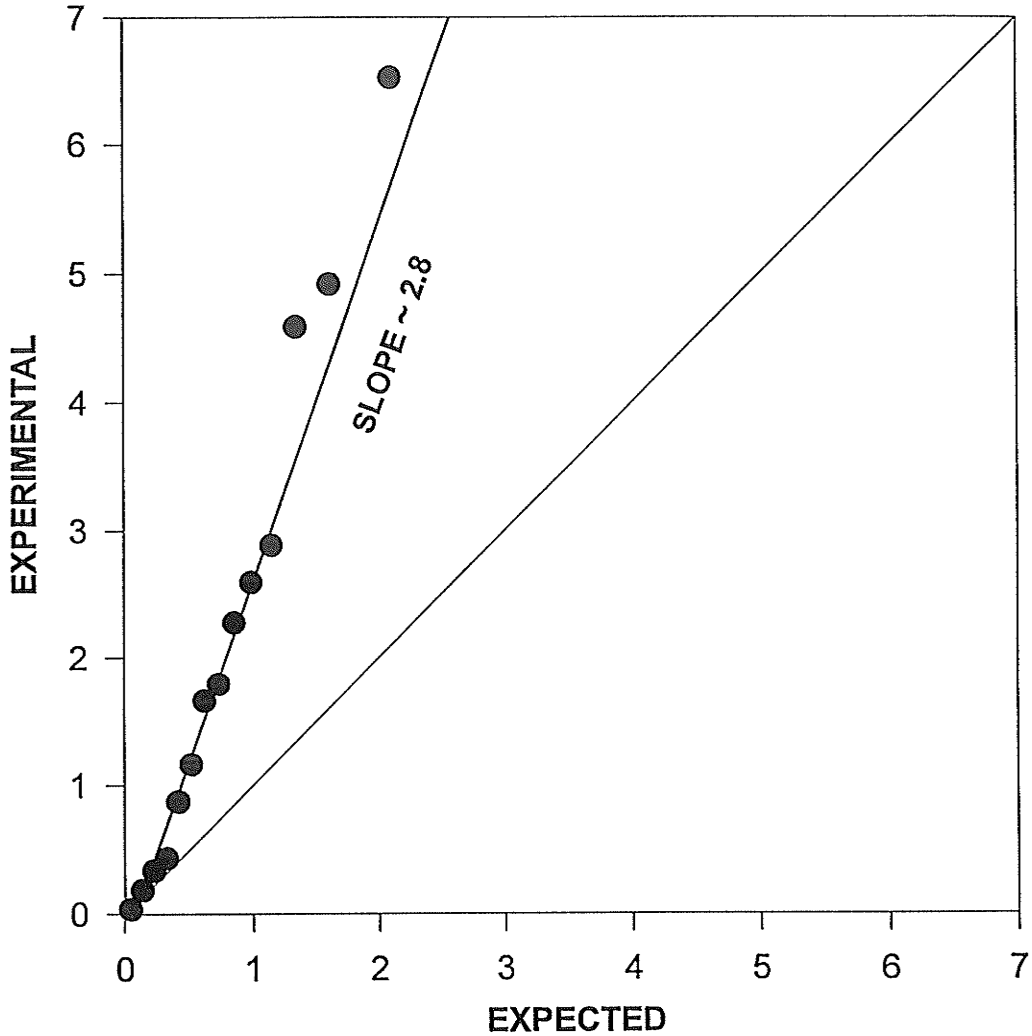

Figure 3-3-1. Half-normal probability plot comparing structural parameters of the 1*M* polytype from single-crystal and the Rietveld refinements.

from single-crystal and Rietveld refinements, respectively, is shown in Figure 3-3-1. The plot shows a linear distribution of the data points. The intercept passes though the origin (within the standard error of estimate) and hence there is no systematic error involved in the two sets of results. However, the slope of 2.8(1) indicates that the standard deviations in the Rietveld refinement are underestimated by a factor of 2.8. This value is higher than that (2.0) in the similar study of muscovite (Liang & Hawthorne 1996). A higher value of the slope indicates greater random error of the Rietveld results (see relevant discussion in Liang & Hawthorne 1996). The stacking disorder, although minor, may be the source of the increases random error.

The unit formula

The refined cation- and F-occupancies for the 1*M* polytype (Table 3-3-4) from single-crystal and Rietveld refinements, respectively, agree closely. The unit formula calculated from the electron-microprobe analysis (Table 3-3-2) indicates the following site-occupancies:

$K^* = 1.006/4 = 0.252$, $Si^* = (Si + 13Al/14)/4 = 0.983$, $Mg^* = 2.979/4 = 0.745$, $F^* = (F + 8(OH)/9)/4 = 0.488$. Corresponding values from the single-crystal refinement are $K^* = 0.25$, $Si^* = 0.973(7)$, $Mg^* = Mg1 + Mg2 = 0.729(7)$, $F^* = 0.486(6)$. It can be seen that the EMPA result and the results from structure refinement agree very closely.

FTIR PAS spectrum at the O-H stretching region (Fig. 3-3-2) shows characteristic O-H stretching near 3710 cm^{-1} (Serratosa & Bradley 1958, Bassett 1960), confirming the existence of O-H groups in the structure of the fluorophlogopite.

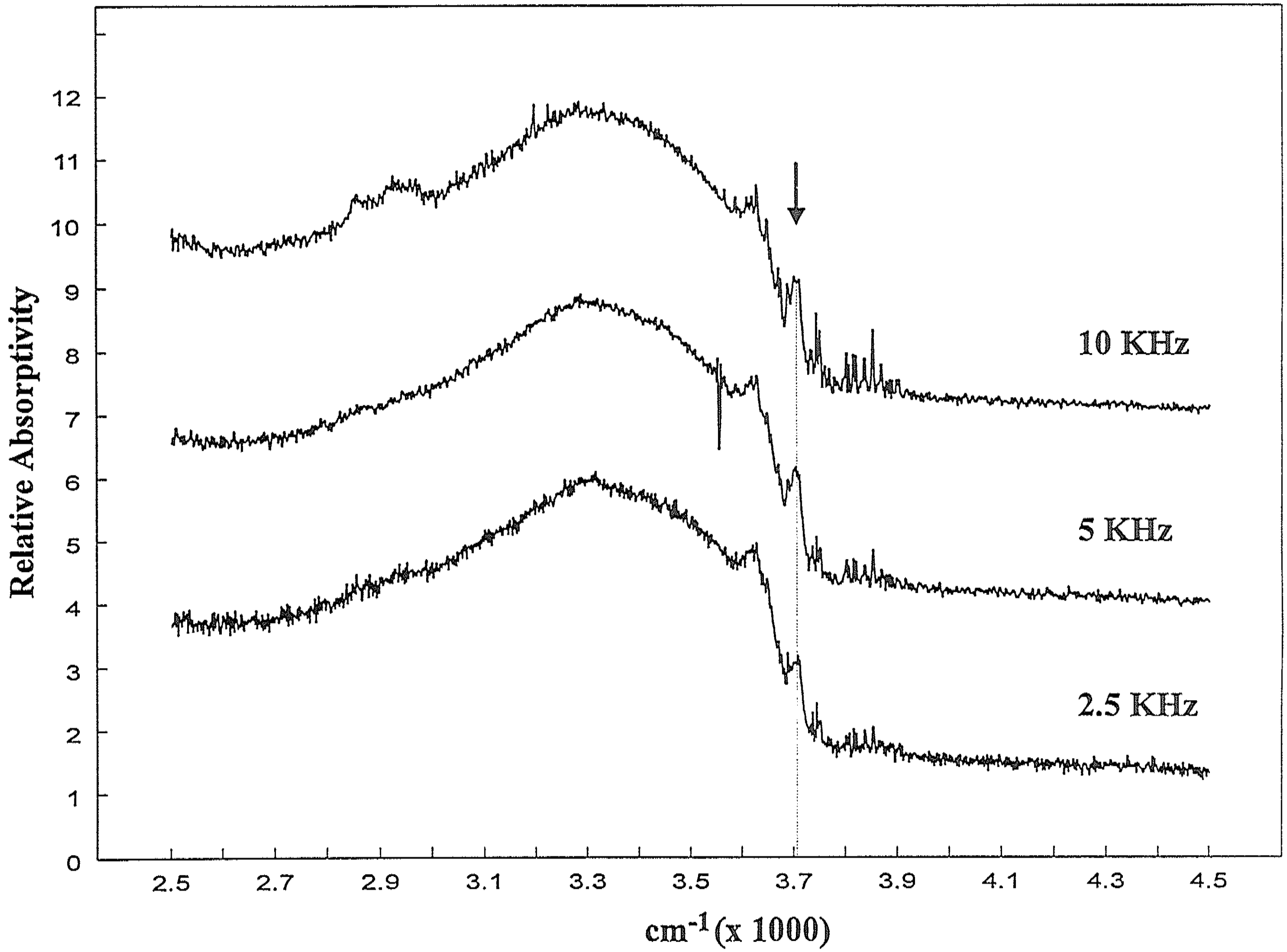

Figure 3-3-2. FTIR PAS spectra of fluorophlogopite at the O-H stretching region. Differing mirror speed (from 10 to 2.5 KHz) represents depth-profiling. The top spectrum corresponds to the experiment that sampled the shallowest from the grain surface, while the bottom spectrum corresponds to the deepest. The O-H stretching band of the fluorophlogopite is marked by an arrow. The other band to the lower wavenumber side may represent fine structure due to F that also occupies the OH site in the phlogopite structure.

Stacking disorder

In the diffraction patterns of the fluorophlogopite (Fig. 3-3-3), certain reflections (both basal and non-basal) are preferentially enhanced, causing residual intensity distribution characteristic of partial stacking disorder (Bailey, 1984). This effect is more evident with the fine grained portion, indicating an increasing stacking disorder as the average grain size decreases.

3.4 Zeolites

Structure refinement of zeolites presents unique problems. Zeolites usually have large unit-cell dimensions. Their structures can be considered to consist of two structural units: (1) the framework configuration; (2) the interstitial constituents. The former consists of corner-sharing $Si(Al)O_4$ tetrahedra that are relatively rigid; the latter includes the usually highly mobile cations (to compensate excess negative charges generated by Al^{3+}/Si^{4+} replacement) and water molecules. It is the purpose of the present section to determine how well the Rietveld method can deal with the two general structure units.

3.4.1. Experimental

Chabazite from Wassons Bluff, Nova Scotia were chosen for the study. Details of electron-microprobe analysis, single-crystal and powder x-ray data collection and their corresponding structure refinements are similar to relevant sections in 3.1.1. Atomic

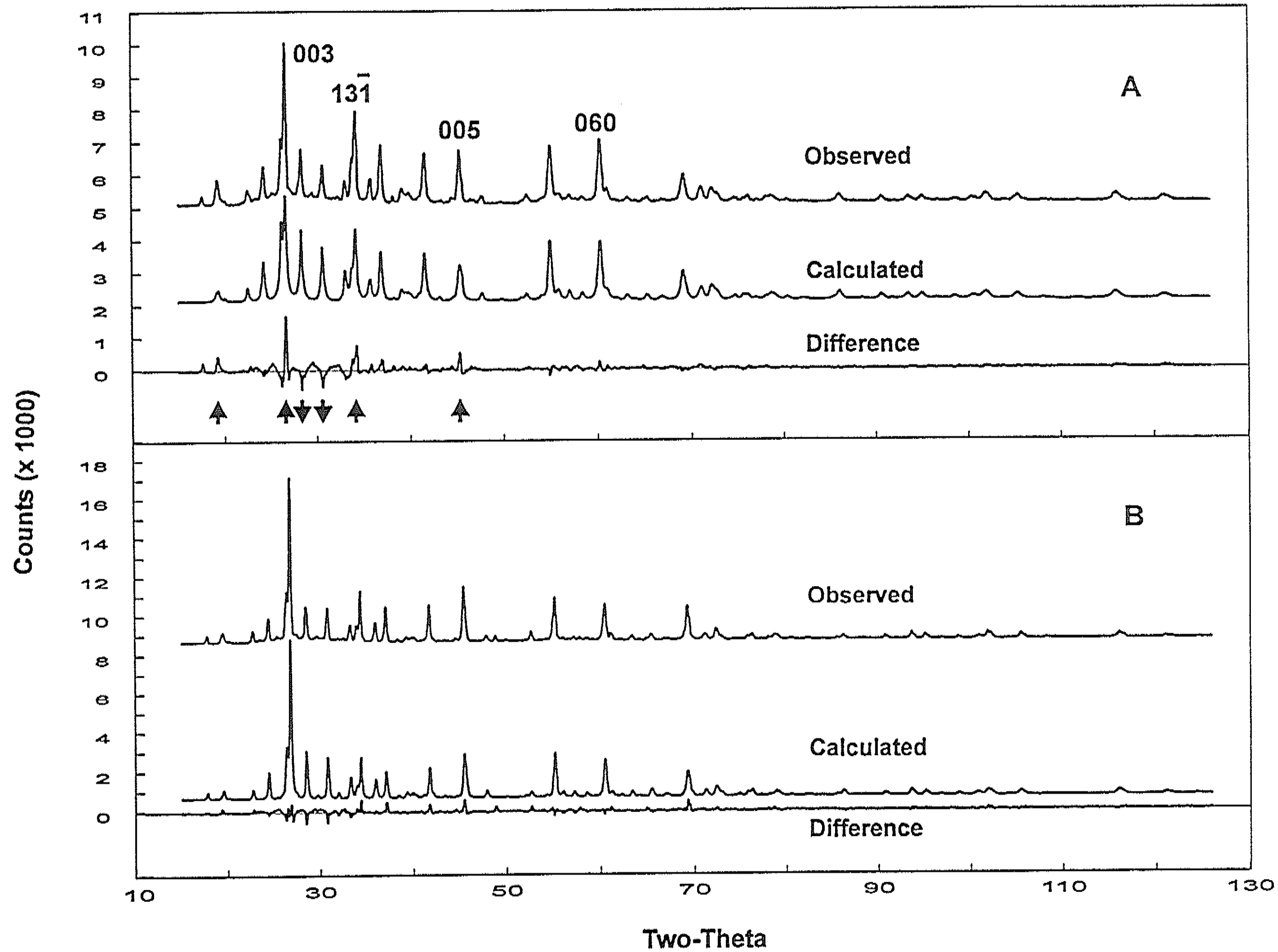

Figure 3-3-3. Observed, calculated and difference X-ray diffraction patterns of the fluorophlogopite.

positions of the charge-compensating cations were determined by difference Fourier method, and the scattering factor of Ca was used for all sites of the charge-compensating cations. The chemical compositions of the zeolites are reported in Table 3-4-1. Details pertinent to the intensity-data collection and structure refinement for single-crystal and Rietveld methods, respectively, are listed in Table 3-4-2 and 3-4-3.

3.4.2 Result and Discussion

The observed and calculated diffraction patterns of chabazite are shown in Figure 3-4-1. The fractional atomic coordinates, refined cation site-occupancies, and interatomic distances and angles of both Rietveld and single-crystal refinements for chabazite are listed in Tables 3-4-4 and 3-4-5. Structure-factors and powder-diffraction step-scan intensities for chabazite are given in Appendix S-5, and Appendix P-25, respectively.

The calculated and observed diffraction patterns

For chabazite, there is a reasonable fit between the calculated and the observed diffraction patterns (Fig. 3-4-1). The residual is, in part, contributed by an impurity phase with minor diffraction peaks near 11, 17 and 30° 2Θ that have no corresponding Bragg reflections in the calculated pattern (Fig. 3-4-1). However, the existence of the impurity phase did not adversely affect the structure refinement of the chabazite, as indicated by the close agreement in atomic coordinates and site occupancies (Table 3-4-5) between the results of Rietveld and single-crystal structure refinement.

TABLE 3-4-1. COMPOSITIONS (WT%) AND UNIT FORMULAE OF CHABAZITE DETERMINED BY ELECTRON MICROPROBE ANALYSIS

SiO_2	52.6
Al_2O_3	16.8
MgO	0.2
CaO	7.7
Na_2O	0.6
K_2O	0.9
SrO	
H_2O*	21.2
Si	9.04
Al	3.40
Mg	0.05
Ca	1.42
Na	0.20
K	0.20
Sr	
H	24.3
O	37

*determined by difference

TABLE 3-4-2. SINGLE-CRYSTAL X-RAY DIFFRACTION DATA COLLECTION AND REFINEMENT INFORMATION FOR CHABAZITE

	Chabazite
a (Å)	13.766(5)
b	13.766(5)
c	14.978(6)
γ/β (°)	120
V (Å^3)	2458.1
Space group	$R\bar{3}m$
Z	3
Crystal size (mm)	0.16 x 0.20 x 0.20
Radiation	Mo$K\alpha$
Monochromator	Graphite
R(azimuthal) %	1.5
Total no. $\|F\|$	902
No. of $\|F\|_{obs}$	890
R_{obs} %	6.5
wR_{obs} %	6.6

$R = \Sigma(|F|-|F|)/\Sigma|F|$

$wR = [\Sigma w(|F|-|F|)^2/\Sigma wF^2]^{0.5}$ $w=1$

TABLE 3-4-3. POWDER INTENSITY DATA COLLECTION AND DETAILS OF RIETVELD STRUCTURE REFINEMENT

a (Å)	13.7796(15)
b (Å)	13.7796(15)
c (Å)	14.9932(11)
β (°)	120
V (Å^3)	2465.48
2θ scan range (°)	10–120
step interval (°2θ)	0.02
integration time/step (s)	20
maximum intensity (counts)	2564
Space group	*R*-3*m*
Unique reflections	491
Structural parameters	26
Experimental parameters	15
N-P	5466
R_P	13.3
R_{WP}	17.4
R_{EXP}	10.5
R_{BRG}	5.6

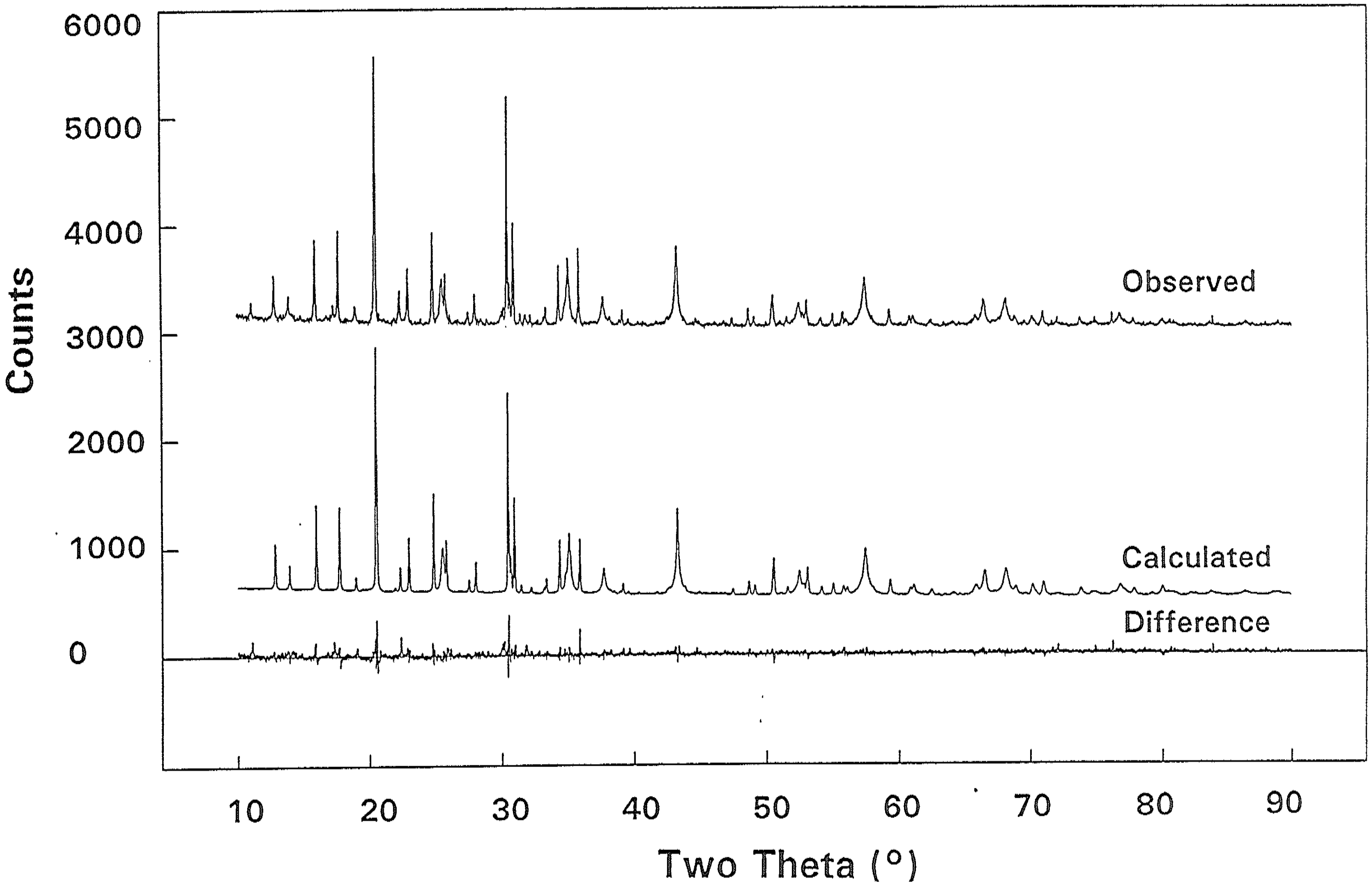

Figure 3-4-1. Observed, calculated and difference X-ray diffraction patterns of chabazite

TABLE 3-4-4. FINAL ATOMIC COORDINATES OF CHABAZITE

	x	y	z	Occupancy	U_{iso}(x1000)
			Rietveld refinement		
T	0.2292(8)	0.0004(9)	0.1038(6)	0.92(3)	–
O1	0.2000(17)	0.1000(8)	0.1261(17)	1/2	–
O2	0.1181(9)	-0.1181(9)	0.1270(14)	1/2	–
O3	0	0.3586(17)	1/2	1/2	–
O4	0.2632(15)	0	0	1/2	–
O5	0	0	0.5790(66)	0.07(1)	–
O6	-0.0986(26)	0.0986(26)	0.5451(45)	0.26(3)	–
Ca1*	1/2	1/2	0	0.08(1)	–
Ca2*	0	0	0.2261(28)	0.08(1)	–
Ca3*	0.2497(29)	-0.2497(29)	0.0143(66)	0.25(2)	–
Ca4*	0	0	0	0.07(1)	–
			Single-crystal refinement		
T	0.2285(1)	-0.0001(1)	0.1048(1)	0.94(1)	12
O1	0.1997(4)	0.0998(2)	0.1254(3)	1/2	39
O2	0.1206(2)	-0.1206(2)	0.1328(3)	1/2	41
O3	0	0.3474	0	1/2	33
O4	0.2618(4)	0	0	1/2	43
O5	0	0	0.5922(8)	0.11(1)	53
O6	-0.1053(10)	0.1053(10)	0.5257(12)	0.32(1)	193
Ca1*	1/2	1/2	0	0.08(1)	169
Ca2*	0	0	0.2333(10)	0.08(1)	105
Ca3*	0.2536(9)	-0.2536(9)	0.0213(20)	0.28(1)	795
Ca4*	0	0	0	0.02(1)	2904

*: Ca, K, Na, and Sr are expected to accompany the same crystallographic sites. The refined site occupancies represent such collective effect of disordered cation site occupancies not those of Ca alone.

TABLE 3-4-5. INTERATOMIC DISTANCES (Å) AND ANGLES (°) FOR CHABAZITE

	Single–crystal	Rietveld
T–O1	1.643(2)	1.65(1)
T–O2	1.636(4)	1.62(1)
T–O3	1.643(2)	1.64(1)
T–O4	1.632(2)	1.62(1)
<T–O>	1.638	1.63
O1–T–O2	108.8(2)	107.2(11)
O1–T–O3	111.1(2)	110.0(13)
O1–T–O4	111.4(2)	112.8(11)
O2–T–O3	106.3(2)	109.1(10)
O2–T–O4	111.1(2)	109.3(11)
O3–T–O4	108.0(2)	108.4(9)
<O–T–O>	109.4	109.5
(Ca1-O2)x2	3.200(5)	3.30(2)
(Ca1-O3)x4	3.462(1)	3.47(1)
(Ca1-O4)x2	3.278(5)	3.26(2)
(Ca1-O6)x2	2.568(15)	2.44(6)
(Ca2-O1)x3	2.877(10)	2.82(3)
(Ca2-O2)x3	3.237(7)	3.19(3)
Ca2-O5	2.614(19)	2.92(11)
(Ca3-O1)x2	3.467(31)	3.35(10)
Ca3-O2	3.590(14)	3.57(6)
(Ca3-O4)x2	3.450(18)	3.36(5)
Ca3-O6a	2.632(34)	2.98(12)
(Ca3-O6b)x2	2.890(25)	2.72(8)
(Ca4-O1)x6	3.032(5)	3.04(2)
(Ca4-O2)x6	3.489(3)	3.40(2)

a: 1/3+x,2/3+y,2/3+z; b:1/3+y,-1/3-x+y,-1/3-z.

Unit-cell dimensions

Unit-cell dimensions determined from Rietveld refinements are slightly greater than single-crystal values. This is similar to the results in the olivine and pyroxene study in 3.1. Nevertheless, the differences are less than 3σ of the single-crystal measurement and the differences are thus insignificant.

Atomic positions by interatomic distances and angles

In chabazite, the T-O distances of the Rietveld refinement agree with the single-crystal results. There are also close agreement in the O-T-O angles. Interatomic distances involving interstitial cations and the water molecules (O_5 and O_6) were not as well determined, giving differences in general of one magnitude greater than those of the T-O distances. Interstitial cations and water molecules in zeolites are highly mobile species (Liang & Sherriff 1993). What diffraction method sees, if the motions are slow enough, is the average electron density distribution of these species. To improve the refinement of atomic positions of these mobile species, it is necessary to couple the Rietveld refinement to MD calculation, in which the time averages of the trajectories of the individual interstitial species are taken as the average atomic positions.

Cation site-occupancies

The refinement of cation site-occupancies can be divided into two groups: that of the framework cations (T-sites) and that of the extra-framework cations (including water). Occupancies of the framework cations agree with the single-crystal results within one-sigma. Refinements of the site-occupancies of the non-framework cations were more difficult. The error ranges from 0 to 7σ.

Error analysis

In the half-normal probability analysis, the data points (Fig. 3-4-2) fall in a linear trend, with some random scattering. This indicates that no systematic error was present in either data set. The slope of ~ 1.4 indicates that the standard deviations in the Rietveld refinement are underestimated by a factor of 1.4.

3.5. Summary

Reliability of Rietveld method in both structural and quantitative studies has been assessed. Three categories of materials were considered in the structural study: (1) anhydrous silicates (olivine and pyroxene); (2) micaceous alumino-silicates (muscovite and phlogopite); (3) porous alumino-silicates (chabazite).

(1) For all three categories of materials, unit-cell dimensions and site-populations determined are compatible to those from single-crystal structure determinations on the same materials.

(2) For the relatively simple structures of category (1) materials, accurate and precise stereochemical details (*i.e.*, atomic positions) can be obtained, given that the phase under study is > 10 wt% in the powder mixture.

(3) For category (2) materials, it is possible to prepare nearly random powder mounts

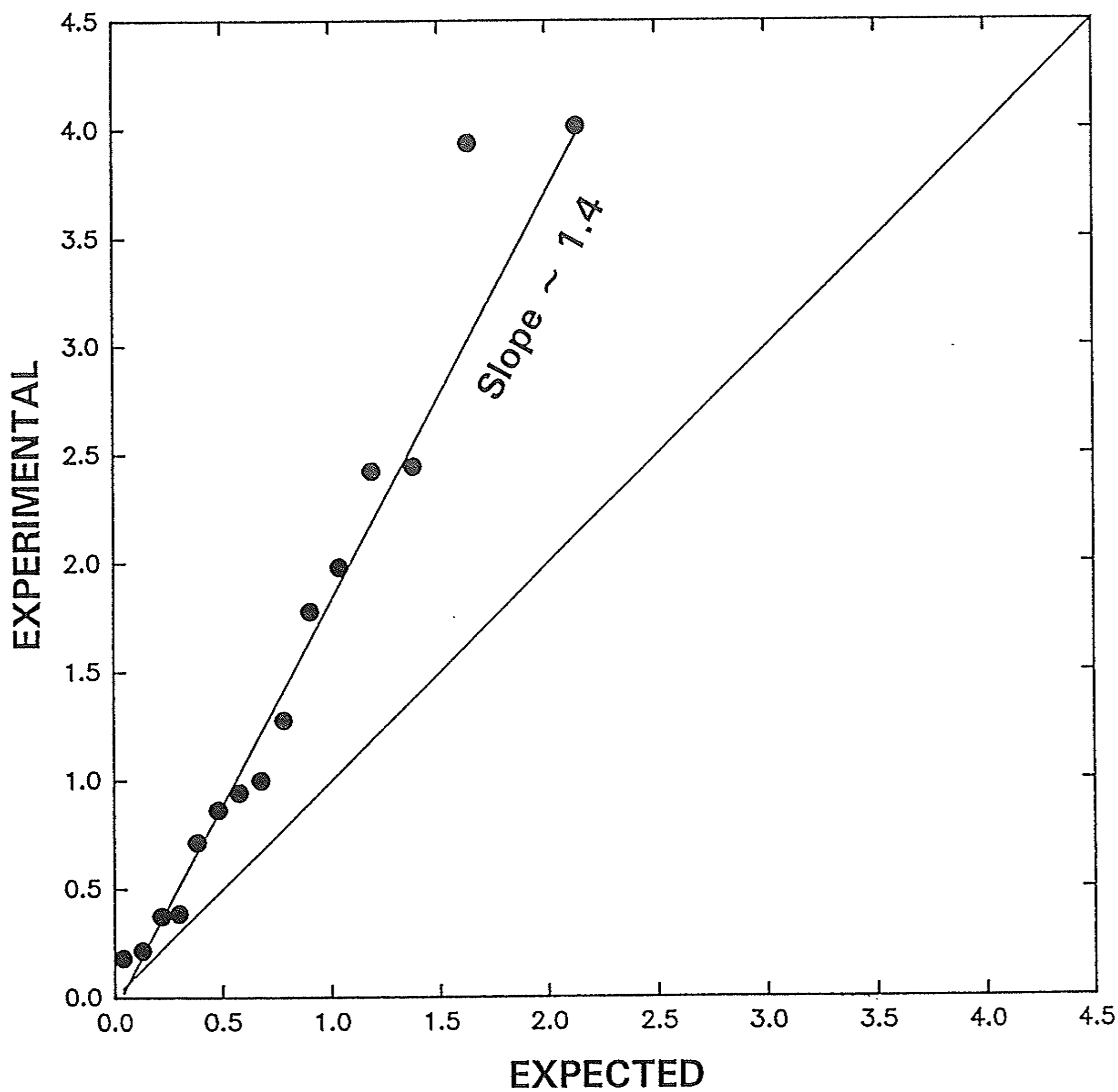

Figure 3-4-2. Half-normal probability analysis of chabazite

for intensity-data collection both in reflection and transmission geometries, which is of vital importance in ensuring successful Rietveld refinement.

(4) For category (3) materials, Rietveld refinement of the framework configuration is compatible to single-crystal refinement. Refinement of the interstitial configuration can still be successful, albeit the accuracy is inferior to that of the framework configuration.

The modal proportions of binary mixtures can be determined with an accuracy of 0.9% absolute and 3.0% relative; this is within the level of the assigned precision. The refined modal proportions are independent of step width over the range of 0.02–0.10° 2θ. However, all conclusions have to be made on the assumption of similar X-ray absorption coefficients for the component phases.

Chapter 4.

The Static Structure-Energy Minimization Method

Two kind of computer simulations of solids are usually used: the Static Structure-Energy Minimization (SSEM) and the Molecular Dynamics (MD) methods. SSEM method searches for minimum structure-energy (static). Vibrational energy, which is most sensitive to sample temperatures, is not considered; MD methods simulate atomic motions by solving Newton's equations of motion for individual atoms in the crystal. Temperature effects can be simulated explicitly with the MD method. However, only the SSEM method is considered here, as it is relatively highly developed and less computer-power demanding.

4.1. Interatomic Interactions

The basic particles in computer simulation of mineral structures are atoms (ions). Therefore, an accurate description of the interatomic interactions is essential in calculating the total energy and simulating atomic motion. The interaction potential, V, can be factored into separate summations (modified from Catlow 1990) as follows:

$$V=\sum_{ij} V'(r_i,r_j)+\sum_{ijk} V'(r_i,r_j,r_k)+\sum_{ijkl} V'(r_i,r_j,r_k,r_l)+ \;\ldots\ldots \qquad \text{4-1}$$

where the first term refers to the sum over all pairs of atoms, the second term to all three-atom interactions, *etc*. The primes indicate that no duplicate be counted in the summation. In silicates, the potential can best be approximated, using a modified ionic model, as (Purton & Catlow 1990)

$$U=U_c+U_R+U_B+U_S \qquad \text{4-2}$$

in which the U's are potentials associated with the Coulomb interaction (U_c), a two-atom repulsion (U_R), a three-atom interaction (U_B) which accounts for the covalency, and polarization (U_S):

$$U_C=\frac{1}{2}\sum_{i}^{(one\ cell)}\sum_{j\neq i}^{(all\ cells)} q_iq_jR_{ij}^{-1} \qquad \text{4-3}$$

$$U_R=\frac{1}{2}\sum_{i}^{(one\ cell)}\sum_{j\neq i}^{(all\ cells)} A_{ij}\exp(-r_{ij}/\rho_{ij})-C_{ij}r^{-6} \qquad \text{4-4}$$

$$U_B = \frac{1}{2}\sum_{ijk} K_{b,ijk}(\theta_{ijk} - \theta_0)^2 \qquad 4\text{-}5$$

$$U_S = k_s d^2 \qquad 4\text{-}6$$

in which i, j, k represent individual atoms (or ions), q_i is the formal charge of the i^{th} ion, r is the internuclear distance, d is the core-shell separation of a polarizable ion (*e.g.*, O^{2-}) approximated by the shell model (Dick & Overhauser 1958), Θ and Θ_0 are the calculated and ideal O-Si-O or O-Al-O bond angles, and (A_{ij}, ρ_{ij}, C_{ij}, $k_{b,ijk}$ and k_s) are the atom-specific parameters which can be obtained either by empirical fitting or by theoretical calculation (see later discussion). The total energy (structure-energy) can be calculated with respect to a given configuration, the starting structure model. The minimum-energy configuration can be sought, usually in the direction of steepest decent of the structure energy through computing the partial derivatives of the total energy with respect to the individual structural parameters.

Among the four interaction terms in eq. 4-2, the Coulombic interaction, U_c, can be calculated explicitly (*c.f.* eq. 4-3) over all atom(ion)-pairs in the system (the whole crystal). There are several ways of formulating the short-range repulsion, U_R. Apart from the Buckingham-type expression (eq. 4-4), there are two additional types of formulation currently in use: the Born-type and the Gilbert-type. The Born-type (Born & Huang 1954) expresses the interaction as

$$U_{ij} = \lambda_{ij}\exp(-r_{ij}/\rho_{ij}) \ , \qquad 4\text{-}7$$

in which U_{ij} is the repulsion between atoms i and j, r_{ij} is the interatomic distance, and λ_{ij} and ρ_{ij} are atom-pair-specific parameters which have to be determined. The Gilbert-type formulation (Gilbert 1968) is of the form

$$U_{ij}=f_0(B_i+B_j)\exp[\frac{A_i+A_j-r_{ij}}{B_i+B_j}] , \qquad 4\text{-}8$$

in which A_i, A_j and B_i, B_j are atom-specific parameters, and f_0 is a constant with a numerical value of 1 and units of $KCal{\cdot}mol^{-1}{\cdot}Å^{-1}$. The conversion between the atom(ion)-pair-specific parameters λ_{ij} and ρ_{ij} in the Born-type equation and the atom(ion)-specific parameters in the Gilbert-type equation (provided that the parameter, λ_{ij}, in the former assumes the unit of $KCal{\cdot}mol^{-1}$) is (Kunz & Armbruster 1992)

$$\begin{aligned}(A_i+A_j)&=\rho_{ij}\ln(\lambda_{ij}/\rho_{ij})\\(B_i+B_j)&=\rho_{ij}\end{aligned} \qquad 4\text{-}9$$

Unlike the summation of Coulombic terms which is over all atom pairs in the crystal, the summation of short-range repulsion terms is only over nearest neighbours, or second-nearest neighbours (when anion-anion interaction is considered).

The three-body interaction term, U_B in eq. 4-2 (*c.f.* eq.4-5), represents the covalency of a given interaction (Sanders *et al.* 1984), and is particularly important for Si-O and Al-O bonds in minerals. Therefore, the simulation in eq. 4-5 will not go beyond the nearest neighbour of a given atom (*e.g.*, Si or Al). The last term in eq. 4-2, the polarization term U_s, describes the polarization (usually of O^{2-} only) using the shell model of Dick & Overhauser (1958). The shell model is a simple mechanical model in which each ion consists of two components, a core of charge X and a shell of charge Y, connected by a harmonic spring. The sum of X and Y comprises the total formal ionic charge. The shell is massless, and the core has the mass of the ion. The ionic polarization is described by the displacement of the centre of the shell from that of the core (*c.f.* eq. 4-6). It is necessary to include polarization effects to study the lattice dynamics, dielectric and defect properties (Catlow 1990). Ionic polarization (and 3-body interaction) is now routinely used in the simulation of silicate minerals (*e.g.*, Bell *et al.* 1992; Collins & Catlow 1992; Winkler *et al.* 1991; Dove 1989; Purton & Catlow 1990).

In minerals containing the hydroxyl group, an intramolecular interaction is usually included, which can be approximated by a Morse function (Saul *et al.* 1985)

$$V_{OH}=D_e\{1-\exp[-\beta(r-r_e)]\}^2 \qquad 4\text{-}10$$

in which D_e is the hydroxyl bond-energy, β is a parameter to be determined, and r and r_e are the observed and the ideal O-H distances, respectively. Coulombic interaction between O and H of the hydroxyl, which assumes effective charges of -1.426 and 0.426 (determined by quantum mechanical calculation, Saul *et al.* 1985), respectively, has to be subtracted, as it is assumed that the Morse potential describes all components of the interactions between the two atoms involved in the calculation.

4.2. Static Structure-Energy Minimization

The Static Structure-Energy Minimization (SSEM) technique searches for a stable structural configuration in terms of the minimum structure energy in the vicinity of an approximate structure configuration. Given a structural configuration (unit-cell size, content and, in many cases, the arrangement of atoms (ions) in the unit-cell) and physical conditions (P, T), the Gibb's free energy of the system can be written (Burnham 1985) as

$$G=H-T\cdot S \qquad \text{4-11}$$

where the enthalpy, H, is

$$\begin{aligned} H&=U+P\cdot V \\ &=U_{coh}+U_{vib}+P\cdot V \end{aligned} \qquad \text{4-12}$$

and the entropy, S, is

$$S=S_{config.}+S_{vib} \qquad \text{4-13}$$

in which U is the internal energy, V the unit-cell volume, and the subscripts '*coh*', '*vib*' and '*config.*' denote cohesive, vibrational and configurational, respectively. In ordered structures (no positional disorder) $S_{config.} = 0$, and at ambient temperature and pressure conditions, the $P{\cdot}V$ term is negligible compared to U. Therefore the cohesive energy, which is termed structure energy here, U_{coh}, dominates the free-energy expression. With the static lattice approximation, similarly bonded structures are assumed to have similar vibrational characteristics. These slightly different structures can thus be compared in terms of structure energy, which is approximated by summing up all the interaction energies from eq. 4-3 to 4-6. A problem arises when calculating the Coulombic interaction term (eq. 4-3), which involves a slowly converging series (Boeyens & Gafner 1969). Ewald (1921) first showed that convergence can be accelerated by summing in reciprocal space. After development by Bertaut (1952), different extensions of the Ewald method appeared (Ohashi & Burnham 1972; Williams 1971). The program WMIN (Busing 1981) uses the Williams formulation of the Coulombic interaction energy:

$$U_c = \frac{1}{2Z}\sum_{i}^{one\ cell}\sum_{j=i}^{all\ cells}\frac{q_i q_j}{r_{ij}}[erfc(a)]$$

$$+\frac{1}{2\pi VZ}\sum_{h\neq 0}^{reciproc.\ latt.}\frac{|F_c(h)|^2}{|h|^2}\exp(-b^2) \qquad 4\text{-}14$$

$$-\frac{k}{Z}\sum_{i}^{one\ cell} q_i^2 ,$$

in which Z is the number of formula units per unit-cell, V is the unit-cell volume, h is the reciprocal-lattice vector, and k is the Ewald constant. The first summation in eq. 4-14 would be identical to the formal Coulombic interaction expression (*c.f.* eq. 4-3) if not for the additional term [*erfc(a)*], an error-function complement. The argument "*a*" increases as the distance r_{ij}, and the value of [*erfc(a)*] decreases from unity to zero. The denominator Z is introduced to ensure that the calculated energy represents that of the unit formula. Convergence is accelerated by the introduction of the error-function complement, but with the trade-off of loosing contributions to the Columbic energy at longer distances.

Such loss is compensated exactly by the second summation in reciprocal space, in which

$$F_c(h) = \sum_{i}^{one\ cell} q_i \exp(2\pi i \boldsymbol{h} \cdot \boldsymbol{x}_i) \qquad 4\text{-}15$$

where $|F_c(\boldsymbol{h})|$ is a structure-factor-like quantity in which the charge q_i replaces the atomic scattering factor in the usual X-ray expression ($\boldsymbol{h} = \{h,k,l\}$, $\boldsymbol{x}_i$ is a vector of coordinates for atom *i*). The convergence of the second sum in eq. 4-15 is accelerated by the term $exp(-b^2)$ whose argument increases as $|\boldsymbol{h}|$ [and $exp(-b^2)$] decreases from unity to zero. The third summation is, in effect, the contributions in the second sum when $\boldsymbol{h} = \boldsymbol{0}$.

After the calculation of the total structure energy, the minimum energy configuration can be sought by different methods. The program WMIN offers three methods: (1) Newton's method, which requires calculation of second derivatives of the energy with respect to the structural parameters; (2) the steepest-decent method, which calculates only the first derivatives; (3) the Rosenbrock search, a vector-search method which requires no derivatives. Newton's method is the best approach to locate a local energy minimum. However, it is easy to fall into false minima. Such method is most suitable when the structure is close to its global minimum-energy configuration. The Rosenbrock method is slower, but offers a better chance to locate true minimum, even from a saddle point (Busing 1981). It is desirable to start the minimization with the Rosenbrock search, and end it with Newton's method, or the method of steepest descent.

4.3. Parameterization of the interatomic potentials

Except for the Coulombic interactions (which can be calculated explicitly), the potential functionals in eq. 4-2 must be parameterized empirically or theoretically. The empirical approach fits the parameters to known structures, making no distinction between different sources of interaction (*e.g.*, ionic or covalent). The theoretical approach uses Modified Electron-Gas (MEG) theory (Muhlhausen & Gordon 1981) which considers purely ionic interaction and is confined to closed-shell systems. A quantum-mechanical approach may also be used to parameterize functions for interactions which cannot be done by empirical or MEG methods (*e.g.*, Morse function for the O-H interaction: Saul *et al.* 1985).

4.3.1. Empirical parameterization

In some simple cases, the short-range repulsion parameters, λ and ρ as in eq. 4-7, can be fitted to compressibility data (Kittel 1971) or vibrational spectra (Lasaga 1980; Bish & Burnham 1980). The more common approach is to fit the parameters to the known structure (Busing 1970; Catlow & James 1982; Catlow *et al.* 1982; Miyamoto & Takeda 1984; Matui & Busing 1984a,b; Kunz & Armbruster 1992). The short-range interaction parameters, q_i, can be adjusted by WMIN in a least-squares procedure (in which one or more related structures are entered as observations) by solving the following equation (Busing 1981):

$$\overline{\boldsymbol{B}}\, \boldsymbol{W} \boldsymbol{B}\, \Delta \boldsymbol{q} = - \overline{\boldsymbol{B}}\, \boldsymbol{W} \boldsymbol{d} \qquad \text{4-16}$$

where $d_i = \partial U/\partial p_i$, and $B_{ij} = \partial^2 U/\partial p_i \partial q_i$ are the derivatives of the energy with respect to structural parameter, p_i, and energy parameter, q_j; W is a weight matrix. The equation is solved for Δq_j, the change in the short-range parameter q_j that tends to minimize the values of d_i.

4.3.2. Parameterization using MEG theory

The Born-type short-range potential functional (eq. 4-7) can be fitted by a least-squares procedure to the results of an MEG calculation which gives the interaction energy of a given cation-anion pair as a function of the interatomic distance (Post & Burnham 1986). The MEG calculation gives the total interaction energy as (Burnham 1990)

$$U = U_C + U_{sr} + U_{se} \tag{4-17}$$

where U_C is a Coulombic interaction energy arising from the interaction of the non-overlap parts of the electron density of two ions, and can be calculated directly as in the standard ionic model for point charges (*c.f.*, eq. 4-3); U_{sr} is the short-range energy, and can be calculated from electron-gas theory (Gordon & Kim 1972; Waldman & Gordon 1979) which assumes that the total charge-density of the cation-anion pair, ρ_{ij}, is simply the direct sum of the individual charge-densities, ρ_i and ρ_j. The charge-density distribution-function ρ_i / ρ_j of the individual ion *i/j* can be calculated using Hartree-Fock Self-Consistent-Field theory. U_{sr} can be separated into three components, the kinetic E_{kin}, exchange E_{ex}, and correlation E_{corr} energies:

$$U_{sr}=F[E_{kin}(\rho),E_{ex}(\rho),E_{corr}(\rho)] \quad 4\text{-}18$$

in which ρ is the direct sum of ρ_i and ρ_j. The density function, ρ, needs to be modified (Waldman & Gordon 1979) from the simple sum in order to correct for errors in the predicted potential-well depths (Gordon & Kim 1972) arising from gradients in non-uniform densities. U_{se} in eq. 4-18 are the ion self-energies, corresponding to the energy differences between free ions and shell-stabilized ions. A shell-stabilized ion is a model (Muhlhausen & Gordon 1981) to account for the isotropic-size change of an ion due to a crystal field (by introducing a valence shell of fixed radius r_0 rather than the ionic radius).

4.3.3. Parameterization through quantum-mechanical calculation

When there is insufficient data to derive a reliable empirical potential, and it is not possible to use MEG theory (which is suitable for closed-shell ionic solids only), it is necessary to use quantum-mechanical calculation to derive the parameters for a given potential. The parameterization of a Morse potential for the OH^- group in crystalline NaOH (Saul *et al.* 1985) is an example. The crystal was divided into two regions: an inner quantum-mechanical cluster and outer point charges. The electronic wave function of the cluster (the inner region, embedded in the outer region of the point-charge model) was calculated with two separate basis sets for O and H, and Na, respectively by the Hartree-Fock Self-Consistent-Field (HF SCF) method. The energy of the cluster ions can thus be obtained from the calculated wavefunction. Such energies (as a function of internuclear separation in this particular case) can then be fitted to a Morse function.

4.4. Application of Static Structure-Energy Minimization: Examples

Quartz

Simulation of the quartz structure using an ionic model (Tossell 1980; Post & Burnham 1986) failed to describe the structure correctly, presumably due to the fact that the bonding in quartz bears strong covalent character. This led to the development of empirical methods that incorporate both ionic and covalent (angle-dependent) features (Sanders *et al.* 1984; Post & Burnham 1986). In the model of Sanders *et al.* (1984), Si and O are assigned their usual formal charge, and covalency is modelled by introducing a bond-bending term (the three-body interaction, *c.f.* eq. 4-5). The model reproduced the quartz structure well, and the simulation results agree well with a recent quantum-mechanical calculation (van Beest *et al.* 1990).

Forsterite

There have been a number of simulations of forsterite, Mg_2SiO_4 (Price & Parker 1984; Post & Burnham 1986; Price *et al.* 1987a,b; Jackson & Gordon 1988). These simulations differ principally with respect to the form and parameterization of the interatomic potentials. The work of Price *et al.* (1987a,b) gave the best fit of the calculated structure to the observed structure. The interatomic-potential parameterizations were adopted from different sources: Mg-O of the Born-Mayer form (Lewis 1985); O-O of the

Buckingham form (Saul *et al.* 1977); and Si-O of the Buckingham form (Sanders *et al.* 1984). In addition, a three-body interaction involving O-Si-O, and polarization effects involving O (approximated by the shell model) were incorporated; they were parameterized by fitting to the structure and elastic constants of quartz (Sanders *et al.* 1984).

Diopside

Diopside, $CaMgSi_2O_6$, is difficult to simulate (Catlow *et al.* 1982; Matsui & Busing 1984a; Post & Burnham 1986). The difficulties arise from the fact that all three O atoms in the asymmetric unit show strong deviations from Pauling's second rule (Burnham 1990). More recent simulations by Dove (1989) gave better results due to the implementation of three-body interactions and polarization effects. Modelling of diopside structure resumed (Winkler *et al.* 1991) with a modified force-constant, k, in the shell model, leading to improved agreement with the experimental structure details.

Al_2SiO_5 polymorphs

The Al_2SiO_5 polymorphs (andalusite, sillimanite and kyanite) have Al in various coordination. Each structure has one [4]-coordinated Si and one [6]-coordinated Al, and one Al in [5]-, [4]-, and [6]-coordination, respectively. The simulation of these minerals will test the transferability of the potential parameterizations and the soundness of the existing simulation model (which involves three-body interactions and polarization effects).

Winkler *et al.* (1991) used the same simulation procedure as for diopside in the simulation of the Al_2SiO_5 polymorphs, except that they had to consider different equilibrium O-Al-O angles for different coordination. The simulated results are generally good, except for discrepancies of 2-3% in the cell dimensions of kyanite and sillimanite. There was also a problem of an exceptionally short O_3-O_3 distance in andalusite (2.06 Å compared to 2.26 Å); this was attributed to an inadequacy in parameterizing the 3-body interaction constant for the [5]-coordinated Al.

Feldspar

The crystal structures of low albite ($NaAlSi_3O_8$), maximum microcline ($NaAlSi_3O_8$), and anorthite ($CaAlSi_2O_8$) were modelled by Purton & Catlow (1990). Emphasis was laid on the comparison between different simulation models and different potential parameterizations. The model that incorporates three-body interaction and polarization effects consistently performed better than the two-body rigid-ion model. It was also found that the MEG potentials for the cation-O interaction fit the feldspar structures better than any other empirical cation-O potentials. T-O-T bond angles are sensitive to different choices of cation-O interaction potentials. It was shown that, at the present level of approximation, the feldspar structure can be simulated accurately.

Micas

Muscovite, phlogopite and octahedrally-substituted phlogopite analogues have been modelled and compared to the structure and elastic and dielectric properties obtained experimentally (Collins & Catlow 1992). The interaction model was essentially identical with the ones used in the simulation of the other minerals (see above). One thing to be noted is that rather than using MEG-derived interatomic potentials for the cation-O interaction as in the feldspar modelling, empirical cation-O parameters were used throughout the work. However, all parameterizations were transferred from previous studies. The interaction within the OH group was approximated by a Morse potential whose parameterization was obtained from a previous *ab initio* study (Catlow 1977). The Si-Al disorder at the tetrahedral sites was approximated using a single hybrid species ($Al_{0.25}Si_{0.75}$) of charge +3.75 and with the short-range interaction of Si. One immediate shortcoming of this average treatment of the Si-Al order-disorder is that potential terms other than the Coulombic term are not averaged. The parameter values (*e.g.* the repulsion parameters) for Si, for example, are used as approximation of the average value. Jones *et al.* (1990) proposed an approach in simulating such disorder explicitly with the split-site model. A particular lattice site can have a fraction x of an ionic species A (*e.g.* Si^{4+}) and a fraction y of an ionic species B (*e.g.* Al^{3+}), where the position of each can be relaxed separately based on their own set of parameters for the various potential functions (see equations 4-3 to 4-9). Such treatment has the advantage that the overall calculation is still confined in the true unit-cell of the mineral under study. More general treatment of Si-Al order-disorder is through the construction of a super-cell in which possible Si-Al order-disorder schemes are treated explicitly in terms of structure-energy minimization (see discussion in the following section on Si-Al order-disorder).

The O-Al-O bond angles involving the [6]-coordinated Al were not considered in the short-range interaction calculation. In general, the simulated cell dimensions are within

1% of the experimental values. T-O bond distances are within 0.02 Å of the experimental values, showing the utility of using hybrid tetrahedral species in calculating short-range repulsions. The calculated O-H bond-distance also agrees closely with the experimental data, indicating the applicability of the Morse-potential model. Other structural details, including the corrugation of the basal surfaces (the departure from coplanarity of the basal O-atoms) and the mean Al-O distances, were also modelled well. Problems with the K-O potential (being too repulsive) was recognized, which cause the O_{basal}-T-O_{apical} angle and the tetrahedral rotation angle to be too small.

Al-Si order-disorder

In a series of papers (Bertram *et al.* 1990; Jones *et al.* 1990; Padlewski *et al.* 1992a,b), Price and coworkers studied Al/Si ordering in sillimanite and mullite. Super-cells consisting 3 to 8 unit-cells were used. In the relatively simple case where three unit- cells were used in the super-cell, there are a total of $\sim 3 \cdot 10^6$ possible configurations of arranging 12 Al and 12 Si atoms at the 24 tetrahedral sites. These configurations were subdivided into 43 groups according to the nature of first, second, third, ... nearest neighbours of the Al atom at the tetrahedral site. At least 3 configurations in each group were considered and full-energy minimization performed. Löwenstein's rule was clearly displayed, as configurations having Al-Al nearest neighbours are either not stable (non-convergent during the EM processes) or give large structure-energies. The energy associated with Al/Si ordering for nearest-neighbour sites is 0.97 eV in the *ab*-plane, and 0.56 eV perpendicular to the *ab*-plane. The interaction of the second-nearest neighbours was significant, whereas that of the more distant neighbours was negligible.

4.5. Summary

Static Structure-Energy Minimization (SSEM) of crystal structure is a semi-empirical method that involves establishing and parameterizing an interaction model. Current SSEM models include individual terms of Coulombic-interaction, repulsion, covalency and polarization, and assumes that the interaction terms are additive. Each interaction is represented by an analytical function with (except the Coulombic term) parameter(s) to be determined. The parameterization can be done by any or all of the following means: (1) fitting to known crystal structures; (2) fitting to the result of calculation of the Modified Electron Gas (MEG) type that consider ionic interaction only between closed-shell ions; (3) fitting to result of quantum-mechanical calculation. Parameterization from all three approaches are in use, and were shown to be transferable between different structures. The current SSEM method is not only capable of reproducing details of crystal structure (unit-cell dimensions and atomic coordinates), with minor modification, it is also capable of reproducing physical properties. The SSEM method can be important prediction tools in crystal-structure studies of powder materials for which experimental data (powder diffraction and spectroscopic observations) may not be in such a resolution that certain structural details, such as the light-atom position, be unambiguously determined.

Chapter. 5

Calculating H-atom Positions in Mica and Clay Structures

Clay minerals are of both geological and environmental importance, and have industrial importance in the oil, paper and ceramic industries. However, the clay minerals are usually very fined-grained. Powder-diffraction methods are usually used in the crystal-structure determination of the clay minerals. However, due to the nature and currently limited resolution of powder-diffraction methods, determination of H-atom positions in the clay structures can be very difficult. Hydrogen atoms, combined with the hydroxyl-oxygens, constitute part of the nearest coordination sphere of the octahedral cations (see later discussion on the clay structures). Difficulty in locating H-atom(s) originated from the fact that H-atom is not a strong X-ray scatterer, and it causes strong incoherent neutron scattering. X-ray diffraction method relies on the different scattering power of an atom to locate that atom in the structure. Hydrogen, as part of the OH-group, has less than one electron associated to it, which makes its scattering power vary weak compared to the other atoms commonly found in clay minerals (Fig. 5-1). Extremely high-quality (free of deformation and stacking-disorder) crystals are needed in order to be able to obtain intensity data to reliably determine the H-atom position(s). However, this is very rarely the case. Stacking disorder is very common in clay minerals (Brindley 1980, see also 3.2.). Neutron diffraction may in some cases offer a solution to the problem (as demonstrated by examples cited in this chapter that are to be discussed later). However, the technique is in many ways limited in its application. Neutron diffractions, especially those with high-flux neutron source, are not as widely available as X-ray diffraction. Furthermore, H causes strong incoherent scattering cross section due to the scattering from the two possible nuclear spin states of ^1H (von Dreele 1989). A diffractogram of high signal-to-noise ratio may be very difficult to obtain because of this exceptionally high incoherent background contribution. Deuterating H-containing materials to replace H by D can eliminate the problem of high incoherent scattering. However, the deuteration process is not only expensive and time-consuming, there is also the problem, for natural H-containing materials, of incomplete deuteration. As D has positive neutron diffraction length, whereas H has negative diffraction length, scattering from residual H will cancel the scattering from D, making the detection of D or H difficult. Therefore, it is necessary, or at least helpful, to use theoretical calculation to assist in locating H-atom positions in clay minerals.

Micas are minerals that closely resemble the clay minerals. However, unlike clay minerals, micas usually occur in large crystals, which makes detailed single-crystal structure study possible. Hydrogen-atom positions in several mica minerals had been determined experimentally using single-crystal neutron diffraction, in conjunction with single-crystal X-ray diffraction experiments. Reproducing these H-atom positions using computer simulation (the SSEM technique) will be a step forward in assisting determining of H-atom positions in clay minerals using powder diffraction method.

Theoretical calculation of H-atom positions or O-H orientations in phyllosilicates began in the early 1970's. The ionic model was used by then and only the electrostatic (Coulombic) energy was calculated with respect to O-H orientation in the structure (Giese 1971). The approach was applied to 31 dioctahedral and trioctahedral hydrated phyllosilicates to determine their O-H orientations (Giese 1979, 1984). This early work was not concerned with O-H distances. Total energies, with the calculation limited to unit cell (in spite of the electrostatic interaction being a very slowly converging quantity in terms of interatomic distance; see equation 4-3), were calculated for a selected number of O-H orientations, and the one that gave the lowest energy was suggested to be the energetically favourable orientation. Such calculation gives qualitative idea of the O-H orientations. The method was further developed (Abbott *et al.* 1989; Abbott 1992) by considering the Born repulsion (equation 4-7) and using energy-minimization techniques in the calculation. The O-H distance is not fixed in this calculation, which includes any number of nearest and non-nearest neighbours of the H-atom in the calculation of the

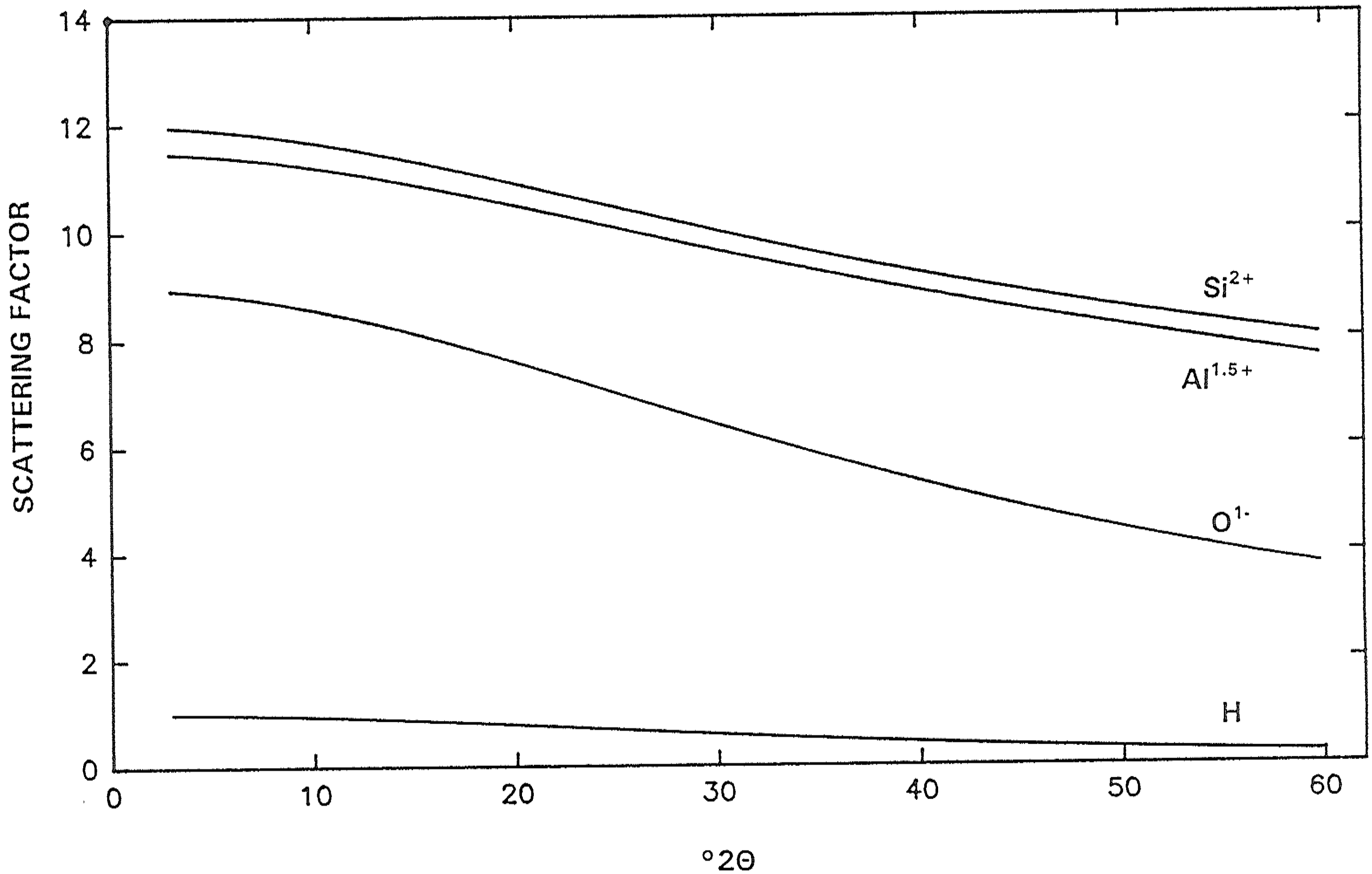

Figure 5-1. X-ray scattering power of H-atom, in comp:)n with those of the other atoms commonly found in clay minerals

electrostatic and repulsion terms. Potential sites (the vicinity of each hydroxyl O-atom) for the H-atoms were considered one at a time. Given an arrangement of the non-H atoms within certain radius from the potential H-atom site, equilibrium (with minimum structure energy) H-atom position can be sought and taken as the calculated H-atom position. This method reproduced H-atom positions in a number of mica and clay species. One problem with this method is that different short-range repulsion parameters have to be used for different environments of the OH-group (environment that corresponds to trioactohedral mica or brucite-type structures). This hinders the general applicability of the method and may raise uncertainty in the final results. Possible sources of the problem may be (1) the truncation of the Coulombic summation at ~ 4.5 Å from the H-atom; (2) omission of three-body interaction term. The method is further limited in that it can consider only one H-atom position at a time. When a structure contains more than one unique H-atom positions, possible strains arising from interaction of the H-atoms cannot be realised.

Developed in parallel is the SSEM method for periodically repeating structures that was reviewed in chapter 4, which had been used to calculate H-atom positions in kaolinite (Collins & Catlow 1991), and, with minor modification, the whole structures and the physical properties of micas (Collins & Catlow 1992). The agreement of the calculated structures and their corresponding physical properties to the observed indicated that the interaction model used in the calculation (including electrostatic, repulsion, polarization, and bond-bending terms) is applicable in general to micas and clay minerals. Although semi-empirical molecular-orbital calculation (Peterson *et al.* 1979) and periodic *ab-initio* Hartree-Fock calculation (Hess and Saunders 1992) have been used to study the O-H orientations and individual H-atom positions, it is chosen here to use the more generally applicable SSEM method for the calculation of H-atom positions in the mica and clay minerals. All H-atom positions in a structure will be considered simultaneously by fixing the rest of the structures (unit-cell dimension, and atomic coordinates of non-H atoms) at the values determined by single-crystal diffraction experiments. One objective of the work is also to resolve uncertainties in the interpretation of structural configurations concerning H-atom positions in several micas and clay minerals.

5.1. Crystal Structures of Micas and Clay Minerals

Micas and clay minerals are members of phyllosilicates in which the TO_4 tetrahedra are interconnected laterally to form two-dimensionally extending sheet of composition T_2O_5 (T = Si, Al, or Fe^{3+}) (Fig. 5-2 and 3). Each tetrahedron shares three of its corners (O-atoms) with the neighbouring tetrahedra, with the fourth corner (the apical O-atom) points in a direction normal to the sheet. These apical O-atoms form part of the octahedral sheet immediately adjacent to the tetrahedral sheet. Apart from the apical O-atoms, the common plan of junction between the tetrahedral and octahedral sheets also consists of OH-groups (may be replaced by F-atoms). In the centre of the octahedra may be Mg, Al, Fe^{2+} and Fe^{3+}, but other atoms (cations) of similar size (Li, Ti, V, Cr, Mn, Co, Ni, Cu and Zn) may also be present. Out of every three octahedra for a given species, the average occupancies of the octahedra can range from 2 to 3, with species at each end termed di- and tri-octahedral, respectively. The tetrahedral and the octahedral sheets

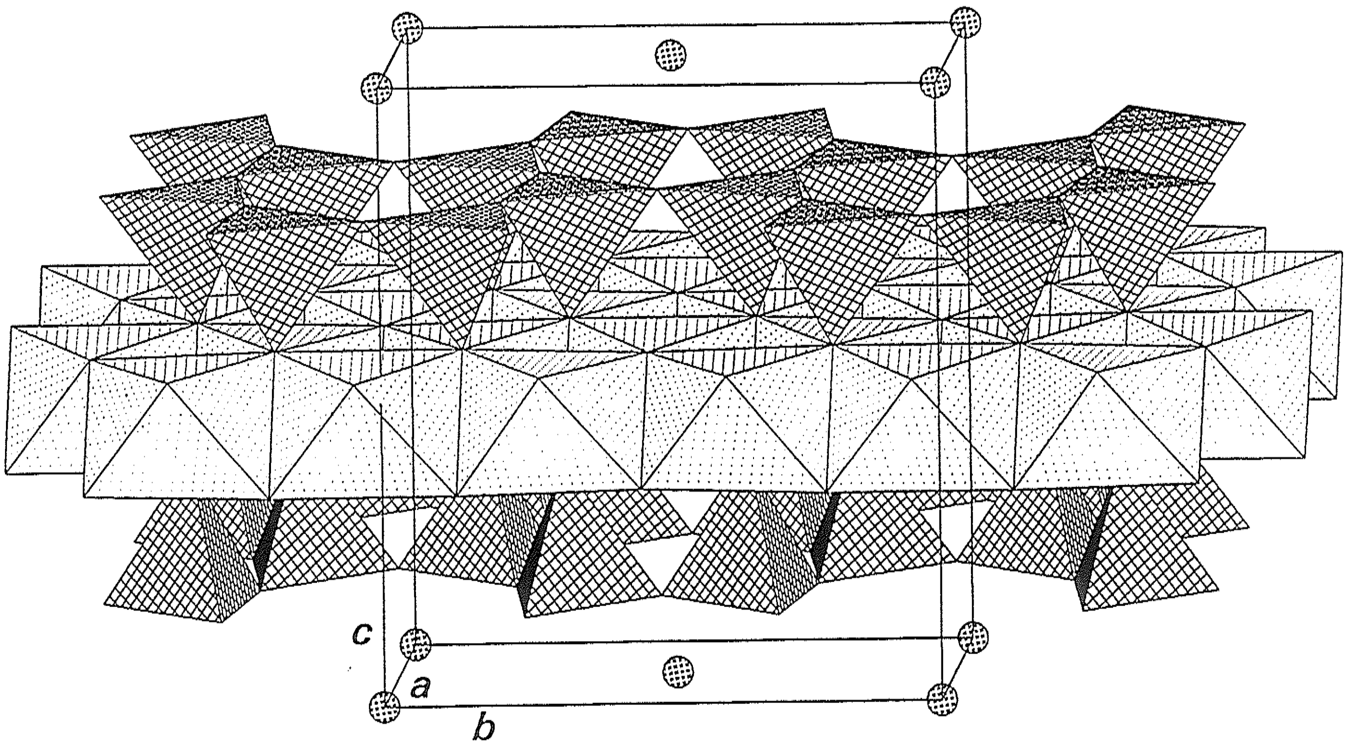

Figure 5-2. Structure model of a 2:1 mica (phlogopite). Structural parameters from Chapter 3.

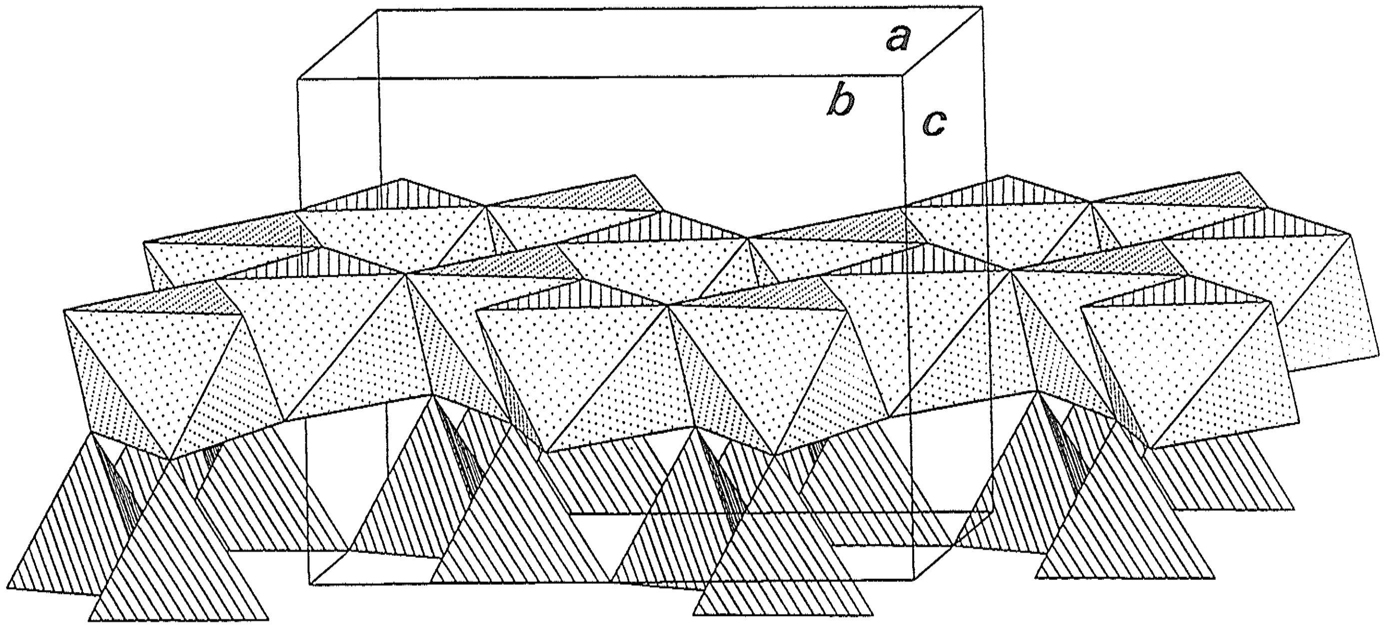

Figure 5-3. Structure model of a 1:1 clay mineral (kaolinite). Structural parameters from Bish (1993)

combine into layers that are basic building blocks of micas and clay minerals. An individual layer may be a 2:1, or an 1:1 layer, depending on the ratio of the number of tetrahedral sheets to that of the octahedral sheet. A 2:1 layer consists of two opposing tetrahedral sheets (with the apices of the tetrahedra in one sheet pointing to those of the other sheet), with an octahedral sheet sandwiched in between (Fig. 5-2). Alkaline or alkaline-earth cations (K, Na, Li, Ca) may be found in between layers. An 1:1 layer consists of one each of the tetrahedral and octahedral sheets (Fig. 5-3), where the plan of anions in the octahedral sheet not shared by the tetrahedral sheet consists entirely of OH-groups (Fig. 5-4).

In real mica or clay structures, individual layers may be stacked to show periodicity in translation or rotation. Different (periodical) stacking sequences give rise to different *polytypes*. Smith & Yoder (1956) and Bailey (1969) showed that there are at least 12 possible polytypes for micas and clay minerals. Six of the relatively common polytypes are shown in Figure 5-5.

The layers can also stack in a random fashion to a certain degree. Diffraction studies of these species will be more difficult.

5.2 The Calculation

The SSEM program used in the present work is WMIN (Busing 1981). A subroutine, THRBD, was added to the original program to include three-body and polarization terms (see equation 4-5 and 4-6), which was tailored for silicate structures.

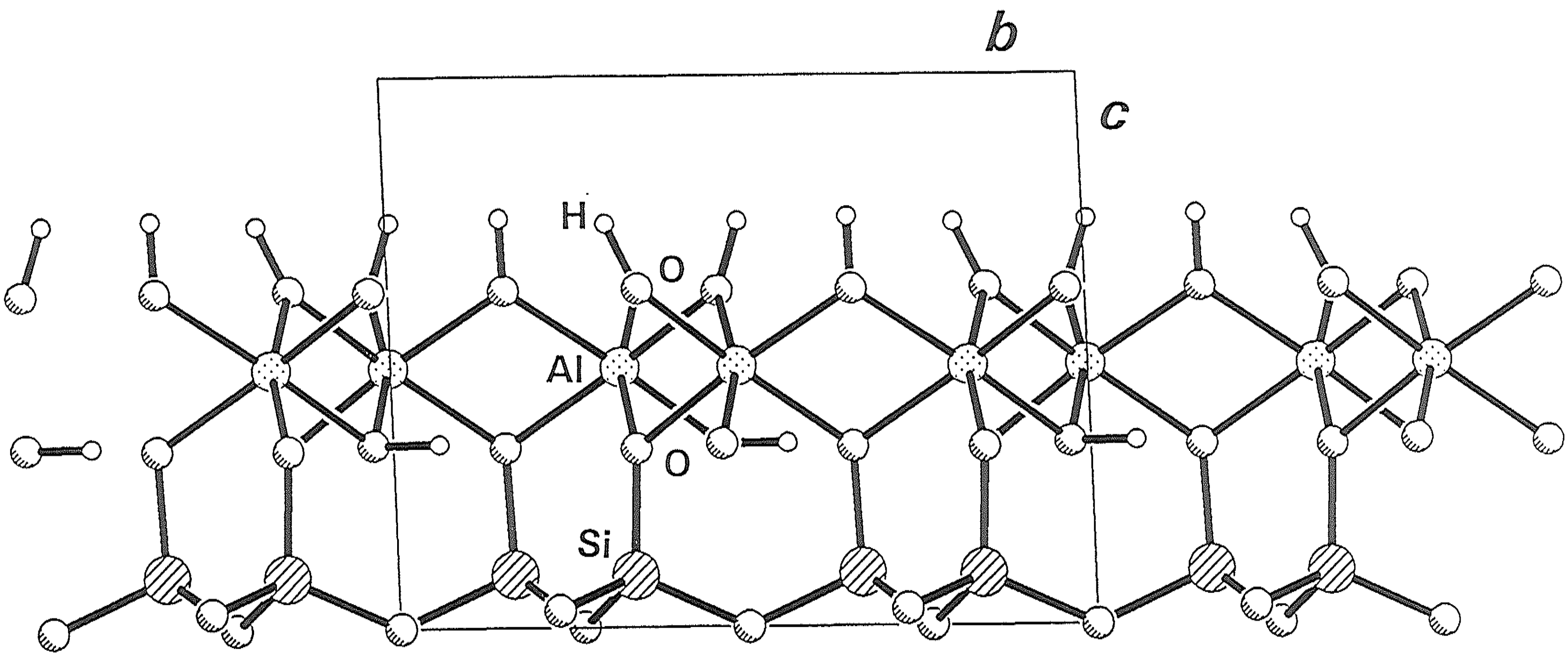

Figure 5-4. Stick-and-ball representation of the 1:1 clay mineral (kaolinite example). Structural parameters from Bish (1993)

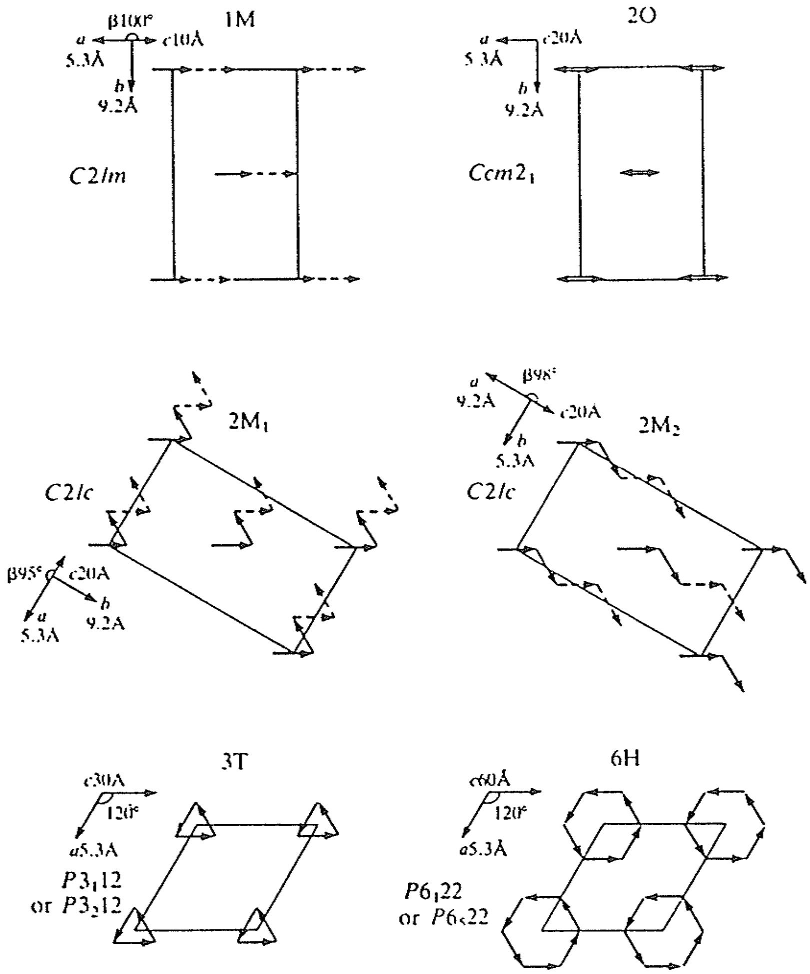

Figure 5-5. The six common polytypes (from Smith & Yoder, 1969) of micas. The arrows are the interlayer stacking vectors. Full line vectors show the layer stacking in one unit cell, whereas broken line vectors show the positions of layers in the next unit cell. The base of the unit cell is shown by thin lines, and the space group and lattice parameters are listed by the side of the diagram in each case.

Minerals selected in the study (Table 5-2-1) have near-end-member chemical compositions and have H-atom positions determined by neutron diffraction. These minerals can be divided into the following groups:

(1) Minerals with non-split H-atoms: phlogopite, chlorite, kaolinite;

(2) Minerals with split H-atom positions: margarite;

(3) Minerals with reasonably well-determined H-atom positions, but with rooms for different interpretation of the results: muscovite, dickite.

All minerals were assumed to have end-member chemical compositions in the calculation. There are two stages in determining the H-atom positions:

Stage 1: locate H-atom position(s) (presumed unknown) in the vicinity of the corresponding hydroxyl O-atom(s). Unit-cell dimensions and non-H atomic coordinates were all fixed at the experimentally determined values. The program was set up such that H-atoms can be positioned on the same site as those of the corresponding hydroxyl O-atoms. Space-group symmetry of the crystal determined experimentally based on the arrangement of the non-H atoms is used, and H-atom(s) are forced, at the stage, to obey this symmetry;

Stage 2: relax the symmetry of the structure, now including the H-atom position(s) located in stage 1, to space-group symmetry $P1$. All H-atoms can vary their positions independently, with the unit-cell dimensions and the non-H atomic positions still fixed at the experimental values. Deviation, if any, of the H-atom positions from the symmetry of the non-H atoms will be detected at this stage (see later discussions on individual species).

Interaction potentials used in the SSEM calculations include Coulombic interaction,

TABLE 5-2-1. MICAS AND CLAY MINERALS SELECTED FOR STUDY

Mineral	Chemical Formula	Polytype	References*
Phlogopite	$KMg_3(AlSi_3)O_{10}(OH)_2$	1*M*	Rayner, 1974
Chlorite	$Mg_{12}[Si_8O_{20}](OH)_{16}$	IIb_4	Joswig *et al.* 1980
Margarite	$Ca_2Al_4(Si_4Al_4)O_{20}(OH)_4$	$2M_1$	Joswig *et al.* 1983
Kaolinite	$Al_2Si_2O_5(OH)_4$	1*M*	Bish, 1993
Muscovite	$KAl_2(AlSi_3)O_{10}(OH)_2$	$2M_1$	Rothbauer, 1971
Dickite	$Al_2Si_2O_5(OH)_4$	1*M*	Bish & Johnston, 1993

* Reference to structure refinements from neutron-diffraction data.

TABLE 5-2-2. POTENTIAL PARAMETERS USED IN THE STRUCTURE-ENERGY CALCULATION

Short-range repulsion: Born/Buckingham-type and Morse potentials*				
	λ (kCal/mol)	ρ (Å)	C (kCal/mol·$Å^{-6}$)	Ref.
$Si^{4+} - O^{2-}$	29607.352	0.3025	245.860	[1]
$Al^{3+} - O^{2-}$	33675.03	0.29912		[2]
$K^{1+} - O^{2-}$	1505142.4	0.2134		[3]
$O^{2-} - O^{2-}$	524946	0.149	642.9	[1]
	D_e (kCal/mol)	r_e (Å)	β ($Å^{-1}$)	
$H^{0.426+}$ - $O^{1.426-}$	162.63	0.9485	2.1986	[4]
Bond-bending interaction**				
	k_B (kCal/rad^2)		θ_O (°)	
$O^{2-} - Si^{4+} - O^{2-}$	48.3631		109.47	[1]
Shell-core interaction between O-shell and O-core***				
		k_P (kCal/Å^2)		
$O(core)^{+0.86902} - O(shell)^{-2.86902}$		1728		[1]

* *c.f.* equations 4-7, 4-4 & 4-10; ** *c.f.* equation 4-5; *** *c.f* equation 4-6

[1] Sanders *et al.* (1984); [2] James (1979); [3] Post & Burnham (1986); [4] Saul *et al.* (1985).

repulsion, covalency and polarization (of the forms of equation 4-3 to 4-6). For the interaction between O and H of the OH groups, a Morse potential was used (*c.f.* equation 4-10). Parameters used in these potentials are given in Table 5-2-2. Isomorphous replacement, such as Al $\rightarrow$ Si in muscovite, was not considered in the energy calculation, except that an effective average formal charge was used for the *T* atoms in the calculation of the Coulombic energy. The potential terms involving (Si,Al)–O were approximated using the parameterization for Si–O. Although such practice has been suggested to be undesirable (*e.g.* Post & Burnham 1986), reasonable success had been reported using this approach in modelling a number of mineral structures (*e.g.* Collins & Catlow 1992, Abbott *et al.* 1989). Furthermore, the calculation focuses on long-range symmetry, rather than the shot-range symmetry, so that the results from the calculation can be compared directly to the results of diffraction experiment, or be verified using diffraction methods.

In the SSEM calculation, 6 cycles of Rosenbrock search was used to reduce the probability of the minimization falling into a local minimum. The search was then switched to Newton's method to speed up the process.

5.3. Results and Discussion

The micas and clay minerals selected in the study are among their most common polytypes (Bailey 1980; *c.f.* Table 5-2-1), and the results and discussions below will be limited to the polytype considered of each mineral.

5.3.1. Phlogopite, Chlorite and Kaolinite

H-atom position(s) calculated with symmetry constraints of *C2/m*, $C\bar{1}$ and *C*1 for phlogopite, chlorite and kaolinite, respectively, are given in Table 5-3-1. H-atom positions calculated with symmetry relaxed to *P*1 are given in Table 5-3-2.

Phlogopite has only one unique H-atom position, and the calculation reproduces the H-atom position determined by neutron diffraction to the third decimal place in the fractional atomic coordinate (Table 5-3-1), which is within 2σ (σ = estimated standard deviation) of the experimental value. For chlorite and kaolinite that have multiple unique H-atom positions in their structures, the accuracy to the third decimal place were still achieved for the bulk of the coordinates, with small proportions of the coordinates giving accuracies to the second decimal place (Table 5-3-1). In chlorite, the difference ranges from 0 to 34σ, with an average of 10σ. Such difference may be attributed to the fact that while the calculation assumed ideal chemical composition (Table 5-1-1), the mineral in the neutron diffraction study shows chemical composition slightly off ideal (Joswig *et al.* 1980). Nevertheless, even the largest difference, at the *x*-coordinate of H_2 of -0.017, represents only a shift along the *a*-axis (axial length of 5.3266 Å) of 0.09 Å, which is about 1/10 of the average O-H distance of 1.00 Å (Shannan 1979). Comparison of the calculated and the observed coordinates for kaolinite is slightly more difficult, as the standard deviations of the observed coordinates, determined by powder neutron diffraction, vary from 0.0001 to 0.003 (by a factor of 30). It should be noted that (1) the calculated coordinates that associate with some of the greatest differences (at $H_1(z)$, $H_3(x)$, $H_4(x)$ of 0.011, -0.016 and 0.041, respectively) correspond to the experimentally determined

TABLE 5-3-1. CALCULATED H-POSITIONS (FIRST ROWS) IN PHLOGOPITE, CHLORITE AND KAOLINITE WITH SYMMETRY CONSTRAINTS, COMPARED TO THOSE DETERMINED EXPERIMENTALLY (SECOND ROWS). DIFFERENCES ARE GIVEN IN THE THIRD ROWS.

		x	*y*	*z*
Phlogopite*	H	**0.0981**	**0.0000**	**0.3050**
$KMg_3(AlSi_3)O_{10}(OH)_2$		0.0992(40)	0.0000	0.3081(15)
		-0.0011		-0.0031
Chlorite**	H_1	**0.7129**	**0.3418**	**0.1405**
$(Mg_{12})(Si_8O_{20})(OH)_{16}$		0.7139(5)	0.3339(3)	0.1399(3)
		-0.0010	0.0079	0.0006
	H_2	**0.1023**	**0.0131**	**0.3632**
		0.1193(5)	0.0054(3)	0.3632(2)
		-0.0170	0.0076	0.0000
	H_3	**0.1406**	**0.3326**	**0.3627**
		0.1301(5)	0.3353(3)	0.3629(2)
		0.0105	-0.0027	-0.0002
	H_4	**0.6184**	**0.1585**	**0.3625**
		0.6143(5)	0.1594(3)	0.3635(2)
		0.0041	-0.0009	-0.0010
Kaolinite***	H_1	**0.152**	**0.0624**	**0.337**
$Al_2Si_2O_5(OH)_4$		0.145(3)	0.0651(1)	0.326(6)
		0.007	-0.0027	0.011
	H_2	**0.063**	**0.1681**	**0.736**
		0.063(3)	0.1638(1)	0.739(1)
		0.000	0.0043	-0.003
	H_3	**0.020**	**0.5111**	**0.731**
		0.036(3)	0.5057(2)	0.732(1)
		-0.016	0.0054	-0.001
	H_4	**0.575**	**0.3201**	**0.736**
		0.534(3)	0.3154(2)	0.728(1)
		0.041	0.0047	0.008

* observed H-position taken from Rayner (1983); ** observed H-position taken from Joswig *et al.* (1980); *** observed H-positions taken from Bish (1993)

TABLE 5-3-2. H-ATOM POSITIONS IN PHLOGOPITE, CHLORITE, AND KAOLINITE PROJECTED BACK INTO THE ASYMMETRIC UNITS AFTER SSEM WITHOUT SYMMETRY CONSTRAINTS

Symmetry operation	*x*	*y*	*z*
		Phlogopite	
H(11) *x, y, z*	.0976	.0000	.3035
H(12) *-x,y,-z*	.0976	.0000	.3035
H(13) *1/2+x,1/2+y,z*	.0976	.0000	.3035
H(14) *1/2-x,1/2+y,-z*	.0972	.0000	.3035
	------	------	------
Mean	**.0975**	**.0000**	**.3035**
Determined with symmetry	.0981	0	.3050
Experimental*	.0992(40)	0	.3081(15)
		Chlorite	
H(11) *x, y, z*	.7134	.3418	.1420
H(12) *1/2+x,1/2+y,z*	.7134	.3418	.1420
H(13) *-x,-y,-z*	.7134	.3418	.1420
H(14) *1/2-x,1/2-y,-z*	.7134	.3418	.1420
	------	------	------
Mean	**.7134**	**.3418**	**.1420**
Determined with symmetry	.7129	.3418	.1405
Experimental**	.7139(5)	.3339(3)	.1399(3)
H(21) *x, y, z*	.1004	.0143	.3616
H(22) *1/2+x,1/2+y,z*	.1004	.0143	.3616
H(23) *-x,-y,-z*	.1004	.0143	.3616
H(24) *1/2-x,1/2-y,-z*	.1004	.0143	.3616
	------	------	------
Mean	**.1004**	**.0143**	**.3616**
Determined with symmetry	.1023	.0131	.3632
Experimental**	.1193(5)	.0054(3)	.3632(2)
H(31) *x, y, z*	.1420	.3326	.3610
H(32) *1/2+x,1/2+y,z*	.1420	.3326	.3610
H(33) *-x,-y,-z*	.1420	.3326	.3610
H(34) *1/2-x,1/2-y,-z*	.1420	.3326	.3610
	------	------	------
Mean	**.1420**	**.3326**	**.3610**
Determined with symmetry	.1406	.3326	.3627
Experimental**	.1303(5)	.3353(3)	.3629(2)

TABLE 5-3-2. (continue)

Symmetry operation	*x*	*y*	*z*
H(41) *x, y, z*	.6171	.1577	.3607
H(42) *1/2+x,1/2+y,z*	.6171	.1577	.3607
H(43) *-x,-y,-z*	.6171	.1577	.3607
H(44) *1/2-x,1/2-y,-z*	.6171	.1578	.3607
	------	------	------
Mean	**.6171**	**.1577**	**.3607**
Determined with symmetry	.6184	.1585	.3625
Experimental**	.6143(5)	.1594(3)	.3635(2)
		Kaolinite	
H(11) *x, y, z*	.155	.0648	.344
H(12) *1/2+x,1/2+y,z*	.155	.0648	.344
	------	------	------
Mean	**.155**	**.0648**	**.344**
Determined with symmetry	.152	.0624	.337
Experimental***	.145(3)	.0651(1)	.326(2)
H(21) *x, y, z*	.062	.1683	.740
H(22) *1/2+x,1/2+y,z*	.062	.1683	.740
	------	------	------
Mean	**.062**	**.1683**	**.740**
Determined with symmetry	.063	.1681	.736
Experimental***	.063(3)	.1638(1)	.739(1)
H(31) *x, y, z*	.020	.5096	.735
H(32) *1/2+x,1/2+y,z*	.020	.5097	.735
	------	------	------
Mean	**.020**	**.5097**	**.735**
Determined with symmetry	.020	.5111	.731
Experimental***	.036(3)	.5057(2)	.732(1)
H(41) *x, y, z*	.577	.3180	.739
H(42) *1/2+x,1/2+y,z*	.577	.3180	.739
	------	------	------
Mean	**.577**	**.3180**	**.739**
Determined with symmetry	.575	.3201	.736
Experimental***	.534(3)	.3154(2)	.728(1)

* Rayner (1974); ** Joswig *et al.* (1980); *** Bish (1993)

coordinates that give the largest standard deviations (0.006, 0.003 and 0.003, respectively); (2) the coordinates (*y*-coordinates of all the H-atoms) determined to a higher precision (with standard deviations of 0.000n) all agree with the calculated to the third decimal place that has been shown to be the accuracy of the SSEM method. These two points suggest that both theoretical and experimental studies with respect to the crystal structure of kaolinite are needed.

After SSEM calculation with symmetry relaxed, the H-atom positions obtained for each of the three minerals (Table 5-3-2) retain the corresponding symmetry of the non-H atom configuration. There is extensive evidence (Farmer & Russel 1964; Rayner 1974; Joswig *et al.* 1980; Johnston *et al.* 1990; Hess & Saunders 1992; Bish 1995), that H atoms in these minerals do obey the symmetry of the non-H atoms. Such a result indicates that the SSEM procedure is reliable in reproducing H-atom positions in environments with site symmetry higher than $P1$.

5.3.2. Margarite

Margarite is unique in that H-atom positions appear in pairs and are so close together that they can be represented by split H-atom model (Joswig *et al.* 1983). Reproducing such split-atom model will be a more stringent test of the SSEM procedure.

From the non-H configuration of Joswig *et al.* (1983), assuming non-split H-atoms that obey the *Cc* symmetry of the non-H atoms, SSEM calculation generated two H-atom positions (Table 5-3-3). It is interesting to note that these two H-atom positions are very close (in errors of ~ 0.01 in fractional coordinates) to H(11B) and H(12B), respectively,

TABLE 5-3-3. H-ATOM POSITIONS IN MARGARITE CALCULATED WITH SYMMETRY CONSTRAINT *Cc* AND ASSUMING NON-SPLIT H-ATOMS

	x	*y*	*z*
H1	**0.449**	**0.581**	**0.107**
H(11B)*	0.439(3)	0.591(2)	0.098(1)
diff.	0.010	-0.010	0.009
H(11A)*	0.3663(7)	0.6550(5)	0.0620(3)
H2	**0.566**	**0.386**	**0.904**
H(12B)*	0.561(4)	0.399(3)	0.905(1)
diff.	0.005	-0.013	0.001
H(12A)*	0.6325(9)	0.3452(5)	0.9396(4)

* Split H-atom positions determined from neutron diffraction experiment (Joswig *et al.*, 1983)

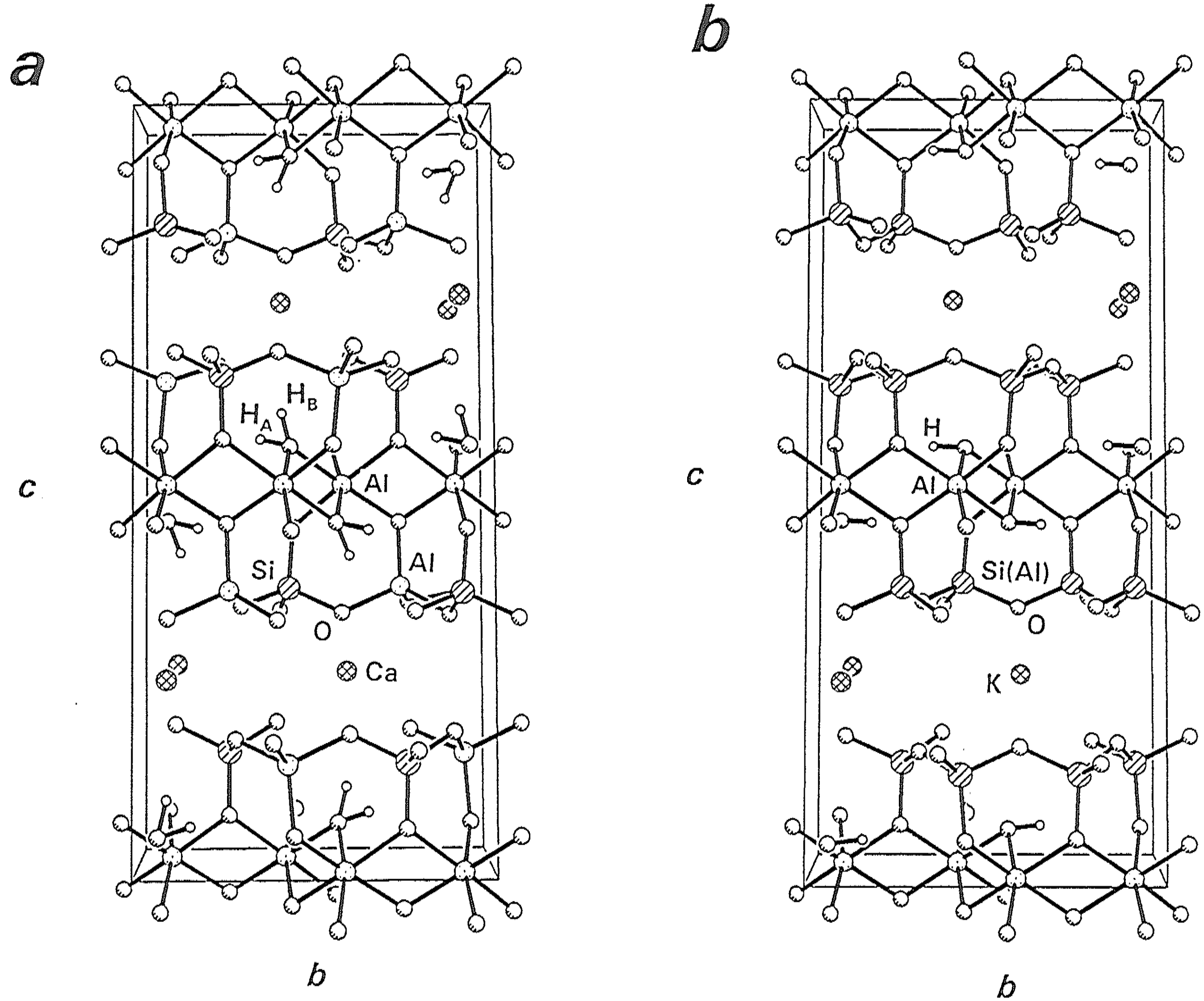

Figure 5-6. Hydroxyl-orientation in margarite (a) as compared to O-H orientations in dioctahedral mica (muscovite, b) and trioctahedral mica (phlogopite, c, next page).

C

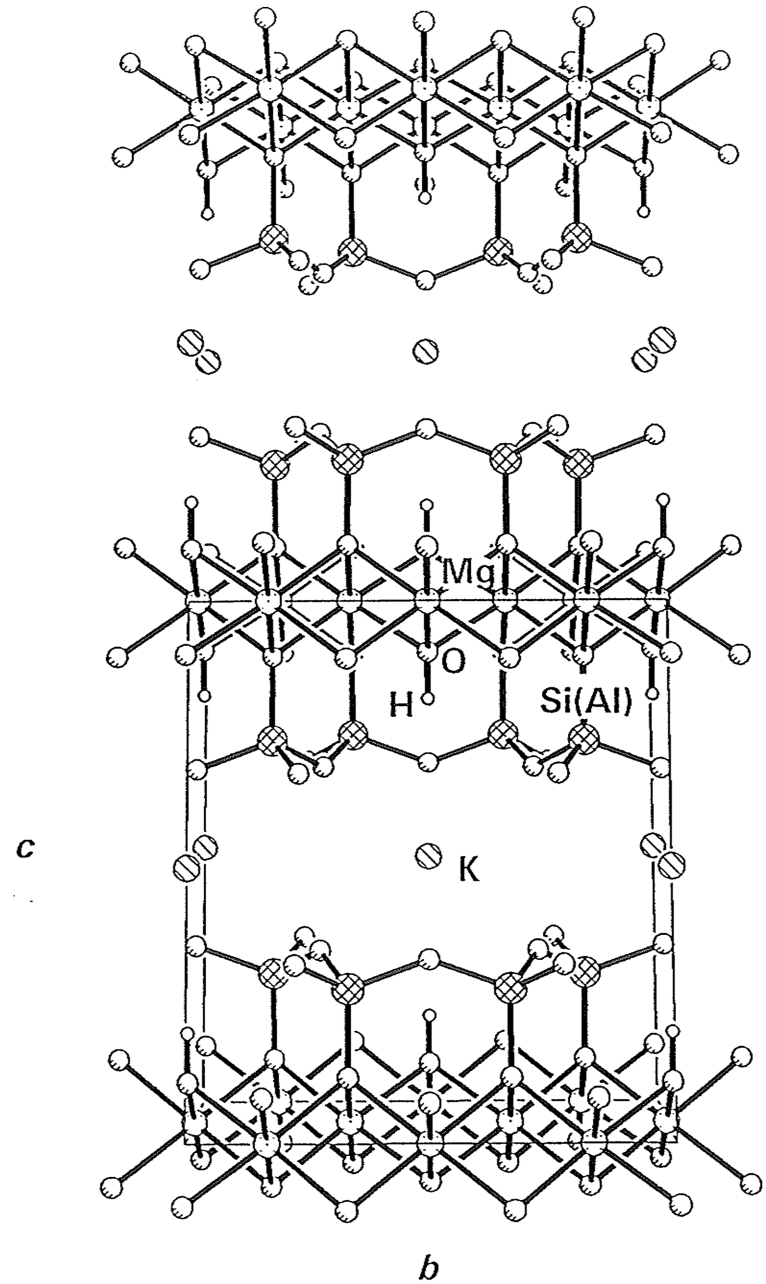

Figure 5-6 (continue).

TABLE 5-3-4. COMPARISON OF CRYSTAL STRUCTURES OF MARGARITE (JOSWIG *et al.* 1983) AND MUSCOVITE (ROTHBAUER, 1971).

	Margarite			Muscovite		
a(Å)	5.108(1)			5.1918(2)		
b(Å)	8.844(2)			9.1053(5)		
c(Å)	19.156(3)			20.0457(7)		
β(°)	95.48(2)			95.735(3)		
Space group	*Cc*			*C2/c*		
	x	*y*	*z*	*x*	*y*	*z*
Ca/K	0.00000	0.0978(5)	0.25000	0.00000	0.0978(5)	0.25000
M1	(omitted from simulation)					
M21	0.2522(4)	0.0851(2)	0.0003(1)	0.2501(6)	0.0838(3)	0.0001(1)
T11	0.4636(4)	0.9279(3)	0.1425(1)	0.4650(5)	0.9291(2)	0.1356(1)
T21	0.4546(3)	0.2565(2)	0.1449(1)	0.4514(5)	0.2581(3)	0.1356(1)
O11	0.3636(2)	0.0978(1)	0.1776(1)	0.4172(4)	0.0929(2)	0.1682(1)
O21	0.2674(2)	0.7786(1)	0.1683(1)	0.2505(4)	0.8106(2)	0.1577(1)
O31	0.2882(3)	0.3906(2)	0.1785(1)	0.2504(4)	0.3702(2)	0.1686(1)
O41	0.4611(2)	0.9455(1)	0.0526(1)	0.4609(4)	0.9428(2)	0.0534(1)
O51	0.3953(2)	0.2545(1)	0.0600(1)	0.3859(3)	0.2514(2)	0.0534(1)
OH11	0.4547(4)	0.5670(2)	0.0517(1)	0.4566(4)	0.5628(2)	0.0502(1)
H11A	0.3663(7)	0.6550(5)	0.0620(3)	0.3656(19)	0.6560(13)	0.0522(10)
H11B	0.439(3)	0.591(2)	0.098(1)			
				Generated by the $\bar{1}$-operation		
M22	0.7480(4)	0.9169(2)	0.9998(1)	0.7499	0.9162	0.9999
T12	0.5350(3)	0.0747(2)	0.8553(1)	0.5350	0.0709	0.8644
T22	0.5468(4)	0.7438(2)	0.8579(1)	0.5486	0.7419	0.8644
O12	0.6376(2)	0.9181(1)	0.8227(1)	0.5828	0.9071	0.8318
O22	0.7122(2)	0.2156(1)	0.8323(1)	0.7495	0.1894	0.8423
O32	0.7352(3)	0.6036(2)	0.8214(1)	0.7496	0.6298	0.8314
O42	0.5451(2)	0.0618(1)	0.9406(1)	0.5391	0.0572	0.9466
O52	0.6200(2)	0.7497(1)	0.9477(1)	0.6141	0.7486	0.9466
OH12	0.5489(3)	0.4361(2)	0.9489(1)	0.5434	0.4372	0.9498
H12A	0.6325(9)	0.3452(5)	0.9396(4)	0.6344	0.3440	0.9478
H12B	0.561(4)	0.399(3)	0.905(1)			

that correspond to the lesser halves (both with 21% site-occupancy) of the split H-atoms of H(11) and H(12) (Joswig *et al.* 1983). In margarite, the A-position constitutes an O-H dipole that forms large angle to the *c*-axis (Fig. 5-6), and correspond to the H-atom position in dioctahedral mica such as in muscovite (compare Fig. 5-6a and b). The B-position constitutes an O-H dipole that forms small angle to the *c*-axis, and corresponds to the H-atom position in trioctahedral mica such as in phlogopite (compare Fig. 5-6a and c). It is important to note that while the simulation was based on the ideal dioctahedral non-H atom configuration (Table 5-3-4), it is the H-position which carries strong trioctahedral character (the B-position), rather than the H-position which carries strong dioctahedral character (associated with A-position), that is energetically favoured. In other words, the occupation of the B-position in margarite by H-atom is not related in the first order to whether the M1-site (the third octahedral site which is empty in dioctahedral mica, but filled in trioctahedral mica) is occupied or not.

The H-atom positions calculated without symmetry constraints, after being transformed back into the asymmetric unit in *Cc*, are given in Table 5-3-5. It can be seen that the space-group symmetry *Cc* is no longer maintained among those positions initially generated from H1 or H2. Among the four positions initially generated from H1, there are two groups: (1) those that are represented by H11 which corresponds to H(11A), and those that are represented by H12 which corresponds to H(11B) in the notation of the work of Joswig *et al.* (1983). Similarly, two groups, H21 and H22, can be identified among the positions generated from H2 that correspond to H(12A) and H(12B), respectively in the work of Joswig *et al.* (1983). The experimentally observed split H-atom model has been

TABLE 5-3-5. H-ATOM POSITIONS IN MARGARITE CALCULATED WITHOUT SYMMETRY CONSTRAINTS

		x	*y*	*z*
H1				
	x, -y, z+1/2	0.3672	0.6633	0.0718
	x+1/2, -y+1/2, z+1/2	0.4186	0.6304	0.0991
		------	------	------
	H11	**0.3929**	**0.6468**	**0.0854**
	H(11A)*	0.3663(7)	0.6550(5)	0.0620(3)
	diff.	0.0266	-0.0082	0.0234
	x, y, z	0.439	0.576	0.104
	x+1/2, y+1/2, z	0.438	0.579	0.103
		------	------	------
	H12	**0.439**	**0.578**	**0.104**
	H(11B)*	0.439(3)	0.591(2)	0.098(1)
	diff.	0.000	-0.013	0.006
H2				
	x, -y, z+1/2	0.5898	0.3657	0.9023
	x+1/2, -y+1/2, z+1/2	0.5903	0.3668	0.9022
		------	------	------
	H21	**0.5900**	**0.3662**	**0.9022**
	H(12A)*	0.6325(9)	0.3452(5)	0.9396(4)
	diff.	-0.0425	0.021	-0.0374
	x, y, z	0.551	0.425	0.896
	x+1/2, y+1/2, z	0.556	0.419	0.898
		------	------	------
	H22	**0.553**	**0.422**	**0.897**
	H(12B)*	0.561(4)	0.399(3)	0.905(1)
	diff.	-0.008	0.023	-0.008

* determined from neutron diffraction (Joswig et al., 1983)

reproduced. However, the agreement between the calculated and experimentally determined coordinates is rather poor with regard to H11 [H(11A)] and H21 [H(12A)]. The differences are in second decimal places, with the largest being -0.0425 (Table 5-3-5). Further examination of the coordinates of the two H-atoms that comprise H11 reveals that the supposedly equivalent coordinates differ by as much as 0.04 along the *x*-axis (equal to 0.2 Å along the *a*-axis of axial length of 5.102 Å). In fact, one of the H-atom positions, which corresponds to the symmetry operation of *x, -y, 1/2+z,* matches very closely the observed H(11A)-position (with difference in the 0.00n level). This raises the possibility of further splitting of the H11 position into H111 and H112 (Table 5-3-6). Such splitting is in accordance to the split H-atom model in the muscovite structure (see 5.3.3. and Chapter 6). Margarite and muscovite have essentially the same structural configuration (Table 5-3-4, Fig. 5-6) except that, in margarite, tetrahedral Al and Si are ordered into different sites and that the interlayer cation is divalent due to greater extent of Al replacement of Si in the tetrahedral sheet. The symmetry of margarite is lowered from *C2/c* (of muscovite) to *Cc* due to the tetrahedral ordering. H-atom positions (the A-positions) calculated in *Cc* symmetry can be compared to those in *C2/c* symmetry by operating on the latter by the $\bar{1}$-symmetry operator (Table 5-3-6). There is a close correspondence of (H111 and H112) in margarite to (H1 and H2) in muscovite. The postulation of further splitting is supported experimentally by the elongated thermal displacement model of H(11A), with U_{33} twice as large as U_{11} and U_{22} (Joswig *et al.* 1983). If H11 [H(11A)] is split, from the quasi-$\bar{1}$ relationship between the two halves of the margarite structure (Table 5-3-4), the quasi-$\bar{1}$ equivalent of H11 [H(11A)], H21

[H(12A)], should also be similarly split into H211 and H212 (Table 5-3-6). However, the coordinates of the two H-atom positions that comprise the H21-position agree to each other so closely that there is hardly room for a further split. In fact, this calculated H21-position corresponds to one hypothetical split, H211, while the experimentally observed position, H(12A), corresponds to the other hypothetical split, H212 (Table 5-3-6). Experimental evidence do exist in support of such further splitting: the thermal displacement model of H(12A) shows similar elongation as H(11A), albeit not as obvious. The fact that such further splitting was not produced by the calculation is probably due to that a non-ideal structure configuration was used. While the calculation assumes ideal dioctahedral structural configuration and complete tetrahedral order of the non-H atoms, the coordinates of these atoms actually came from a sample that displays minor trioctahedral character (minor M1-site occupancy) and partial tetrahedral compositional (Al, Si) disorder (Joswig *et al.* 1983). Substantial effort is needed before such partial site-occupancy/disorder can be simulated explicitly using SSEM method.

On assuming multiple split H-atom model, the differences in fractional coordinates between the experimentally determined and the calculated positions are, in general, in the third decimal place (Table 5-3-6).

5.3.3. Muscovite

The calculated H-atom position in muscovite in the space group *C2/c* is given in Table 5-3-7. The eight H-atom positions determined with the symmetry relaxed to *P*1 are listed in Table 5-3-8 (projected back into the asymmetric unit of the *C2/c* structure). There

TABLE 5-3-6. SPLIT H-ATOM POSITIONS IN MARGARITE AS COMPARED TO MUSCOVITE (CHAPTER 6).

	Margarite				Muscovite		
	x	*y*	*z*		*x*	*y*	*z*
H111	**0.3672**	**0.6633**	**0.0718**	H1	0.3656(19)	0.6560(13)	0.0522(10)
H11A*	0.3663(7)	0.6550(5)	0.0620(3)				
diff.	0.0009	0.0083	0.0098				
H112	**0.4186**	**0.6304**	**0.0991**	H2	0.3883(25)	0.6380(17)	0.0720(15)
H12	**0.439**	**0.578**	**0.104**				
H11B*	0.439(3)	0.591(2)	0.098(1)				
diff.	0.00 0	-0.013	0.006				
				Generated by the $\bar{1}$-operation from H1 & H2			
H211†	0.6328	0.3367	0.9282	H1'	0.6344	0.3440	0.9478
H12A*	0.6325(9)	0.3452(5)	0.9396(4)				
H212	**0.5900**	**0.3662**	**0.9022**	H2'	0.6117	0.3620	0.9280
H212†	0.5814	0.3696	0.9009				
H22	**0.553**	**0.422**	**0.897**				
H12B*	0.561(4)	0.399(3)	0.905(1)				
diff.	-0.008	0.023	-0.008				

* from Joswig et al., 1983; † hypothetical, derived from the $\bar{1}$ equivalent of H111 or H112. The highlighted are the H-atom positions calculated in margarite.

TABLE 5-3-7. H-ATOM COORDINATES IN MUSCOVITE IN THE SPACE GROUP *C*2/*c*

	Calculated	Experimental*	Difference
x	0.3987	0.3727(7)	0.0260
y	0.6322	0.6499(4)	-0.0177
z	0.0815	0.0599(2)	0.0216
O-H (Å)	0.956	0.928(5)	0.028

*Rothbauer (1971)

TABLE 5-3-8. THE EIGHT H-ATOM POSITIONS PROJECTED BACK INTO THE ASYMMETRIC UNIT OF THE *C2/c* MUSCOVITE CELL

Symmetry operation	*x*	*y*	*z*
H(11) *x, y, z*	0.3629	0.6509	0.0643
H(12) *-x,-y,-z*	0.3642	0.6515	0.0642
H(13) *1/2+x,1/2+y,z*	0.3629	0.6509	0.0643
H(14) *1/2-x,1/2-y,-z*	0.3646	0.6516	0.0642
	------	------	------
H1	**0.3637**	**0.6512**	**0.0642**
H(21) *-x,y,1/2-z*	0.3932	0.6438	0.0766
H(22) *x,-y,1/2+z*	0.3942	0.6442	0.0766
H(23) *1/2-x,1/2+y,1/2-z*	0.3961	0.6436	0.0772
H(24) *1/2+x,1/2-y,1/2+z*	0.3944	0.6445	0.0765
	------	------	------
H2	**0.3945**	**0.6440**	**0.0767**
H-position calculated in *C2/c*	0.3987	0.6322	0.0815
H-position observed*	0.3727(7)	0.6499(4)	0.0599(2)

* Rothbauer, 1971

is a reasonable agreement between the calculated and the experimentally determined H-atom positions in the *C2/c* muscovite structure (Table 5-3-7). However, if the symmetry is relaxed to *P*1 in the calculation, there are eight independent H-atom positions. If each of these positions is transferred back to the *x y z* position of the asymmetric unit of the *C2/c* muscovite structure (Table 5-3-8), the H-atom positions fall into two sets labelled H_{1j} and H_{2j} (j=1,4) in Table 5-3-8. The average values of the *x* and *y* coordinates for each set bracket the experimental values (Table 5-3-8). The slightly greater difference of the *z*-coordinates is probably related to the inadequate description of H bonding in the calculation (Collins & Catlow 1991), or average description of the Si-Al substitution that assumes total disorder. Overall, the result is in accord with the anisotropic displacement model of Rothbauer (1971) in which the H-atom shows very anisotropic displacement behaviour; the result of the *P*1 calculation indicates this anisotropic model to be an envelope of two positions of the split-H atom, separated by 0.44 Å. The result for the split-site model is in accord with the work of Abbott *et al.* (1989) who also gave two general OH orientations (two H-atom positions) in the muscovite structure. They based their prediction on calculations for 18 different local arrangements of Al and Si over the tetrahedral sites surrounding the H-atom in the *C2/c* muscovite structure. As no apparent long-range Si-Al ordering has been observed (Güven 1971, Richardson & Richardson 1982, Schultz *et al.* 1989, see also 3.2.), all the above 18 arrangement are equally possible in muscovite structure. Therefore, two H-atom positions are expected according to the calculation of Abbott *et al.* (1989). Furthermore, the H2 position has very similar atomic coordinates to those of the single H-atom position calculated with symmetry constraints

(Table 5-3-8). This suggests that H2 is energetically more favourable than H1. Careful examination of the relative positions of H1 and H2 indicated that H2 corresponds to the "type-2" minimum of Abbott *et al.* (1989), which is energetically more favourable than the "Type-1" minimum (corresponding to H1 position in the present work). These remarkably similar results produced by the two different approaches prompted experimental verification, which will be described in the following chapter (Chapter 6).

5.3.4. Dickite

The calculated H-atom positions in dickite in the space group *Cc* are shown in Table 5-3-9. The 16 H-atom positions determined with the symmetry relaxed to *P*1 are listed in Table 5-3-10 (projected back into the asymmetric unit of the *Cc* structure). When the symmetry of *Cc* was used, the agreement between the calculated and observed coordinates is rather poor (Table 5-3-9). Most differences are in the second decimal places, with the highest [of H1(*z*)] being -0.0402. After optimization with *P*1 symmetry, 6 unique H-atom positions can be identified (Table 5-3-10). Among the 16 H-atom positions in the dickite unit-cell, those that are initially generated from H1 and H2, respectively, of the asymmetric unit (4 for each of the H1 and H2 atoms) still maintain (with a spread of 0.02 in fractional coordinates) the *Cc* symmetry. The H-atom positions initially generated from H3 can be divided into two groups, H31 and H32, with a principal separation of 0.07 in the *x*-coordinate (corresponding to 0.36 Å). H-atom positions initially generated from H4 can be similarly grouped into H41 and H42, with a principal separation of 0.26 Å along the *a*-axis (*x*-coordinate). It is important to notice that after optimization

TABLE 5-3-9. CALCULATED (FIRST ROWS) AND EXPERIMENTALLY DETERMINED* (SECOND ROWS) H-POSITIONS IN DICKITE (CALCULATION WITH SYMMETRY *Cc*, ASSUMING NON-SPLIT H-ATOMS). THE DIFFERENCES ARE GIVEN IN THIRD ROWS.

	x	*y*	*z*
H1	**0.4911**	**0.2014**	**0.1147**
	0.4795(9)	0.1848(4)	0.1549(5)
	0.0116	0.0166	-0.0402
H2	**0.3077**	**0.2543**	**0.3615**
	0.2957(8)	0.2558(5)	0.3627(3)
	0.0120	-0.0015	-0.0012
H3	**0.297**	**0.9329**	**0.3596**
	0.326(1)	0.9456(5)	0.3515(4)
	-0.029	-0.0127	0.0081
H4	**0.2690**	**0.5739**	**0.3595**
	0.2891(9)	0.5813(6)	0.3605(3)
	-0.0201	-0.0074	-0.0010

* Bish & Johnston, 1993

TABLE 5-3-10. H-POSITIONS IN DICKITE CALCULATED WITH *P*1 SYMMETRY

		x	y	z
H1				
	x, y, z	0.4898	0.1744	0.1580
	x, -y, z+1/2	0.4794	0.1803	0.1669
	x+1/2, y+1/2, z	0.4900	0.1743	0.1580
	x+1/2, -y+1/2, z+1/2	0.4786	0.1805	0.1667
		------	------	------
	H1	**0.4844**	**0.1774**	**0.1624**
	H1*	0.4795(9)	0.1848(4)	0.1549(5)
	diff.	0.0049	-0.0074	0.0075
H2				
	x, y, z	0.2952	0.2605	0.3664
	x, -y, z+1/2	0.3170	0.2535	0.3636
	x+1/2, y+1/2, z	0.2951	0.2605	0.3664
	x+1/2, -y+1/2, z+1/2	0.3170	0.2465	0.3636
		------	------	------
	H2	**0.3061**	**0.2552**	**0.3650**
	H2*	0.2957(8)	0.2558(5)	0.3627(3)
	diff.	0.0104	-0.0006	0.0023
H3				
	x, y, z	0.328	0.9340	0.3589
	x+1/2, y+1/2, z	0.328	0.9341	0.3588
		------	------	------
	H31	**0.328**	**0.9340**	**0.3588**
	H3*	0.326(1)	0.9456(5)	0.3515(4)
	diff.	0.002	-0.0116	0.0073
	x, -y, z+1/2	0.253	0.9281	0.3643
	x+1/2, -y+1/2, z+1/2	0.253	0.9285	0.3643
		------	------	------
	H32	**0.253**	**0.9283**	**0.3643**

TABLE 5-3-10. (continued)

	x	*y*	*z*
H4			
x, y, z	0.2463	0.5656	0.3585
x+1/2, y+1/2, z	0.2462	0.5656	0.3585
	-------	------	------
H41	**0.2462**	**0.5656**	**0.3585**
x, -y, z+1/2	0.2971	0.5802	0.3658
x+1/2, -y+1/2, z+1/2	0.2972	0.5802	0.3658
	------	------	------
H42	**0.2972**	**0.5802**	**0.3658**
H4*	0.2891(9)	0.5813(6)	0.3605(3)
diff.	0.0081	-0.0011	0.0053

* determined from neutron diffraction (Bish & Johnston, 1993)

by considering each of the 16 H-atoms explicitly (in *P*1 symmetry), the agreement between the calculated and the observed atomic coordinates of the H1 and H2 improves substantially by a factor of 10 (compare Table 5-3-9 and 5-3-10). There is also a similar improvement in the agreement between the calculated and observed coordinates of H3 and H4, given that the two observed H-atoms correspond to H31 and H42, respectively, of the calculated. Such agreement level conforms to the accuracy of the SSEM calculation (see earlier discussion). The results indicate (1) instead of representing all 4 H-atoms non-split in space group *Cc*, two of the H-atoms (H3 and H4) should be represent split; (2) interactions between H-atoms can be important in determining equilibrium H-atom positions in the structure. This is especially true when the structure contain many H-atoms.

The result that there are probably 6 unique H-atom positions in the dickite structure helps explain apparent disagreement between the diffraction and vibrational spectroscopic studies on the OH-groups in dickite. It had long been a mystery (Farmer & Russel 1964; Johnston *et al.* 1990; Joswig & Drits 1986; Prost, *et al.* 1989; Sen Gupta, *et al.* 1984) that, whereas infrared (IR) spectroscopy shows 6 O-H stretching bands (corresponding to at least 6 unique OH-groups and hence 6 H-atom positions) in the low-temperature IR spectra of dickite (Fig. 5-7), diffraction experiments can locate only 4 unique H-atom positions. The strong bands (Figure 5-7) at 3620, 3655 and 3731 cm^{-1} can be explained by the 4 H-atom positions located by the diffraction experiments (the band at 3655 cm^{-1} is known to be the overlap of two O-H (O-H2 and O-H4) stretching bands), but the two weak bands at 3619 and 3717 cm^{-1} were left unassigned. The postulation that H3 and H4 split into (H31, H32) and (H41, H42) explains the existence of the two additional bands.

The O-H stretching frequency is strongly influenced by details of H-bonding (Nakamoto *et al.* 1955). Longer H...O distance and smaller O-H...O angle will give higher stretching frequency, and *vice versa*. This relationship is maintained in the correspondence of the H...O distances and O-H...O angles of the four experimentally-observed H-atoms (assuming that H3 = H31 and H4 = H42, Table 5-3-11, also refer to Table 5-3-10), and their assignment to the IR-bands. The H32...O distance decreases from 2.28 (2.36) of H31...O (H..3...O) to 2.15, and the O-H32...O angle increases from 144° (140°) of O-H31...O (O-H3...O) to 176°. Such difference will cause the O-H32 band to shift from 3731 cm^{-1} of O-H31 (O-H3) toward a lower frequency, most likely one of the weak bands at 3717 and 3619 cm^{-1}. In fact, the band at 3717 cm^{-1} had already been suggested to be a split of H3 based on the large thermal displacement factor and some anisotropy of the H3-site in the neutron diffraction data (Bish & Johnston 1993). On the contrary, the H...O distance and O-H...O angle associated with H41 increase to 1.96 Å and decreases to 156°, respectively, from those related to H42 (equivalent to H4) of 1.96 Å and 156°, respectively. This means that the O-H41 stretching band will increase in frequency relative to that of O-H42 (O-H4), from 3655 to probably 3619 cm^{-1}.

The excessive intensity of the band at 3731 cm^{-1} is still found puzzling. For similar populations of IR-active (O-H stretching) vibration, IR-intensity is inversely proportional to the frequency due, mostly, to the modulation of a transition dipole moment function (Steele 1971) which is an inverse linear function over vibrational frequency (Hermansson *et al.* 1991, Burns & Hawthorne, 1994). Site-population of H3 (H31) is similar or less than those of H1, H2, or H4. Since the stretching frequency of O-H3 (O-H31) is the

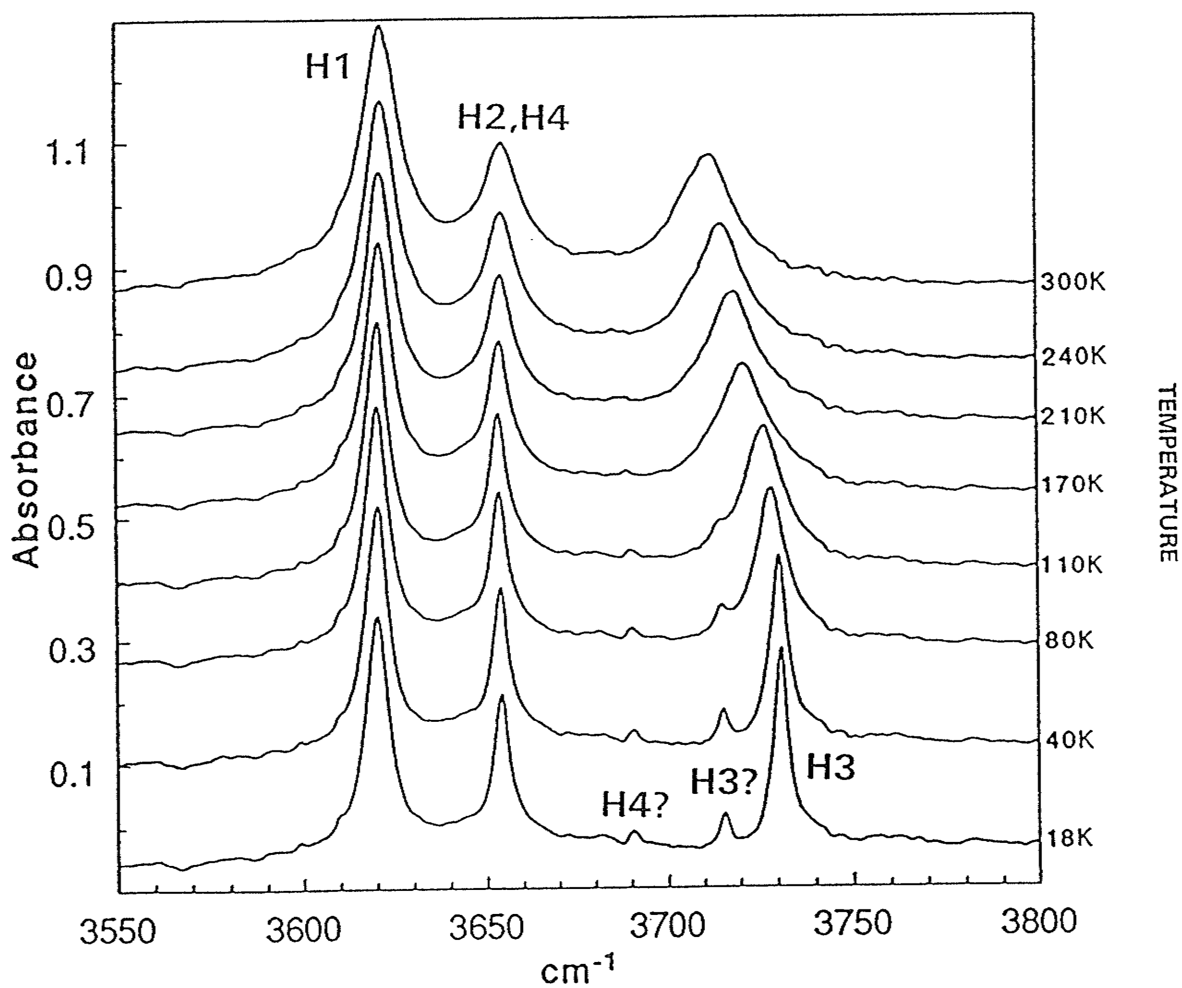

Figure 5-7. Variable-temperature FT-IR spectra of dickite (adapted from Johnston & Bish, 1993)

TABLE 5-3-11. HYDROGEN BONDS IN DICKITE

	$d_{O\text{-}H}$(Å)	$d_{H...O}$(Å)		∠O-H...O(°)
OH1	0.99			
	0.94*			
OH2	1.00	...O1	1.93	166
	0.96*		1.97*	164*
OH31	0.99	...O3	2.28	144
	0.95*		2.36	140*
OH32	0.99		2.15*	176
OH41	1.00	...O2	1.96	156
OH42	1.00		1.92	167
	0.94*		1.99*	166*

* determined by neutron diffraction (Bish & Johnston, 1993)

highest in the spectrum, its intensity should be smaller than any of the two major bands that represent the stretching vibration associated with H1, H2 and H4(H42). However, this is not the case (Fig. 8). Further vibrational study is needed using Raman spectroscopy which gives vibrational intensity independent of transition dipole moment (Sherwood 1972), such that a more realistic picture of the vibrational intensity distribution can be obtained.

5.4. Summary

Using the SSEM calculation, with the input of space group symmetry, unit-cell dimensions, and non-H atomic coordinates, H-atom positions of the O-H group(s) in micas and clay minerals can be located to the accuracy to the third decimal place in atomic coordinates. Split H-atom model can be reliably reproduced, and relative energies of the split positions can also be resolved.

The non-split H-atom in muscovite as determined by diffraction experiment is predicted to be split, with the split position closer to the *c*-axis energetically more favourable than the split position closer to the basal plane. Similar splitting is predicted for the structurally similar mineral, margarite.

In addition to the diffraction-determined 4 unique H-atom positions in dickite, 2 more H-atom positions were shown possible in the dickite structure, with the experimentally determined H3 and H4 split into (H31, H32) and (H41, H42), respectively. The total of 6 unique H-atom positions helps to explain the existence of 6 O-H stretching bands on vibrational spectra of dickite.

Chapter 6.

The Split H-atom position Model in Muscovite: Experimental Verification

Locating H atoms in muscovite has been difficult. Being a very weak X-ray scatterer, H was usually omitted in X-ray structure studies (Güven 1971, Richardson & Richardson 1982, see also 3.2.). Even in the study of Schultz *et al.* (1989) in which the H atom was included, only isotropic-displacement factors for the H-atom position could be refined. Single-crystal neutron diffraction (Rothbauer 1971) gave accurate information about the H-atom position in muscovite. However, the exceptionally large anisotropic-displacement of the H-atom (amplitude up to 14 times greater than those of other atoms in the structure) was not explained. Vibrational spectroscopic studies (IR and Raman) can provide indirect information on H-atom positions by detecting the relative orientation of the OH dipoles in the structure. Despite extensive work (Serratosa & Bradley 1958, Basset 1960, Vedder & Mcdonald 1963, Wada & Kamitakahara 1991), the question of OH orientation and even the number of unique OH groups in muscovite remains unclear.

H-atom in muscovite had been predicted split in space group C2/c by SSEM calculation (Chapter 5). As part of the effort to better understanding of crystal chemistry of micas and clay minerals, it is necessary to test such theoretical prediction by experiments.

6.1. Experimental

6.1.1. Single-crystal neutron-diffraction study at room temperature

The program SHELXTL PC™ was used for the structure-refinement. The coherent neutron scattering-lengths (in fm[1]) were b_O = 5.803, b_H = -3.7409, b_{Si} = 4.1491, b_{Al} = 3.449, b_K = 3.71 (Koester 1977).

The single-crystal neutron-diffraction data of Rothbauer (1971) were used to refine the H-atom position in the structure; all 625 reflections in the original study were included. The space group, unit-cell dimensions and non-H atom positional parameters of Rothbauer (1971) were used as input parameters. However, two H-atoms were inserted in the starting model, both with fractional occupancy of 0.5. During the initial structure-refinement, only the positional, displacement and site-occupancy parameters of the two H-

[1]: fm = 10^{-15} m. Scattering length takes the unit of length.

atom positions were varied. The isotropic-displacement factors of the two H sites were refined independently and the site occupancies were refined without constraint. The complete structure, including position and anisotropic-displacement parameters for all atoms, was refined in the final cycle of refinement.

6.1.2. Neutron diffraction at 12 K

Powder neutron-diffraction data for muscovite was collected at 12 K in a liquid-He cryostat using the same sample as in 3.2, loaded into a vanadium can. The intensity data were collected over a 48-hour period on the high-resolution powder diffractometer at the C2 beam-hole of the NRU reactor at the Chalk River Laboratories, Ontario. A wave-length of 1.5022(1) Å, calibrated with Al_2O_3 powder, was used in the data collection. The detector collects data simultaneously over an 80° range of scattering angles with an angular separation of the wires of 0.1°. The scattering range of 8 to 118° was covered by setting the detector in low- and high-angle positions in sequence. A second set of data was collected with the detector at positions 0.05° offset to those of the first set, giving intensity data at a step interval of 0.05° 2Θ.

The structure at 12 K was refined using the program LHPM3. Details of the procedure are similar to those in 3.2. Parameters pertinent to the refinement are listed in Table 6-1.

TABLE 6-1. POWDER-DIFFRACTION INTENSITY-DATA COLLECTION AND DETAILS OF RIETVELD REFINEMENT OF MUSCOVITE AT 12 K

2Θ scan-angle (°)	16-117
step interval (°2Θ)	0.05
maximum intensity (counts)	7234
Refinement details	
No. of unique reflections	779
No. of structural parameters	46
No. of experimental parameters	9
N-P	1968
R_p	1.8
R_{WP}	2.4
R_{EXP}	1.6
R_{BRG}	0.46
Space group	*C2/c*
Unit-cell dimensions	
a(Å)	5.1628(7)
	5.1765(4)*
	5.1918(2)**
b(Å)	8.962(1)
	8.9872(6)*
	9.1053(5)**
c(Å)	19.977(3)
	20.072(1)*
	20.0457(7)**
β(°)	95.738(12)
	95.756(6)*
	95.735(3)**

*room-temperature (from 3.2);
**room-temperature (Rothbauer 1971).

6.1.3. Fourier-Transform Infrared Photo-Acoustic Spectroscopy (FT-IR PAS) at room temperature

Fourier-Transform Infrared Photo-Acoustic Spectroscopy (FT-IR PAS) differs from conventional FT IR spectroscopy in that the IR band-intensity distribution is not only a function of absorbability of the sample and IR frequency (as in transmission IR spectroscopy), but is also strongly dependent on the thermal-diffusion length, μ_s, of the sample (Spencer 1986; Choquet *et al.* 1986), which is defined as

$$\mu_s=\sqrt{(2k/\rho C\omega)} \qquad 6\text{-}1$$

where k, ρ, *C* are the thermal conductivity, density and specific heat of the sample, respectively, and ω is the modulation frequency of the light:

$$\omega=2\pi V\nu \quad \textit{(for a Michelson interferometer)} \qquad 6\text{-}2$$

in which ν is the IR frequency and *V* is the mirror velocity of the interferometer. The intensity ratio of two adjacent IR bands will change in response to varying mirror speed; as the mirror speed decreases, the intensity of the band at higher wavenumber increases relative to the band at lower wavenumber. This is the property of FT-IR PAS that was used here to show that there is more than one O-H stretching band in the IR spectrum of muscovite.

The spectra were collected with a Bio-Rad FTS-60A (Bio-Rad, Cambridge, MA) spectrometer. An MTEC Model 200 photoacoustic cell (MTEC, Ames, IA) with its accompanying preamplifier and power supply was used to acquire all the spectra. The sample tray was filled with the powder sample without attempting to compact the powder. The photoacoustic cell (with the sample) was purged with dry helium. A high-surface-area carbon-black sample (MTEC) was used as the reference material for all spectra. Different interferometer mirror speeds, corresponding to average modulation frequencies of 5, 10, 50, 100, 400 and 2500 Hz, respectively, were used in the collection of the spectra. The number of scans was varied depending on the mirror speed (modulation frequency) used. The resolution of the spectra is 4 cm^{-1}. Other experimental details can be found in Sowa & Mantsch (1994).

6.1.4. Precession photography

A single-crystal precession camera was used to obtain zero-level precession photos of a crystal of the same muscovite sample that was used in the low-temperature neutron-diffraction experiment. Exposures of up to one week were used to examine possible deviations from *C*2/*c* symmetry. Photos corresponding to μ-angles of 25 and 30°, respectively, were obtained to identify any double diffraction effects as a double diffraction cannot occur at two different μ-angles.

6.1.5. Peak-profiling of very weak reflections using single-crystal diffractometer

The same muscovite crystal used in the precession work was mounted on a fully automated single-crystal diffractometer. Peak profiles of the very weak *h*0*l* (*l*=odd) reflections were obtained by step-scanning the corresponding peaks. For each weak reflection that may span a 2θ-range of up to 2°, between 100 to 120 steps were taken, with a counting time of 5 minutes at each step. For one of such reflection, $20\bar{1}$, scans in different orientations, corresponding to varying psi-angle, were taken to ensure that the reflection observed was not a double diffraction. A double-diffraction can only be observed at one specific psi angle, whereas a Bragg diffraction is observed throughout the complete range of psi angles.

6.2. Results

6.2.1. Neutron-diffraction study at room temperature

The H-atom positions determined by structure-refinement using the neutron-diffraction data of Rothbauer (1971) at room temperature are listed in Table 6-2, and the final positional parameters of the muscovite structure are given in Table 6-3. Structure-refinement using a single H-atom model gave an *R*-index of 3.9% and a weighted *R*-index of 4.3%; refinement using a split H-atom model gave essentially the same R-values of 3.9% (R) and 4.2% (weighted *R*), respectively. The non-H atom part of the structure is not significantly affected by the different models for the H-atom site (Table 6-3). There is approximately a 50:50 occupancy of the split-site H-atom sites. There is also a very close correspondence between the experimentally determined split H-atom sites and the sites predicted from the SSEM calculation (Table 6-2).

TABLE 6-2. H POSITIONS DETERMINED FROM NEUTRON-DIFFRACTION DATA AT ROOM TEMPERATURE WITH THE NON-H ATOMS FIXED

	Experimental	Calculated*	Difference
H1			
x	0.3652(19)	0.3637	0.0015
y	0.6560(12)	0.6512	0.0048
z	0.0521(10)	0.0642	-0.0121
O-H(Å)	0.967(12)	0.988	-0.021
H2			
x	0.3883(24)	0.3945	-0.0062
y	0.6384(16)	0.6440	-0.0056
z	0.0720(14)	0.0767	-0.0047
O-H(Å)	0.899(20)	0.979	-0.080

* Chapter 5

TABLE 6-3. ATOMIC COORDINATES OF THE FINAL REFINED STRUCTURE OF MUSCOVITE

	x	*y*	*z*	occupancy
		Room temperature		
Al	0.2501(6)	0.0838(3)	0.0001(1)	1.10(2)
T(1)	0.4650(5)	0.9291(2)	0.1356(1)	0.96(2)
T(2)	0.4514(5)	0.2581(3)	0.1356(1)	0.99(2)
O1	0.4172(4)	0.0929(2)	0.1682(1)	1
O2	0.2505(4)	0.8106(2)	0.1577(1)	1
O3	0.2504(4)	0.3702(2)	0.1686(1)	1
O4	0.4609(4)	0.9428(2)	0.0534(1)	1
O5	0.3859(3)	0.2514(2)	0.0534(1)	1
OH	0.4566(4)	0.5628(2)	0.0502(1)	1
K	0	0.0978(5)	1/4	0.50(1)
H(1)	0.3656(19)	0.6560(13)	0.0522(10)	0.50(6)
H(2)	0.3883(25)	0.6380(17)	0.0720(15)	0.36(6)
		12 K		
Al	0.264(6)	0.082(2)	0.001(2)	0.94(3)
T(1)	0.464(4)	0.930(2)	0.137(1)	0.92(4)
T(2)	0.449(4)	0.261(3)	0.134(1)	0.99(5)
O1	0.406(8)	0.091(12)	0.167(1)	1
O2	0.253(10)	0.801(8)	0.157(1)	1
O3	0.247(3)	0.368(2)	0.167(1)	1
O4	0.457(3)	0.949(2)	0.052(1)	1
O5	0.382(4)	0.253(2)	0.054(1)	1
OH	0.460(5)	0.560(2)	0.050(1)	1
K	0	0.092(4)	1/4	0.48(2)
H(1)	0.392(4)	0.668(2)	0.052(5)	0.49(6)
H(2)	0.402(3)	0.632(2)	0.088(3)	0.41(5)
		Rothbauer (1971)		
Al	0.2502(4)	0.0835(2)	0.00008(8)	1.11(1)
T(1)	0.4646(3)	0.9291(2)	0.13553(8)	0.96(1)
T(2)	0.4516(3)	0.2581(2)	0.13559(8)	0.97(1)
O1	0.4167(3)	0.0927(1)	0.16829(6)	1
O2	0.2505(3)	0.8107(1)	0.15783(7)	1
O3	0.2502(3)	0.3703(1)	0.16869(6)	1
O4	0.4610(2)	0.9432(1)	0.05343(6)	1
O5	0.3859(2)	0.2515(1)	0.05348(5)	1
OH	0.4566(3)	0.5627(2)	0.05018(6)	1
K	0	0.0980(3)	1/4	0.50(1)
H	0.3727(7)	0.6499(4)	0.0599(2)	0.88(1)

6.2.2. Neutron-diffraction study at 12 K

The unit-cell dimensions of muscovite at 12 K are compared to those at room temperature in Table 6-1; final atomic coordinates and cation occupancies are given in Table 6-3. Selected interatomic distances and angles in muscovite at different temperatures are given in Table 6-4. The observed and calculated diffraction patterns, along with their difference, are shown in Figure 6-1. A comparison of the nuclear density distribution for the H sites at room temperature and at 12 K is given in Figure 6-2. Powder-diffraction step-scan intensity is given in Appendix P-27.

There is a contraction in cell dimensions upon cooling (Table 6-1); the contraction in the *c*-dimension (0.1 Å) is an order of magnitude larger than that in the *a*- (0.01 Å) and *b*- (0.02 Å) dimensions, a feature characteristic of hydrous phyllosilicates (Bish & Johnston 1993, Bish 1995, Bish & Von Dreele 1989).

6.2.3. Precession photos and profiles of the weak reflections

Precession photos with μ = 25 and 30° are shown in Figure 6-3. The corresponding indexing is given in Figure 6-4. Profiles of a selected number of *h*0*l* (*l*=odd) reflections are shown in Figure 6-5. Profiles for one of such reflection, $20\bar{1}$, at different psi-angles, are given in Figure 6-6.

6.2.4. The IR-spectra

The photoacoustic FT-IR spectrum between 500 and 4000 cm^{-1} of the same muscovite sample as used in the low-temperature neutron-diffraction experiment is shown

TABLE 6-4. SELECTED INTERATOMIC DISTANCES (Å) AND ANGLES (°) OF MUSCOVITE AT ROOM TEMPERATURE AND 12 K

	room temperature	12 K
<T(1)-O>	1.644(1)	1.65(3)
<O-T(1)-O>	109.4(8)	109.5(13)
<T(2)-O>	1.643(1)	1.63(4)
<O-T(2)-O>	109.4(8)	109.4(10)
<Al-O>	1.930(1)	1.92(1)
<K_{inner}-O>	2.859(1)	2.83(3)
<K_{outer}-O>	3.363(2)	3.39(2)
H(1)-O	0.967(12)	1.04(10)
H(2)-O	0.899(20)	1.06(7)
H(1)-H(2)	0.44(3)	0.78(12)

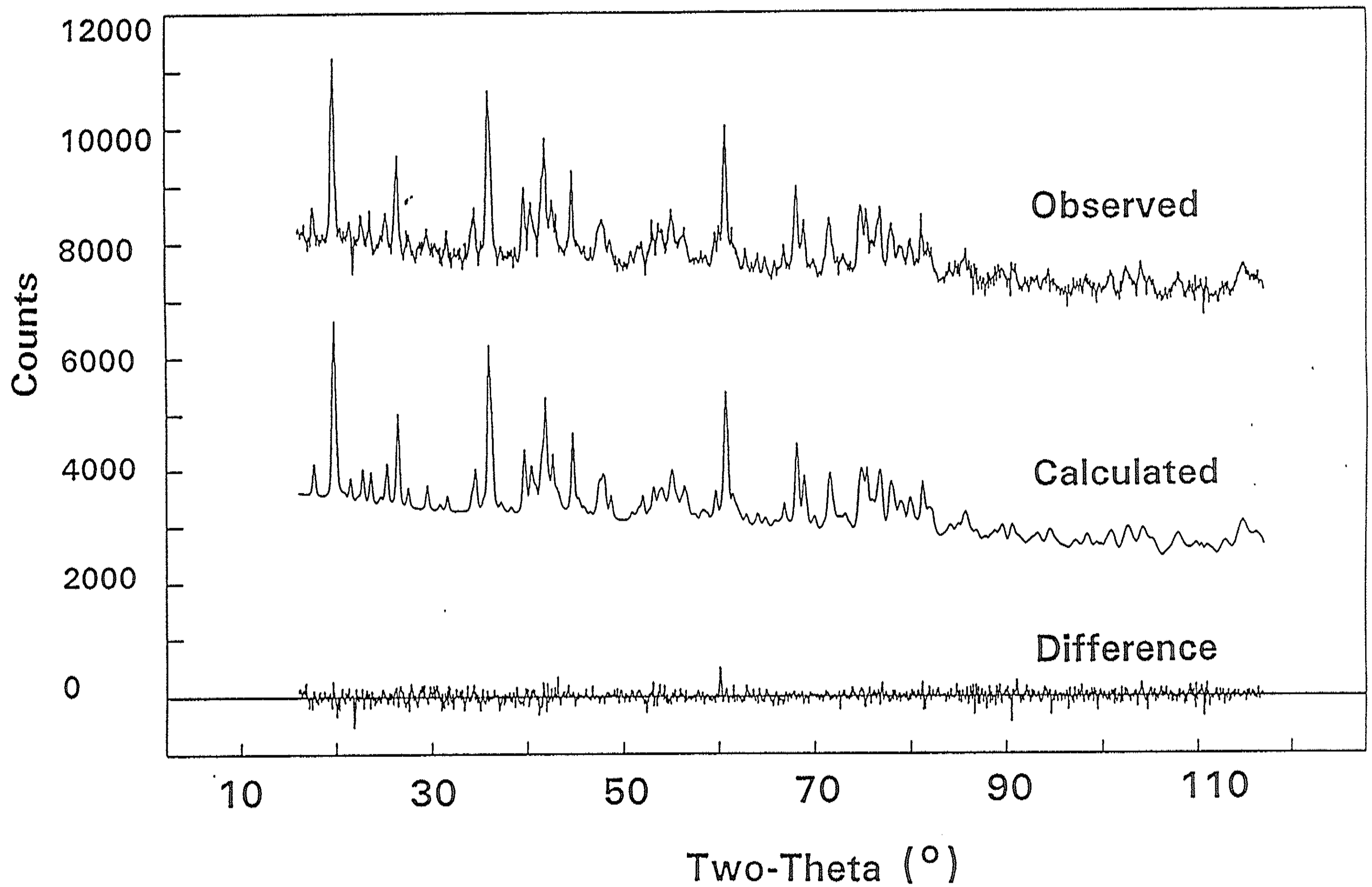

Figure 6-1. Observed and calculated neutron-diffraction patterns of muscovite at 12 K. The observed diffraction-pattern has been increased by 5000 counts to avoid pattern overlap.

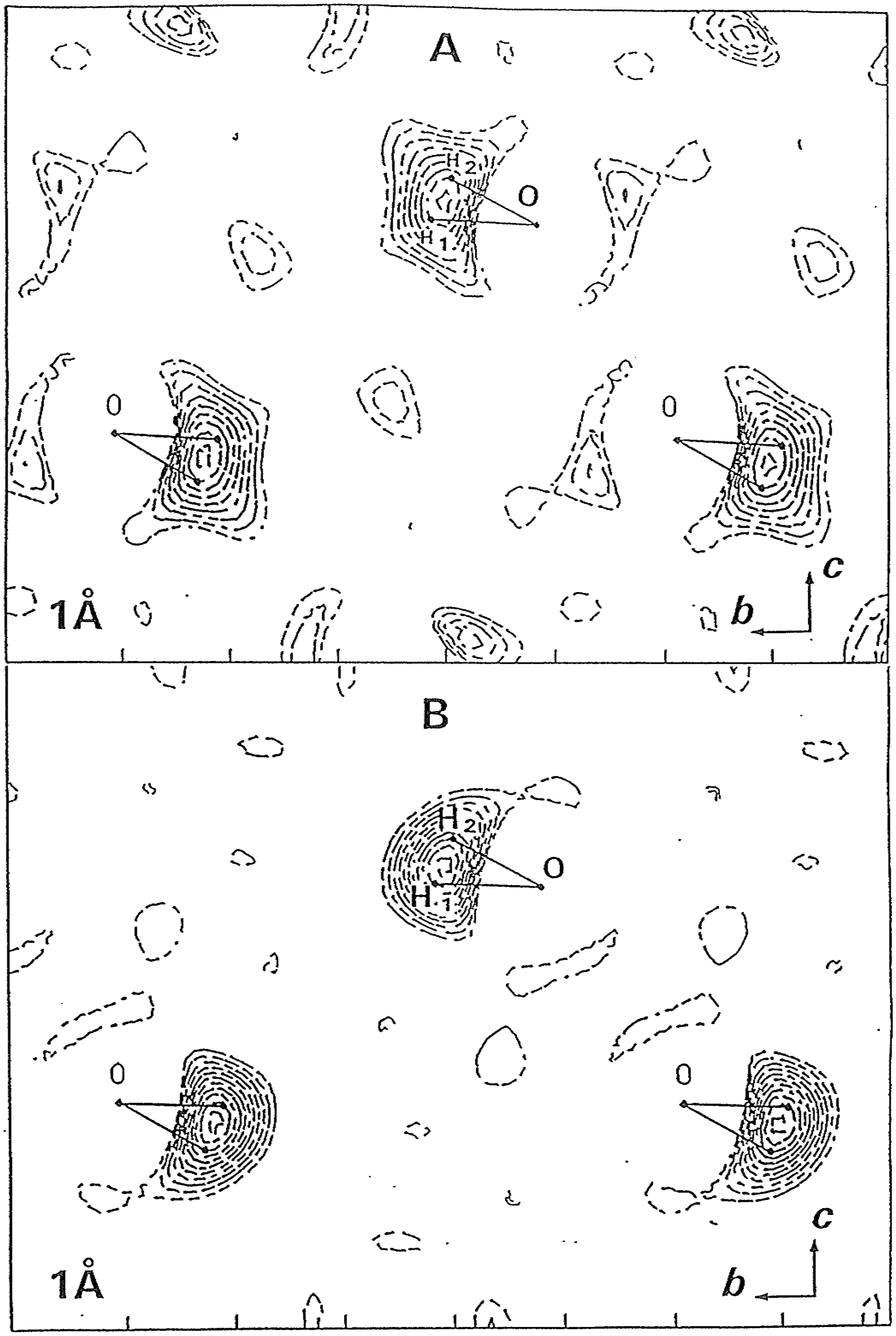

Figure 6-2. Difference-Fourier maps, with H removed from the refinement model, projected down [100] showing the H-density distribution in muscovite at A: room temperature (contours from -10.0 to -2.0) and B: at 12 K (contours from -11.0 to -1.0). The contour interval is 0.1. Arbitrary unit.

in Figure 6-7. The interferometer-mirror speed (in modulation frequency) used in collecting the spectrum was 2.5 KHz. Spectra in the OH-stretching region of 3200 to 3900 cm^{-1} are given in Figure 6-8. The mirror speed for these spectra ranges from 5 Hz to 2.5 KHz.

6.3. Discussion

6.3.1. H-atom positions at room temperature

Although the calculation of H-atom positions in muscovite (see section 5.3.4) was not done at room temperature because the vibrational energy was ignored, the fact that the unit-cell dimensions and the non-H atomic positions were fixed at room-temperature values made the result of the calculation close to an analogous calculation at room temperature. When *C2/c* symmetry was applied to the H atoms derived from the refinement, the calculation reproduced that of the latest of the kind (Collins & Catlow 1992). However, this gives a difference an order of magnitude greater than that observed when *C2/c* symmetry was removed (*c.f.* Tables 6-2 and 5-2-5). There is much closer agreement between calculated and observed H-atom positions when the split H-atom model is used.

6.3.2. H-atom position at 12 K

At 12 K, an elongated nuclear-density distribution for the H atom was observed (Fig. 6-2), similar to that observed at room temperature. The sample used in the present

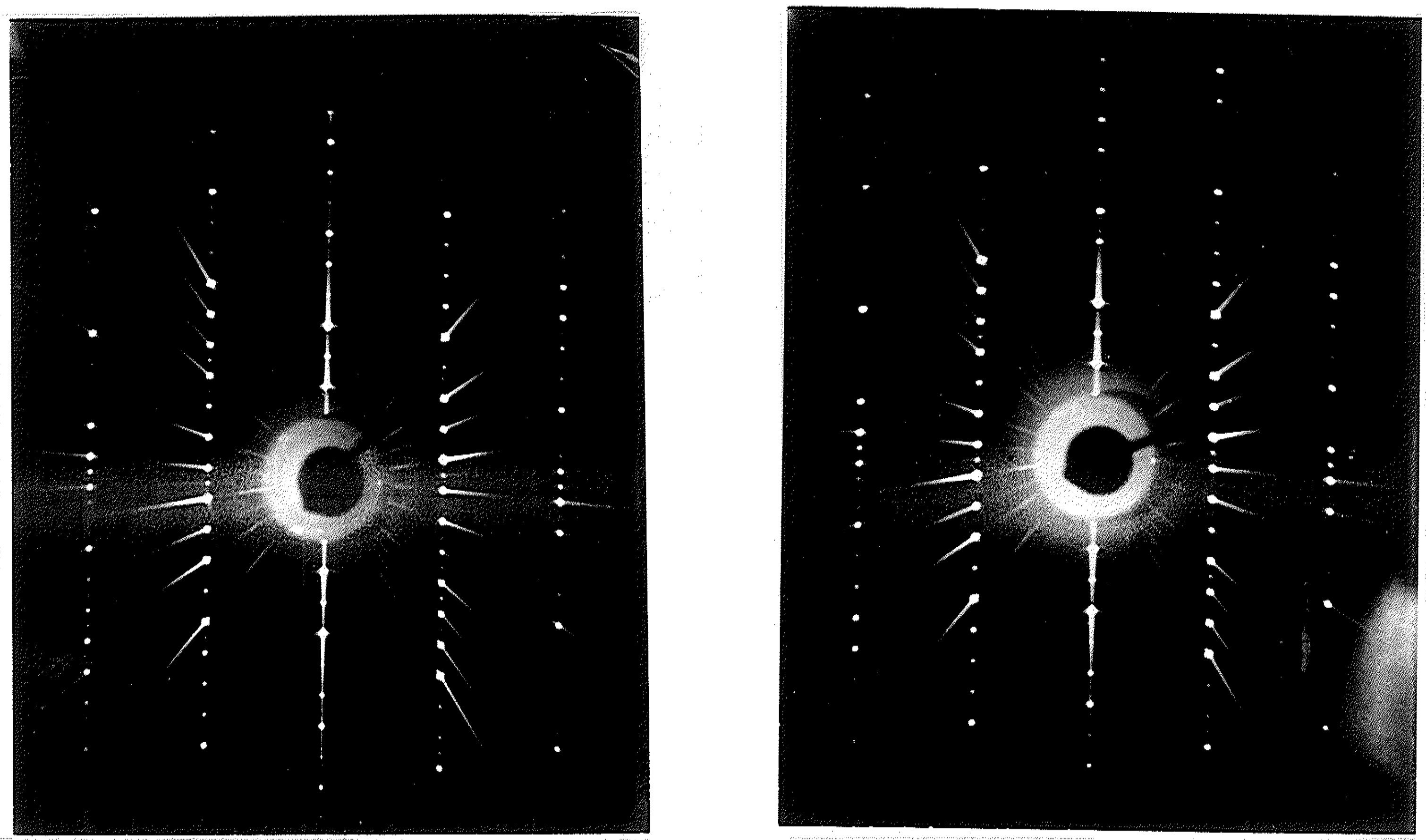

Figure 6-3. Precession photos of muscovite with $\mu = 25$ and $30°$, respectively

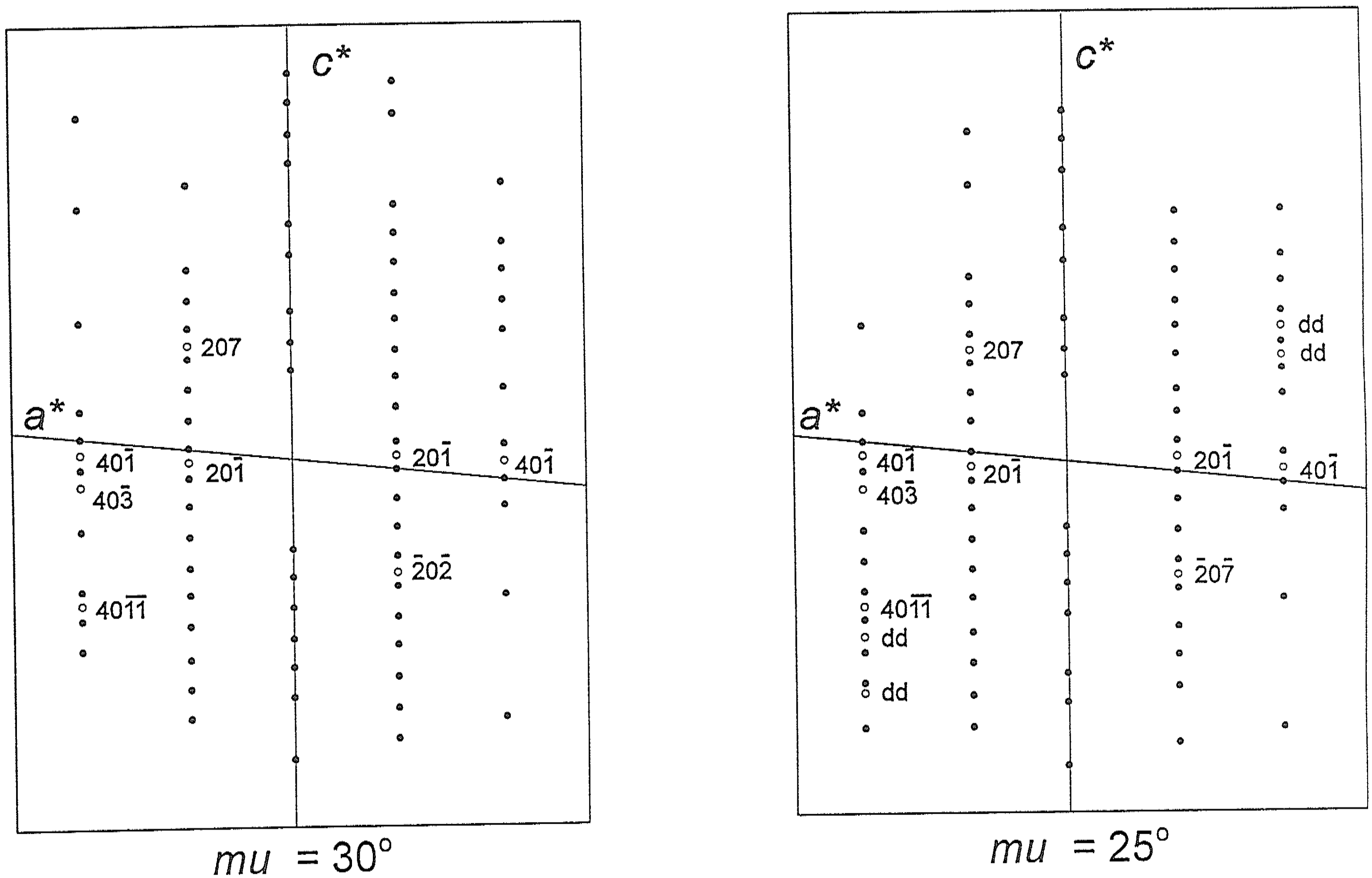

Figure 6-4. Partial indexing of the precession photos of muscovite in Figure 6-3. Solid circles represent reflections conform to the symmetry of *C2/c*. Open circles represent reflections violating the *c*-glide symmetry. Note the existence of double

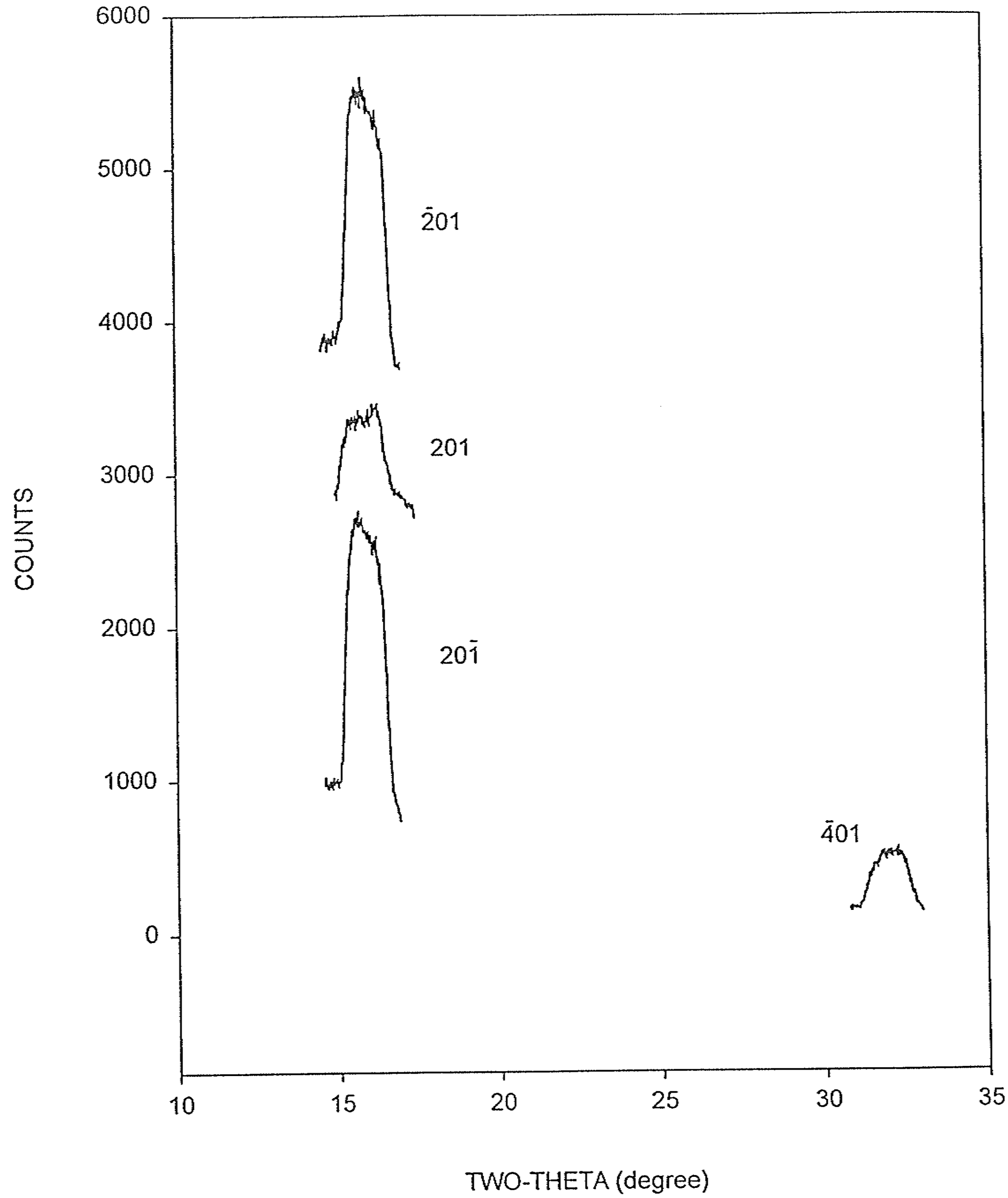

Figure 6-5. Peak profiles of selected $h0l$ (l=odd) reflections in muscovite. Intensities of 201 and 201 were raised by 2600 and 3600 counts, respectively.

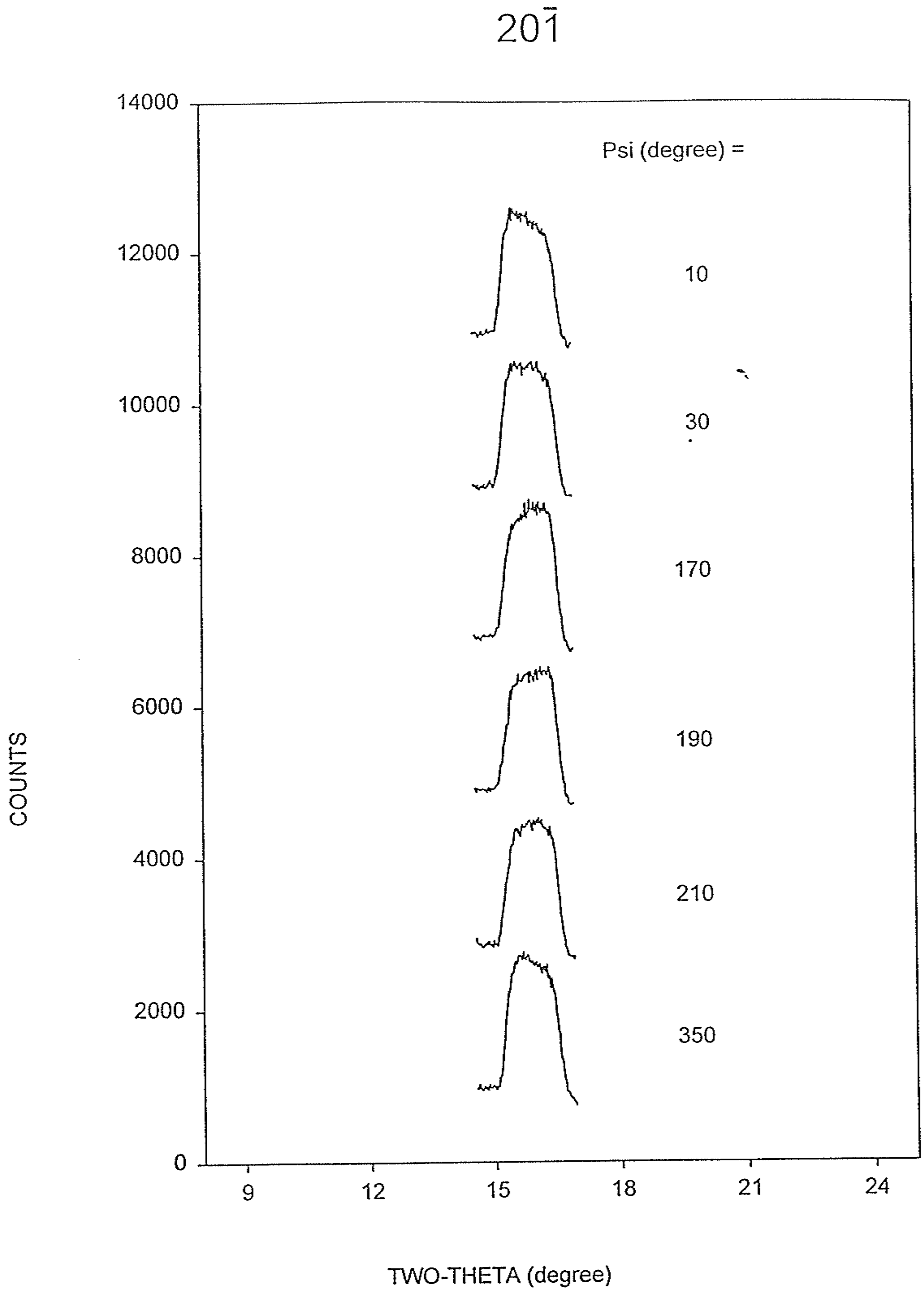

Figure 6-6. Peak profiles of $20\bar{1}$ of muscovite with different Psi-angles. Intensities for all profiles, except the one at psi = 350°, were raised appropriately.

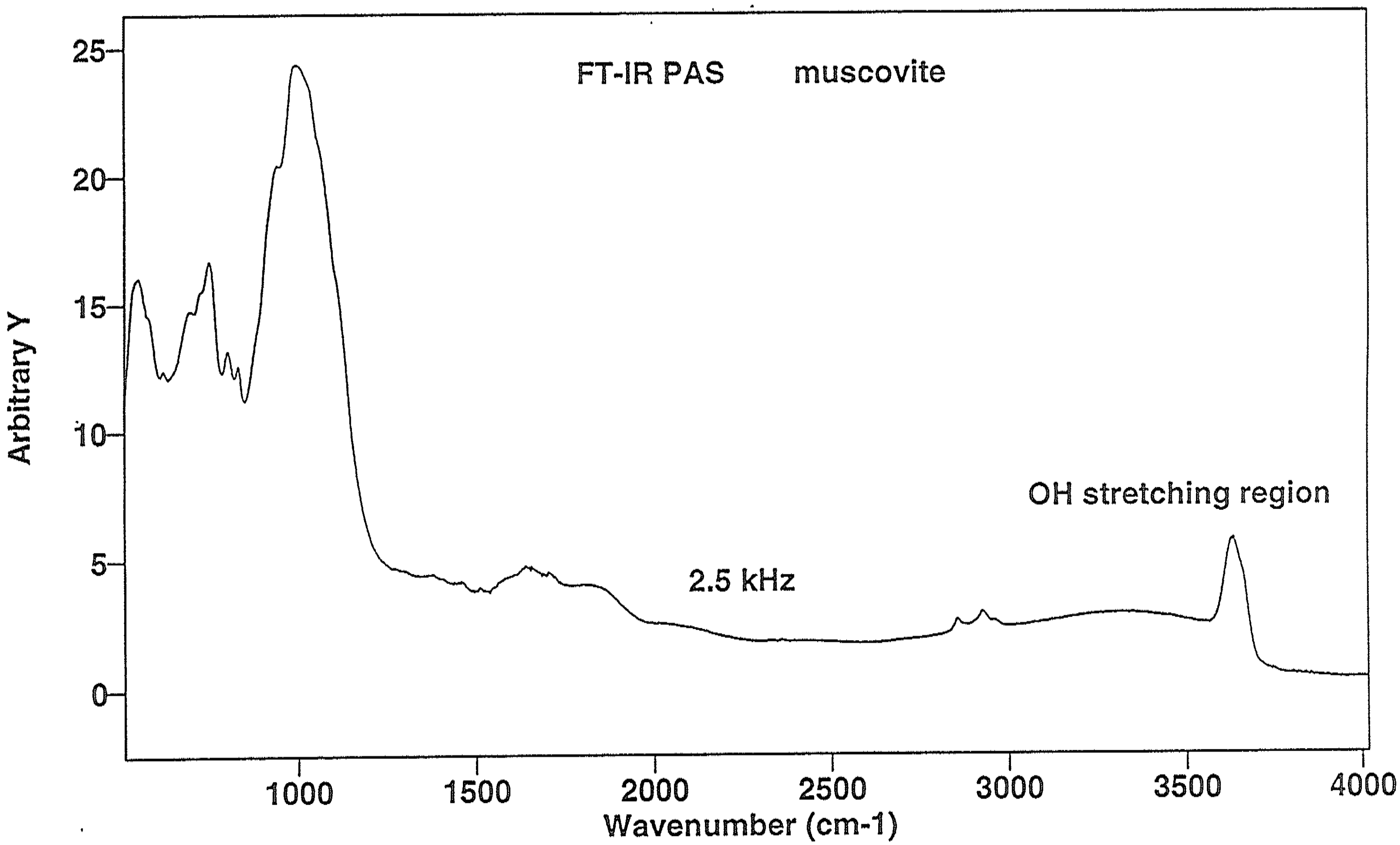

Figure 6-7. FT-IR PAS of muscovite at room temperature

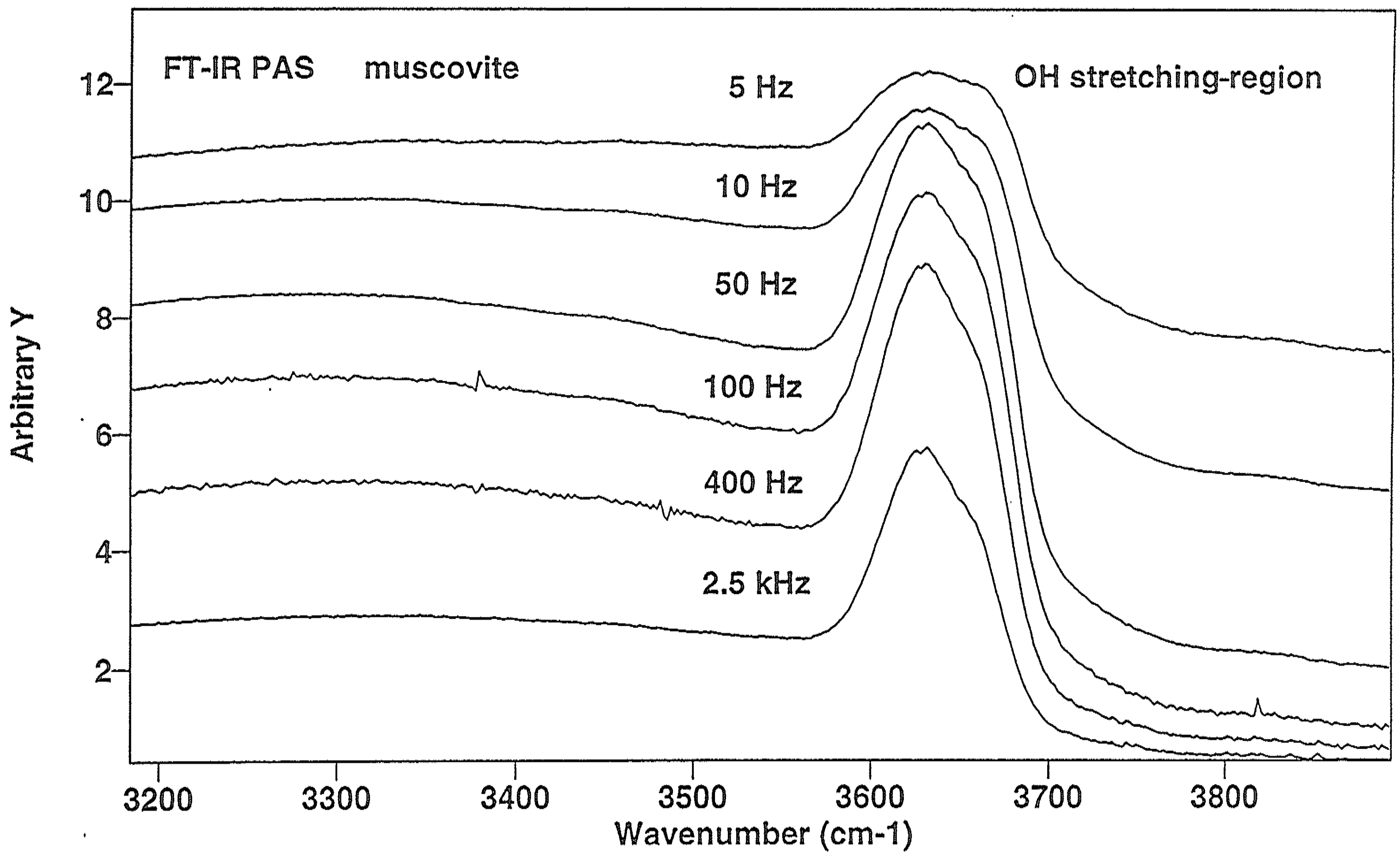

Figure 6-8. FT-IR PAS spectra of the OH-stretching region of muscovite at room temperature

study has a chemical composition similar to the sample used by Rothbauer (1971), although the unit-cell parameters of the two samples do differ somewhat. Although the individual O-H distances at 12 K are not significantly different from those at room temperature, the H(1)-H(2) separation is significantly larger at low temperature (0.78 Å) than at room temperature (0.44 Å). Such an increase in separation at low temperature supports the split H-atom model. Nevertheless, even with such a separation, it was still not possible to resolve two maxima (Fig. 6-2).

The occupancy of the Al site (Table 6-3) was persistently low during the Rietveld refinement. It could be related to the fact that the isotropic-displacement factors from the room-temperature structure refinement were used and fixed in the low-temperature refinement. Attempts to refine individual displacement factors were not successful.

6.3.3. Infrared spectroscopy

There is evidence from infrared spectroscopy (Serratosa & Bradley 1958, Basset 1960, Vedder & McDonald 1963, Rouxhel 1970) of more than one OH-orientation in the muscovite structure. The FWHM of the O-H stretching band of muscovite is almost twice as large as that of phlogopite (Rouxhel 1970, Basset 1960 , Serratosa & Bradley 1958), irrespective of sample temperature (from 273 to 77 K). In fact, two O-H orientations were suggested by Serratosa & Bradley (1958), in analogy to the O-H orientations in lepidolite. The FT-IR PAS spectrum of muscovite in the present work (Fig. 6-7) shows similar width of the OH-stretching band at high mirror-speed (2.5 KHz). In this spectrum, there is a shoulder to the high-frequency side of the absorption envelope and it is separated from the principal maximum by an inflection point; this indicates the presence of (at least) two distinct bands in the spectrum. This conclusion is reinforced by the series of spectra collected with gradually decreasing interferometer-mirror speed (Fig. 6-8). The intensity of the high-frequency shoulder increase relative to the maximum intensity of the envelope as the mirror speed decreases from 2.5 KHz to 5 Hz. Note that wave number increases toward the right-hand side in Figure 6-8, and that slower mirror speed favours higher IR frequencies (see 6.1.3.). The increase in relative intensity of the right shoulder of the envelope indicates that there are two (or more) unique bands in the muscovite spectrum, in turn indicating more than one symmetrically distinct OH group.

6.3.4. Possibility of symmetry lower than *C2/c*

The two sets of H-atom positions (Table 5-3-8) calculated from the structure-energy minimization are related to each other (in the original *C2/c* structure) by the *c*-glide. This suggests that the true symmetry of muscovite is either $C\bar{1}$ or *C*2. In the precession photos (Fig. 6-3), there are very weak (*h*0*l*) (*l*=odd) reflections violating the *c*-glide restriction. Peak-profiles (Fig. 6-4 and 5) of these 'violating' reflections are slightly asymmetric but still well-defined. The presence of these reflections indicate that the space group symmetry of muscovite is *C*2 or $C\bar{1}$ rather than *C2/c*. Similar violating reflections were observed by Schultz *et al.* (1989) on Weissenberg photographs of rose muscovite.

6.4. Discussion and Interpretation

FT IR PAS spectra give evidence that (at least) two symmetrically distinct OH groups, and therefore two unique H atom positions, exist in muscovite structure. The two H-atom positions can either be explained by a dynamic, positional disorder model in space group *C*2/*c*, or by a long-range order model in a subgroup of *C*2/*c* (*C*2 or $C\bar{1}$). Weak reflections of *h*0*l* (*l*=odd) observed on precession photos and on single-crystal diffractometer indicate the lack of *c*-glide symmetry that are necessary in the *C*2/*c* space group. Therefore, the true space group symmetry of muscovite should be *C*2 or $C\bar{1}$ rather than *C*2/*c*. Further experiment, such as second-harmonic generation, is needed to determine if a centre of symmetry exists or not, so as to determine the exact symmetry of muscovite of *C*2 (no centre of symmetry) or $C\bar{1}$ (with centre of symmetry).

It should be noted that the existence of *h*0*l* (*l*=odd) reflections had been explained (Schultz *et al.* 1989) not by the unique ($C\bar{1}$ or *C*2) H-atom arrangement with respect to the other atoms, but by postulating partial trioctahedral character of the structure in which *M*(1) was partially occupied by Li in rose muscovite, with *M*(1') (the symmetry equivalent of *M*(1) in *C*2/*c*) empty. However, the concentration of Li in the (rose) muscovite sample was not sufficient to account for the observed scattering.

Keeping in mind that the *M*(1)-site, which is nominally vacant in dioctahedral mica (Fig. 6-9), is one of the potential directions in which the OH group can point, the residual electron density observed near the *M*(1)-site (Schultz *et al.* 1989, Güven 1971) may be accounted for by relaxing the symmetry of *C*2/*c* to *C*2 or $C\bar{1}$ with respect to the

H positions.

6.5. Summary

There are two positions for H atom in the muscovite structure. The two positions can be represented by a split H-atom site model in space group *C2/c*. A subgroup of *C*2 or $C\overline{1}$ for the overall structure is also possible. The occupancies of the two split-sites are approximately equal.

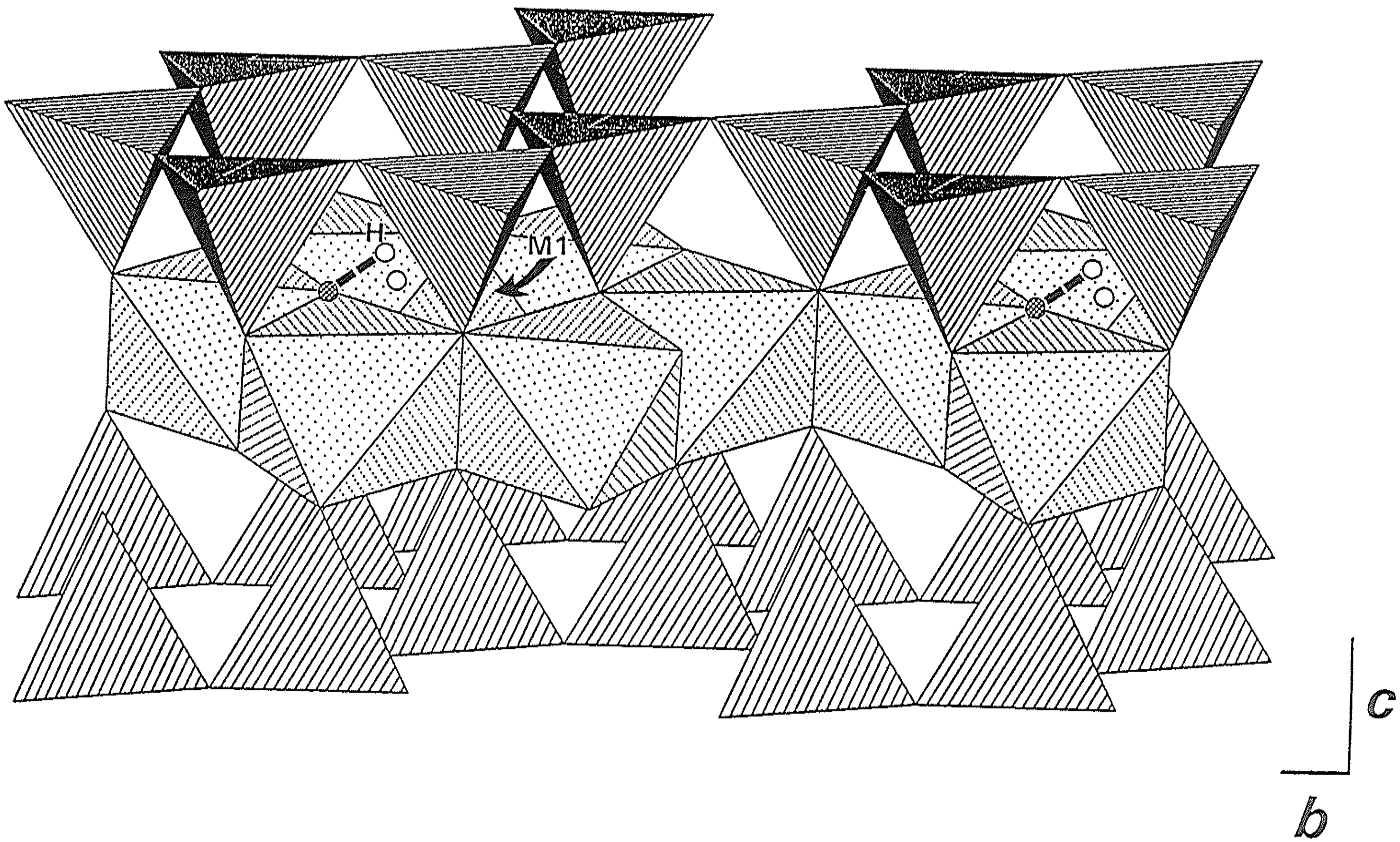

Figure 6-9. Spatial relationship between the OH orientation and the nominally vacant M1 site in the muscovite structure.

Chapter 7

Coupled Rietveld--Static Structure-Energy Minimization Method

In Rietveld refinement, there are cases where the powder-diffraction data is of insufficient resolution to allow accurate refinement, or the starting model leads to convergence at a local minimum. As a result, stereo-chemistries that are crystal-chemically unreasonable may be generated. Soft constraints, in the form of prescribed bond-distances (Cartlidges & Meier 1984; McCusker *et al.* 1985; Bish & Von Dreele 1989) and angles (Marler *et al.* 1993), must be used in order to avoid such unreasonable results. Prescribing bond-length and bond-angle constraints is somewhat subjective, and removing these constraints as the Rietveld refinement progresses is often not successful (McCusker *et al.*

1985; Marler *et al.* 1993); thus it is possible to introduce subjective bias into the final result. The issue becomes more difficult when one wants to refine structures at very low or high temperatures (see, for example, Cartlidge & Meier 1984), since there are usually not sufficient empirical data to enable prescribing bond-length and angle constraints.

Calculation (Catlow & Price 1990; Burnham 1990) of crystal-structure arrangements using Static-Structure Energy Minimization (the SSEM method) has been fairly successful in recent years (Collins & Catlow 1992; Winkler *et al.* 1991; Purton & Catlow 1990; Dove 1989; Price *et al.* 1987; Sanders *et al.* 1985, see also Chapter 5). Current models involving electrostatic- and repulsive-interaction terms, with certain higher order corrections (see 4.1), are capable of predicting atomic positions with an accuracy of 1-3% for simple ordered structures (Purton & Catlow 1990). In more complicated structures, the differences tend to be larger than 5%. This problem with complicated structures is common to other simulation techniques such as Molecular Dynamics (MD). However, the problem can be ameliorated by introducing experimental constraints from diffraction experiments (Brünger *et al.* 1987; Fujinaga *et al.* 1989; Brünger & Karplus 1991) or NMR (van Gunsteren & Mark 1992).

Rietveld refinement using powder-diffraction data can potentially provide experimental constraints in computer simulation of crystal structures. At the same time, computer simulation is sufficiently accurate to constrain Rietveld refinement. This suggests that Rietveld refinement and computer simulation can be coupled together to enhance the effectiveness of the Rietveld method in dealing with complex structures while avoiding possible bias that can be introduced by using soft distance and angle constraints. As a first step towards this goal, the Rietveld method is to be coupled with SSEM such that Rietveld refinement of difficult structures at room temperature can be effectively constrained.

7.1. Rietveld and SSEM programs: modification in the present study

The Rietveld and the SSEM programs used here are LHPM3 and WMIN, respectively. LHPM3 was further modified to correct for sample-displacement error. The correction is of the form (Parrish *et al.* 1986)

$$\Delta 2\Theta = s \cdot \cos\theta \;/\; R \qquad \text{7-1}$$

in which s and R (in mm) are the displacement of the sample surface from the focusing circle and the diffractometer radius, respectively, and $\Delta 2\Theta$ is in radians. The correction is applied to the positions of the calculated Bragg-reflections which, together with the corresponding intensities, are then used in the calculation of step intensities.

The SSEM program, WMIN, as modified in Chapter 4, was used in the coupling of the Rietveld and the SSEM methods.

7.2. Coupling Rietveld refinement with static-structure energy minimization

To couple the Rietveld and SSEM calculations, both quantities to be minimized are considered simultaneously in the form of a sum

$$E_{sum} = E_{EM} + W \cdot R_{wp} \qquad 7\text{-}2$$

in which W is a weight (to be discussed later), E_{EM} is the static-structure energy, and R_{wp} is the weighted R-squared value (*c.f.* equation 2-13), usually formulated in Rietveld refinement as

$$R_{wp} = \frac{R}{\sum_i w_i \, Y_{io}} = \frac{\sum_i w_i \, (Y_{io} - Y_{ic})^2}{\sum_i w_i \, Y_{io}} \qquad 7\text{-}3$$

where Y_{io} and Y_{ic} are the observed and calculated step intensities, respectively, and w_i are the assigned weights. The use of R_{wp}, rather than R, is to ensure that the combined quantity is relatively independent of the absolute values of the raw step intensities in the powder-diffraction experiment.

The weight, W, in equation 7-2 scales R_{wp} with respect to the structure energy, E_{EM}. There is no theoretical justification for what form that W should take, or what value it should have. A pragmatic view suggests that W will vary with the adequacy of the potential model and the degree of resolution of the diffraction data. Work (Fujinaga *et al.* 1989) coupling single-crystal diffraction data with structure simulation (both SSEM and MD) has used the reciprocal of the square of the calculated structure factor as a weight. There was also the suggestion (Brünger *et al.* 1991) to use a weight such that the magnitudes of the first derivatives of R_{wp} with respect to the structural parameters be similar to those of the structure energy, E_{EM}. These approaches are either not applicable to powder-diffraction data, or are not sufficiently efficient and flexible.

The form of the weight used in this work was determined by trial-and-error, using the coupled method and different weighing schemes to refine the structures of well-characterized single-phase olivine and pyroxene whose structures are easy to refine using the Rietveld method alone (see 3.1). It was found that R_{BRG} (the Bragg-R) makes a good weight. For multiphase refinement, the weight takes the form

$$W = {}^{1}R_{BRG} + {}^{2}R_{BRG} + \ldots \qquad 7\text{-}4$$

The use of R_{BRG} has evolved the weight W from the function of being a simple scaling factor, to enabling the refinement not only to consider the overall agreement between the observed and the calculated diffraction patterns, but to consider the agreement between the "observed" and calculated Bragg intensities as well, which may not always be implied by the consideration of R_{WP} (or R).

It may seem that the use of R_{BRG} as a weight will give less weight to powder-diffraction data (the Rietveld part) as the refinement progresses, as we expect a successful refinement to converge (giving smaller R's). However, as the CRSSEM method is developed mostly to work with refinements that initially converge into a false minimum (see examples later in the chapter), the R-values are small at the beginning of the CRSSEM refinement, and become larger as the refinement progresses, giving more weight to the powder data (the Rietveld part). The tendency R-values to increase in the CRSSEM refinement is caused by certain instrument-related factors (*e.g.* asymmetry that is more outstanding in high-resolution diffraction experiments) and non-periodical structural features (*e.g.* stacking disorder in layered structures) which cannot be adequately modeled in Rietveld method at present (see detailed discussion in the heulandite example).

Therefore, the CRSSEM method actually seeks a balance between the two quantities in equation 7-2, E_{EM} and R_{WP}, while trying to obtain a smaller sum of the two quantities.

The combined quantity in equation 7-2 is minimized and the structure refined as outlined in Figure 7-1. An approximate structure model (usually refined using Rietveld method alone) is input to two functional blocks, R and W, respectively to calculate the two quantities, E_{EM} and R_{WP}, in equation 7-2. The static-structure energy, E_{EM}, is calculated in block W (implemented by the subroutine WCALC in WMIN). The core positions of the O atoms used in the calculation correspond to those of the input model, and the shellpositions are adjusted independent of (at least not directly related to) the powder-diffraction data. In the R-block, R_{wp} is calculated in the modified subroutine ITER of the Rietveld program, which can calculate the structure factors and evaluate the difference while keeping all instrumental and structural parameters fixed at the input values. The R_{BRG}, used as W in equation 7-2, is calculated for each call to ITER by a subroutine BRAGG written in this study. At fixed interval, the instrumental parameters for the Rietveld refinement are adjusted by the Rietveld program alone while keeping all structural parameters fixed. A sum, E_{sum}, is then formed from the quantities E_{EM} and R_{wp} obtained from the two functional blocks. This sum will be the basis for the optimization routines residing in the program WMIN. When the modified Rosenbrock search routine is chosen, this sum will be minimized by adjusting the structural-parameters through repeated entries of the R and W blocks such that only the parameter shifts that lower E_{sum}, which contains contributions from the structure energy E_{EM} and the Rietveld difference R_{WP}, will be accepted. A cycle of refinement is completed when shifts for all structural

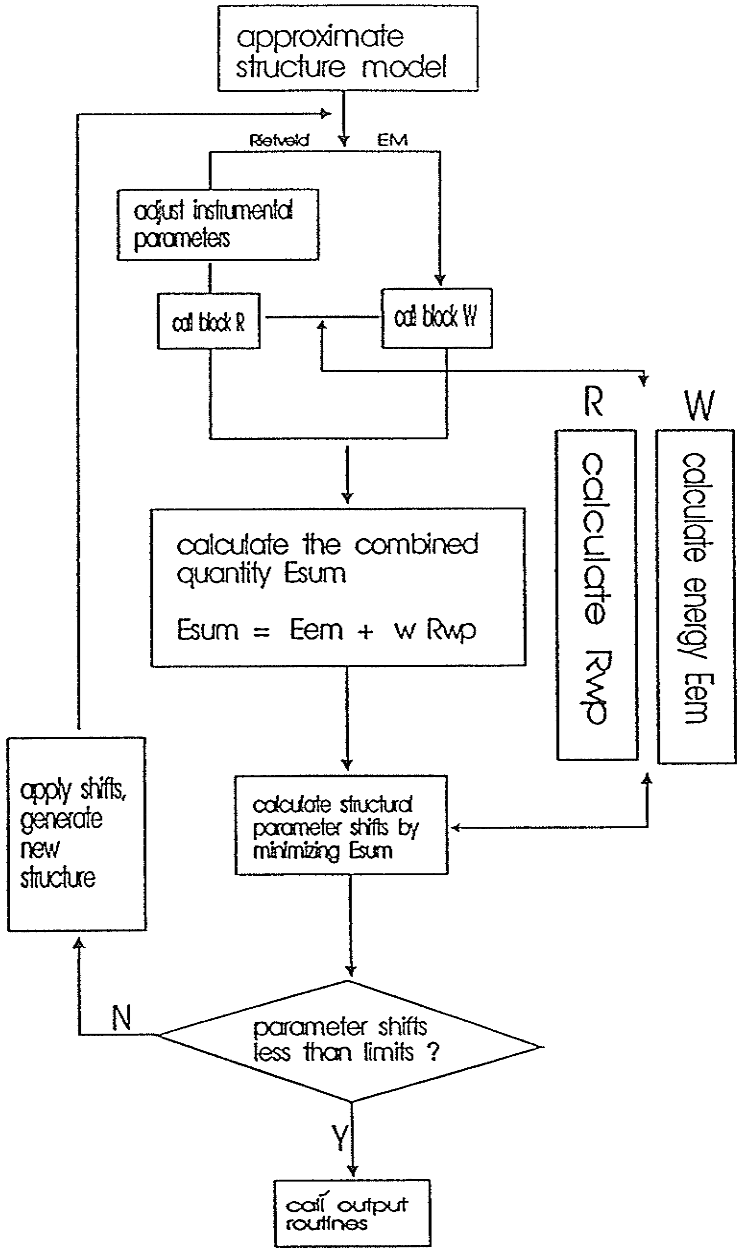

Figure 7-1. Schematic representation of the coupled Rietveld--static-structure energy minimization refinement method.

parameters are calculated. If any of these shifts is greater than certain limit (0.001 along any axes of the fractional coordinate system), the shifts are applied and a new cycle of refinement is started. Usually, only several cycles are needed to achieve convergence if the starting model is reasonably close to the final one.

If Newton's method of minimization is chosen, the first and second derivatives needed for the minimization will be calculated numerically, i.e., variations of the total energy corresponding to finite increments and decrements of structural parameters will be calculated by actually calling the R and W blocks. Optimization is done by solving for structural parameter shift, **Δp** (**Δp** = Δp_i, i = 1 ... n in the equation):

$$\boldsymbol{B}\ \Delta \boldsymbol{p} = -\boldsymbol{d} \qquad 7\text{-}5$$

in which $B_{ij} = \partial^2 E_{sum}/\partial p_i \partial p_j$, $d_i = \partial E_{sum}/\partial p_i$, i,j = 1 ... n. This method is faster, but is more prone to the problem of optimization falling into local minima. The computer program had been set up in this study such that optimization can start with a Rosenbrock search and finish with searches using Newton's method.

7.3. Examples of structure refinement using the CRSSEM method

7.3.1. Minor phases in binary mixtures

It was shown in section 3.1. that when the minor phase is ~ 10 wt% or less, the refined structural parameters of the minor phase deviate significantly from the correct values. It is tempting to try to improve the refinement results using the Coupled Rietveld--

Static-Structure Energy Minimization (CRSSEM) method. Here, two cases are considered, one with a mixture of 10 wt% olivine and 90 wt% pyroxene, and the other with a mixture of 10 wt% pyroxene and 90 wt% olivine; the intensity data are from section 3.1. The coefficients used for the potential function in the SSEM calculation are listed in Table 7-1. The starting structure-models were those obtained by Rietveld refinement alone. Isomorphous replacement of Mg^{2+} by Fe^{2+} in olivine, and Ca^{2+} by Mg^{2+} and Fe^{2+} in pyroxene are not considered explicitly in the structure-energy calculation; the potential parameters for (Mg,Fe)-O and (Ca,Mg,Fe)-O atom pairs were those for Mg-O and Ca-O, respectively. In the minimization of E_{sum} (equation 7-2) with the Rosenbrock search, five stages were used in each cycle; the structure parameters were first adjusted one at a time (the exploratory search) to determine the direction of shift, followed by a vector search in which all parameters were adjusted at the same time in the direction determined in the exploratory search. Results of these refinements are listed in Table 7-2, where they are compared with the results of Rietveld refinement alone, and also the results of single-crystal structure-refinement. A dramatic improvement (although similar improvement may also be achieved using Rietveld method with soft distance constraints) in the refined structure of olivine in the 10 wt% olivine - 90 wt% pyroxene mixture was obtained by the coupled method. This is most easily seen by comparing the Si-O distances (Table 7-2); the values are no longer obviously unrealistic, and are ordered in the same way as the single-crystal values. There is also an improvement in the structure refinement of the pyroxene in the 10 wt% pyroxene - 90 wt% olivine mixture, albeit not as dramatic as in the case of olivine. The short Si-O distances produced here are related to a deficiency in

Table 7-1. POTENTIAL PARAMETERS USED IN THE STRUCTURE ENERGY CALCULATION OF OLIVINE AND PYROXENE

Short-range repulsion of Born/Buckingham-type potentials*

	λ (KCal/mol)	ρ (Å)	C(KCal/mol·Å^{-6}	Ref
Si^{4+}-O^{2-}	29607.352	0.3025	245.860	[1]
Ca^{2+}-O^{2-}	160461	0.2516		[2]
Mg^{2+}-O^{2-}	32942	0.2945		[3]
O^{2-}-O^{2-}	524946	0.149	642.9	[1]

Bond-bending interaction**

	k_B (Kcal/rad^2)	Θ_0 (°)	Ref
O^{2-}-Si^{4+}-O^{2-}	48.3631	109.47	[1]

Shell-core interaction between O-shell and O-core***

	k_p (KCal/Å^2)	Ref
$O_{core}^{+0.86902}$-$O_{shell}^{-2.86902}$	1728	[1]

* *cf.* equations. 4-7 & 4-4; ** *cf.* equation 4-5; *** *cf.* equation. 4-6

[1] Sanders et al. (1984)

[2] Post & Burnham (1986)

[3] Price & Parker (1988)

TABLE 7-2. COMPARISON OF CRYSTAL-STRUCTURE REFINEMENTS BY THE RIETVELD METHOD AND BY THE COUPLED RIETVELD--STATIC-STRUCTURE ENERGY MINIMIZATION METHOD

	Olivine			Pyroxene		
	Rietveld method	CRSSEM	single crystal	Rietveld alone	CRSSEM method	single crystal
a (Å)	4.767(2)	4.767(2)	4.764(1)	9.747(4)	9.747(3)	9.743(2)
b (Å)	10.249(4)	10.249(4)	10.226(3)	8.914(3)	8.914(4)	8.916(2)
c (Å)	6.000(2)	6.000(2)	6.004(2)	5.259(2)	5.260(3)	5.256(1)
β (°)				105.90(3)	105.90(4)	105.88(2)
Selected interatomic distances (Å)						
Si-O1	1.71(9)	1.60(8)	1.620(2)	1.64(4)	1.52(5)	1.604(2)
Si-O2	1.82(3)	1.65(6)	1.653(2)	1.60(5)	1.50(5)	1.588(2)
Si-O3a	1.86(4)	1.62(8)	1.637(2)	1.59(6)	1.62(7)	1.668(2)
Si-O3b	1.86(4)	1.62(6)	1.637(2)	1.83(6)	1.69(6)	1.689(2)

the current potential models when applied to the pyroxene structure. Calculation of the pyroxene structure by the SSEM method alone (Dove 1989) with the same potential model and the same parameterization gave even shorter Si-O distances.

7.3.2. Structure refinement of synthetic zeolite ZSM-23

The crystal structure of ZSM-23 was refined from synchrotron X-ray powder-diffraction data using the Rietveld method, together with 146 bond-distance and angle constraints (Marler *et al.* 1993). These constraints assumed a mean Si-O distance of 1.602 Å (this constraint itself is very material-dependent) and a mean Si-O-Si angle of 151° (*c.f.* the ZSM-22 structure; Marler 1987) as the corresponding ideal values in the ZSM-23 structure. The refinement converged to R_{wp} = 0.085 and R_{BRG} = 0.132. However, the constraints could not be removed as the refinement progressed.

In the present study, the same set of synchrotron data was used. The structure of Marler *et al.* (1993) was used as input to the coupled Rietveld--static-structure minimization procedure. Potential parameters were those that are relevant in Table 7-1, except that repulsion for the Si-O pair was calculated using the Born model (see equation 4-1) with the coefficients of Kunz & Armbruster (1992):

$$\lambda_{Si\text{-}O} = 399628.6 \text{ KCal/mol}$$

$$\rho_{Si\text{-}O} = 0.197 \text{ Å}$$

The NH_4^+ and F^- ions were omitted from the structure-energy calculation. This is feasible because (1) the framework of the zeolite structure is neutral, and (2) the amount of NH_4F in the unit cell is very small. Therefore, the existence of NH_4F in the zeolite channel can be considered as a minor perturbation of the structure energy, and can be compensated, along with other insufficiencies in the potential model, by the pseudo-energy term from the Rietveld part of the coupled method.

The refinement results using the coupled method are shown in Tables 7-5, 7-6 and 7-7; the powder pattern is shown in Figure 7-2. There is a good fit between the observed and calculated patterns as indicated by the low R_{BRG} and the relatively low R_{wp} (there is a second unknown phase present, and this was not modelled). The corresponding R-values from the work of Marler *et al.* (1993) are rather different. Difference in R_{wp} and R_{exp} in between the two works may be explained by the different weighting schemes used in calculating these R-values. However, R_{BRG} is only slightly affected by the type of weighting scheme and its formulation has little variation between different Rietveld codes. As R_{BRG} is a measure of the correspondence between the calculated structure model and the observed data (the Bragg reflections in the powder-diffraction pattern), the lower R_{BRG} obtained in this study indicates that a better model was derived by the CRSSEM method.

The refined structure is slightly different from that of Marler *et al.* (1993) in terms of unit-cell parameters (Table 7-5) and atomic coordinates (Table 7-6). However, most of the interatomic distances and angles agree within 1σ (Table 7-7). Differences are observed in Si-O-Si angles and F-N distances. Whereas the lower ranges of Si-O-Si angles are similar in the two refinements, the range of angles is greater in the present refinement; many recent single-crystal structure-refinements of the ZSM series (van Koningsveld 1990; van Koningsveld *et al.* 1989, van Koningsveld *et al.* 1987) show Si-O-Si angles in the range of 140-176°, in good agreement with the present work.

TABLE 7-3. REFINEMENT DETAILS OF THE ZSM-23 STRUCTURE

	This work	Marler et al. (1993)
Wavelength (Å)	1.1999	1.1999
Profile range (°2Θ)	5.80 - 61.385	5.80 - 61.385
step size (°2Θ)	0.005	0.005
exclude regions (°2Θ)	16.6 - 17.5	16.6 - 17.5
	20.0 - 21.0	20.0 - 21.0
a (Å)	11.1486(2)	11.129(1)
b (Å)	5.0330(1)	5.025(1)
c (Å)	21.5585(3)	21.519(1)
β (°)	89.838(1)	89.85(4)
R_{BRG}	0.056	0.132
R_{wp}	0.189	0.085
R_e	0.065	0.033

TABLE 7-4. THE FINAL ATOMIC COORDINATES OF THE ZSM-23 STRUCTURE

	This work			Marler et al. (1993)		
Atom	X	Y	Z	X	Y	Z
SI1	-.008(4)	-.015(15)	.456(2)	-0.009(2)	-0.02(1)	0.4578(9)
SI2	.726(4)	-.082(13)	.425(2)	0.726(2)	-0.082(8)	0.425(1)
SI3	.228(4)	-.114(13)	.384(2)	0.228(2)	-0.112(8)	0.384(1)
SI4	.312(3)	0	.251(2)	0.312(2)	0	0.251(1)
SI5	.479(3)	.503(12)	.250(2)	0.476(2)	0.503(4)	0.249(1)
SI6	.348(4)	.393(13)	.435(2)	0.346(2)	0.390(8)	0.434(1)
SI7	.603(3)	.417(12)	.378(2)	0.600(2)	0.417(8)	0.378(1)
SI8	-.010(4)	-.099(14)	.044(2)	-0.010(2)	-0.10(1)	0.0422(9)
SI9	.727(4)	-.010(14)	.079(2)	0.726(2)	-0.012(9)	0.077(1)
SI10	.231(4)	-.076(13)	.120(2)	0.232(2)	-0.077(7)	0.118(1)
SI11	.355(4)	.424(14)	.063(2)	0.355(2)	0.424(8)	0.063(1)
SI12	.603(4)	.487(12)	.120(2)	0.603(2)	0.487(8)	0.120(1)
O1	.012(7)	.270(22)	.489(4)	0.012(5)	0.27(1)	0.487(2)
O2	.865(7)	-.020(24)	.424(3)	0.866(2)	-0.02(1)	0.422(2)
O3	.093(7)	-.090(23)	.408(3)	0.093(3)	-0.09(1)	0.408(2)
O4	.683(7)	-.040(24)	.495(3)	0.683(4)	-0.04(1)	0.495(1)
O5	.655(7)	.125(21)	.383(7)	0.655(4)	0.122(9)	0.381(2)
O6	.237(6)	-.050(25)	.312(4)	0.231(4)	-0.05(1)	0.311(1)
O7	.315(7)	.092(19)	.419(4)	0.317(4)	0.085(9)	0.41((2)
O8	.370(6)	.296(16)	.254(4)	0.368(3)	0.292(4)	0.254(3)
O9	.563(6)	.488(22)	.309(4)	0.564(4)	0.49(1)	0.308(1)
O10	.487(6)	.440(24)	.422(4)	0.486(2)	0.44(1)	0.423(2)
O11	.866(7)	-.069(23)	.079(3)	0.866(2)	-0.07(1)	0.079(2)
O12	.102(7)	-.050(23)	.089(3)	0.100(3)	-0.05(1)	0.089(2)
O13	.680(7)	-.030(23)	.008(3)	0.679(4)	-0.03(1)	0.008(1)
O14	.228(6)	-.030(21)	.192(4)	0.226(3)	-0.03(1)	0.192(1)
O15	.553(7)	.440(21)	.189(4)	0.553(4)	0.43(1)	0.189(1)
O16	.496(7)	.460(23)	.073(4)	0.497(2)	0.46(1)	0.071(2)
O17	.706(7)	.283(20)	.103(3)	0.708(3)	0.28(1)	0.103(2)
O18	.322(7)	.133(21)	.087(4)	0.322(4)	0.130(8)	0.086(2)
O19	-.001(7)	.113(23)	-.012(4)	-0.001(5)	0.11(1)	-0.014(2)
O20	.699(7)	.626(20)	.402(4)	0.701(3)	0.621(9)	0.401(2)
O21	.271(7)	.587(19)	.394(4)	0.269(4)	0.584(8)	0.392(2)
O22	.420(6)	.796(14)	.246(4)	0.422(2)	0.797(5)	0.246(3)
O23	.652(7)	.785(21)	.119(4)	0.652(4)	0.786(9)	0.120(2)
O24	.286(7)	.635(20)	.106(4)	0.285(4)	0.632(8)	0.106(2)
F	.933(7)	.557(19)	.215(4)	0.938(8)	0.55(3)	0.215(5)
N	.910(9)	.085(24)	.255(7)	0.89(1)	0.06(4)	0.261(9)

TABLE 7-5. RANGES OF DISTANCES (Å) AND BOND-ANGLES (°) OF ZSM-23

	This work	Marler et al. (1993)
Si-O	1.58(8) - 1.63(8)	1.59 - 1.60
<Si-O>	1.59(1)	1.60
Si-Si	2.99(7) - 3.20(5)	3.00 - 3.15
<Si-Si>	3.03(1)	3.08
O-O	2.54(10) - 2.67(13)	2.56 - 2.65
<O-O>	2.60(1)	2.61
F-N	2.54(12) and 2.82(13)	2.74 and 2.76
O-Si-O	106(6) - 114(5)	106 - 112
<O-Si-O>	109(1)	109
Si-O-Si	142(6) - 174(7)	140 - 159
<Si-O-Si>	152(1)	149

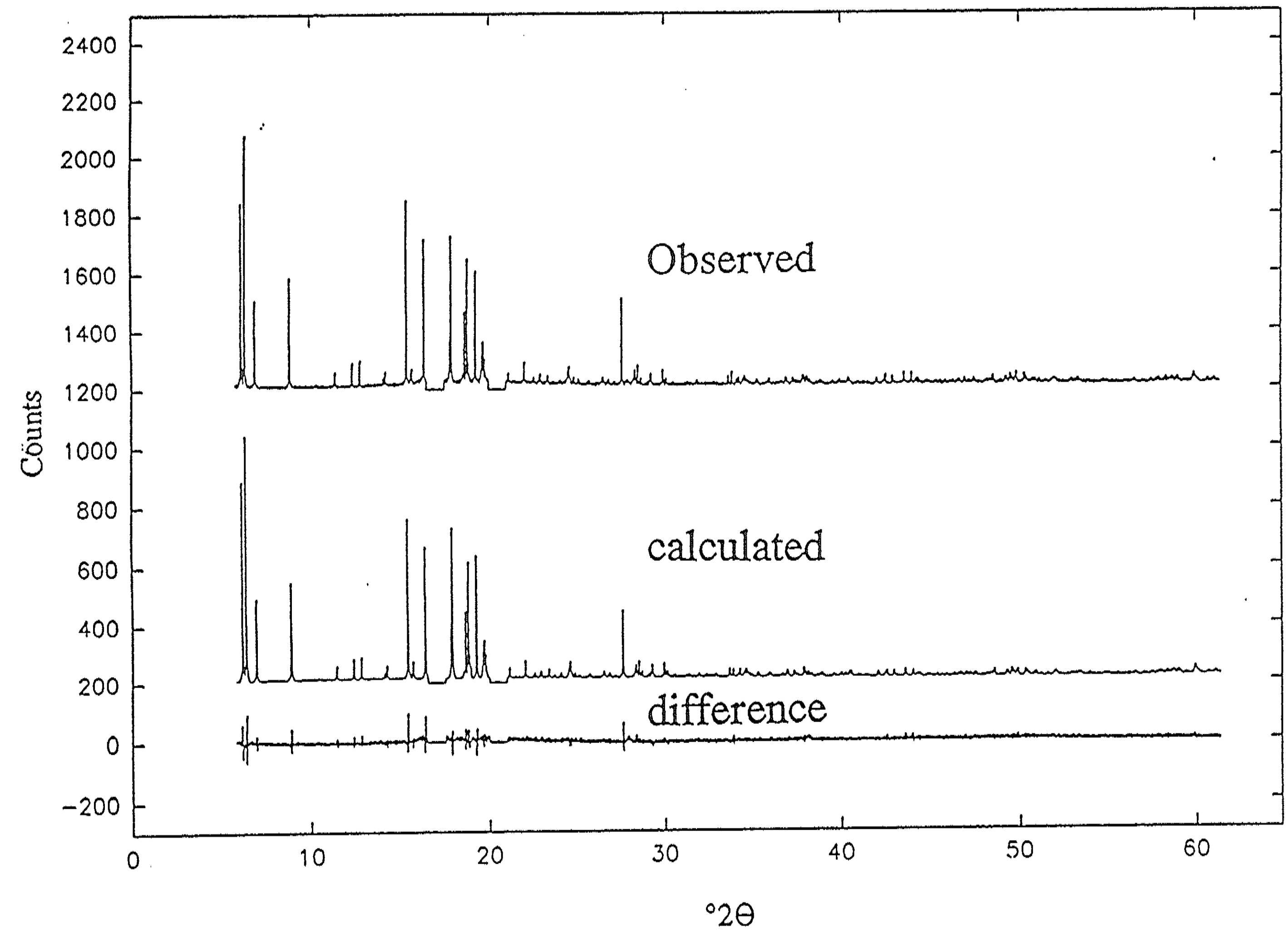

Figure 7-2. Observed (A), calculated (B) and the difference (C) powder diffraction patterns of ZSM-23

7.4. Summary

Coupled Rietveld--Static-Structure Energy Minimization (CRSSEM) refinement is a viable solution to the problem of crystal-structure refinement using powder-diffraction data when the latter is not of sufficient resolution to allow adequate structure refinement using the Rietveld method alone. Such situations can arise when the material of interest occurs as a minor phase in a mixture, or when the structure is very complex, such as those of the synthetic zeolites. The core of the coupled method is the minimization of the sum of two quantities: (1) the difference between the observed and calculated powder-diffraction patterns; (2) the static-structure energy. Such minimization scheme is hopefully a more objective solution to this problem than the use of distance and angle constraints.

Chapter 8

Refining Crystal Structures of Boromuscovite Polytypes Using the CRSSEM Method

8.1. Boromuscovite: a new mineral

Boromuscovite was described as a new mineral species by Foord *et al.* (1991). It has an ideal formula $KAl_2(Si_3B)O_{10}(OH)_2$, and the chemical composition reported by Foord *et al.* (1991) is very close to that of the end-member; the key chemical feature is the occurrence of a significant amount of B at the tetrahedral site(s) of the structure. However, no crystal-structure refinement has yet been done because of the fine-grained nature of the mineral. Furthermore, boromuscovite occurs as a mixture of 1*M* and $2M_1$ polytypes, further complicating the problem of structural characterization.

Rietveld method is the ideal method for structure refinement of this new mineral, not only for the obvious reason that the mineral was a fine-grained powder in diffraction intensity- data collection, but also for the method's ability to simultaneously refine more than a single phase. With the development of the Coupled Rietveld--Static Structure-Energy Minimization (CRSSEM) method, the chance of success in refining simultaneously the structures of both polytypes is increased.

8.2. Experimental

The material used here is from Řečice granitic pegmatite, Czech Republic, supplied by Milan Novák at the Department of Mineralogy, Moravian Museum, Czech Republic.

8.2.1. Chemical analysis

Electron-microprobe analysis was done in wavelength-dispersion mode on a Cameca SX–50 instrument with a beam diameter of 5 μm and an accelerating potential of 15 kV. Other experimental details are as described in section 3.1.1.

Quantitative ion-microprobe analysis for Li, Be and B was done by Luisa Ottolini at the CNR Centro di Studio per la Cristallochimica e la Cristallografia, Pavia, Italy. The instrument used is a CAMECA IMS 4F, using a primary beam of $^{16}O^{-}$ ions (5–15 μm diameter) at 12.5 keV and 5–10 nA current intensity. Secondary ions at masses 7 (Li), 9

(Be), 11 (B), and 30 (Si) as the reference isotope for the matrix, were collected under an ion-imaged field of 25 μm diameter, contrast diaphragm of 400 μm and field aperture of 1800 μm. Analytical reproducibility was checked on a standard sample (natural Macusani-rhyolite glass), resulting typically in a few percent variation over the span of a day. Energy filtering was used to monitor secondary ions: medium- to high-energy ions of ~100 ± 25 eV energies were selected in this experimental configuration. This approach is very effective in minimizing matrix effects for the light lithophile elements, Li, Be and B, over a wide range of concentration (Ottolini *et al.* 1993). It is a particularly effective method for B, and careful experiments show that an accuracy of 3% relative is possible (Hawthorne *et al.* 1995). Further details of this method as applied to micas are given in Černý *et al.* (1995).

8.2.2. Powder-diffraction data collection

The intensity-data collection procedure was similar to that described in section 3.2.1. Details of the data collection are listed in Table 8-1. Powder-diffraction step-scan intensities are given in Appendix P-28.

8.3. Structure refinement of two polytypes of boromuscovite

The refinement used the muscovite structure of Richardson & Richardson (1982) as a starting model for the $2M_1$ polytype, and the structure of Sidorenko *et al.* (1975) for the $1M$ polytype. Initial refinement was done using the modified Rietveld program

TABLE 8-1. INTENSITY DATA COLLECTION AND DETAILS OF STRUCTURE REFINEMENT

	$2M_1$	$1M$
a (Å)	5.090(1)	5.102(4)
b (Å)	8.822(2)	8.788(7)
c (Å)	19.819(5)	10.076(7)
β (°)	95.62(1)	101.23(3)
V (Å^3)	885.67	443.12
2θ scan range (°)	17–122	
step interval (°2θ)	0.02	
integration time/step (s)	20	
maximum intensity (counts)	1720	
Unique reflections	747	397
Structural parameters	38	24
Experimental parameters	12	
N-P	5177	
R_P	10.8	
R_{WP}	13.8	
R_{EXP}	7.9	
R_{BRG}	3.8	3.8

LHPM3. Details of the Rietveld refinement are similar to those in 3.2.1., and are summarized in Table 8-1. During structure refinement, when the atomic coordinates of the minor phase (the 1*M* polytype) were fixed, the structure of the dominant $2M_1$ phase could be refined, but resulted in unrealistic *T*–O distances. When attempting to refine the structure of the minor 1*M* phase, the refinement did not converge. Computer simulation (SSEM) of the 1*M* structure suggested the presence of a mirror plane, and refinement in the space group *C*2/*m* (rather than *C*2 of the starting model) did converge. However, unrealistic *T*–O distances occurred in both phases.

At this stage, the CRSSEM method was used. The coefficients for the various potential functions (equations 4–3 to 4-8) are those used in Chapter 5. Isomorphous replacement, such as B $\rightarrow$ Si and Al $\rightarrow$ Si, was not considered explicitly in the energy calculation, except that an effective charge of 3.75^+ (based on the chemical analysis) instead of 4^+ was used for the *T* atoms in the calculation of Coulombic energy. The potential terms involving (Si,B,Al)–O, (Al,Mg)–O, (K,Na)–O were approximated using parameterizations for Si–O, Al–O and K–O, respectively. The isomorphous replacements can be compensated for by the Rietveld part of the CRSSEM method.

It should be emphasized here that the potential parameterization involves only Si, Al, K, H and O, and energy minimization alone would result in the muscovite structure. Thus information on the 'boromuscovite' character of the sample (*i.e.*, short T–O distances, low T-site scattering, smaller cell dimensions) come entirely from the Rietveld component of the CRSSEM procedure. However, in the absence of the constraint of the energy minimization, the Rietveld refinement alone resulted in impossible individual T–O distances. Hence, it is apparent that the constraints of the energy minimization play an important role in the extraction of the boromuscovite features of the sample from the X-ray data *via* Rietveld refinement.

8.4. Results

The chemical composition and unit formula of boromuscovite are listed in Table 8-2. The refined atomic positions are shown in Table 8-3, selected bond-distances and angles are listed in Table 8-4, and site occupancies are given in Table 8-5. The overall fit between the calculated and the observed diffraction patterns is shown in Figure 8-1.

The chemical composition is very similar to that reported by Foord *et al.* (1991). The structural formulae of boromuscovite, calculated on the basis of 12 [O+OH+F], is $(K_{0.89}Na_{0.01})(Al_{1.99}Li_{0.01})(Si_{3.10}B_{0.68}Al_{0.22})O_{10.0}[(OH)_{1.98}F_{0.02}]$. The cell dimensions for both $2M_1$ and $1M$ polytypes are similar to those given by Foord *et al.* (1991). Based on the refined cell-parameters and scale factors of the two polytypes in the powder, the relative weight percentage of the $2M_1$ polytype can be calculated from (*c.f.* eq. 2-18)

$$W_{2M_1} = \frac{S_{2M_1}\ (ZMV)_{2M_1}}{S_{2M_1}\ (ZMV)_{2M_1} + S_{1M}\ (ZMV)_{1M}} \cdot 100\% \qquad 8\text{-}1$$

in which S, Z, M and V are the refined scale-factor, number of formula units in the unit cell, the mass of the formula unit, and the cell volume, respectively. The results of the present refinement give

TABLE 8-2. CHEMICAL ANALYSIS (wt%) AND UNIT FORMULA OF BOROMUSCOVITE

	present work*	Foord *et al.* (1991)
SiO_2	48.21	48.1
Al_2O_3	29.19	28.1
B_2O_3	6.12	7.0
FeO	0.04	0.1
MnO	–	0.08
MgO	0.03	0.15
BaO	0.11	—
CaO	–	0.01
Li_2O	0.03	0.05
K_2O	10.93	11.0
Na_2O	0.06	—
Rb_2O	0.03	0.52
Cs_2O	0.02	0.05
H_2O	4.61**	4.77
F	0.11	0.76
O=F	–0.05	0.32
Total	99.44	100.46

TABLE 8-2. (CONTINUE)

	present work*	Foord *et al.* (1991)
Si	3.10	3.06
Al	0.22	0.16
B	0.68	0.78
Al	1.99	1.94
Mg	–	0.01
Li	0.01	0.01
Ca	–	0.01
K	0.89	0.89
Rb	–	0.01
Na	0.01	—
O	10	10
OH	1.98	2.02
F	0.02	0.16

* P, Ti, Sc, Sr, Zn, Be, Mn not detected

** estimated by stoichiometry

– = not detected

— = not determined

TABLE 8-3. FINAL ATOMIC COORDINATES OF BOROMUSCOVITE POLYTYPES

	x	y	z	Displacement factor
		$2M_1$ polytype		
A1	0.251(3)	0.079(2)	–0.0002(7)	0.47
T1	0.442(3)	0.254(2)	0.1351(7)	0.12
T2	0.045(3)	0.426(2)	0.3640(7)	0.17
K	0	0.113(2)	1/4	0.26
O	0.039(5)	0.072(4)	0.4541(6)	0.35
O1	0.385(5)	0.248(4)	0.0569(12)	0.37
O2	0.043(4)	0.438(3)	0.4466(13)	0.29
O3	0.419(4)	0.090(3)	0.1655(10)	0.38
O4	0.229(6)	0.364(3)	0.1636(10)	0.68
O5	0.270(5)	0.314(2)	0.3466(12)	0.32
		$1M$ polytype		
Al	0	0.666(8)	0	0.62
T	0.437(11)	0.674(5)	0.272(5)	0.12
K	1/2	0	1/2	0.26
OH	0.433(16)	0	0.100(8)	0.35
O1	0.347(12)	0.715(6)	0.116(8)	0.37
O2	0.192(14)	0.726(7)	0.332(8)	0.68
O3	0.520(17)	1/2	0.587(9)	0.38

TABLE 8-4. INTERATOMIC DISTANCES (Å) AND ANGLES (°) IN BOROMUSCOVITE

$2M_1$ POLYTYPE

T1–O1	1.55(2)	T2–O2	1.64(2)
T1–O3	1.58(3)	T2–O3c	1.58(3)
T1–O4	1.58(3)	T2–O4e	1.56(3)
T1–O5	1.57(2)	T2–O5	1.57(3)
<T1–O>	1.57	<T2–O>	1.59
O1–O3	2.56(4)	O2–O3c	2.62(4)
O1–O4	2.53(3)	O2–O4e	2.56(3)
O1–O5	2.53(4)	O2–O5	2.63(3)
O3–O4	2.58(4)	O3c–O4e	2.57(4)
O3–O5	2.56(4)	O3c–O5	2.62(4)
O4–O5	2.61(4)	O4e–O5	2.56(4)
<O–O>T1	2.56	<O–O>T2	2.59
O1–T1–O3	109.8(21)	O2–T2–O3c	108.9(17)
O1–T1–O4	108.2(14)	O2–T2–O4e	106.1(14)
O1–T1–O5	108.6(13)	O2–T2–O5	109.5(14)
O3–T1–O4	109.4(13)	O3c–T2–O4e	109.8(16)
O3–T1–O5	108.8(15)	O3c–T2–O5	112.5(15)
O4–T1–O5	112.0(16)	O4e–T2–O5	109.6(15)
<O–T1–O>	109.5	<O–T2–O>	109.4
Al–O1	1.96(3)	K–O3 x2	2.84(2)
Al–O1a	1.98(3)	K–O4g x2	2.99(2)
Al–O2b	1.91(2)	K–O5 x2	2.92(2)
Al–O2c	1.88(3)	<K–O$_{inner}$>	2.92
Al–OHd	1.89(3)		
Al–OH	1.81(2)	K–O3f x2	3.25(2)
<Al–O>	1.90	K–O4 x2	3.14(2)
		K–O5g x2	3.46(2)
		<K–O$_{outer}$>	3.28

TABLE 8-4. (CONTINUE)

1*M* POLYTYPE

T–O1	1.59(7)	Al–O1	1.97(6)
T–O2	1.56(7)	Al–O1i	1.85(8)
T–O2h	1.59(7)	Al–OHj	1.84(6)
T–O3	1.59(5)	<Al–O>	1.89
<T–O>	1.58		
O1–O2	2.46(9)	O1–T–O2	103(4)
O1–O2h	2.57(10)	O1–T–O2h	108(4)
O1–O3	2.60(10)	O1–T–O3	110(4)
O2–O2h	2.59(2)	O2–T–O2h	110(4)
O2–O3	2.69(9)	O2–T–O3	118(5)
O2h–O3	2.57(8)	O2h–T–O3	108(4)
<O–O>T	2.56	<O–T–O>	109.5
K–O2k x4	3.17(6)		
K–O2l x4	2.90(7)		
K–O3m x2	2.92(9)		
<K–O>	3.00		

a: 1/2–x, 1/2–y, –z; b: 1/2+x, 1/2–y, 1/2+z; c: 1/2–x, 1/2+y, 1/2–z; d: x, –y, –1/2+z; e: –x, y, 1/2–z; f: 1–x, y, 1/2–z; g: 1/2–x, –1/2+y, 1/2–z; h: 1/2+x, 1/2–y+1, z; i: 1/2–x, 1/2–y+1, –z; j: 1/2–x, 1/2+y, –z; k: x, 1–y, z; l: 1/2+x, 1/2+y, z; m: –1/2+x, –1/2+y, z.

TABLE 8-5. REFINED SITE-OCCUPANCIES AND ASSIGNED SPECIES IN BOROMUSCOVITE POLYTYPES

	Refined occupancy	Assigned from formula unit
	$2M_1$ polytype	
Al	0.96(2) Al	1.99 Al
T1	0.78(3) Si + 0.22(3) B	3.10 Si + 0.22 Al + 0.68 B
T2	0.72(3) Si + 0.28(3) B	
K	0.41(1) K	0.89 K
	$1M$ polytype	
Al	0.41(5) Al	1.99 Al
T	0.75(13) Si + 0.25(13) B	3.10 Si + 0.22 Al + 0.68 B
K	0.20 K	0.89 K

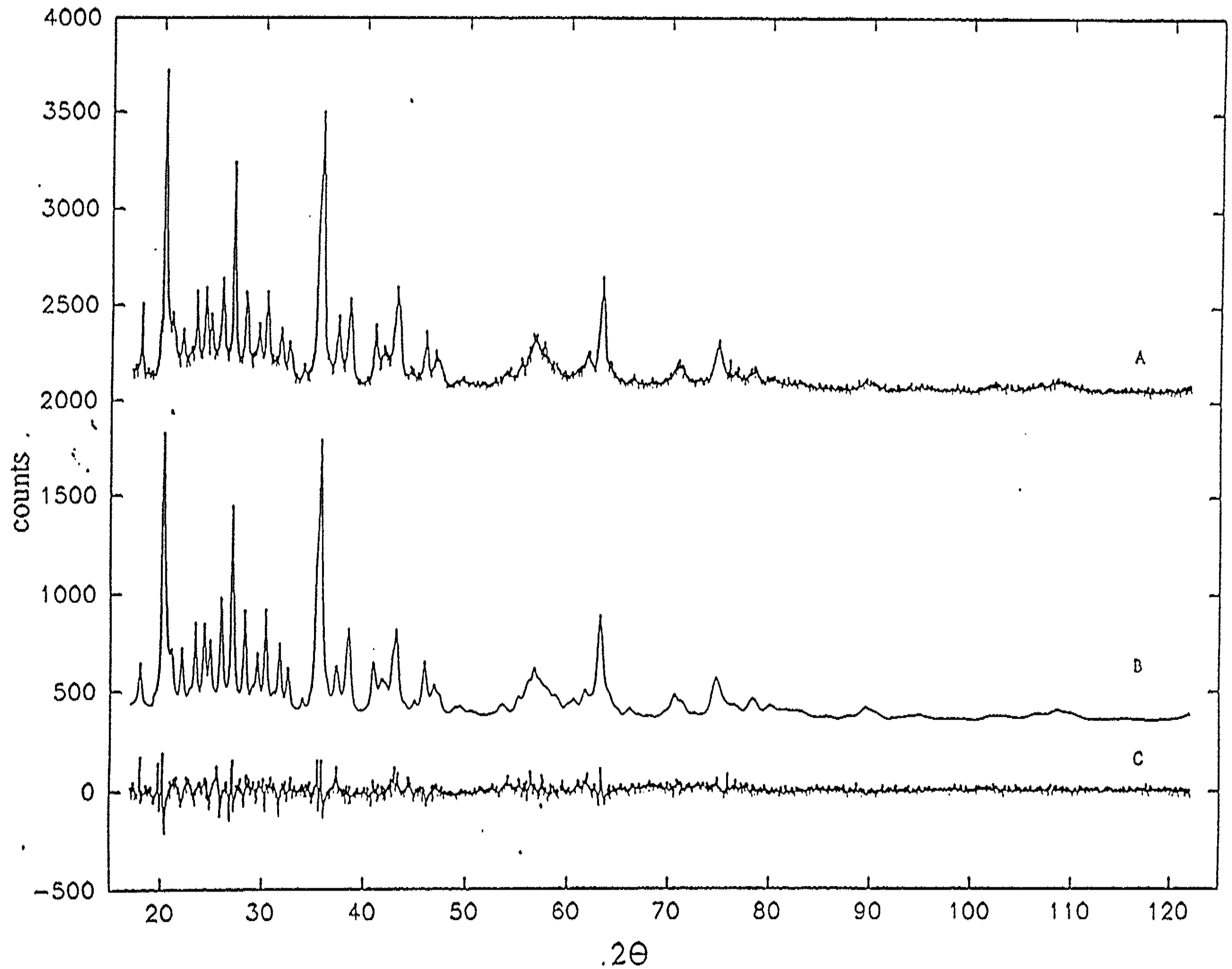

Figure 8-1. Observed (A), calculated (B) and the difference (C) powder-diffraction patterns of boromuscovite.

$$W_{2M1} = 83 \text{ wt\%} \text{ and } W_{1M} = 100 - 83 = 17 \text{ wt\%} .$$

This result differs significantly from that of Foord *et al.* (1991) who gave a 50:50 ratio of the two polytypes in the mixture from California based on visual estimation.

8.5. Discussion

In the $2M_1$ polytype, the <*T1*–O> distance is slightly shorter than the <*T2*–O> distance (Table 8-4). The difference arises from the different T–O_{nbr} distances. The $T1$–O_{nbr} is shorter, whereas $T2$–O_{nbr} is greater than T–O_{br}, respectively. The T–O_{br} distances are similar within individual polytypes and between polytypes, and are close to 1.57 Å. The refined T-site occupancies for (Si+Al) and B agree well with results of the chemical analysis. On a plot relating B-content and <*T*–O> distance (Fig. 8-2), the *T1* and *T2* sites fall on the trend suggested by Fleet (1992). The <*T*–O> distance (1.58 Å) in the 1*M* polytype is equal to the average of those in the $2M_1$ polytype, indicating no preferred partitioning of B into either polytype. The refined *T*-site occupancy of (Si+Al) is not as reliable as those in the $2M_1$ polytype, as there was strong correlation between the site occupancy and scale factor during refinement.

8.6. Summary

(1) Boromuscovite from Řečice granitic pegmatite, Czech Republic is a mixture of 83 wt% $2M_1$ and 17 wt% 1*M* polytypes.

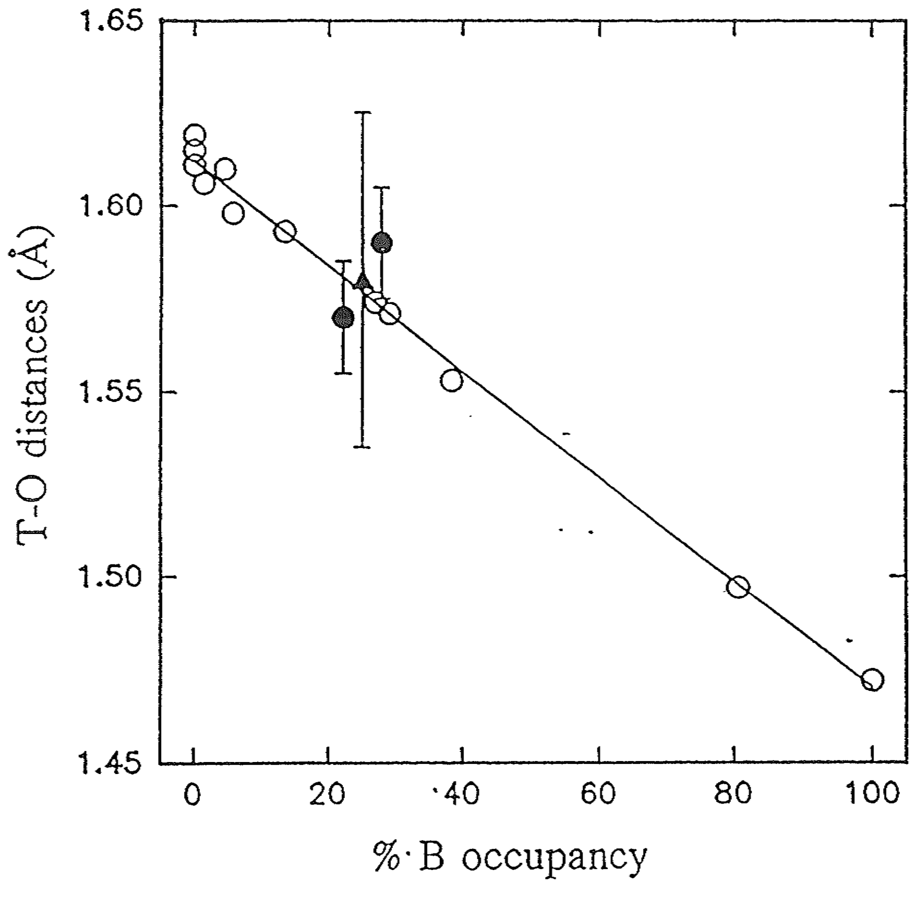

Figure 8-2. The relationship between <*T*–O> distances and B content; solid circle: boromuscovite ($2M_1$); solid triangle: boromuscovite (1*M*); open circle: data points from Fleet (1992); line: linear regression of data points from Fleet (1992).

(2) Crystal structures of both polytypes were successfully refined using the Coupled Rietveld--Static-Structure-Energy Minimization (CRSSEM) method. Simultaneous structure refinement of the two polytypes converged to R_{wp} = 13.8% (R_{exp} = 7.9%), R_{BRG} ($2M_1$) = 3.8% and R_{BRG} ($1M$) = 3.8%.

(3) The CRSSEM method allows much more accurate determination of modal amounts and crystal-structure details of mixtures of polytypes than has hitherto been possible.

Chapter 9

Conclusions and Potential Development

Some generalizations, based on the present work, can be made regarding the reliability and applicability of the Rietveld method in crystal-chemical studies of minerals.

The Rietveld method can refine crystal structures accurately within the level of the assigned precision. For single-phase anhydrous materials (without profound tendency of preferred orientation), such as olivine and diopside, the Rietveld method can give crystal structures statistically identical to those of single-crystal work (although of lower precision). For materials that tend to give strong preferred orientation, such as micas, a combination of careful sample preparation and a preferred-orientation correction (using the March model) will enable the Rietveld method to give structure refinements to the same reliability level as that of olivine and diopside. For materials that host species with large thermal displacement (such as water molecules and charge-compensating cations in zeolites), structure refinement of the relatively rigid framework can still be successful. Refinement of cation site-occupancies by the Rietveld method, based on fixed isotropic thermal displacements, reproduces the results by single-crystal refinement and chemical analysis. The above-stated reliability applies to multi-phase Rietveld refinement, given that the minor phase is greater than 10 wt%.

The role of computer simulation in crystal-chemical studies of fine-grained materials is to assist in locating and determining the light elements, such as H, in the structure, although it may find other roles such as setting up a starting structure model of a new mineral species from the structure of a topologically similar mineral. With the combination of Rietveld refinement, computer simulation and spectroscopic studies, H-atom positions in the structure of powder materials can be determined.

The capability of the Rietveld method can be extended when it is coupled with computer simulation. The problem of insufficient experimental resolution (*e.g.* in crystal-structure studies of minor phases in mixtures and minerals with large complicated structures) can be ameliorated by considering inter-atomic interactions through computer simulation of the structure. The Coupled Rietveld--Static Structure-Energy Minimization (CRSSEM) method is most useful in determining similar structures co-existing in a powder mixture, such as a mixture of the $2M_1$ and $1M$ polytypes of a mica species. Determination of large zeolite structures, such as most of the synthetic zeolite structures, can be another area of application of the CRSSEM method.

The thesis work also identified areas for further work. In the Rietveld refinement, unrealistic thermal-displacement parameters often occur even when only isotropic displacement factors are allowed to refine. Site occupancies tend to correlate strongly with thermal-displacement parameters, and hence reliable determination of displacement parameters is of vital interest to crystal-chemical studies of crystalline materials. Coupling Rietveld refinement with *Molecular Dynamics* (MD) may be an answer to the problem. Trajectories of individual atoms, in response to a given temperature and structural configuration, can be calculated explicitly based on current atomic-interaction models. These trajectories can serve as a basis of Rietveld refinement of displacement parameters. The advantage of dynamic coupling of MD with Rietveld refinement is that calculation of the trajectories and the refinement of displacement parameters, which can both be uncertain when being considered alone, will regulate each other to give results that are closer to the true values.

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Appendix P-1: step-intensity data of pure diopside

18.00	.05	138.00		pure diopside					
26.	31.	32.	25.	27.	28.	30.	25.	27.	23.
35.	27.	32.	19.	23.	36.	23.	31.	29.	40.
32.	31.	35.	35.	39.	36.	34.	33.	27.	34.
33.	30.	30.	41.	53.	40.	55.	67.	92.	124.
124.	88.	63.	56.	50.	55.	48.	28.	25.	25.
31.	25.	26.	26.	28.	25.	25.	32.	26.	38.
24.	18.	18.	26.	25.	29.	27.	26.	30.	23.
18.	18.	27.	23.	29.	24.	30.	23.	24.	26.
25.	26.	20.	23.	21.	27.	29.	20.	21.	23.
18.	22.	24.	26.	13.	24.	30.	22.	21.	13.
35.	24.	30.	30.	30.	24.	23.	18.	20.	19.
23.	23.	29.	24.	22.	25.	28.	24.	18.	21.
36.	29.	24.	26.	41.	54.	81.	106.	92.	76.
51.	43.	36.	25.	31.	30.	34.	23.	17.	23.
28.	38.	29.	31.	26.	20.	25.	26.	23.	36.
37.	35.	25.	28.	36.	36.	24.	39.	30.	29.
27.	24.	27.	31.	32.	44.	40.	38.	40.	59.
78.	119.	177.	274.	340.	280.	201.	129.	92.	71.
62.	48.	49.	69.	25.	57.	62.	81.	85.	136.
277.	460.	676.	792.	830.	595.	369.	181.	135.	74.
60.	53.	44.	42.	23.	42.	41.	39.	41.	38.
38.	40.	53.	43.	63.	23.	38.	46.	32.	51.
54.	44.	47.	54.	56.	48.	71.	94.	119.	154.
177.	201.	231.	311.	451.	700.	1239.	1952.	2602.	2796.
2299.	1518.	918.	614.	508.	650.	912.	983.	940.	638.
401.	266.	179.	177.	212.	267.	383.	671.	902.	1046.
924.	664.	422.	240.	131.	104.	70.	55.	62.	65.
58.	56.	71.	83.	65.	60.	41.	50.	47.	32.
30.	32.	27.	40.	41.	38.	21.	34.	21.	29.
33.	24.	31.	21.	33.	21.	29.	26.	22.	28.
26.	33.	25.	28.	31.	23.	22.	21.	31.	31.
27.	24.	28.	32.	20.	32.	29.	33.	28.	38.
25.	24.	36.	29.	40.	46.	41.	42.	61.	59.
48.	54.	64.	60.	88.	95.	141.	182.	278.	465.
659.	752.	690.	536.	348.	261.	281.	334.	499.	869.
1197.	1383.	1460.	1592.	1576.	1409.	1130.	809.	531.	322.
186.	156.	113.	96.	73.	58.	74.	52.	42.	47.
34.	46.	50.	40.	36.	51.	28.	27.	44.	27.
31.	37.	28.	24.	19.	31.	29.	29.	27.	43.
27.	32.	52.	87.	72.	64.	61.	57.	41.	32.
33.	32.	23.	32.	33.	29.	40.	33.	22.	36.
48.	41.	37.	44.	45.	48.	30.	55.	54.	84.
127.	195.	328.	462.	512.	408.	316.	195.	131.	91.
68.	58.	50.	33.	49.	40.	30.	37.	34.	36.
29.	27.	31.	36.	27.	31.	39.	42.	44.	61.
63.	88.	148.	205.	275.	352.	292.	248.	219.	228.
268.	295.	288.	268.	205.	148.	83.	59.	68.	55.
56.	49.	57.	42.	50.	62.	98.	160.	217.	311.
380.	330.	309.	237.	193.	203.	271.	405.	602.	597.
515.	375.	268.	150.	126.	128.	134.	201.	275.	329.
292.	241.	195.	118.	99.	76.	57.	65.	69.	73.
55.	57.	75.	70.	74.	64.	72.	57.	47.	47.
47.	69.	63.	75.	99.	123.	205.	329.	488.	546.
496.	415.	284.	190.	165.	116.	131.	178.	187.	251.
347.	368.	332.	333.	307.	251.	220.	166.	115.	80.
75.	65.	59.	47.	49.	63.	38.	64.	78.	82.
99.	142.	208.	209.	182.	159.	101.	77.	67.	40.
55.	42.	46.	59.	43.	35.	33.	41.	28.	17.
28.	28.	30.	21.	30.	36.	29.	20.	39.	29.
16.	29.	33.	36.	33.	38.	27.	24.	32.	36.
28.	39.	28.	25.	17.	23.	27.	32.	36.	32.
28.	41.	36.	47.	44.	23.	30.	38.	46.	81.
58.	78.	69.	62.	60.	61.	40.	40.	43.	57.
60.	104.	139.	237.	246.	267.	231.	220.	170.	135.
101.	77.	62.	62.	60.	91.	107.	114.	120.	93.

74.	62.	52.	36.	42.	37.	42.	38.	44.	37.
24.	40.	31.	24.	28.	42.	28.	39.	39.	50.
52.	53.	53.	52.	42.	40.	44.	43.	38.	67.
76.	100.	172.	264.	315.	414.	317.	235.	212.	135.
94.	72.	61.	57.	44.	42.	38.	44.	36.	32.
25.	41.	47.	52.	69.	58.	72.	81.	61.	64.
62.	49.	41.	41.	31.	28.	32.	28.	24.	23.
28.	25.	32.	30.	37.	28.	29.	44.	50.	47.
58.	65.	77.	72.	66.	85.	102.	130.	172.	184.
142.	123.	141.	101.	106.	119.	133.	156.	174.	127.
140.	100.	82.	60.	45.	51.	65.	43.	40.	59.
44.	45.	40.	56.	64.	70.	97.	130.	151.	180.
272.	457.	559.	744.	743.	595.	535.	439.	344.	283.
279.	235.	223.	199.	144.	88.	75.	75.	66.	55.
54.	43.	43.	33.	39.	35.	38.	39.	34.	50.
54.	51.	64.	69.	97.	82.	62.	62.	61.	40.
39.	49.	25.	35.	34.	43.	30.	36.	41.	36.
70.	102.	121.	142.	126.	109.	94.	90.	54.	70.
77.	83.	103.	144.	150.	129.	123.	134.	98.	67.
63.	54.	70.	50.	48.	53.	60.	74.	97.	123.
179.	176.	162.	212.	245.	251.	263.	233.	212.	182.
150.	115.	96.	96.	83.	66.	72.	90.	112.	131.
110.	198.	249.	320.	279.	257.	252.	202.	155.	105.
96.	92.	71.	93.	96.	103.	107.	119.	111.	156.
157.	121.	113.	100.	89.	59.	43.	57.	45.	43.
45.	40.	42.	41.	51.	45.	51.	50.	49.	30.
54.	40.	65.	63.	63.	78.	70.	52.	49.	42.
46.	32.	41.	36.	43.	58.	83.	104.	81.	78.
94.	89.	87.	76.	76.	62.	52.	52.	53.	50.
45.	53.	40.	58.	70.	64.	95.	134.	136.	183.
263.	341.	434.	491.	431.	405.	338.	339.	288.	219.
169.	141.	131.	122.	137.	164.	283.	271.	291.	304.
242.	228.	166.	165.	121.	102.	71.	51.	55.	59.
56.	55.	58.	52.	59.	114.	118.	98.	130.	93.
95.	89.	71.	53.	52.	43.	46.	33.	35.	37.
43.	49.	60.	69.	107.	83.	71.	63.	64.	62.
44.	35.	33.	30.	35.	35.	29.	22.	25.	21.
27.	25.	28.	23.	27.	24.	27.	35.	23.	34.
24.	23.	22.	27.	28.	30.	42.	41.	51.	43.
64.	64.	45.	48.	57.	55.	50.	50.	48.	52.
56.	82.	66.	100.	135.	166.	153.	180.	154.	176.
202.	223.	203.	230.	181.	172.	132.	135.	122.	107.
82.	100.	115.	104.	91.	73.	71.	72.	62.	45.
56.	52.	38.	30.	35.	31.	28.	22.	26.	33.
28.	27.	33.	21.	37.	41.	25.	24.	33.	34.
49.	71.	54.	43.	46.	64.	62.	68.	118.	135.
123.	117.	145.	98.	137.	126.	132.	176.	202.	190.
185.	163.	131.	166.	116.	100.	64.	65.	70.	44.
48.	44.	36.	46.	42.	42.	50.	47.	81.	73.
85.	94.	110.	131.	158.	115.	134.	139.	111.	98.
80.	67.	85.	62.	50.	54.	57.	44.	46.	57.
49.	48.	66.	80.	116.	157.	177.	184.	160.	142.
126.	121.	99.	82.	46.	42.	55.	34.	41.	40.
32.	33.	37.	50.	68.	57.	47.	44.	41.	31.
37.	32.	23.	30.	25.	31.	43.	35.	40.	32.
39.	34.	39.	49.	41.	50.	44.	50.	42.	38.
56.	45.	42.	56.	61.	75.	77.	93.	65.	64.
60.	58.	59.	45.	31.	24.	41.	19.	30.	25.
28.	36.	43.	48.	34.	36.	32.	32.	36.	34.
37.	34.	29.	27.	42.	30.	41.	35.	41.	34.
38.	31.	29.	42.	23.	34.	23.	32.	23.	27.
34.	34.	26.	38.	24.	25.	26.	33.	22.	28.
32.	37.	31.	24.	39.	43.	34.	38.	36.	36.
47.	59.	52.	51.	54.	79.	78.	47.	44.	39.
47.	45.	38.	27.	16.	20.	16.	18.	18.	24.
15.	24.	15.	22.	16.	21.	23.	16.	31.	37.
28.	16.	31.	31.	37.	40.	45.	35.	49.	41.
58.	70.	76.	69.	74.	75.	99.	94.	79.	77.
89.	77.	52.	54.	49.	52.	33.	39.	26.	30.

26.	28.	27.	23.	28.	34.	25.	16.	20.	29.
25.	33.	38.	40.	42.	38.	37.	34.	34.	31.
34.	26.	32.	29.	29.	24.	21.	21.	22.	33.
41.	29.	37.	31.	31.	40.	30.	25.	27.	28.
19.	27.	25.	20.	18.	29.	24.	35.	38.	32.
38.	38.	26.	24.	36.	38.	23.	27.	25.	25.
33.	42.	52.	46.	33.	39.	40.	34.	29.	27.
28.	23.	26.	31.	28.	25.	28.	34.	31.	35.
20.	31.	29.	28.	25.	36.	35.	34.	35.	28.
36.	20.	21.	30.	25.	21.	22.	22.	30.	19.
34.	40.	26.	31.	25.	27.	35.	45.	41.	44.
45.	50.	54.	51.	67.	80.	64.	83.	57.	51.
72.	57.	64.	46.	50.	44.	56.	72.	51.	72.
95.	117.	154.	241.	209.	213.	151.	149.	178.	236.
275.	254.	214.	171.	137.	146.	152.	142.	124.	117.
119.	122.	145.	128.	123.	150.	109.	128.	108.	93.
101.	84.	95.	82.	77.	71.	51.	45.	45.	58.
36.	52.	37.	43.	47.	47.	49.	44.	43.	50.
60.	59.	70.	57.	86.	92.	78.	95.	59.	68.
72.	82.	79.	72.	69.	76.	82.	57.	75.	63.
46.	69.	53.	65.	49.	51.	74.	58.	52.	61.
88.	103.	110.	69.	47.	56.	73.	60.	50.	71.
41.	43.	42.	34.	28.	33.	32.	28.	28.	35.
25.	25.	28.	36.	29.	42.	43.	50.	52.	53.
62.	61.	45.	61.	34.	50.	33.	53.	43.	35.
34.	45.	38.	29.	27.	40.	38.	40.	47.	41.
41.	47.	49.	51.	48.	51.	58.	52.	38.	53.
55.	44.	56.	62.	74.	84.	76.	65.	50.	61.
64.	50.	66.	42.	51.	41.	40.	36.	41.	44.
48.	39.	38.	45.	43.	40.	52.	50.	60.	61.
47.	52.	55.	51.	68.	74.	67.	81.	66.	75.
76.	65.	82.	110.	85.	88.	70.	51.	55.	48.
58.	48.	50.	26.	43.	33.	34.	37.	30.	30.
24.	24.	29.	24.	37.	35.	50.	27.	39.	30.
34.	38.	46.	62.	72.	67.	67.	48.	41.	39.
44.	49.	58.	37.	33.	39.	37.	32.	34.	35.
41.	45.	36.	40.	39.	52.	44.	33.	37.	44.
40.	35.	35.	48.	46.	37.	51.	70.	75.	80.
79.	61.	52.	56.	42.	72.	70.	51.	43.	47.
40.	24.	40.	36.	32.	25.	40.	49.	40.	38.
35.	45.	37.	47.	64.	50.	44.	40.	46.	46.
52.	43.	56.	72.	62.	54.	73.	55.	58.	79.
85.	105.	80.	73.	72.	65.	89.	79.	78.	75.
62.	65.	61.	40.	38.	49.	51.	45.	35.	54.
34.	28.	28.	21.	26.	26.	23.	30.	22.	16.
31.	14.	24.	23.	23.	20.	27.	18.	20.	28.
39.	19.	22.	26.	28.	21.	24.	17.	20.	18.
21.	22.	24.	26.	17.	14.	20.	27.	23.	26.
29.	27.	34.	29.	36.	34.	43.	36.	43.	32.
26.	37.	53.	42.	44.	53.	46.	41.	38.	39.
32.	46.	42.	61.	61.	63.	55.	41.	52.	45.
54.	61.	43.	62.	47.	44.	39.	41.	46.	25.
42.	32.	25.	38.	24.	36.	37.	32.	30.	31.
26.	25.	18.	25.	32.	27.	31.	24.	27.	20.
27.	21.	28.	29.	25.	31.	37.	34.	37.	42.
37.	52.	45.	36.	49.	37.	37.	34.	49.	50.
58.	76.	85.	97.	106.	111.	72.	61.	83.	84.
79.	97.	100.	84.	114.	86.	71.	80.	78.	66.
79.	69.	74.	93.	67.	98.	123.	113.	105.	111.
94.	85.	74.	77.	98.	87.	81.	74.	61.	56.
41.	46.	51.	48.	43.	48.	40.	36.	24.	27.
33.	36.	23.	43.	25.	37.	37.	32.	35.	27.
33.	22.	32.	25.	28.	33.	43.	33.	32.	36.
28.	30.	23.	25.	27.	22.	25.	32.	16.	24.
26.	23.	28.	25.	30.	21.	19.	23.	16.	27.
25.	28.	22.	32.	26.	31.	25.	27.	40.	31.
32.	24.	36.	36.	28.	38.	26.	41.	30.	33.
34.	29.	34.	20.	29.	36.	37.	22.	35.	27.
27.	36.	33.	31.	39.	42.	39.	40.	45.	48.

55.	48.	54.	49.	40.	55.	55.	41.	41.	64.
45.	50.	39.	45.	36.	42.	49.	39.	41.	58.
40.	53.	58.	67.	76.	57.	41.	39.	48.	44.
33.	39.	51.	35.	40.	39.	46.	29.	28.	30.
32.	38.	32.	47.	49.	40.	36.	32.	45.	41.
25.	33.	34.	48.	36.	58.	51.	55.	59.	57.
72.	61.	58.	55.	40.	54.	48.	45.	56.	63.
60.	57.	57.	60.	39.	44.	48.	44.	46.	47.
47.	40.	45.	47.	35.	52.	46.	54.	58.	64.
62.	48.	46.	59.	47.	59.	37.	45.	57.	59.
67.	59.	60.	65.	57.	76.	80.	74.	70.	47.
42.	47.	36.	37.	46.	38.	45.	54.	47.	38.
36.	31.	37.	31.	39.	26.	26.	29.	30.	50.
39.	47.	50.	55.	44.	67.	39.	39.	39.	35.
39.	46.	44.	47.	34.	38.	48.	59.	32.	43.
34.	28.	33.	31.	31.	31.	39.	34.	33.	26.
32.	29.	21.	23.	39.	27.	37.	26.	35.	26.
32.	30.	27.	26.	32.	28.	24.	30.	28.	33.
22.	30.	29.	25.	25.	34.	24.	33.	36.	27.
25.	33.	30.	26.	31.	14.	30.	33.	23.	23.
33.	27.	25.	32.	27.	27.	29.	40.	41.	38.
42.	38.	46.	39.	36.	29.	32.	28.	36.	27.
36.	37.	42.	33.	34.	36.	27.	34.	32.	35.
35.	42.	45.	37.	32.	39.	47.	37.	35.	56.
42.	61.	41.	43.	45.	41.	38.	46.	34.	37.
47.	34.	39.	57.	50.	59.	64.	48.	54.	52.
42.	52.	52.	66.	66.	76.	72.	75.	65.	73.
56.	52.	49.	45.	69.	51.	49.	45.	61.	54.
71.	58.	51.	56.	54.	47.	53.	49.	67.	48.
56.	49.	64.	52.	45.	43.	48.	51.	58.	35.
47.	56.	46.	59.	46.	51.	47.	59.	68.	59.
66.	62.	66.	68.	74.	63.	60.	52.	52.	54.
65.	58.	66.	51.	75.	63.	61.	76.	68.	71.
59.	44.	58.	52.	37.	53.	39.	46.	47.	57.
50.	41.	34.	44.	41.	43.	38.	41.	52.	31.
28.	39.	31.	54.	44.	41.	41.	45.	53.	36.
49.	33.	42.	52.	33.	42.	35.	34.	44.	33.
31.									

Appendix P-2: step-intensity data of the 10 wt% olivine mixture of Ol+Py

16.0000	.0500136.0000		10%-olivine mixture						
38.	30.	35.	31.	36.	31.	26.	42.	31.	38.
34.	31.	40.	33.	31.	25.	33.	31.	20.	23.
41.	29.	37.	34.	36.	40.	46.	43.	48.	58.
78.	54.	42.	36.	43.	49.	31.	33.	42.	25.
26.	36.	40.	36.	27.	35.	32.	36.	30.	34.
24.	33.	37.	26.	36.	24.	32.	26.	39.	30.
41.	37.	43.	35.	40.	27.	27.	36.	45.	34.
37.	33.	38.	29.	40.	38.	55.	44.	74.	104.
121.	111.	81.	57.	75.	58.	57.	62.	37.	50.
37.	32.	27.	23.	25.	36.	36.	23.	33.	31.
25.	29.	27.	38.	24.	25.	27.	25.	30.	34.
32.	34.	32.	20.	30.	30.	31.	32.	31.	19.
27.	33.	36.	29.	28.	38.	22.	33.	36.	22.
22.	39.	30.	39.	41.	59.	67.	104.	114.	139.
116.	101.	70.	71.	50.	35.	51.	28.	27.	29.
30.	38.	26.	35.	30.	41.	42.	44.	46.	55.
68.	60.	49.	39.	43.	67.	51.	86.	73.	98.
91.	64.	34.	41.	39.	35.	40.	30.	32.	27.
34.	17.	33.	35.	35.	40.	42.	53.	58.	77.
100.	88.	88.	83.	62.	45.	56.	37.	36.	34.
32.	22.	31.	28.	37.	38.	40.	31.	47.	55.
76.	103.	158.	214.	284.	350.	330.	290.	192.	126.
79.	74.	64.	45.	58.	62.	76.	56.	93.	122.
177.	317.	445.	611.	661.	702.	601.	445.	253.	150.
99.	85.	51.	54.	55.	52.	49.	36.	33.	42.
38.	40.	45.	55.	56.	59.	49.	44.	54.	47.
45.	47.	66.	57.	50.	63.	61.	98.	106.	152.
162.	178.	232.	257.	349.	524.	881.	1415.	2044.	2626.
2824.	2581.	1980.	1280.	801.	727.	723.	820.	863.	874.
694.	505.	354.	269.	203.	219.	325.	513.	713.	889.
927.	863.	718.	515.	341.	235.	159.	108.	106.	70.
79.	76.	71.	57.	71.	71.	69.	58.	44.	52.
61.	50.	57.	68.	82.	129.	145.	181.	169.	117.
97.	86.	52.	44.	42.	39.	42.	42.	33.	40.
40.	33.	36.	36.	36.	31.	39.	32.	33.	33.
34.	26.	38.	33.	32.	33.	33.	27.	26.	51.
36.	37.	36.	37.	44.	44.	35.	51.	58.	50.
54.	60.	51.	71.	78.	109.	122.	164.	249.	358.
511.	670.	686.	653.	566.	474.	395.	373.	520.	721.
1017.	1348.	1539.	1663.	1708.	1574.	1521.	1323.	995.	729.
435.	266.	197.	130.	116.	91.	112.	104.	143.	168.
232.	254.	228.	204.	140.	112.	87.	67.	60.	43.
42.	37.	34.	42.	29.	37.	46.	39.	36.	30.
42.	48.	65.	69.	52.	94.	78.	76.	65.	56.
53.	47.	51.	48.	60.	59.	61.	65.	63.	41.
42.	58.	63.	55.	42.	57.	57.	73.	87.	89.
125.	176.	269.	353.	455.	452.	454.	353.	263.	170.
135.	121.	118.	121.	148.	133.	121.	111.	97.	105.
97.	84.	87.	103.	69.	67.	76.	60.	82.	66.
78.	99.	130.	156.	217.	289.	298.	321.	301.	251.
291.	334.	329.	331.	285.	233.	180.	125.	86.	67.
68.	68.	60.	70.	85.	106.	126.	143.	194.	283.
338.	349.	334.	298.	253.	246.	287.	352.	454.	539.
592.	480.	439.	279.	206.	196.	171.	186.	216.	251.
263.	263.	289.	230.	195.	133.	94.	77.	77.	73.
92.	87.	85.	89.	78.	107.	96.	64.	71.	42.
46.	80.	72.	95.	113.	127.	194.	327.	452.	499.
505.	459.	386.	277.	220.	178.	158.	185.	224.	286.
322.	366.	386.	411.	371.	371.	315.	213.	173.	121.
97.	92.	73.	75.	64.	48.	53.	68.	73.	94.
105.	127.	156.	194.	235.	187.	153.	133.	96.	64.
73.	66.	57.	63.	57.	73.	36.	37.	30.	36.
34.	37.	31.	38.	32.	33.	25.	39.	34.	37.
28.	42.	43.	39.	43.	35.	28.	37.	47.	39.

41.	39.	30.	34.	39.	30.	23.	51.	37.	46.
53.	47.	40.	29.	44.	39.	35.	51.	59.	87.
83.	88.	99.	94.	76.	75.	49.	47.	59.	63.
67.	101.	147.	195.	217.	260.	274.	243.	234.	207.
160.	131.	105.	91.	83.	100.	118.	128.	127.	120.
131.	119.	81.	69.	58.	63.	62.	68.	55.	58.
39.	41.	45.	36.	40.	36.	25.	43.	35.	42.
68.	62.	70.	66.	49.	58.	59.	60.	93.	70.
95.	131.	220.	336.	450.	487.	469.	476.	360.	310.
269.	179.	122.	105.	86.	82.	77.	78.	68.	60.
40.	51.	63.	47.	71.	83.	66.	89.	82.	83.
65.	55.	61.	57.	48.	43.	37.	32.	33.	37.
32.	34.	51.	28.	41.	39.	49.	39.	36.	66.
65.	92.	92.	90.	95.	107.	121.	143.	191.	181.
189.	190.	164.	140.	117.	145.	136.	137.	163.	156.
154.	137.	115.	102.	76.	76.	77.	66.	59.	70.
79.	88.	76.	87.	80.	98.	112.	106.	169.	194.
275.	422.	588.	735.	833.	769.	751.	636.	558.	429.
380.	358.	294.	213.	194.	153.	123.	109.	73.	69.
59.	60.	70.	52.	63.	63.	58.	57.	63.	58.
52.	70.	67.	89.	94.	84.	100.	79.	67.	59.
66.	60.	56.	64.	64.	63.	62.	50.	68.	58.
62.	77.	110.	134.	155.	158.	130.	129.	88.	82.
72.	91.	87.	133.	175.	166.	166.	145.	122.	113.
100.	72.	61.	41.	54.	62.	93.	71.	110.	137.
178.	183.	184.	242.	258.	287.	306.	268.	235.	230.
227.	146.	152.	128.	112.	108.	125.	112.	130.	160.
169.	232.	305.	345.	331.	328.	335.	349.	270.	227.
182.	181.	134.	124.	147.	114.	136.	128.	130.	161.
151.	187.	176.	165.	160.	144.	114.	102.	117.	114.
90.	70.	60.	63.	54.	69.	73.	62.	43.	61.
50.	53.	55.	76.	71.	73.	62.	67.	69.	60.
56.	58.	45.	60.	45.	71.	83.	79.	104.	119.
93.	103.	105.	86.	80.	81.	83.	70.	93.	73.
64.	65.	65.	60.	63.	74.	80.	96.	176.	151.
198.	314.	394.	433.	478.	471.	415.	347.	358.	292.
230.	175.	160.	157.	166.	186.	238.	318.	330.	346.
284.	264.	263.	226.	179.	157.	133.	103.	103.	77.
103.	91.	69.	106.	100.	94.	138.	155.	160.	137.
106.	102.	87.	86.	76.	63.	59.	55.	53.	55.
54.	55.	72.	75.	90.	81.	86.	86.	80.	78.
73.	61.	40.	43.	48.	39.	39.	38.	43.	31.
26.	46.	32.	42.	31.	51.	47.	48.	45.	64.
58.	61.	52.	65.	58.	51.	51.	40.	55.	64.
61.	78.	66.	55.	61.	50.	54.	50.	54.	64.
61.	72.	83.	85.	125.	177.	185.	174.	186.	203.
231.	250.	237.	216.	225.	190.	178.	160.	160.	138.
124.	113.	131.	127.	152.	111.	102.	99.	82.	78.
56.	56.	47.	56.	45.	30.	37.	36.	41.	36.
47.	41.	31.	28.	30.	41.	45.	37.	45.	50.
54.	72.	60.	64.	60.	80.	84.	96.	88.	130.
151.	142.	155.	137.	130.	150.	162.	172.	180.	248.
240.	224.	207.	193.	159.	136.	130.	91.	72.	68.
76.	72.	59.	64.	66.	60.	82.	67.	84.	92.
105.	129.	132.	130.	146.	155.	134.	144.	123.	154.
119.	127.	110.	101.	82.	86.	65.	60.	68.	58.
60.	60.	72.	82.	102.	153.	194.	161.	183.	161.
161.	145.	122.	90.	94.	51.	64.	60.	47.	46.
47.	47.	61.	67.	76.	69.	54.	55.	51.	61.
50.	45.	42.	31.	33.	37.	37.	58.	44.	55.
62.	57.	50.	69.	56.	44.	60.	57.	43.	57.
48.	55.	51.	58.	75.	79.	81.	109.	99.	86.
87.	72.	63.	52.	59.	58.	34.	17.	28.	35.
36.	44.	32.	42.	33.	36.	31.	40.	44.	39.
46.	30.	33.	37.	33.	46.	29.	35.	47.	52.
46.	51.	46.	56.	61.	44.	43.	54.	36.	37.
37.	46.	35.	50.	40.	51.	28.	30.	36.	45.
30.	29.	43.	39.	38.	39.	59.	41.	52.	52.
52.	68.	64.	79.	80.	84.	94.	90.	63.	50.

55.	58.	56.	43.	47.	44.	36.	26.	31.	29.
38.	45.	35.	35.	24.	27.	26.	34.	28.	41.
34.	46.	40.	32.	48.	43.	60.	41.	45.	56.
65.	72.	93.	87.	97.	95.	119.	114.	104.	96.
92.	90.	79.	67.	53.	60.	65.	47.	47.	44.
37.	32.	42.	36.	28.	35.	46.	48.	42.	33.
51.	43.	50.	38.	66.	55.	49.	41.	58.	52.
51.	52.	43.	36.	38.	39.	39.	35.	48.	38.
36.	34.	43.	39.	36.	38.	35.	44.	42.	39.
43.	24.	37.	41.	45.	30.	29.	44.	42.	27.
51.	44.	39.	42.	22.	30.	40.	29.	28.	46.
46.	62.	64.	63.	56.	55.	66.	47.	49.	50.
41.	51.	37.	30.	43.	43.	35.	51.	45.	51.
48.	43.	45.	39.	41.	50.	35.	50.	26.	47.
38.	32.	36.	38.	39.	27.	29.	41.	29.	41.
31.	30.	29.	26.	41.	39.	50.	52.	46.	51.
45.	64.	64.	64.	71.	83.	96.	92.	90.	75.
76.	83.	75.	62.	54.	70.	74.	53.	86.	91.
121.	124.	172.	205.	244.	239.	241.	157.	200.	248.
301.	307.	274.	266.	196.	174.	180.	173.	163.	187.
149.	155.	153.	188.	204.	182.	133.	134.	161.	131.
116.	102.	113.	110.	108.	77.	63.	65.	58.	62.
44.	58.	51.	50.	49.	46.	36.	54.	59.	66.
72.	73.	73.	92.	94.	90.	85.	81.	75.	76.
67.	90.	78.	65.	76.	88.	77.	76.	63.	80.
65.	54.	70.	70.	60.	54.	53.	61.	82.	86.
87.	119.	99.	81.	84.	70.	83.	88.	89.	81.
53.	49.	46.	38.	49.	44.	56.	43.	28.	40.
32.	32.	33.	44.	39.	45.	57.	48.	53.	66.
49.	68.	70.	65.	47.	61.	51.	54.	59.	42.
48.	43.	43.	39.	43.	50.	43.	55.	57.	60.
60.	51.	61.	61.	45.	62.	61.	60.	69.	64.
59.	63.	70.	66.	75.	111.	95.	88.	68.	65.
64.	77.	61.	70.	51.	55.	38.	46.	54.	64.
59.	49.	60.	40.	59.	65.	49.	57.	72.	68.
61.	88.	61.	66.	78.	73.	82.	86.	90.	81.
90.	98.	105.	114.	104.	102.	68.	85.	60.	62.
78.	73.	54.	60.	50.	41.	43.	46.	38.	44.
50.	43.	40.	49.	28.	45.	30.	33.	44.	41.
38.	40.	59.	64.	65.	58.	84.	59.	51.	47.
55.	58.	49.	55.	64.	41.	47.	57.	44.	52.
50.	45.	41.	46.	50.	36.	65.	57.	57.	62.
55.	42.	51.	42.	52.	65.	57.	89.	87.	100.
84.	75.	66.	80.	61.	76.	55.	57.	66.	64.
48.	50.	47.	50.	47.	43.	43.	53.	51.	67.
56.	63.	53.	46.	50.	68.	59.	53.	59.	62.
50.	51.	52.	66.	73.	60.	62.	58.	63.	92.
98.	110.	119.	110.	101.	106.	94.	114.	109.	124.
95.	95.	75.	69.	84.	65.	67.	58.	67.	49.
42.	51.	50.	38.	36.	61.	42.	28.	40.	35.
26.	35.	21.	34.	22.	33.	28.	32.	27.	25.
34.	34.	22.	27.	24.	24.	30.	27.	30.	27.
37.	41.	31.	43.	35.	36.	30.	32.	45.	33.
36.	42.	40.	34.	52.	52.	52.	44.	54.	36.
54.	45.	57.	54.	50.	59.	51.	51.	56.	44.
54.	45.	52.	64.	70.	67.	56.	53.	70.	64.
61.	64.	75.	57.	63.	53.	48.	47.	37.	59.
67.	59.	45.	44.	33.	40.	41.	51.	38.	47.
39.	33.	36.	35.	31.	40.	36.	32.	40.	42.
43.	47.	37.	40.	40.	40.	38.	44.	33.	47.
46.	45.	59.	41.	50.	53.	66.	56.	64.	66.
63.	71.	75.	91.	110.	90.	107.	105.	87.	93.
97.	118.	84.	125.	109.	124.	102.	85.	92.	93.
80.	85.	85.	77.	97.	99.	80.	133.	137.	120.
115.	103.	106.	93.	99.	91.	108.	91.	74.	70.
65.	58.	64.	47.	50.	56.	50.	48.	54.	41.
43.	50.	41.	40.	51.	40.	47.	28.	32.	42.
46.	38.	36.	30.	38.	50.	49.	37.	42.	34.
50.	40.	29.	35.	35.	27.	35.	28.	42.	37.

42.	31.	27.	29.	33.	38.	38.	37.	36.	42.
29.	45.	37.	41.	46.	44.	44.	49.	47.	42.
44.	44.	39.	41.	41.	52.	40.	39.	41.	43.
45.	37.	39.	32.	33.	38.	39.	28.	35.	31.
35.	40.	51.	47.	43.	33.	47.	49.	52.	45.
54.	47.	46.	44.	42.	40.	47.	55.	70.	53.
67.	67.	65.	55.	57.	55.	52.	44.	63.	41.
67.	55.	67.	76.	86.	66.	49.	52.	40.	61.
53.	47.	50.	62.	71.	55.	60.	41.	53.	41.
48.	49.	46.	45.	43.	62.	33.	42.	39.	51.
33.	45.	52.	61.	53.	59.	61.	62.	60.	82.
76.	69.	74.	54.	57.	66.	74.	73.	72.	78.
92.	60.	72.	80.	64.	80.	53.	56.	57.	49.
68.	46.	65.	54.	71.	60.	69.	65.	63.	66.
82.	82.	63.	62.	64.	61.	58.	57.	61.	65.
73.	59.	67.	58.	73.	79.	79.	91.	78.	60.
54.	70.	44.	49.	60.	49.	64.	60.	54.	53.
34.	47.	45.	35.	25.	36.	53.	33.	61.	56.
55.	53.	60.	68.	68.	63.	50.	60.	58.	54.
62.	46.	53.	49.	59.	68.	57.	58.	52.	55.
50.	50.	58.	46.	43.	30.	45.	46.	56.	39.
50.	51.	47.	48.	47.	51.	53.	39.	43.	49.
45.	44.	37.	39.	38.	34.	49.	33.	40.	52.
53.	37.	47.	40.	36.	38.	41.	31.	48.	29.
34.	33.	40.	37.	44.	50.	35.	32.	35.	39.
43.	43.	36.	43.	38.	46.	43.	42.	39.	50.
55.	55.	48.	39.	41.	35.	53.	39.	46.	49.
55.	61.	52.	58.	53.	47.	49.	49.	54.	45.
48.	43.	45.	51.	58.	38.	44.	57.	50.	54.
65.	53.	65.	47.	60.	61.	50.	47.	47.	43.
56.	58.	59.	60.	61.	68.	69.	61.	63.	65.
62.	60.	67.	74.	82.	79.	84.	77.	79.	81.
70.	62.	56.	62.	51.	68.	58.	64.	71.	62.
61.	64.	64.	51.	53.	61.	64.	59.	69.	79.
69.	80.	68.	49.	56.	71.	66.	68.	53.	57.
64.	86.	51.	82.	71.	84.	72.	66.	77.	82.
78.	83.	70.	85.	91.	87.	79.	74.	77.	71.
76.	83.	65.	91.	77.	98.	77.	95.	87.	62.
59.									

Appendix P-3: step-intensity data of the 20 wt% olivine mixture of Ol+Py

16.00	.05	136.00		20% olivine mixture					
33.	33.	40.	40.	31.	44.	25.	36.	37.	27.
39.	41.	40.	32.	26.	25.	36.	29.	33.	35.
54.	42.	40.	53.	64.	59.	83.	84.	112.	126.
96.	63.	41.	36.	37.	41.	31.	32.	36.	33.
35.	25.	28.	32.	45.	44.	24.	32.	43.	22.
27.	43.	23.	24.	26.	29.	41.	41.	39.	33.
39.	37.	45.	22.	41.	31.	29.	39.	40.	44.
38.	42.	39.	39.	47.	50.	37.	76.	97.	114.
88.	96.	98.	80.	70.	54.	56.	44.	43.	33.
30.	29.	38.	32.	31.	35.	33.	31.	27.	36.
31.	41.	32.	22.	35.	30.	24.	32.	32.	35.
29.	31.	37.	34.	40.	21.	30.	29.	28.	29.
26.	32.	45.	50.	27.	31.	30.	31.	41.	36.
41.	50.	53.	57.	73.	107.	180.	193.	231.	228.
196.	145.	79.	68.	46.	49.	34.	37.	33.	37.
40.	37.	29.	46.	42.	54.	84.	101.	102.	112.
84.	66.	55.	54.	56.	62.	93.	100.	98.	67.
65.	51.	34.	26.	40.	43.	37.	31.	31.	31.
45.	33.	36.	41.	33.	54.	57.	110.	124.	136.
157.	172.	121.	115.	100.	73.	52.	34.	34.	33.
34.	36.	42.	39.	44.	37.	40.	35.	66.	52.
107.	113.	189.	270.	271.	286.	268.	191.	132.	90.
79.	69.	38.	57.	44.	46.	72.	83.	98.	168.
270.	433.	534.	631.	644.	595.	474.	276.	159.	97.
79.	63.	57.	50.	52.	42.	28.	55.	39.	38.
51.	36.	41.	63.	44.	62.	42.	45.	57.	42.
41.	43.	59.	48.	51.	83.	76.	96.	140.	117.
177.	213.	276.	386.	504.	836.	1261.	1761.	2116.	2426.
2181.	1858.	1238.	854.	667.	645.	741.	929.	986.	727.
503.	339.	227.	220.	202.	261.	437.	652.	758.	929.
915.	768.	591.	364.	239.	156.	122.	83.	73.	72.
75.	74.	85.	91.	75.	65.	58.	49.	44.	55.
55.	55.	90.	126.	224.	259.	311.	354.	266.	226.
108.	86.	64.	57.	45.	43.	35.	38.	30.	44.
40.	36.	35.	39.	32.	30.	42.	29.	37.	25.
34.	37.	34.	30.	29.	37.	35.	27.	49.	36.
39.	58.	36.	34.	42.	46.	52.	40.	53.	63.
59.	66.	72.	83.	109.	133.	137.	194.	299.	419.
512.	662.	629.	579.	441.	346.	318.	393.	544.	825.
1101.	1375.	1604.	1829.	1762.	1710.	1517.	1168.	769.	517.
340.	202.	158.	133.	128.	95.	135.	174.	295.	338.
404.	432.	393.	286.	205.	134.	94.	68.	75.	50.
49.	48.	45.	38.	48.	46.	48.	43.	43.	56.
44.	62.	60.	73.	81.	70.	75.	71.	63.	58.
56.	43.	55.	61.	84.	78.	96.	86.	76.	93.
69.	61.	57.	54.	59.	65.	86.	98.	117.	112.
162.	222.	290.	387.	476.	436.	371.	225.	179.	144.
134.	147.	179.	203.	201.	195.	194.	150.	141.	154.
182.	175.	192.	134.	112.	100.	63.	74.	68.	65.
97.	97.	143.	247.	230.	272.	314.	279.	239.	214.
280.	289.	321.	275.	211.	139.	144.	98.	82.	62.
49.	76.	77.	89.	90.	117.	162.	204.	285.	303.
323.	315.	281.	215.	217.	210.	289.	420.	483.	533.
480.	404.	308.	216.	157.	158.	159.	204.	229.	300.
289.	273.	218.	159.	120.	100.	79.	71.	66.	75.
67.	84.	91.	87.	88.	79.	56.	54.	40.	59.
58.	62.	60.	86.	108.	150.	203.	302.	373.	439.
422.	399.	336.	254.	184.	134.	154.	148.	235.	256.
310.	328.	355.	359.	311.	303.	270.	204.	148.	120.
86.	76.	48.	66.	52.	45.	52.	48.	42.	64.
101.	138.	164.	221.	205.	140.	116.	120.	93.	75.
71.	65.	77.	60.	74.	71.	46.	54.	34.	37.
29.	31.	29.	33.	36.	33.	37.	29.	26.	36.
24.	30.	39.	36.	42.	41.	25.	44.	42.	31.

41.	38.	47.	32.	43.	38.	51.	54.	60.	74.
54.	61.	50.	45.	42.	42.	58.	42.	63.	72.
88.	95.	79.	64.	55.	59.	43.	52.	70.	66.
76.	107.	145.	218.	202.	249.	250.	230.	186.	173.
127.	87.	76.	79.	71.	130.	117.	129.	114.	127.
108.	97.	63.	52.	73.	68.	64.	57.	50.	52.
53.	46.	37.	46.	37.	45.	31.	40.	50.	53.
60.	56.	84.	72.	60.	77.	79.	87.	102.	108.
126.	194.	318.	405.	523.	615.	634.	544.	379.	335.
274.	211.	184.	158.	135.	89.	90.	75.	74.	70.
61.	40.	39.	74.	85.	69.	93.	62.	68.	68.
68.	58.	63.	55.	53.	34.	40.	29.	33.	36.
36.	31.	32.	34.	46.	43.	45.	37.	56.	76.
55.	63.	75.	87.	111.	121.	160.	183.	177.	224.
208.	159.	133.	117.	112.	96.	157.	158.	177.	158.
124.	103.	102.	72.	83.	70.	70.	72.	79.	89.
95.	92.	133.	117.	125.	120.	146.	141.	168.	231.
341.	500.	606.	751.	813.	803.	684.	555.	441.	386.
316.	235.	199.	196.	154.	126.	112.	91.	71.	91.
64.	55.	78.	65.	69.	62.	58.	56.	73.	71.
86.	69.	82.	102.	101.	84.	69.	85.	78.	63.
71.	66.	69.	71.	71.	79.	80.	71.	74.	68.
73.	85.	119.	118.	118.	100.	104.	97.	70.	65.
79.	97.	121.	156.	139.	167.	148.	126.	125.	105.
94.	54.	58.	57.	69.	68.	63.	90.	106.	141.
135.	161.	203.	220.	238.	224.	268.	249.	241.	204.
180.	160.	141.	131.	127.	109.	136.	130.	139.	148.
176.	253.	252.	291.	360.	342.	352.	313.	301.	236.
222.	187.	149.	143.	116.	140.	131.	131.	198.	179.
227.	242.	245.	234.	219.	204.	173.	137.	114.	105.
92.	76.	56.	78.	73.	66.	52.	92.	43.	51.
80.	62.	65.	83.	80.	72.	80.	70.	54.	61.
55.	44.	43.	55.	48.	66.	74.	91.	94.	95.
84.	93.	107.	100.	100.	94.	92.	91.	78.	62.
54.	60.	59.	63.	71.	85.	94.	125.	140.	181.
267.	379.	436.	406.	426.	458.	400.	335.	288.	278.
184.	161.	132.	147.	176.	166.	212.	266.	280.	244.
269.	247.	225.	194.	135.	135.	127.	127.	110.	123.
121.	108.	121.	105.	128.	118.	152.	149.	113.	134.
128.	113.	104.	70.	71.	58.	47.	59.	48.	59.
55.	59.	70.	83.	88.	94.	68.	87.	76.	67.
55.	52.	43.	33.	34.	39.	40.	31.	39.	41.
34.	47.	42.	37.	47.	47.	64.	94.	91.	85.
92.	134.	99.	83.	78.	81.	55.	78.	55.	56.
87.	57.	65.	71.	57.	51.	49.	48.	60.	72.
67.	60.	100.	103.	141.	173.	198.	181.	201.	192.
263.	232.	243.	198.	182.	183.	180.	145.	135.	127.
141.	139.	150.	149.	119.	129.	118.	101.	94.	84.
71.	46.	44.	45.	65.	48.	46.	43.	41.	34.
42.	43.	43.	37.	50.	43.	54.	47.	48.	57.
62.	87.	71.	70.	67.	68.	65.	108.	128.	137.
119.	118.	127.	125.	140.	139.	148.	165.	207.	229.
237.	190.	181.	158.	152.	136.	94.	68.	69.	55.
58.	50.	54.	64.	49.	63.	70.	73.	103.	79.
113.	95.	121.	144.	152.	155.	136.	148.	137.	136.
121.	79.	102.	91.	85.	64.	66.	80.	73.	65.
63.	61.	69.	93.	117.	165.	207.	199.	176.	158.
140.	137.	119.	85.	83.	55.	49.	44.	50.	37.
41.	57.	43.	55.	55.	50.	59.	63.	46.	54.
52.	50.	38.	39.	40.	42.	46.	50.	60.	68.
53.	49.	66.	50.	57.	54.	51.	57.	50.	62.
60.	65.	49.	57.	68.	77.	79.	91.	88.	67.
78.	53.	54.	45.	47.	40.	39.	27.	38.	35.
34.	29.	35.	37.	38.	34.	32.	39.	30.	42.
37.	47.	53.	31.	43.	48.	42.	51.	39.	40.
58.	46.	65.	40.	49.	66.	45.	50.	40.	48.
39.	43.	47.	35.	45.	32.	36.	44.	33.	36.
36.	36.	42.	32.	45.	41.	59.	50.	45.	44.
52.	62.	57.	77.	54.	70.	78.	76.	63.	67.

59.	58.	48.	48.	39.	45.	36.	41.	38.	29.
50.	38.	27.	28.	32.	32.	34.	42.	36.	31.
56.	46.	62.	52.	48.	59.	62.	62.	54.	75.
74.	84.	74.	90.	91.	112.	122.	108.	97.	88.
77.	88.	83.	70.	49.	53.	57.	61.	67.	41.
43.	49.	49.	44.	44.	53.	59.	51.	43.	43.
57.	55.	42.	56.	45.	49.	56.	57.	52.	45.
44.	43.	47.	38.	39.	36.	56.	34.	33.	52.
45.	46.	50.	34.	51.	45.	42.	37.	44.	40.
38.	41.	29.	28.	40.	48.	39.	40.	40.	35.
48.	52.	38.	35.	39.	34.	44.	39.	29.	42.
52.	54.	71.	44.	49.	52.	44.	41.	53.	56.
45.	33.	40.	44.	45.	49.	57.	47.	58.	59.
55.	65.	45.	52.	48.	39.	38.	41.	41.	32.
39.	29.	34.	22.	24.	29.	18.	36.	36.	33.
35.	41.	51.	49.	31.	46.	46.	47.	50.	60.
70.	57.	62.	71.	83.	106.	94.	80.	78.	96.
90.	89.	80.	67.	68.	74.	66.	101.	78.	95.
134.	145.	213.	238.	243.	215.	195.	196.	195.	243.
262.	262.	246.	200.	164.	150.	156.	181.	175.	139.
137.	146.	179.	159.	162.	172.	142.	132.	114.	128.
112.	114.	103.	88.	78.	88.	79.	81.	71.	61.
60.	46.	53.	42.	57.	50.	57.	40.	58.	62.
63.	85.	85.	80.	114.	99.	92.	83.	76.	88.
72.	76.	75.	83.	71.	84.	72.	70.	55.	72.
73.	70.	56.	64.	83.	67.	67.	74.	72.	86.
100.	94.	108.	91.	98.	72.	81.	118.	72.	78.
59.	69.	39.	63.	40.	64.	60.	42.	49.	34.
25.	40.	27.	34.	49.	39.	49.	49.	70.	73.
69.	60.	69.	50.	46.	50.	55.	58.	58.	48.
36.	42.	41.	54.	61.	52.	70.	59.	68.	77.
70.	65.	64.	70.	67.	67.	56.	59.	56.	66.
54.	65.	81.	57.	79.	98.	87.	83.	67.	66.
52.	68.	68.	58.	65.	48.	45.	53.	53.	48.
49.	46.	50.	62.	60.	53.	58.	55.	54.	57.
74.	69.	49.	71.	71.	88.	78.	83.	76.	88.
88.	101.	92.	113.	104.	84.	85.	73.	70.	48.
77.	50.	67.	66.	43.	47.	50.	57.	34.	22.
39.	44.	55.	31.	52.	39.	57.	52.	37.	44.
44.	58.	49.	60.	76.	63.	63.	47.	57.	59.
62.	61.	54.	37.	53.	48.	44.	47.	41.	40.
55.	65.	33.	53.	50.	58.	47.	46.	56.	74.
52.	68.	60.	56.	59.	59.	72.	72.	90.	86.
82.	69.	64.	67.	56.	78.	50.	52.	66.	58.
57.	55.	44.	67.	47.	49.	44.	39.	38.	55.
49.	55.	54.	57.	57.	81.	55.	53.	57.	56.
62.	51.	70.	56.	54.	57.	70.	60.	75.	82.
95.	101.	104.	108.	88.	89.	108.	86.	95.	92.
75.	75.	74.	68.	71.	62.	61.	62.	51.	66.
33.	46.	40.	43.	48.	52.	37.	32.	34.	29.
41.	35.	30.	35.	25.	27.	42.	29.	36.	26.
23.	24.	35.	38.	27.	36.	34.	30.	29.	28.
33.	38.	24.	28.	36.	45.	46.	43.	43.	35.
42.	36.	39.	42.	36.	44.	52.	45.	46.	38.
36.	47.	34.	66.	50.	60.	51.	57.	47.	49.
66.	67.	51.	52.	62.	60.	59.	60.	67.	63.
58.	59.	59.	75.	56.	42.	42.	55.	63.	43.
53.	46.	34.	39.	42.	44.	36.	49.	46.	43.
51.	39.	36.	41.	32.	44.	36.	42.	51.	43.
48.	58.	54.	44.	36.	38.	50.	54.	52.	54.
64.	62.	48.	49.	49.	42.	48.	68.	66.	62.
79.	81.	83.	99.	108.	124.	102.	109.	89.	90.
82.	107.	98.	97.	101.	92.	101.	85.	74.	83.
77.	93.	85.	79.	71.	95.	95.	111.	115.	73.
90.	82.	88.	78.	90.	93.	86.	104.	80.	60.
47.	57.	71.	55.	66.	43.	41.	50.	37.	48.
36.	44.	45.	37.	44.	51.	37.	42.	38.	38.
41.	56.	42.	43.	49.	51.	38.	45.	46.	46.
36.	29.	33.	41.	56.	40.	42.	29.	44.	37.

37.	44.	37.	32.	27.	24.	27.	25.	27.	34.
39.	37.	38.	35.	41.	34.	45.	49.	51.	42.
35.	33.	36.	34.	34.	45.	40.	41.	45.	39.
47.	46.	46.	36.	48.	38.	35.	36.	38.	43.
40.	40.	36.	38.	49.	38.	47.	55.	51.	49.
53.	65.	73.	58.	73.	47.	58.	50.	64.	65.
71.	61.	49.	56.	46.	39.	41.	57.	43.	63.
67.	60.	76.	74.	91.	65.	51.	53.	52.	43.
48.	48.	58.	65.	53.	50.	66.	63.	51.	44.
56.	50.	56.	43.	58.	69.	63.	57.	63.	41.
38.	44.	37.	58.	47.	56.	56.	58.	74.	68.
76.	57.	67.	56.	54.	58.	67.	68.	75.	70.
72.	67.	60.	60.	61.	59.	51.	68.	63.	64.
69.	70.	67.	53.	83.	67.	50.	65.	64.	76.
63.	71.	73.	57.	67.	57.	48.	52.	61.	70.
63.	66.	62.	59.	68.	81.	81.	89.	63.	73.
58.	49.	45.	41.	59.	46.	62.	59.	55.	46.
42.	48.	36.	34.	38.	32.	43.	38.	51.	46.
55.	45.	50.	42.	64.	76.	44.	55.	52.	56.
69.	57.	58.	72.	78.	70.	48.	51.	52.	61.
46.	53.	67.	56.	55.	42.	44.	56.	34.	49.
44.	48.	38.	54.	31.	37.	54.	63.	44.	50.
49.	51.	52.	40.	48.	42.	37.	43.	42.	48.
39.	48.	41.	48.	48.	45.	44.	38.	55.	37.
35.	40.	44.	38.	32.	47.	46.	55.	40.	35.
44.	47.	37.	40.	56.	41.	57.	48.	47.	52.
52.	57.	51.	51.	53.	44.	49.	55.	52.	45.
56.	43.	52.	56.	39.	55.	41.	39.	38.	43.
42.	48.	41.	52.	44.	62.	46.	55.	56.	61.
76.	52.	55.	66.	70.	55.	55.	51.	57.	65.
45.	69.	71.	49.	63.	62.	63.	71.	59.	56.
56.	54.	55.	74.	94.	89.	62.	91.	59.	68.
73.	70.	70.	69.	34.	60.	61.	53.	56.	61.
55.	46.	62.	64.	52.	63.	74.	82.	63.	63.
77.	51.	68.	50.	55.	50.	61.	55.	76.	66.
66.	55.	74.	70.	88.	70.	59.	71.	86.	86.
101.	76.	90.	78.	66.	66.	67.	77.	82.	64.
71.	63.	85.	75.	81.	88.	96.	101.	112.	76.
61.									

Appendix P-4: step-intensity data of the 30 wt% olivine mixture of Ol+Py

19.00 139.00 .05 30% olivine mixture

38.	42.	47.	31.	22.	42.	44.	39.	49.	33.
41.	46.	38.	36.	43.	41.	57.	55.	76.	89.
84.	102.	70.	63.	63.	61.	51.	42.	41.	45.
36.	33.	38.	34.	34.	37.	41.	31.	29.	34.
34.	42.	37.	32.	33.	36.	30.	29.	31.	34.
32.	26.	41.	38.	36.	41.	38.	26.	38.	33.
28.	23.	40.	33.	39.	32.	30.	31.	33.	47.
47.	54.	66.	66.	111.	155.	220.	358.	415.	414.
291.	244.	130.	109.	79.	53.	42.	60.	39.	49.
42.	40.	46.	48.	53.	73.	104.	147.	174.	161.
122.	108.	65.	61.	50.	64.	81.	85.	97.	79.
62.	42.	38.	51.	44.	48.	40.	39.	30.	45.
40.	43.	41.	43.	65.	52.	75.	104.	171.	219.
238.	239.	244.	163.	123.	86.	68.	71.	44.	43.
35.	33.	35.	40.	47.	37.	36.	48.	54.	62.
59.	109.	160.	234.	268.	266.	204.	149.	99.	87.
69.	59.	62.	44.	57.	53.	59.	69.	87.	142.
188.	347.	534.	646.	561.	497.	365.	218.	122.	98.
68.	46.	54.	45.	51.	44.	41.	43.	42.	55.
47.	31.	57.	61.	55.	57.	52.	59.	53.	43.
55.	57.	53.	52.	76.	66.	74.	93.	104.	117.
152.	210.	262.	306.	445.	691.	1029.	1515.	2057.	2332.
2097.	1649.	1055.	681.	460.	557.	667.	775.	715.	546.
338.	262.	182.	176.	185.	202.	265.	503.	672.	721.
757.	599.	464.	291.	153.	131.	96.	78.	81.	65.
53.	63.	64.	74.	66.	61.	56.	56.	44.	70.
86.	89.	107.	162.	287.	425.	495.	555.	460.	313.
190.	111.	83.	65.	51.	53.	44.	36.	35.	31.
41.	30.	33.	44.	39.	35.	35.	33.	40.	20.
30.	33.	34.	35.	39.	43.	35.	32.	39.	29.
45.	28.	55.	43.	37.	31.	51.	42.	62.	47.
54.	62.	70.	78.	98.	109.	131.	178.	289.	424.
531.	648.	566.	503.	366.	346.	319.	339.	455.	751.
1094.	1279.	1514.	1762.	1829.	1690.	1427.	1004.	676.	418.
302.	193.	153.	129.	154.	126.	185.	237.	454.	625.
687.	655.	578.	373.	288.	180.	134.	109.	82.	68.
57.	64.	39.	45.	43.	56.	34.	38.	43.	45.
42.	50.	63.	64.	66.	76.	101.	67.	54.	61.
51.	54.	80.	69.	89.	117.	127.	122.	107.	72.
71.	50.	70.	62.	63.	112.	109.	132.	139.	120.
173.	203.	328.	362.	381.	405.	322.	238.	150.	127.
157.	212.	264.	304.	382.	321.	281.	246.	253.	284.
318.	291.	268.	187.	140.	109.	79.	71.	63.	59.
83.	102.	145.	189.	292.	304.	272.	250.	210.	184.
226.	278.	254.	224.	155.	113.	111.	87.	70.	63.
48.	71.	83.	115.	153.	194.	258.	251.	317.	317.
267.	262.	245.	197.	161.	173.	243.	321.	426.	433.
388.	266.	214.	164.	129.	105.	129.	160.	210.	228.
246.	204.	151.	113.	104.	91.	85.	67.	71.	60.
72.	81.	64.	72.	62.	80.	57.	53.	44.	50.
65.	60.	57.	72.	110.	107.	179.	294.	428.	424.
441.	377.	286.	213.	162.	136.	123.	156.	201.	263.
322.	285.	301.	309.	289.	245.	221.	165.	120.	91.
60.	59.	42.	50.	38.	41.	55.	56.	56.	80.
85.	132.	168.	191.	192.	140.	134.	87.	84.	67.
80.	80.	82.	70.	70.	66.	54.	47.	55.	41.
39.	36.	42.	40.	22.	35.	27.	38.	37.	23.
35.	43.	32.	39.	38.	31.	28.	31.	29.	42.
35.	42.	47.	37.	42.	56.	61.	75.	65.	78.
71.	51.	62.	56.	45.	43.	51.	43.	66.	73.
63.	72.	77.	82.	50.	67.	41.	42.	44.	48.
69.	101.	147.	170.	190.	230.	238.	191.	164.	169.
114.	84.	95.	63.	63.	133.	119.	134.	104.	136.
85.	61.	62.	53.	59.	61.	71.	71.	67.	67.

63.	55.	59.	49.	41.	46.	42.	52.	58.	46.
51.	70.	54.	79.	53.	73.	86.	93.	108.	127.
161.	259.	394.	585.	737.	758.	700.	513.	462.	385.
330.	245.	230.	202.	168.	107.	97.	103.	78.	70.
59.	58.	55.	62.	75.	87.	87.	76.	85.	78.
64.	55.	42.	47.	42.	39.	39.	39.	40.	34.
41.	38.	23.	29.	30.	39.	46.	47.	48.	58.
76.	71.	88.	115.	108.	129.	166.	186.	200.	209.
167.	173.	142.	107.	106.	112.	137.	155.	127.	153.
114.	121.	74.	71.	80.	64.	72.	74.	77.	111.
128.	167.	163.	147.	166.	139.	149.	154.	170.	201.
298.	416.	550.	682.	623.	661.	572.	392.	324.	315.
254.	200.	182.	151.	125.	101.	87.	85.	86.	87.
67.	72.	70.	64.	62.	77.	67.	77.	80.	72.
77.	86.	54.	93.	92.	95.	92.	80.	73.	93.
88.	90.	90.	100.	77.	88.	88.	86.	84.	79.
103.	109.	130.	116.	111.	99.	94.	80.	68.	60.
58.	82.	101.	119.	112.	141.	116.	116.	82.	70.
64.	67.	60.	61.	63.	75.	74.	73.	105.	120.
134.	166.	165.	184.	214.	249.	238.	214.	190.	192.
172.	136.	148.	136.	117.	123.	113.	148.	168.	159.
209.	244.	286.	365.	318.	322.	358.	340.	318.	280.
246.	217.	166.	148.	162.	126.	152.	128.	158.	215.
224.	263.	340.	294.	263.	276.	234.	161.	153.	132.
86.	79.	78.	77.	65.	54.	68.	71.	66.	78.
67.	70.	66.	69.	82.	86.	64.	56.	68.	53.
50.	58.	58.	47.	68.	59.	71.	71.	76.	78.
73.	81.	89.	96.	103.	91.	68.	76.	69.	58.
59.	58.	57.	68.	55.	61.	86.	113.	130.	171.
156.	276.	341.	394.	348.	310.	282.	277.	247.	180.
160.	118.	133.	125.	115.	161.	183.	220.	243.	255.
203.	199.	179.	152.	161.	141.	161.	180.	159.	181.
153.	153.	132.	118.	124.	133.	163.	152.	165.	145.
121.	104.	82.	81.	72.	67.	53.	48.	51.	61.
55.	75.	75.	85.	87.	80.	99.	75.	75.	55.
58.	63.	49.	47.	35.	30.	44.	41.	55.	41.
54.	45.	42.	45.	52.	49.	79.	124.	168.	141.
113.	137.	145.	148.	135.	88.	86.	75.	91.	89.
68.	72.	61.	50.	64.	51.	56.	50.	50.	59.
60.	61.	70.	82.	115.	135.	163.	152.	152.	178.
196.	196.	177.	214.	149.	171.	172.	145.	137.	147.
154.	172.	154.	177.	147.	152.	108.	106.	98.	77.
65.	55.	57.	52.	36.	44.	40.	44.	34.	40.
42.	43.	39.	32.	50.	45.	41.	72.	61.	80.
63.	61.	78.	85.	79.	71.	71.	94.	112.	122.
138.	150.	111.	99.	109.	110.	122.	163.	186.	199.
165.	163.	153.	121.	137.	120.	109.	76.	56.	46.
36.	49.	39.	53.	62.	51.	62.	68.	85.	88.
90.	95.	128.	124.	120.	120.	134.	126.	111.	107.
118.	82.	97.	64.	90.	68.	61.	53.	74.	70.
70.	72.	93.	78.	96.	148.	171.	171.	149.	155.
110.	128.	115.	77.	72.	62.	56.	47.	47.	44.
47.	50.	48.	59.	57.	62.	50.	51.	44.	52.
50.	63.	49.	45.	40.	45.	60.	56.	69.	59.
49.	53.	61.	67.	45.	48.	45.	49.	50.	41.
55.	50.	56.	48.	60.	86.	84.	67.	67.	71.
64.	69.	50.	67.	30.	44.	46.	33.	28.	32.
32.	37.	39.	28.	40.	46.	36.	37.	30.	32.
46.	47.	35.	34.	32.	37.	32.	44.	40.	48.
56.	52.	48.	72.	58.	37.	49.	62.	50.	50.
50.	37.	34.	30.	43.	32.	35.	33.	31.	34.
35.	35.	34.	40.	40.	39.	40.	41.	46.	44.
62.	61.	65.	67.	76.	87.	63.	62.	65.	75.
76.	82.	66.	49.	48.	55.	47.	59.	34.	29.
43.	41.	36.	32.	37.	33.	36.	32.	41.	54.
57.	47.	51.	42.	60.	54.	47.	59.	60.	69.
83.	72.	76.	97.	86.	96.	96.	122.	89.	95.
81.	78.	85.	77.	54.	67.	66.	68.	67.	72.
65.	52.	64.	58.	48.	60.	66.	64.	67.	66.

66.	53.	57.	57.	67.	57.	39.	47.	49.	40.
40.	35.	34.	49.	48.	49.	57.	46.	54.	57.
60.	73.	60.	41.	33.	38.	50.	43.	28.	28.
43.	44.	33.	45.	37.	33.	43.	44.	42.	36.
43.	38.	45.	41.	30.	44.	37.	38.	26.	41.
29.	58.	47.	58.	51.	39.	43.	51.	51.	37.
41.	38.	48.	40.	33.	59.	64.	72.	68.	70.
50.	53.	55.	45.	45.	49.	51.	41.	42.	22.
30.	48.	39.	36.	49.	42.	19.	24.	27.	32.
37.	38.	40.	35.	50.	51.	41.	48.	55.	55.
72.	60.	83.	73.	89.	88.	82.	98.	73.	81.
85.	69.	79.	67.	79.	66.	87.	79.	80.	91.
106.	123.	144.	193.	166.	160.	172.	142.	177.	181.
182.	243.	193.	176.	137.	131.	142.	117.	156.	110.
106.	128.	129.	118.	138.	157.	125.	111.	100.	89.
108.	95.	85.	86.	67.	81.	60.	52.	44.	45.
62.	55.	42.	36.	58.	54.	51.	40.	67.	68.
85.	63.	89.	88.	80.	86.	90.	77.	65.	79.
75.	66.	62.	59.	76.	76.	70.	74.	79.	63.
59.	64.	59.	56.	48.	62.	67.	68.	70.	84.
83.	100.	84.	86.	79.	87.	104.	130.	127.	83.
70.	70.	70.	69.	74.	61.	55.	39.	39.	30.
43.	39.	46.	28.	45.	57.	57.	57.	61.	70.
65.	65.	73.	57.	63.	49.	57.	60.	45.	56.
40.	48.	50.	55.	52.	81.	89.	74.	75.	87.
90.	68.	81.	65.	58.	53.	64.	72.	66.	70.
49.	55.	53.	71.	97.	91.	93.	63.	65.	56.
40.	60.	59.	60.	60.	58.	48.	38.	62.	48.
65.	44.	40.	57.	47.	57.	51.	55.	53.	63.
54.	61.	55.	65.	71.	84.	90.	92.	100.	84.
83.	55.	69.	90.	97.	81.	70.	60.	59.	71.
62.	64.	51.	61.	44.	47.	52.	48.	50.	43.
32.	30.	41.	43.	38.	42.	41.	60.	36.	41.
41.	41.	58.	61.	54.	59.	60.	62.	58.	46.
57.	62.	50.	49.	44.	46.	45.	36.	56.	43.
41.	40.	35.	50.	52.	49.	51.	58.	63.	55.
70.	61.	58.	75.	62.	52.	65.	87.	78.	88.
73.	49.	63.	75.	55.	72.	61.	49.	55.	43.
65.	62.	62.	51.	65.	34.	55.	53.	53.	62.
55.	53.	54.	47.	49.	75.	75.	54.	51.	48.
39.	60.	62.	68.	43.	52.	60.	58.	53.	81.
91.	90.	82.	82.	76.	81.	103.	106.	72.	73.
69.	57.	68.	60.	58.	59.	60.	63.	56.	47.
50.	49.	41.	33.	36.	37.	23.	38.	33.	28.
36.	38.	30.	33.	37.	32.	27.	37.	37.	23.
33.	25.	34.	24.	36.	26.	35.	31.	41.	31.
47.	43.	45.	34.	33.	44.	39.	43.	33.	43.
43.	33.	34.	45.	39.	48.	52.	47.	48.	52.
42.	56.	44.	52.	53.	47.	43.	51.	39.	61.
77.	69.	72.	72.	51.	60.	73.	55.	65.	68.
73.	68.	74.	62.	49.	56.	35.	43.	64.	63.
47.	63.	57.	36.	43.	55.	39.	49.	61.	50.
29.	55.	34.	38.	46.	42.	48.	53.	44.	41.
35.	50.	66.	74.	64.	63.	66.	37.	51.	47.
50.	56.	82.	66.	55.	51.	41.	68.	64.	72.
67.	82.	103.	94.	95.	95.	74.	83.	98.	94.
93.	85.	89.	94.	89.	90.	90.	68.	78.	75.
77.	65.	83.	83.	87.	79.	97.	90.	106.	94.
83.	89.	70.	83.	80.	82.	86.	81.	76.	55.
50.	54.	56.	59.	43.	39.	53.	39.	40.	40.
49.	42.	43.	48.	47.	42.	46.	44.	47.	33.
46.	48.	46.	51.	49.	74.	58.	49.	56.	38.
32.	37.	44.	39.	33.	47.	48.	41.	30.	38.
28.	28.	29.	39.	26.	21.	28.	37.	33.	47.
49.	58.	37.	54.	41.	36.	43.	57.	41.	43.
47.	50.	44.	31.	41.	30.	48.	51.	36.	44.
53.	34.	51.	34.	43.	29.	45.	36.	33.	42.
33.	38.	42.	47.	34.	41.	44.	41.	52.	48.
62.	57.	52.	58.	50.	46.	58.	47.	52.	54.

66.	51.	48.	52.	38.	49.	53.	47.	42.	52.
58.	62.	54.	68.	61.	80.	54.	52.	45.	48.
40.	41.	62.	61.	52.	45.	47.	69.	53.	53.
63.	59.	49.	48.	47.	52.	51.	55.	57.	72.
43.	45.	61.	43.	55.	45.	49.	69.	53.	58.
67.	70.	57.	67.	66.	91.	74.	74.	53.	90.
78.	67.	69.	68.	59.	62.	62.	58.	55.	66.
54.	71.	64.	69.	73.	54.	55.	60.	64.	69.
75.	81.	53.	64.	60.	56.	67.	57.	56.	67.
61.	71.	59.	56.	56.	75.	77.	69.	58.	65.
37.	62.	39.	46.	40.	47.	41.	49.	42.	40.
51.	36.	45.	35.	35.	45.	46.	35.	30.	41.
46.	35.	55.	61.	63.	53.	48.	45.	54.	57.
68.	84.	76.	74.	65.	60.	66.	53.	59.	44.
55.	46.	56.	59.	58.	55.	48.	40.	44.	39.
30.	40.	38.	43.	47.	49.	57.	41.	53.	47.
64.	46.	55.	43.	43.	39.	50.	50.	46.	58.
51.	58.	46.	52.	49.	51.	45.	39.	33.	45.
49.	36.	34.	56.	51.	45.	54.	46.	46.	64.
40.	63.	63.	51.	66.	58.	57.	54.	51.	52.
56.	48.	54.	64.	56.	40.	51.	66.	45.	54.
58.	42.	51.	53.	45.	60.	50.	48.	49.	47.
45.	45.	35.	48.	52.	55.	53.	68.	57.	60.
58.	54.	69.	60.	60.	52.	72.	51.	56.	58.
54.	86.	84.	62.	67.	73.	57.	58.	72.	63.
68.	54.	45.	61.	71.	96.	75.	78.	64.	63.
71.	66.	42.	52.	47.	56.	61.	59.	64.	54.
59.	69.	79.	61.	55.	48.	53.	76.	63.	73.
64.	80.	49.	58.	50.	46.	43.	54.	60.	53.
66.	77.	85.	73.	75.	86.	93.	82.	90.	83.
65.	79.	74.	83.	78.	90.	77.	80.	88.	90.
83.	59.	79.	76.	88.	88.	91.	89.	83.	89.
89.	78.	62.	74.	84.	90.	99.	100.	112.	73.
79.	65.	78.	57.	69.	61.	62.	64.	72.	75.
64.	75.	70.	68.	55.	54.	56.	72.	57.	62.
46.	52.	44.	60.	46.	49.	49.	47.	46.	62.
44.	37.	40.	53.	48.	42.	44.	52.	48.	46.
55.	41.	40.	37.	43.	38.	48.	49.	52.	56.
45.									

Appendix P-5: step-intensity data of the 40 wt% olivine mixture of Ol+Py

19.00	.05	139.00		40% olivine mixture					
87.	78.	87.	78.	74.	74.	84.	88.	76.	66.
87.	94.	81.	88.	75.	85.	98.	134.	128.	135.
156.	150.	119.	119.	74.	103.	82.	92.	75.	80.
80.	67.	81.	85.	74.	76.	75.	81.	67.	64.
55.	73.	56.	73.	73.	63.	67.	52.	63.	62.
69.	53.	75.	80.	62.	62.	65.	72.	67.	71.
84.	57.	77.	78.	72.	58.	61.	61.	76.	72.
110.	102.	141.	184.	223.	327.	435.	577.	670.	642.
609.	435.	287.	173.	151.	98.	83.	78.	82.	77.
68.	80.	92.	99.	82.	149.	189.	237.	270.	286.
259.	199.	170.	117.	111.	136.	144.	139.	132.	104.
96.	93.	76.	74.	60.	62.	75.	80.	59.	63.
75.	73.	85.	86.	83.	125.	143.	182.	278.	380.
414.	432.	383.	315.	252.	214.	153.	103.	94.	77.
78.	69.	63.	71.	72.	64.	61.	87.	78.	78.
117.	164.	237.	275.	334.	317.	302.	248.	162.	153.
131.	96.	95.	95.	73.	103.	95.	106.	116.	172.
293.	476.	627.	697.	728.	665.	506.	318.	220.	151.
126.	85.	85.	91.	65.	75.	65.	72.	80.	64.
58.	73.	73.	85.	78.	65.	66.	84.	78.	79.
69.	81.	84.	91.	112.	90.	100.	125.	179.	174.
224.	291.	401.	488.	655.	916.	1474.	2051.	2590.	2965.
2764.	2212.	1607.	1110.	884.	830.	929.	936.	951.	779.
610.	433.	323.	254.	292.	276.	421.	617.	791.	899.
938.	890.	697.	460.	326.	200.	166.	115.	99.	105.
96.	114.	110.	121.	112.	85.	105.	97.	92.	114.
107.	150.	207.	291.	473.	694.	784.	853.	777.	622.
434.	244.	169.	137.	122.	100.	80.	75.	80.	80.
79.	60.	61.	57.	71.	62.	63.	68.	62.	78.
66.	62.	70.	58.	45.	51.	59.	65.	47.	78.
67.	69.	47.	64.	54.	78.	71.	84.	105.	92.
97.	99.	114.	136.	134.	153.	195.	273.	366.	456.
687.	834.	837.	776.	599.	485.	493.	534.	766.	1002.
1373.	1717.	2223.	2607.	2605.	2628.	2346.	1876.	1247.	869.
561.	395.	307.	237.	254.	215.	329.	452.	689.	912.
1076.	1275.	1100.	817.	601.	437.	317.	199.	155.	125.
86.	95.	69.	75.	78.	70.	66.	61.	66.	74.
73.	91.	118.	103.	124.	114.	113.	116.	83.	92.
103.	92.	105.	121.	138.	194.	186.	191.	181.	145.
136.	116.	90.	110.	120.	141.	186.	204.	213.	211.
215.	302.	391.	459.	511.	553.	451.	381.	298.	222.
322.	349.	445.	478.	564.	542.	470.	483.	387.	415.
416.	404.	441.	337.	319.	192.	154.	127.	125.	107.
104.	149.	190.	257.	295.	329.	344.	341.	303.	312.
325.	350.	351.	279.	260.	208.	156.	129.	109.	86.
100.	107.	144.	181.	234.	290.	351.	350.	380.	391.
393.	370.	355.	287.	233.	249.	326.	446.	489.	594.
578.	453.	406.	293.	192.	174.	199.	228.	248.	330.
311.	307.	264.	212.	173.	144.	129.	132.	118.	123.
104.	112.	129.	102.	97.	101.	87.	77.	85.	83.
83.	102.	103.	119.	132.	219.	268.	374.	478.	580.
532.	473.	408.	389.	257.	231.	204.	226.	305.	330.
408.	430.	467.	413.	415.	393.	302.	265.	210.	148.
117.	90.	100.	69.	71.	84.	55.	71.	72.	106.
144.	148.	234.	215.	198.	197.	193.	141.	128.	111.
105.	126.	131.	141.	107.	112.	102.	84.	82.	64.
57.	58.	56.	55.	51.	55.	65.	43.	58.	48.
47.	47.	53.	56.	55.	55.	60.	60.	56.	56.
49.	57.	67.	51.	52.	70.	86.	110.	95.	127.
117.	117.	111.	67.	77.	82.	92.	79.	95.	85.
107.	112.	119.	120.	95.	95.	80.	77.	74.	79.
87.	119.	171.	203.	270.	319.	265.	244.	239.	216.
162.	125.	99.	112.	115.	145.	179.	156.	176.	183.
175.	102.	98.	111.	101.	90.	100.	113.	109.	106.

105.	85.	99.	76.	77.	65.	63.	58.	70.	76.
69.	96.	79.	103.	109.	92.	97.	127.	174.	184.
292.	390.	575.	754.	962.	1115.	1108.	949.	839.	698.
593.	533.	418.	366.	271.	224.	178.	154.	143.	131.
108.	104.	94.	89.	107.	90.	112.	115.	108.	100.
97.	97.	74.	69.	63.	49.	46.	65.	56.	63.
60.	57.	63.	48.	51.	66.	59.	74.	65.	91.
95.	136.	115.	151.	177.	194.	262.	315.	278.	352.
287.	260.	232.	205.	155.	187.	191.	240.	243.	184.
163.	177.	128.	129.	100.	102.	107.	101.	120.	156.
187.	188.	228.	219.	251.	251.	222.	241.	256.	280.
371.	550.	762.	846.	938.	977.	856.	765.	616.	560.
458.	340.	299.	247.	182.	184.	153.	122.	118.	120.
150.	108.	105.	109.	109.	120.	116.	120.	140.	117.
103.	109.	110.	123.	120.	126.	110.	93.	110.	129.
138.	158.	148.	163.	148.	165.	157.	145.	174.	138.
129.	165.	152.	179.	136.	153.	133.	137.	105.	104.
79.	117.	121.	165.	152.	164.	152.	155.	134.	106.
95.	95.	99.	92.	86.	89.	97.	117.	139.	151.
185.	229.	223.	254.	297.	293.	310.	330.	288.	268.
260.	246.	227.	233.	213.	206.	167.	195.	224.	214.
271.	324.	394.	473.	500.	568.	611.	608.	528.	518.
401.	405.	302.	289.	238.	210.	211.	226.	284.	250.
346.	386.	477.	502.	458.	436.	413.	306.	268.	231.
175.	139.	113.	126.	124.	92.	90.	107.	78.	117.
103.	92.	91.	97.	97.	96.	87.	90.	86.	85.
80.	83.	64.	80.	73.	91.	93.	101.	103.	110.
123.	129.	143.	150.	133.	155.	134.	116.	133.	126.
88.	95.	76.	78.	93.	110.	122.	126.	170.	203.
248.	341.	390.	461.	476.	453.	466.	396.	345.	295.
235.	187.	198.	166.	175.	249.	289.	268.	321.	350.
307.	329.	286.	258.	229.	227.	269.	260.	299.	243.
282.	263.	240.	233.	215.	228.	288.	266.	221.	232.
214.	169.	169.	133.	114.	89.	75.	67.	88.	83.
94.	108.	90.	108.	123.	137.	102.	130.	119.	111.
87.	74.	85.	77.	78.	65.	68.	60.	63.	66.
68.	77.	99.	87.	90.	119.	137.	166.	215.	218.
239.	250.	231.	256.	219.	192.	159.	116.	128.	138.
129.	100.	98.	77.	85.	75.	83.	75.	85.	72.
88.	91.	111.	140.	151.	189.	187.	220.	198.	239.
254.	274.	276.	255.	262.	238.	221.	208.	203.	232.
233.	238.	259.	253.	213.	220.	206.	178.	165.	128.
114.	96.	86.	63.	73.	62.	66.	57.	53.	68.
57.	56.	60.	55.	62.	91.	100.	100.	87.	96.
116.	111.	114.	102.	95.	103.	105.	116.	141.	181.
195.	188.	156.	183.	176.	187.	176.	186.	245.	259.
278.	249.	205.	216.	188.	163.	156.	99.	86.	83.
78.	81.	88.	69.	84.	92.	102.	106.	123.	133.
133.	167.	189.	213.	173.	171.	181.	200.	196.	176.
168.	131.	121.	140.	131.	96.	115.	101.	94.	105.
101.	118.	97.	128.	150.	179.	216.	208.	257.	178.
168.	167.	188.	154.	110.	90.	78.	69.	85.	62.
72.	60.	64.	93.	78.	79.	93.	81.	77.	75.
78.	74.	74.	67.	76.	88.	93.	92.	86.	109.
81.	78.	82.	78.	78.	87.	67.	84.	76.	92.
64.	71.	65.	75.	97.	102.	85.	124.	113.	96.
77.	87.	74.	66.	61.	49.	63.	52.	56.	49.
53.	53.	43.	52.	47.	62.	42.	55.	49.	56.
55.	56.	54.	45.	54.	34.	59.	57.	77.	48.
78.	102.	107.	109.	98.	97.	87.	86.	92.	65.
61.	71.	67.	45.	50.	56.	47.	41.	62.	47.
55.	53.	51.	65.	67.	72.	66.	77.	70.	75.
84.	81.	79.	110.	97.	121.	114.	105.	104.	103.
122.	126.	97.	87.	89.	74.	96.	86.	75.	74.
70.	65.	57.	54.	53.	62.	69.	67.	77.	103.
94.	98.	86.	99.	90.	95.	92.	82.	74.	93.
116.	124.	125.	123.	116.	130.	128.	153.	138.	139.
120.	120.	99.	103.	84.	110.	90.	97.	103.	109.
100.	97.	77.	100.	95.	101.	110.	89.	87.	101.

89.	82.	98.	103.	81.	75.	77.	82.	77.	54.
75.	57.	59.	58.	74.	71.	75.	73.	82.	80.
94.	73.	79.	82.	53.	63.	48.	55.	46.	69.
63.	69.	55.	75.	70.	72.	73.	66.	68.	77.
68.	58.	47.	46.	60.	59.	49.	61.	40.	66.
79.	70.	85.	89.	92.	78.	78.	74.	68.	74.
44.	49.	61.	58.	90.	87.	94.	119.	90.	95.
83.	94.	87.	84.	84.	78.	72.	62.	59.	49.
54.	53.	56.	59.	49.	59.	43.	42.	53.	49.
42.	70.	47.	58.	59.	73.	74.	71.	81.	76.
79.	103.	124.	119.	115.	126.	119.	123.	132.	125.
122.	112.	114.	101.	102.	104.	139.	107.	116.	150.
165.	188.	231.	241.	247.	242.	248.	237.	229.	255.
286.	335.	291.	252.	209.	191.	177.	203.	213.	190.
197.	200.	199.	198.	208.	193.	184.	160.	153.	150.
157.	116.	119.	122.	109.	108.	78.	80.	73.	71.
80.	71.	79.	66.	72.	57.	69.	73.	82.	83.
98.	108.	92.	124.	114.	115.	117.	111.	100.	97.
97.	95.	97.	94.	107.	104.	96.	99.	97.	109.
99.	77.	95.	97.	89.	91.	76.	103.	102.	124.
121.	129.	123.	143.	135.	152.	166.	202.	156.	138.
134.	113.	114.	111.	100.	91.	84.	89.	70.	66.
48.	69.	69.	63.	58.	69.	73.	75.	75.	94.
84.	86.	89.	92.	84.	72.	72.	80.	87.	84.
78.	78.	76.	95.	104.	103.	137.	114.	105.	124.
113.	115.	117.	104.	115.	91.	96.	80.	75.	81.
81.	76.	81.	94.	118.	101.	103.	95.	99.	72.
68.	78.	90.	69.	89.	74.	77.	83.	83.	74.
77.	67.	75.	86.	99.	78.	70.	78.	89.	88.
91.	70.	94.	100.	117.	107.	111.	104.	115.	121.
111.	126.	132.	130.	146.	133.	113.	117.	90.	113.
95.	96.	92.	86.	79.	71.	89.	84.	76.	53.
66.	67.	77.	75.	73.	68.	49.	64.	53.	60.
55.	88.	77.	80.	97.	92.	75.	79.	87.	102.
97.	94.	87.	79.	79.	76.	79.	67.	78.	66.
66.	69.	74.	69.	95.	71.	88.	105.	95.	97.
101.	88.	91.	98.	95.	69.	108.	118.	128.	116.
122.	118.	92.	96.	92.	94.	106.	84.	83.	105.
89.	102.	87.	75.	89.	94.	88.	70.	87.	81.
70.	85.	80.	71.	67.	79.	70.	96.	51.	96.
79.	81.	81.	86.	91.	81.	91.	89.	78.	95.
118.	152.	129.	135.	126.	117.	115.	105.	136.	118.
108.	86.	93.	91.	76.	76.	86.	80.	82.	86.
75.	61.	64.	70.	47.	49.	47.	55.	61.	36.
47.	55.	62.	49.	33.	57.	48.	48.	47.	61.
41.	41.	41.	62.	58.	46.	54.	54.	68.	66.
67.	62.	63.	56.	52.	59.	48.	66.	55.	52.
45.	72.	61.	66.	80.	81.	70.	64.	56.	52.
69.	52.	75.	84.	77.	74.	71.	67.	81.	75.
101.	97.	110.	100.	89.	100.	93.	100.	87.	109.
103.	103.	108.	106.	89.	83.	81.	78.	72.	70.
71.	92.	63.	77.	74.	64.	77.	60.	78.	73.
78.	76.	56.	68.	72.	79.	73.	77.	82.	76.
92.	109.	98.	122.	96.	81.	71.	96.	89.	87.
88.	100.	90.	68.	75.	70.	94.	88.	107.	100.
104.	120.	141.	157.	178.	154.	137.	126.	133.	123.
125.	143.	132.	132.	136.	121.	137.	109.	120.	122.
110.	112.	108.	104.	123.	113.	154.	136.	155.	131.
132.	106.	131.	116.	137.	113.	126.	123.	88.	94.
86.	75.	90.	92.	93.	56.	59.	61.	61.	62.
59.	64.	57.	66.	58.	70.	55.	60.	73.	67.
60.	74.	70.	73.	90.	93.	78.	92.	77.	67.
75.	68.	77.	58.	70.	74.	59.	55.	54.	63.
50.	40.	37.	45.	46.	52.	43.	44.	56.	75.
67.	73.	65.	72.	60.	79.	76.	79.	57.	78.
70.	61.	72.	61.	54.	68.	68.	63.	82.	56.
73.	70.	59.	54.	45.	49.	55.	44.	60.	61.
46.	56.	58.	41.	56.	55.	73.	51.	71.	69.
54.	92.	86.	70.	58.	62.	64.	65.	73.	80.

62.	77.	83.	68.	56.	61.	66.	69.	66.	59.
50.	89.	97.	87.	98.	74.	81.	81.	66.	62.
61.	64.	70.	80.	87.	83.	106.	89.	83.	88.
82.	68.	72.	85.	84.	82.	90.	82.	72.	98.
74.	88.	77.	78.	69.	75.	83.	90.	102.	106.
97.	103.	105.	100.	98.	113.	109.	115.	117.	107.
100.	129.	125.	99.	100.	113.	91.	83.	94.	99.
90.	97.	103.	89.	103.	118.	86.	101.	81.	84.
88.	98.	99.	106.	98.	90.	91.	97.	103.	77.
93.	97.	82.	74.	85.	90.	87.	90.	90.	90.
80.	70.	65.	77.	53.	68.	89.	57.	77.	69.
54.	69.	66.	60.	43.	61.	63.	69.	65.	67.
70.	69.	78.	76.	88.	91.	84.	91.	100.	90.
95.	109.	101.	111.	112.	91.	77.	106.	88.	80.
74.	81.	74.	87.	97.	72.	66.	62.	56.	63.
49.	65.	64.	64.	56.	76.	73.	80.	74.	81.
88.	101.	91.	70.	64.	60.	57.	92.	77.	72.
77.	86.	89.	69.	69.	80.	71.	57.	58.	47.
68.	69.	69.	57.	78.	90.	78.	69.	64.	76.
72.	91.	87.	97.	96.	78.	73.	72.	84.	82.
86.	78.	78.	80.	95.	78.	87.	79.	82.	87.
88.	102.	88.	74.	68.	86.	51.	61.	66.	66.
62.	72.	79.	70.	99.	75.	83.	99.	88.	92.
99.	103.	93.	113.	124.	104.	97.	91.	81.	79.
96.	113.	80.	120.	98.	89.	108.	87.	95.	95.
83.	95.	87.	79.	71.	102.	89.	107.	94.	84.
99.	95.	99.	80.	59.	85.	82.	92.	83.	81.
89.	82.	94.	76.	83.	78.	102.	82.	99.	96.
90.	75.	98.	93.	84.	86.	96.	81.	89.	101.
89.	111.	104.	111.	132.	105.	122.	109.	135.	116.
136.	101.	103.	145.	132.	124.	108.	120.	114.	117.
113.	106.	126.	128.	107.	122.	116.	124.	93.	109.
128.	117.	122.	111.	113.	142.	170.	138.	130.	128.
127.	123.	102.	109.	107.	87.	87.	100.	90.	112.
111.	104.	97.	118.	113.	107.	79.	116.	97.	79.
86.	75.	67.	70.	91.	70.	84.	83.	78.	57.
71.	81.	67.	85.	70.	67.	73.	55.	66.	71.
65.	63.	80.	57.	83.	65.	63.	65.	89.	88.
85.									

Appendix P-6: step-intensity data of the 50 wt% olivine mixture of Ol+Py

16.00	.05	136.00	50% olivine mixture						
104.	90.	81.	96.	92.	93.	113.	69.	97.	90.
98.	95.	84.	104.	99.	83.	121.	86.	82.	110.
109.	136.	116.	122.	161.	219.	341.	409.	474.	385.
304.	184.	130.	120.	114.	90.	99.	101.	97.	85.
78.	77.	82.	105.	79.	96.	91.	83.	71.	90.
73.	78.	86.	87.	80.	80.	75.	85.	82.	102.
98.	88.	85.	77.	102.	98.	83.	81.	82.	91.
91.	82.	101.	82.	96.	83.	89.	115.	146.	161.
179.	157.	155.	101.	115.	114.	106.	89.	63.	85.
87.	79.	104.	82.	95.	72.	82.	78.	81.	60.
85.	76.	59.	88.	76.	78.	75.	72.	79.	73.
73.	63.	69.	82.	85.	70.	71.	68.	96.	74.
81.	77.	71.	69.	90.	78.	85.	83.	89.	105.
103.	144.	167.	223.	246.	400.	655.	911.	1105.	1061.
771.	471.	352.	183.	165.	120.	107.	97.	99.	79.
102.	92.	101.	108.	131.	170.	233.	322.	393.	359.
346.	227.	147.	105.	114.	129.	119.	145.	135.	113.
87.	79.	62.	62.	62.	72.	74.	55.	67.	75.
73.	82.	103.	73.	117.	125.	192.	261.	382.	516.
607.	501.	516.	416.	294.	226.	140.	117.	82.	104.
78.	74.	82.	70.	70.	88.	88.	106.	83.	98.
100.	149.	208.	269.	325.	385.	298.	216.	156.	122.
109.	83.	66.	87.	83.	89.	102.	96.	147.	174.
254.	423.	564.	826.	791.	669.	451.	278.	152.	123.
97.	86.	73.	71.	70.	68.	68.	91.	66.	72.
72.	92.	90.	66.	77.	64.	76.	69.	93.	84.
88.	85.	93.	104.	114.	113.	109.	138.	165.	175.
251.	299.	388.	530.	654.	932.	1405.	2090.	2638.	3001.
2662.	1783.	1170.	724.	589.	637.	842.	947.	984.	747.
504.	319.	253.	222.	225.	258.	380.	571.	840.	1050.
1010.	766.	506.	330.	227.	177.	146.	122.	109.	90.
121.	111.	109.	113.	140.	113.	92.	106.	114.	139.
149.	209.	235.	386.	615.	982.	1267.	1368.	1032.	698.
413.	266.	145.	130.	131.	98.	98.	82.	99.	82.
86.	75.	69.	69.	64.	60.	62.	80.	54.	74.
59.	58.	85.	70.	85.	75.	60.	68.	73.	66.
77.	79.	83.	64.	72.	74.	83.	70.	86.	90.
96.	93.	118.	133.	140.	171.	195.	242.	350.	463.
589.	747.	741.	693.	541.	433.	400.	478.	669.	956.
1370.	1819.	2409.	2775.	2963.	2948.	2474.	1688.	1097.	634.
445.	347.	302.	240.	273.	309.	405.	569.	895.	1332.
1633.	1683.	1363.	1120.	705.	430.	306.	223.	163.	126.
116.	92.	100.	99.	84.	74.	79.	82.	82.	103.
77.	96.	122.	131.	127.	134.	145.	132.	123.	93.
103.	116.	125.	161.	233.	267.	293.	262.	256.	158.
147.	95.	111.	103.	135.	171.	221.	267.	278.	279.
265.	274.	363.	450.	566.	487.	416.	304.	264.	243.
272.	388.	627.	670.	735.	739.	584.	472.	456.	562.
668.	719.	634.	506.	350.	235.	166.	138.	112.	104.
135.	143.	172.	246.	337.	320.	357.	340.	266.	266.
288.	345.	328.	326.	230.	204.	148.	113.	113.	99.
107.	135.	154.	222.	301.	371.	429.	459.	432.	466.
445.	381.	293.	278.	228.	209.	282.	396.	481.	524.
496.	407.	304.	227.	161.	161.	171.	202.	247.	279.
316.	281.	250.	184.	136.	129.	124.	131.	113.	112.
122.	129.	132.	105.	109.	122.	76.	74.	83.	89.
87.	92.	88.	115.	135.	178.	244.	359.	516.	594.
554.	522.	432.	309.	226.	225.	208.	200.	248.	374.
401.	390.	372.	339.	321.	361.	293.	226.	216.	108.
95.	98.	72.	71.	68.	79.	82.	80.	92.	84.
149.	166.	212.	241.	223.	187.	157.	122.	100.	102.
111.	135.	122.	116.	123.	104.	104.	75.	98.	78.
64.	54.	64.	57.	52.	43.	48.	54.	53.	48.
46.	51.	52.	47.	55.	71.	60.	43.	52.	59.

63.	66.	62.	59.	62.	77.	105.	138.	147.	146.
158.	110.	123.	98.	88.	97.	99.	96.	94.	101.
145.	131.	125.	92.	101.	88.	71.	72.	81.	79.
85.	124.	154.	226.	274.	319.	320.	243.	213.	201.
149.	126.	98.	110.	126.	179.	194.	211.	201.	184.
163.	127.	107.	98.	95.	90.	123.	127.	160.	146.
133.	109.	86.	111.	76.	69.	65.	83.	81.	97.
104.	102.	112.	111.	120.	128.	150.	150.	212.	255.
298.	459.	667.	1096.	1338.	1505.	1336.	1122.	961.	807.
670.	525.	449.	405.	296.	254.	231.	197.	155.	165.
99.	114.	106.	102.	106.	108.	99.	111.	103.	88.
74.	79.	73.	66.	84.	76.	66.	52.	53.	54.
69.	57.	61.	67.	62.	60.	68.	76.	68.	80.
107.	118.	136.	166.	185.	244.	328.	375.	375.	347.
335.	294.	236.	166.	168.	154.	196.	202.	234.	192.
178.	141.	128.	107.	101.	103.	122.	99.	143.	212.
226.	325.	351.	334.	325.	279.	280.	224.	235.	274.
340.	510.	694.	888.	915.	916.	898.	770.	634.	522.
419.	323.	277.	229.	213.	157.	148.	143.	128.	131.
132.	123.	119.	120.	115.	124.	143.	145.	139.	170.
124.	135.	132.	136.	163.	128.	115.	106.	124.	126.
169.	174.	216.	207.	178.	188.	204.	199.	162.	143.
135.	139.	152.	159.	159.	143.	117.	122.	107.	81.
101.	80.	107.	149.	177.	180.	154.	145.	114.	97.
83.	108.	82.	81.	96.	117.	107.	129.	131.	172.
188.	225.	212.	208.	269.	299.	297.	298.	242.	298.
253.	258.	254.	257.	211.	239.	230.	233.	243.	275.
320.	381.	434.	505.	589.	587.	682.	649.	626.	593.
529.	395.	323.	307.	275.	236.	221.	209.	250.	308.
392.	485.	616.	684.	619.	628.	494.	426.	316.	263.
188.	138.	150.	122.	139.	120.	137.	101.	129.	101.
90.	106.	104.	104.	95.	111.	85.	94.	78.	65.
72.	70.	74.	81.	98.	98.	105.	118.	115.	123.
124.	102.	146.	139.	147.	130.	154.	145.	130.	114.
107.	82.	87.	92.	99.	98.	107.	134.	169.	200.
242.	319.	412.	480.	540.	554.	489.	352.	383.	305.
204.	170.	158.	130.	165.	202.	250.	333.	309.	312.
314.	350.	261.	228.	281.	253.	273.	329.	331.	380.
299.	272.	258.	234.	251.	232.	280.	248.	226.	229.
214.	159.	137.	133.	93.	83.	85.	84.	71.	87.
98.	90.	98.	130.	120.	126.	122.	94.	114.	95.
85.	74.	95.	61.	77.	54.	58.	62.	72.	69.
79.	86.	90.	98.	102.	122.	189.	225.	290.	335.
311.	329.	295.	314.	271.	221.	160.	162.	135.	142.
112.	107.	103.	92.	73.	71.	85.	76.	71.	81.
77.	90.	114.	125.	141.	160.	184.	191.	209.	210.
234.	223.	221.	222.	165.	213.	210.	182.	184.	243.
274.	253.	275.	277.	226.	261.	205.	184.	163.	153.
129.	93.	107.	84.	67.	62.	63.	58.	55.	59.
61.	58.	63.	80.	66.	91.	112.	112.	107.	117.
92.	108.	119.	117.	108.	111.	90.	115.	159.	134.
156.	159.	141.	162.	140.	146.	153.	192.	203.	222.
260.	197.	198.	191.	158.	131.	109.	100.	59.	88.
72.	83.	64.	88.	88.	109.	124.	130.	123.	143.
133.	143.	144.	165.	178.	170.	157.	157.	173.	160.
151.	161.	154.	129.	134.	99.	129.	99.	81.	86.
112.	106.	124.	129.	168.	201.	278.	220.	180.	192.
192.	185.	152.	126.	106.	93.	100.	86.	73.	84.
58.	67.	65.	93.	90.	82.	95.	70.	83.	92.
91.	95.	65.	86.	76.	85.	75.	91.	106.	117.
76.	86.	80.	81.	84.	86.	76.	95.	84.	93.
64.	76.	73.	69.	79.	91.	106.	105.	115.	72.
100.	96.	90.	89.	72.	45.	48.	43.	48.	49.
50.	53.	49.	58.	55.	52.	47.	44.	55.	38.
55.	60.	47.	61.	58.	69.	60.	53.	63.	78.
84.	112.	117.	108.	103.	120.	98.	100.	72.	69.
70.	73.	47.	61.	57.	78.	58.	53.	63.	53.
53.	64.	52.	62.	63.	61.	75.	82.	73.	61.
80.	87.	83.	110.	98.	141.	123.	104.	111.	133.

127.	136.	122.	105.	89.	107.	87.	96.	84.	74.
78.	59.	78.	78.	62.	68.	74.	87.	92.	97.
119.	87.	91.	88.	99.	102.	77.	106.	90.	96.
86.	140.	128.	120.	122.	147.	143.	126.	146.	113.
122.	114.	115.	115.	96.	122.	90.	105.	125.	118.
118.	113.	97.	100.	126.	105.	126.	137.	138.	100.
111.	92.	122.	92.	103.	83.	70.	67.	76.	74.
83.	63.	86.	56.	86.	108.	90.	88.	93.	87.
91.	96.	87.	95.	69.	56.	71.	75.	73.	61.
72.	77.	82.	97.	76.	74.	59.	81.	83.	72.
54.	60.	69.	52.	50.	64.	62.	51.	50.	63.
79.	61.	111.	105.	92.	75.	70.	71.	68.	69.
61.	54.	64.	82.	81.	93.	114.	125.	126.	112.
117.	95.	107.	100.	96.	101.	75.	63.	75.	58.
45.	49.	50.	66.	52.	51.	46.	45.	56.	54.
45.	45.	56.	64.	68.	71.	66.	63.	67.	82.
85.	106.	108.	117.	102.	137.	143.	130.	124.	116.
139.	140.	147.	132.	103.	117.	95.	118.	137.	163.
151.	205.	201.	267.	276.	241.	190.	194.	197.	235.
252.	252.	261.	217.	176.	173.	163.	190.	166.	163.
188.	192.	202.	194.	203.	180.	171.	163.	159.	138.
150.	97.	120.	97.	93.	109.	90.	60.	74.	70.
69.	64.	67.	53.	85.	57.	91.	83.	84.	92.
114.	116.	107.	106.	112.	133.	127.	111.	94.	92.
96.	86.	107.	88.	78.	98.	91.	91.	78.	79.
67.	81.	101.	82.	84.	88.	96.	99.	93.	98.
134.	124.	126.	108.	131.	168.	164.	229.	204.	182.
143.	133.	111.	120.	134.	127.	101.	71.	75.	65.
62.	59.	59.	60.	57.	79.	62.	75.	85.	73.
103.	83.	97.	95.	66.	77.	81.	63.	67.	65.
73.	77.	86.	106.	114.	129.	154.	148.	125.	105.
101.	107.	115.	130.	123.	105.	86.	87.	84.	82.
101.	93.	86.	88.	111.	138.	143.	104.	105.	87.
83.	85.	90.	97.	70.	58.	65.	82.	88.	65.
79.	88.	90.	85.	79.	76.	88.	82.	80.	88.
76.	85.	93.	97.	92.	110.	115.	137.	145.	126.
123.	105.	136.	141.	109.	127.	117.	111.	96.	81.
96.	101.	98.	95.	76.	103.	88.	98.	79.	67.
59.	75.	80.	82.	79.	65.	75.	51.	50.	65.
61.	54.	74.	91.	102.	84.	79.	71.	89.	106.
71.	89.	75.	81.	79.	82.	70.	68.	76.	71.
60.	70.	72.	59.	90.	87.	67.	80.	89.	109.
91.	103.	87.	91.	76.	88.	100.	102.	116.	107.
103.	89.	62.	87.	80.	87.	109.	83.	97.	92.
91.	108.	106.	101.	97.	70.	79.	82.	78.	102.
79.	93.	75.	86.	80.	85.	76.	87.	82.	86.
90.	95.	91.	75.	69.	70.	85.	87.	96.	94.
106.	136.	148.	112.	105.	89.	102.	128.	122.	125.
107.	103.	116.	76.	82.	66.	81.	103.	68.	61.
64.	73.	48.	55.	55.	60.	60.	52.	52.	45.
48.	54.	44.	57.	47.	53.	42.	45.	48.	62.
55.	50.	53.	43.	65.	63.	64.	71.	70.	65.
66.	8.	67.	79.	63.	68.	54.	64.	66.	59.
66.	65.	54.	68.	67.	71.	68.	79.	70.	72.
61.	71.	71.	83.	63.	77.	67.	79.	88.	100.
123.	107.	111.	99.	98.	95.	116.	99.	102.	79.
93.	103.	113.	117.	90.	83.	76.	85.	61.	85.
106.	85.	89.	78.	78.	57.	83.	88.	98.	79.
82.	65.	61.	71.	77.	82.	90.	86.	80.	94.
105.	137.	132.	129.	118.	95.	78.	93.	92.	102.
109.	104.	105.	92.	105.	63.	86.	87.	85.	94.
99.	105.	102.	137.	133.	106.	105.	122.	118.	130.
125.	130.	136.	110.	106.	129.	114.	129.	103.	112.
108.	104.	121.	114.	118.	120.	124.	140.	130.	115.
121.	98.	127.	135.	118.	129.	119.	106.	98.	97.
87.	81.	73.	84.	86.	67.	73.	57.	75.	73.
47.	68.	61.	79.	54.	65.	70.	44.	60.	81.
85.	71.	92.	77.	101.	87.	106.	83.	96.	76.
88.	71.	82.	79.	96.	89.	90.	65.	56.	61.

46.	56.	52.	58.	62.	46.	65.	50.	73.	67.
77.	80.	75.	83.	85.	70.	72.	76.	80.	70.
81.	74.	80.	65.	63.	57.	81.	79.	63.	59.
69.	62.	53.	53.	50.	56.	58.	65.	62.	55.
56.	67.	51.	49.	60.	57.	68.	55.	79.	62.
73.	60.	68.	65.	63.	71.	71.	68.	88.	85.
73.	69.	75.	81.	65.	54.	54.	66.	83.	76.
71.	66.	80.	94.	97.	88.	93.	88.	61.	64.
63.	72.	70.	81.	80.	96.	88.	115.	94.	101.
87.	73.	78.	98.	87.	80.	103.	87.	92.	79.
79.	85.	86.	82.	73.	81.	80.	87.	88.	90.
107.	99.	99.	105.	103.	109.	116.	110.	107.	113.
106.	110.	111.	115.	109.	100.	110.	118.	97.	105.
100.	103.	113.	147.	125.	126.	103.	92.	87.	101.
96.	99.	116.	103.	131.	98.	91.	107.	94.	88.
75.	94.	77.	106.	91.	96.	88.	78.	71.	90.
70.	56.	64.	71.	63.	70.	77.	52.	63.	67.
47.	73.	62.	63.	62.	58.	69.	55.	67.	65.
66.	86.	77.	99.	88.	104.	80.	85.	77.	85.
99.	122.	141.	128.	116.	105.	85.	89.	96.	89.
94.	86.	92.	86.	89.	89.	73.	88.	65.	70.
87.	74.	66.	83.	77.	72.	92.	103.	115.	89.
92.	119.	91.	84.	64.	67.	80.	87.	73.	75.
103.	91.	81.	88.	72.	50.	71.	78.	89.	70.
75.	78.	79.	92.	80.	89.	91.	83.	73.	87.
97.	98.	93.	114.	104.	93.	96.	95.	86.	83.
81.	85.	82.	96.	89.	89.	81.	89.	88.	111.
97.	86.	78.	68.	63.	76.	81.	78.	74.	69.
71.	85.	88.	86.	81.	86.	106.	86.	119.	101.
101.	83.	103.	119.	97.	98.	86.	90.	83.	101.
91.	113.	121.	101.	86.	108.	107.	96.	86.	91.
80.	102.	75.	86.	87.	97.	107.	99.	99.	98.
101.	83.	91.	76.	86.	81.	66.	70.	68.	74.
73.	81.	88.	82.	101.	87.	97.	80.	87.	80.
82.	84.	99.	79.	78.	69.	89.	83.	88.	95.
107.	112.	129.	113.	140.	132.	122.	121.	107.	136.
113.	116.	132.	115.	109.	121.	116.	106.	135.	121.
120.	123.	110.	129.	139.	127.	131.	121.	104.	117.
117.									

Appendix P-7: step-intensity data of the 60 wt% olivine mixture of Ol+Py

16.00	.05	136.00		60% olivine mixture					
97.	96.	89.	90.	93.	106.	78.	103.	101.	92.
103.	85.	90.	90.	100.	88.	82.	90.	109.	95.
112.	124.	138.	181.	211.	346.	465.	509.	434.	338.
246.	197.	151.	125.	91.	115.	98.	91.	96.	98.
77.	80.	71.	93.	82.	85.	102.	82.	74.	73.
86.	65.	80.	84.	76.	71.	97.	77.	82.	85.
69.	91.	88.	91.	81.	90.	78.	80.	83.	96.
84.	75.	77.	84.	83.	99.	88.	127.	134.	153.
119.	117.	112.	100.	109.	93.	79.	97.	89.	92.
96.	90.	112.	96.	95.	73.	93.	83.	84.	75.
68.	77.	71.	75.	78.	103.	68.	77.	62.	75.
70.	65.	73.	71.	76.	60.	74.	56.	79.	68.
83.	67.	77.	85.	90.	83.	70.	95.	75.	113.
108.	164.	191.	278.	381.	581.	806.	1055.	1132.	962.
653.	448.	295.	209.	174.	103.	99.	70.	103.	92.
85.	98.	92.	138.	165.	215.	281.	390.	403.	354.
284.	228.	162.	138.	107.	125.	114.	131.	118.	107.
93.	75.	80.	83.	77.	70.	65.	80.	76.	69.
73.	86.	116.	113.	125.	168.	253.	401.	536.	567.
629.	616.	519.	431.	318.	210.	126.	127.	96.	91.
83.	73.	72.	51.	81.	86.	80.	83.	90.	97.
118.	147.	193.	285.	289.	269.	213.	180.	122.	98.
87.	99.	76.	75.	75.	69.	102.	95.	154.	186.
316.	497.	586.	637.	558.	510.	314.	210.	139.	103.
83.	77.	86.	65.	76.	61.	69.	81.	68.	79.
71.	78.	80.	82.	65.	79.	79.	82.	80.	96.
69.	90.	98.	83.	82.	109.	117.	118.	148.	187.
232.	289.	378.	538.	658.	1015.	1391.	1826.	2233.	2121.
1694.	1217.	750.	587.	518.	618.	727.	768.	654.	532.
373.	289.	215.	197.	203.	260.	369.	581.	729.	764.
722.	551.	384.	270.	191.	136.	120.	108.	107.	94.
102.	105.	102.	111.	123.	101.	107.	107.	129.	142.
185.	228.	327.	535.	960.	1353.	1567.	1378.	1128.	720.
383.	280.	168.	124.	115.	104.	102.	97.	98.	60.
73.	70.	82.	71.	77.	82.	66.	74.	77.	64.
65.	76.	58.	73.	60.	54.	69.	70.	60.	76.
75.	66.	78.	76.	94.	74.	83.	68.	89.	94.
96.	121.	136.	141.	134.	198.	199.	223.	356.	495.
627.	620.	659.	496.	432.	400.	387.	503.	651.	923.
1235.	1760.	2311.	2643.	2760.	2390.	1960.	1331.	922.	610.
422.	310.	271.	267.	340.	353.	506.	818.	1246.	1682.
1905.	1799.	1408.	975.	651.	435.	324.	208.	173.	129.
99.	101.	107.	80.	102.	89.	84.	96.	77.	78.
98.	99.	89.	130.	125.	123.	120.	116.	125.	82.
103.	108.	130.	198.	288.	291.	290.	262.	201.	153.
138.	118.	96.	135.	179.	207.	242.	295.	265.	245.
259.	293.	368.	412.	454.	425.	361.	296.	284.	284.
373.	578.	753.	834.	862.	737.	608.	504.	557.	667.
637.	684.	583.	475.	339.	234.	175.	138.	126.	126.
104.	155.	172.	242.	266.	261.	271.	217.	212.	242.
248.	268.	285.	238.	191.	137.	131.	103.	101.	103.
102.	151.	188.	282.	322.	382.	460.	418.	439.	415.
401.	320.	279.	249.	194.	197.	268.	402.	448.	477.
387.	358.	275.	198.	169.	145.	141.	168.	205.	240.
253.	183.	161.	150.	119.	102.	114.	105.	125.	107.
103.	96.	119.	116.	119.	103.	91.	76.	92.	78.
71.	83.	105.	114.	129.	151.	297.	333.	444.	520.
437.	390.	327.	250.	201.	193.	166.	186.	251.	271.
299.	378.	357.	378.	364.	286.	234.	166.	133.	109.
88.	74.	69.	77.	61.	77.	75.	80.	79.	91.
105.	175.	186.	169.	175.	137.	125.	134.	123.	112.
117.	117.	141.	170.	118.	116.	90.	102.	84.	55.
82.	56.	40.	47.	63.	47.	55.	56.	64.	45.
67.	56.	68.	44.	58.	44.	53.	47.	50.	51.

68.	56.	63.	64.	68.	80.	127.	171.	164.	168.
142.	117.	97.	89.	71.	75.	81.	96.	96.	96.
112.	108.	103.	85.	99.	80.	80.	87.	83.	85.
106.	124.	171.	233.	240.	264.	242.	239.	190.	182.
135.	139.	109.	126.	130.	166.	200.	186.	167.	166.
112.	117.	111.	89.	98.	118.	120.	153.	136.	144.
131.	106.	100.	80.	79.	96.	78.	83.	90.	105.
103.	89.	101.	103.	105.	131.	135.	161.	234.	267.
397.	543.	847.	1193.	1364.	1387.	1245.	1199.	1050.	892.
725.	590.	466.	398.	334.	299.	239.	197.	154.	149.
139.	109.	85.	112.	98.	110.	90.	95.	87.	84.
82.	68.	68.	74.	49.	76.	59.	60.	55.	52.
70.	53.	54.	60.	52.	54.	88.	69.	77.	95.
74.	135.	138.	147.	217.	239.	278.	350.	360.	330.
320.	246.	210.	156.	146.	142.	147.	160.	133.	137.
157.	122.	115.	112.	96.	100.	111.	138.	178.	276.
283.	325.	369.	356.	291.	272.	241.	235.	218.	292.
367.	628.	638.	704.	841.	809.	733.	671.	568.	430.
375.	277.	297.	220.	205.	170.	156.	139.	125.	114.
120.	115.	146.	133.	127.	135.	137.	145.	127.	171.
164.	128.	128.	138.	102.	130.	113.	128.	102.	123.
148.	216.	210.	210.	201.	189.	187.	189.	174.	141.
166.	141.	155.	146.	128.	131.	87.	74.	88.	77.
67.	109.	125.	151.	144.	145.	156.	161.	128.	97.
81.	79.	76.	86.	79.	103.	119.	115.	132.	147.
181.	209.	220.	224.	238.	244.	261.	265.	244.	234.
271.	249.	258.	230.	265.	236.	221.	214.	231.	245.
310.	407.	449.	466.	490.	525.	637.	682.	598.	559.
523.	390.	332.	281.	236.	217.	220.	239.	314.	354.
486.	610.	741.	732.	714.	619.	555.	412.	316.	273.
232.	147.	122.	143.	122.	124.	144.	118.	121.	121.
99.	112.	82.	104.	92.	87.	88.	71.	62.	86.
68.	70.	69.	55.	93.	88.	87.	104.	96.	121.
100.	115.	100.	155.	164.	155.	133.	154.	128.	126.
98.	114.	92.	83.	83.	73.	87.	159.	137.	183.
210.	278.	385.	360.	352.	345.	341.	325.	230.	209.
196.	154.	162.	141.	146.	178.	239.	262.	265.	254.
270.	267.	236.	214.	203.	229.	323.	354.	356.	342.
351.	325.	242.	253.	235.	213.	308.	277.	251.	210.
205.	170.	149.	119.	106.	96.	98.	81.	69.	82.
80.	100.	100.	112.	91.	102.	112.	100.	122.	83.
84.	87.	82.	82.	71.	81.	60.	75.	69.	80.
88.	81.	94.	118.	111.	171.	187.	273.	353.	357.
327.	318.	317.	305.	259.	197.	198.	165.	172.	143.
127.	90.	90.	77.	81.	73.	65.	57.	87.	81.
81.	100.	88.	129.	150.	176.	207.	188.	197.	182.
203.	213.	204.	202.	176.	183.	166.	195.	214.	240.
265.	297.	309.	287.	258.	247.	178.	177.	178.	145.
106.	104.	89.	77.	61.	73.	66.	66.	81.	54.
71.	57.	70.	75.	91.	81.	95.	135.	105.	111.
115.	126.	120.	118.	98.	107.	85.	111.	96.	135.
152.	133.	142.	119.	137.	130.	134.	187.	177.	220.
182.	162.	146.	161.	142.	117.	89.	86.	83.	72.
62.	69.	81.	72.	92.	107.	100.	132.	126.	134.
111.	135.	140.	143.	172.	167.	172.	164.	166.	170.
162.	146.	128.	119.	116.	99.	112.	112.	93.	112.
84.	96.	110.	143.	137.	163.	191.	213.	157.	179.
193.	160.	141.	131.	95.	84.	75.	78.	87.	97.
65.	69.	73.	79.	76.	84.	102.	86.	76.	82.
79.	65.	84.	77.	83.	87.	89.	115.	93.	106.
71.	77.	72.	81.	66.	67.	59.	66.	66.	81.
75.	66.	63.	54.	59.	80.	81.	98.	79.	82.
84.	93.	70.	57.	44.	67.	57.	43.	42.	37.
46.	52.	56.	41.	49.	56.	53.	46.	42.	57.
58.	53.	49.	63.	46.	63.	51.	52.	64.	75.
80.	120.	130.	123.	129.	127.	117.	115.	83.	88.
85.	50.	67.	57.	57.	66.	51.	47.	55.	51.
60.	53.	59.	63.	61.	70.	68.	74.	76.	86.
81.	82.	91.	99.	113.	138.	114.	118.	125.	122.

142.	130.	114.	94.	104.	94.	88.	81.	79.	71.
65.	65.	63.	77.	64.	88.	70.	99.	111.	115.
115.	98.	103.	103.	104.	103.	89.	86.	107.	110.
108.	137.	116.	122.	111.	129.	152.	134.	135.	139.
124.	122.	110.	97.	93.	132.	96.	120.	136.	129.
123.	148.	118.	114.	109.	140.	133.	140.	157.	111.
108.	116.	112.	114.	91.	98.	79.	80.	61.	67.
68.	65.	76.	77.	103.	112.	104.	95.	113.	89.
73.	87.	72.	78.	76.	71.	70.	57.	67.	83.
92.	95.	76.	93.	96.	84.	98.	89.	73.	58.
64.	59.	50.	65.	62.	52.	46.	55.	58.	71.
55.	79.	75.	76.	75.	79.	60.	76.	74.	80.
69.	84.	63.	72.	92.	117.	120.	157.	143.	118.
128.	102.	108.	138.	101.	65.	79.	72.	64.	55.
57.	54.	60.	52.	54.	44.	41.	51.	49.	58.
45.	58.	58.	72.	62.	79.	90.	66.	59.	86.
85.	103.	91.	105.	102.	139.	142.	132.	119.	116.
145.	116.	116.	112.	103.	125.	114.	110.	152.	146.
172.	194.	216.	242.	235.	190.	171.	184.	202.	236.
228.	249.	196.	145.	135.	153.	128.	170.	156.	159.
167.	179.	186.	197.	184.	160.	165.	152.	129.	123.
154.	116.	112.	108.	85.	87.	79.	76.	60.	64.
83.	75.	82.	53.	56.	74.	68.	77.	83.	82.
106.	94.	84.	116.	117.	118.	95.	91.	97.	86.
96.	83.	84.	83.	75.	91.	75.	88.	81.	75.
82.	61.	80.	79.	83.	91.	82.	105.	90.	108.
109.	129.	116.	131.	145.	175.	226.	219.	214.	192.
155.	132.	135.	139.	128.	102.	103.	80.	74.	71.
86.	54.	64.	53.	58.	67.	77.	70.	87.	74.
106.	93.	92.	78.	83.	92.	68.	79.	82.	75.
88.	79.	92.	106.	143.	159.	188.	131.	175.	137.
128.	115.	140.	133.	121.	98.	92.	98.	88.	88.
68.	91.	85.	84.	115.	106.	112.	109.	79.	101.
83.	81.	84.	85.	78.	71.	83.	80.	75.	83.
103.	106.	110.	98.	100.	77.	89.	87.	95.	96.
77.	73.	96.	106.	92.	117.	149.	116.	130.	131.
108.	101.	110.	112.	127.	129.	107.	102.	90.	91.
89.	80.	89.	70.	94.	106.	89.	94.	70.	65.
71.	72.	67.	77.	76.	60.	57.	51.	54.	75.
46.	62.	92.	83.	91.	89.	94.	86.	82.	104.
84.	94.	90.	91.	75.	86.	72.	74.	86.	73.
60.	68.	64.	73.	76.	92.	89.	91.	124.	126.
111.	99.	97.	106.	77.	90.	116.	111.	136.	113.
108.	79.	88.	70.	103.	94.	89.	94.	77.	100.
117.	107.	116.	125.	93.	86.	93.	73.	80.	88.
95.	86.	79.	89.	73.	77.	87.	74.	69.	82.
76.	74.	65.	69.	57.	68.	73.	86.	74.	92.
107.	132.	124.	132.	92.	115.	101.	101.	111.	121.
99.	92.	101.	78.	67.	72.	70.	74.	73.	74.
71.	72.	55.	50.	65.	60.	51.	64.	49.	45.
49.	47.	35.	39.	44.	48.	47.	53.	50.	48.
52.	53.	49.	42.	62.	51.	52.	64.	65.	58.
66.	72.	65.	59.	63.	53.	62.	71.	55.	69.
65.	62.	77.	63.	63.	81.	64.	77.	60.	50.
62.	67.	81.	55.	87.	76.	63.	78.	91.	95.
104.	124.	115.	105.	92.	89.	86.	89.	100.	89.
110.	117.	118.	97.	84.	86.	72.	65.	78.	86.
88.	82.	85.	63.	68.	78.	84.	89.	110.	102.
78.	77.	61.	71.	77.	88.	81.	94.	80.	109.
101.	119.	157.	147.	156.	97.	93.	75.	100.	88.
113.	113.	85.	89.	84.	75.	89.	76.	76.	86.
83.	88.	108.	124.	130.	127.	142.	100.	127.	126.
100.	135.	116.	115.	114.	109.	132.	104.	99.	97.
105.	114.	143.	116.	101.	98.	121.	121.	119.	106.
115.	104.	120.	127.	99.	97.	89.	103.	96.	78.
94.	86.	77.	83.	82.	63.	71.	71.	62.	70.
72.	60.	70.	72.	67.	71.	95.	64.	66.	69.
66.	71.	76.	85.	83.	114.	96.	103.	110.	88.
82.	74.	67.	75.	74.	77.	74.	72.	59.	70.

64.	47.	56.	49.	49.	63.	66.	66.	60.	84.
92.	91.	87.	86.	76.	75.	93.	73.	91.	66.
78.	71.	74.	61.	66.	66.	80.	79.	58.	75.
81.	76.	58.	57.	60.	48.	48.	64.	51.	45.
63.	48.	61.	57.	61.	60.	69.	49.	61.	79.
61.	87.	78.	66.	59.	63.	59.	57.	73.	77.
69.	70.	67.	67.	47.	54.	63.	71.	63.	54.
58.	73.	70.	86.	70.	69.	69.	74.	62.	53.
67.	84.	73.	79.	82.	79.	110.	110.	105.	93.
92.	95.	97.	77.	94.	86.	80.	82.	84.	78.
80.	60.	72.	66.	58.	109.	78.	83.	85.	87.
89.	72.	94.	95.	88.	143.	103.	114.	106.	89.
110.	134.	100.	121.	128.	92.	103.	99.	98.	97.
101.	107.	147.	137.	127.	104.	121.	100.	90.	94.
96.	106.	90.	124.	108.	96.	105.	69.	79.	68.
83.	87.	87.	78.	90.	76.	90.	85.	73.	63.
56.	70.	71.	62.	68.	83.	69.	80.	60.	64.
59.	53.	62.	60.	64.	61.	61.	75.	55.	62.
82.	64.	64.	94.	62.	104.	93.	79.	72.	79.
117.	124.	127.	108.	125.	115.	93.	83.	88.	96.
87.	99.	104.	93.	83.	79.	80.	88.	66.	71.
76.	68.	76.	88.	86.	85.	98.	83.	101.	90.
97.	89.	95.	74.	75.	72.	65.	90.	83.	88.
81.	117.	82.	95.	86.	62.	58.	76.	76.	67.
78.	70.	75.	85.	90.	67.	84.	89.	93.	99.
106.	117.	112.	115.	111.	113.	96.	86.	90.	87.
81.	81.	105.	92.	85.	82.	77.	121.	116.	101.
92.	88.	90.	86.	78.	76.	80.	81.	72.	81.
73.	86.	91.	98.	88.	91.	70.	102.	98.	111.
105.	97.	105.	115.	95.	113.	96.	84.	89.	86.
112.	99.	114.	107.	106.	104.	101.	87.	92.	95.
89.	81.	76.	95.	94.	102.	81.	107.	97.	85.
75.	74.	73.	73.	75.	66.	78.	80.	83.	74.
73.	75.	73.	87.	86.	87.	71.	83.	100.	104.
90.	111.	84.	78.	71.	81.	73.	83.	83.	92.
88.	118.	103.	140.	149.	143.	121.	161.	123.	119.
100.	122.	100.	111.	113.	121.	116.	117.	130.	135.
129.	94.	127.	107.	119.	118.	119.	125.	117.	111.
114.									

Appendix P-8: step-intensity data of the 70 wt% olivine mixture of Ol+Py

16.00 .05 136.00 70% olivine mixture

114.	125.	115.	132.	115.	121.	106.	109.	95.	123.
127.	124.	118.	103.	109.	109.	126.	105.	134.	135.
142.	153.	172.	205.	280.	443.	604.	682.	630.	546.
441.	311.	245.	175.	153.	139.	115.	120.	123.	109.
114.	120.	107.	125.	118.	125.	104.	101.	106.	111.
112.	139.	109.	111.	102.	108.	91.	112.	117.	112.
103.	131.	98.	118.	121.	118.	119.	102.	120.	94.
102.	114.	104.	131.	93.	107.	110.	126.	139.	150.
160.	155.	130.	133.	127.	151.	112.	114.	98.	103.
122.	120.	121.	120.	138.	117.	91.	94.	93.	86.
90.	109.	102.	88.	93.	93.	101.	88.	88.	102.
84.	113.	101.	99.	79.	88.	106.	100.	100.	118.
95.	110.	105.	76.	115.	98.	108.	107.	130.	135.
175.	174.	255.	361.	471.	746.	1100.	1424.	1505.	1415.
1203.	870.	560.	318.	271.	202.	161.	139.	122.	112.
126.	166.	149.	164.	204.	267.	390.	491.	597.	589.
488.	386.	292.	212.	136.	157.	153.	155.	161.	140.
111.	108.	100.	100.	102.	103.	108.	93.	103.	98.
112.	123.	132.	138.	149.	191.	270.	444.	647.	794.
854.	865.	744.	639.	518.	382.	287.	183.	163.	125.
110.	96.	110.	84.	96.	103.	100.	102.	130.	128.
141.	177.	199.	246.	285.	297.	251.	240.	186.	127.
134.	91.	112.	87.	107.	112.	109.	132.	122.	189.
277.	371.	500.	577.	565.	507.	421.	333.	235.	168.
115.	117.	102.	95.	94.	91.	107.	89.	70.	92.
92.	99.	105.	96.	94.	115.	104.	110.	104.	108.
117.	117.	95.	108.	133.	114.	128.	163.	183.	185.
261.	311.	425.	558.	700.	931.	1343.	1780.	2123.	2204.
2045.	1543.	1113.	741.	533.	618.	771.	738.	720.	518.
444.	340.	225.	243.	231.	265.	340.	533.	630.	768.
743.	651.	494.	363.	253.	249.	182.	143.	128.	131.
127.	136.	130.	147.	141.	121.	139.	138.	176.	192.
219.	300.	417.	623.	1066.	1635.	2013.	1997.	1773.	1312.
860.	541.	366.	254.	195.	164.	149.	138.	111.	92.
114.	103.	103.	109.	95.	76.	87.	74.	93.	82.
94.	75.	91.	72.	74.	113.	85.	70.	91.	87.
94.	98.	99.	105.	86.	93.	102.	100.	113.	87.
129.	123.	141.	170.	211.	210.	231.	250.	338.	457.
559.	637.	669.	596.	503.	475.	506.	531.	712.	958.
1363.	1840.	2500.	3142.	3426.	3295.	2819.	2275.	1527.	1050.
706.	541.	424.	413.	432.	506.	650.	973.	1577.	2389.
2703.	2703.	2352.	1728.	1375.	897.	614.	402.	267.	242.
180.	168.	147.	141.	121.	114.	122.	114.	113.	122.
99.	96.	132.	141.	146.	172.	178.	141.	132.	132.
165.	148.	171.	248.	342.	432.	438.	403.	330.	267.
237.	181.	171.	166.	208.	282.	311.	374.	397.	388.
317.	323.	349.	430.	445.	443.	392.	390.	321.	393.
459.	669.	947.	1115.	1236.	1213.	983.	824.	806.	921.
999.	967.	909.	779.	520.	400.	276.	190.	160.	176.
126.	150.	150.	207.	253.	240.	270.	264.	235.	235.
268.	245.	277.	240.	212.	189.	157.	143.	129.	148.
152.	178.	222.	345.	404.	530.	611.	642.	595.	496.
425.	367.	323.	284.	198.	224.	304.	336.	439.	422.
408.	372.	291.	207.	190.	168.	155.	182.	189.	234.
215.	229.	181.	148.	142.	130.	161.	152.	136.	140.
165.	156.	118.	149.	119.	110.	112.	102.	96.	109.
105.	110.	112.	117.	114.	176.	209.	334.	429.	503.
504.	564.	505.	380.	315.	267.	207.	198.	228.	245.
277.	306.	294.	316.	270.	283.	209.	163.	157.	137.
109.	83.	85.	99.	80.	77.	67.	69.	97.	99.
127.	142.	212.	227.	193.	179.	158.	134.	135.	159.
171.	162.	191.	191.	165.	143.	132.	120.	118.	99.
95.	92.	72.	78.	71.	62.	69.	69.	62.	86.
71.	57.	58.	72.	59.	74.	66.	67.	65.	67.

70.	78.	91.	70.	102.	120.	185.	203.	219.	246.
220.	179.	178.	146.	118.	123.	129.	99.	127.	136.
143.	150.	103.	120.	116.	106.	102.	93.	84.	112.
106.	137.	185.	200.	238.	233.	255.	269.	221.	167.
175.	135.	131.	148.	152.	201.	220.	212.	232.	221.
169.	157.	144.	144.	120.	150.	149.	190.	204.	182.
186.	159.	128.	149.	104.	94.	104.	114.	106.	109.
115.	114.	151.	154.	143.	162.	187.	219.	261.	355.
443.	656.	1010.	1406.	1822.	1908.	1892.	1747.	1560.	1350.
1198.	944.	805.	661.	521.	471.	366.	334.	256.	206.
215.	175.	127.	148.	115.	130.	126.	130.	105.	101.
106.	97.	102.	79.	81.	81.	79.	80.	110.	72.
79.	84.	66.	63.	76.	85.	93.	80.	100.	99.
131.	120.	144.	171.	201.	327.	363.	438.	502.	486.
448.	359.	324.	222.	196.	161.	177.	191.	167.	194.
176.	116.	167.	121.	125.	144.	156.	154.	232.	283.
370.	464.	488.	505.	457.	399.	339.	318.	298.	332.
384.	449.	626.	778.	899.	937.	919.	830.	658.	636.
518.	373.	339.	268.	252.	179.	174.	172.	160.	183.
148.	161.	180.	152.	158.	154.	178.	224.	217.	233.
208.	182.	176.	169.	159.	176.	111.	162.	165.	180.
225.	254.	310.	317.	326.	329.	320.	257.	265.	250.
191.	198.	158.	164.	166.	150.	132.	99.	106.	85.
103.	113.	129.	167.	158.	139.	158.	151.	128.	112.
114.	115.	108.	104.	103.	128.	145.	133.	164.	159.
178.	188.	251.	268.	240.	263.	312.	286.	318.	317.
324.	359.	331.	325.	318.	330.	315.	342.	343.	337.
401.	457.	487.	614.	628.	698.	813.	992.	984.	916.
826.	719.	566.	477.	434.	295.	300.	290.	344.	375.
528.	678.	1146.	1187.	1074.	1092.	1020.	807.	596.	501.
361.	283.	187.	167.	182.	166.	173.	165.	154.	165.
129.	118.	131.	124.	135.	106.	102.	79.	97.	96.
94.	76.	70.	84.	92.	91.	91.	115.	130.	122.
115.	139.	160.	180.	205.	212.	225.	202.	178.	158.
130.	117.	123.	106.	93.	104.	123.	127.	148.	199.
185.	283.	285.	366.	411.	318.	318.	280.	280.	215.
208.	172.	197.	143.	175.	199.	262.	265.	287.	293.
309.	303.	289.	277.	266.	324.	403.	470.	563.	556.
487.	453.	422.	357.	320.	333.	355.	396.	383.	302.
301.	267.	217.	170.	147.	121.	136.	98.	109.	92.
136.	115.	137.	112.	146.	126.	150.	132.	140.	121.
109.	110.	97.	101.	96.	98.	101.	88.	103.	100.
126.	123.	112.	135.	150.	187.	293.	384.	426.	492.
514.	456.	512.	462.	399.	331.	308.	241.	207.	155.
165.	136.	97.	91.	107.	92.	84.	80.	90.	86.
102.	95.	116.	104.	157.	183.	210.	192.	210.	211.
209.	209.	216.	242.	228.	195.	210.	211.	259.	304.
354.	386.	382.	395.	351.	329.	308.	285.	243.	204.
168.	139.	109.	96.	95.	88.	68.	94.	79.	77.
77.	69.	91.	90.	123.	121.	133.	167.	181.	179.
151.	147.	138.	134.	123.	124.	119.	116.	110.	136.
137.	128.	159.	157.	144.	154.	160.	164.	188.	233.
221.	192.	189.	182.	153.	152.	114.	99.	100.	81.
80.	95.	90.	91.	127.	115.	129.	150.	145.	136.
143.	169.	172.	190.	183.	182.	183.	192.	193.	219.
209.	185.	179.	151.	157.	158.	126.	149.	121.	131.
145.	146.	152.	165.	161.	197.	219.	218.	220.	221.
186.	200.	195.	170.	148.	133.	125.	120.	101.	107.
82.	89.	96.	76.	116.	101.	107.	102.	94.	91.
117.	117.	107.	114.	110.	109.	142.	137.	155.	123.
117.	116.	96.	137.	102.	94.	66.	86.	98.	91.
92.	71.	77.	83.	111.	84.	103.	91.	92.	82.
84.	72.	86.	83.	66.	65.	65.	67.	55.	57.
53.	60.	70.	64.	58.	56.	61.	55.	66.	84.
58.	57.	60.	57.	82.	65.	65.	71.	79.	94.
104.	147.	140.	167.	169.	171.	152.	124.	130.	91.
99.	106.	84.	76.	84.	67.	67.	65.	80.	58.
70.	58.	76.	73.	66.	82.	89.	89.	89.	90.
110.	102.	125.	127.	169.	153.	142.	120.	153.	146.

194.	211.	176.	159.	143.	151.	129.	125.	115.	123.
110.	118.	87.	99.	113.	108.	122.	110.	160.	178.
174.	166.	145.	165.	152.	126.	118.	108.	129.	133.
133.	178.	146.	141.	140.	149.	160.	179.	172.	144.
118.	132.	121.	128.	129.	161.	160.	176.	178.	193.
178.	163.	178.	180.	178.	198.	191.	213.	204.	170.
146.	143.	142.	141.	151.	131.	101.	107.	104.	84.
94.	89.	96.	118.	140.	132.	142.	149.	120.	113.
132.	122.	114.	114.	84.	83.	87.	91.	91.	91.
111.	122.	147.	131.	130.	102.	105.	114.	98.	108.
101.	81.	88.	61.	70.	72.	59.	55.	72.	77.
76.	93.	88.	108.	91.	81.	103.	84.	80.	83.
79.	79.	74.	88.	112.	131.	182.	192.	211.	187.
164.	123.	142.	125.	137.	107.	106.	100.	92.	95.
71.	68.	63.	58.	69.	61.	61.	66.	56.	62.
62.	67.	72.	85.	83.	88.	91.	95.	101.	94.
107.	107.	152.	130.	166.	167.	184.	187.	169.	154.
149.	155.	170.	168.	159.	174.	163.	162.	182.	211.
215.	223.	232.	265.	292.	233.	246.	223.	228.	248.
242.	253.	223.	214.	158.	188.	155.	172.	159.	181.
192.	197.	201.	204.	173.	182.	178.	171.	155.	168.
152.	127.	128.	125.	119.	96.	87.	84.	76.	91.
86.	78.	93.	93.	80.	92.	99.	109.	101.	93.
122.	117.	109.	123.	123.	112.	117.	116.	115.	111.
115.	116.	92.	100.	81.	110.	115.	78.	88.	94.
85.	85.	81.	94.	111.	98.	102.	106.	101.	105.
154.	132.	124.	148.	170.	210.	298.	321.	307.	284.
252.	218.	199.	189.	193.	187.	138.	132.	118.	82.
107.	79.	84.	81.	84.	92.	83.	107.	90.	98.
96.	95.	88.	101.	85.	100.	101.	109.	97.	105.
104.	118.	129.	143.	147.	195.	207.	217.	195.	183.
173.	164.	161.	169.	151.	138.	121.	124.	122.	84.
92.	100.	119.	97.	111.	130.	142.	121.	119.	106.
99.	104.	119.	112.	108.	127.	83.	94.	87.	94.
120.	95.	112.	107.	114.	88.	97.	106.	104.	120.
143.	110.	122.	115.	126.	108.	155.	187.	209.	177.
147.	142.	127.	152.	147.	171.	158.	111.	126.	113.
116.	121.	99.	121.	120.	118.	110.	119.	120.	103.
102.	99.	88.	112.	94.	90.	93.	76.	69.	83.
75.	70.	89.	102.	107.	100.	115.	98.	121.	140.
141.	140.	116.	116.	110.	108.	107.	115.	105.	94.
113.	85.	96.	79.	104.	112.	112.	133.	138.	163.
152.	157.	123.	127.	109.	128.	139.	149.	146.	184.
134.	123.	102.	123.	103.	101.	122.	104.	112.	116.
129.	155.	150.	172.	143.	127.	114.	112.	107.	119.
135.	131.	128.	115.	100.	89.	118.	110.	107.	99.
79.	101.	96.	100.	82.	95.	99.	85.	106.	111.
122.	143.	134.	109.	112.	123.	125.	128.	129.	123.
135.	122.	111.	100.	84.	124.	84.	100.	80.	92.
80.	88.	97.	73.	88.	65.	58.	72.	64.	79.
68.	59.	55.	74.	44.	60.	69.	80.	77.	77.
63.	66.	56.	50.	88.	66.	72.	79.	94.	94.
103.	99.	103.	90.	84.	95.	99.	85.	114.	104.
101.	93.	85.	89.	92.	84.	71.	84.	68.	80.
68.	96.	69.	86.	92.	100.	117.	104.	109.	113.
136.	164.	154.	120.	131.	120.	125.	115.	125.	127.
122.	133.	149.	168.	123.	106.	90.	92.	102.	96.
104.	126.	88.	104.	106.	111.	119.	122.	143.	132.
141.	107.	108.	129.	99.	123.	139.	134.	137.	137.
147.	171.	183.	184.	186.	147.	141.	122.	109.	139.
134.	147.	160.	126.	116.	93.	81.	116.	109.	119.
116.	112.	113.	147.	151.	143.	118.	146.	159.	135.
159.	148.	129.	126.	121.	125.	129.	132.	108.	123.
112.	120.	133.	131.	149.	138.	128.	164.	127.	147.
139.	129.	141.	161.	138.	128.	119.	127.	117.	114.
117.	123.	105.	110.	82.	81.	73.	92.	87.	86.
97.	91.	103.	82.	85.	92.	87.	84.	100.	79.
106.	97.	113.	114.	142.	146.	142.	172.	119.	131.
109.	99.	101.	99.	117.	108.	110.	111.	80.	68.

90.	67.	70.	82.	80.	66.	77.	70.	94.	94.
94.	116.	117.	107.	99.	98.	99.	87.	112.	123.
98.	94.	98.	80.	75.	82.	107.	90.	88.	73.
92.	92.	86.	76.	71.	76.	78.	58.	100.	76.
72.	48.	81.	67.	64.	69.	68.	67.	80.	79.
62.	59.	76.	93.	75.	74.	78.	76.	90.	89.
79.	97.	81.	72.	82.	82.	76.	62.	86.	71.
87.	90.	76.	92.	94.	100.	86.	77.	76.	78.
89.	80.	105.	95.	111.	113.	105.	135.	138.	132.
127.	120.	127.	114.	127.	120.	121.	100.	129.	124.
100.	113.	91.	115.	102.	105.	101.	115.	110.	120.
110.	119.	139.	139.	134.	150.	168.	178.	164.	169.
170.	147.	166.	172.	156.	134.	158.	115.	124.	150.
149.	160.	154.	209.	185.	162.	117.	128.	130.	115.
124.	137.	126.	131.	114.	143.	129.	113.	99.	115.
96.	105.	94.	95.	93.	110.	95.	110.	84.	99.
80.	86.	81.	74.	94.	79.	93.	103.	78.	77.
75.	81.	66.	74.	63.	69.	86.	87.	88.	80.
91.	90.	106.	109.	112.	92.	106.	106.	104.	134.
147.	169.	155.	162.	153.	152.	134.	108.	121.	115.
128.	120.	126.	115.	109.	143.	107.	99.	80.	97.
103.	91.	93.	100.	106.	116.	117.	120.	129.	148.
128.	155.	141.	116.	111.	92.	119.	117.	116.	106.
152.	134.	123.	135.	123.	123.	89.	108.	100.	88.
92.	93.	103.	140.	122.	121.	110.	126.	128.	117.
152.	175.	151.	164.	137.	158.	157.	130.	135.	117.
108.	130.	129.	140.	152.	105.	136.	143.	152.	138.
99.	121.	102.	110.	100.	82.	97.	116.	113.	102.
102.	94.	118.	114.	104.	107.	112.	130.	143.	110.
154.	137.	129.	173.	158.	146.	121.	116.	121.	129.
148.	145.	145.	153.	123.	133.	113.	123.	103.	98.
94.	105.	121.	136.	115.	121.	123.	136.	113.	97.
95.	118.	87.	80.	98.	92.	94.	88.	86.	102.
100.	109.	100.	107.	104.	110.	92.	114.	92.	88.
127.	110.	106.	124.	89.	102.	105.	118.	129.	153.
125.	153.	151.	190.	202.	161.	193.	187.	145.	145.
144.	139.	151.	129.	158.	162.	171.	187.	162.	172.
175.	160.	142.	156.	155.	143.	118.	140.	141.	147.
126.									

Appendix P-9: step-intensity data of the 80 wt% olivine mixture of Ol+Py

19.00 .05 139.00 80% olivine mixture

116.	103.	115.	99.	124.	106.	101.	115.	114.	97.
102.	87.	115.	107.	110.	89.	120.	115.	125.	144.
130.	130.	126.	122.	104.	118.	115.	108.	119.	124.
116.	134.	112.	146.	118.	118.	123.	104.	103.	106.
97.	111.	93.	113.	87.	104.	99.	94.	96.	81.
111.	126.	109.	113.	114.	103.	99.	96.	101.	114.
113.	100.	93.	113.	90.	122.	109.	130.	116.	138.
181.	197.	312.	386.	506.	763.	1059.	1335.	1589.	1667.
1530.	1239.	919.	612.	429.	296.	208.	156.	133.	145.
147.	146.	153.	215.	217.	314.	405.	506.	557.	616.
589.	491.	416.	305.	242.	170.	156.	135.	123.	137.
131.	117.	114.	101.	95.	98.	94.	116.	101.	99.
121.	127.	127.	149.	174.	257.	368.	517.	696.	839.
976.	1006.	1013.	866.	728.	537.	412.	300.	200.	143.
135.	115.	127.	100.	83.	104.	109.	113.	121.	109.
113.	136.	173.	188.	196.	227.	199.	164.	170.	135.
144.	106.	108.	89.	119.	120.	91.	113.	119.	131.
206.	271.	357.	413.	410.	397.	367.	249.	219.	169.
138.	105.	98.	85.	107.	94.	106.	91.	112.	94.
105.	98.	114.	100.	118.	87.	95.	102.	90.	112.
116.	110.	116.	110.	125.	127.	129.	145.	190.	191.
255.	290.	400.	524.	715.	932.	1151.	1337.	1517.	1629.
1630.	1392.	1072.	813.	584.	540.	511.	542.	450.	446.
381.	306.	258.	207.	215.	222.	300.	397.	464.	501.
525.	457.	479.	353.	309.	170.	128.	135.	123.	146.
131.	112.	119.	137.	141.	137.	187.	180.	162.	212.
240.	357.	545.	884.	1351.	1685.	2120.	2212.	2154.	1770.
1264.	860.	566.	380.	261.	176.	174.	166.	126.	141.
125.	146.	93.	115.	114.	92.	88.	94.	93.	92.
98.	89.	86.	93.	77.	103.	98.	90.	96.	96.
80.	86.	100.	77.	115.	101.	122.	119.	103.	89.
126.	130.	148.	177.	183.	195.	203.	244.	290.	371.
375.	433.	538.	522.	525.	435.	489.	536.	700.	834.
1174.	1854.	2348.	2693.	3130.	3010.	2866.	2355.	1926.	1274.
927.	651.	533.	455.	480.	607.	804.	1224.	1881.	2422.
2904.	2916.	2740.	2397.	1819.	1259.	901.	601.	437.	326.
271.	195.	185.	161.	129.	157.	121.	100.	116.	124.
122.	117.	143.	138.	166.	177.	202.	185.	183.	193.
184.	200.	231.	319.	337.	434.	473.	463.	436.	345.
275.	234.	216.	221.	302.	298.	383.	415.	447.	436.
453.	397.	382.	375.	359.	408.	357.	336.	332.	448.
592.	811.	1038.	1392.	1431.	1443.	1346.	1213.	1179.	1044.
1113.	1151.	1067.	920.	710.	582.	384.	243.	208.	193.
163.	147.	168.	215.	221.	253.	212.	229.	227.	229.
246.	207.	220.	211.	221.	187.	159.	124.	161.	160.
154.	212.	314.	371.	499.	582.	621.	648.	653.	572.
480.	418.	335.	247.	246.	219.	221.	248.	270.	309.
300.	295.	233.	186.	178.	147.	142.	158.	176.	199.
211.	226.	191.	161.	147.	128.	143.	153.	169.	161.
173.	170.	164.	140.	125.	111.	118.	119.	104.	95.
116.	103.	108.	114.	147.	179.	206.	291.	393.	422.
443.	438.	413.	385.	284.	240.	227.	184.	196.	211.
272.	275.	279.	285.	243.	220.	182.	189.	152.	119.
119.	94.	87.	84.	83.	83.	88.	78.	89.	110.
132.	144.	158.	159.	162.	175.	130.	152.	158.	229.
174.	201.	253.	189.	188.	184.	181.	133.	119.	95.
86.	92.	80.	84.	71.	67.	76.	81.	66.	92.
66.	65.	86.	72.	66.	81.	77.	81.	85.	81.
91.	74.	120.	90.	106.	161.	187.	216.	252.	238.
262.	246.	196.	190.	146.	134.	111.	119.	137.	122.
137.	120.	128.	116.	103.	100.	96.	103.	98.	117.
119.	129.	159.	157.	180.	206.	230.	191.	176.	179.
146.	141.	143.	147.	169.	201.	257.	249.	247.	217.
203.	182.	180.	163.	157.	201.	195.	233.	228.	224.

225.	186.	174.	148.	150.	115.	129.	105.	127.	140.
118.	129.	142.	162.	162.	205.	221.	267.	337.	398.
610.	908.	1299.	1614.	2028.	2296.	2268.	2041.	1962.	1637.
1423.	1250.	1020.	846.	690.	571.	458.	408.	329.	287.
262.	210.	162.	159.	140.	126.	142.	141.	93.	127.
100.	102.	104.	108.	87.	93.	92.	82.	94.	83.
76.	87.	82.	81.	93.	94.	101.	98.	112.	131.
133.	148.	170.	238.	305.	384.	419.	502.	500.	534.
492.	360.	330.	257.	215.	178.	163.	171.	190.	192.
137.	162.	150.	126.	160.	136.	157.	242.	291.	373.
470.	486.	554.	541.	522.	461.	385.	350.	330.	351.
417.	483.	635.	758.	853.	937.	903.	862.	751.	668.
578.	452.	382.	273.	232.	224.	166.	188.	207.	189.
181.	181.	165.	186.	188.	201.	232.	236.	239.	259.
226.	213.	187.	168.	149.	162.	173.	163.	179.	216.
289.	320.	366.	368.	382.	363.	315.	301.	298.	242.
226.	197.	188.	170.	157.	144.	111.	101.	116.	103.
112.	129.	135.	146.	143.	158.	137.	140.	143.	111.
111.	111.	104.	112.	128.	143.	150.	157.	182.	166.
175.	199.	208.	197.	218.	249.	243.	260.	289.	341.
340.	365.	411.	391.	368.	365.	394.	365.	399.	414.
460.	514.	588.	653.	762.	959.	977.	1023.	1051.	1038.
949.	785.	688.	645.	471.	389.	393.	402.	393.	499.
666.	952.	1055.	1109.	1151.	1080.	1017.	920.	688.	511.
432.	384.	255.	230.	220.	205.	192.	217.	169.	153.
149.	170.	150.	130.	140.	100.	144.	106.	109.	97.
98.	102.	95.	90.	94.	114.	92.	101.	118.	146.
135.	184.	158.	195.	199.	205.	225.	210.	196.	176.
157.	162.	123.	114.	107.	106.	129.	128.	145.	160.
185.	217.	253.	281.	262.	272.	234.	267.	210.	217.
176.	144.	153.	184.	156.	189.	206.	207.	261.	262.
245.	267.	306.	293.	330.	424.	514.	569.	620.	573.
632.	534.	518.	466.	446.	468.	447.	403.	384.	342.
313.	304.	208.	202.	168.	128.	114.	125.	116.	115.
129.	125.	154.	150.	147.	165.	154.	167.	140.	148.
124.	148.	122.	115.	123.	96.	116.	129.	107.	136.
131.	159.	148.	172.	196.	270.	385.	496.	619.	638.
658.	627.	577.	545.	538.	421.	340.	304.	270.	204.
216.	150.	139.	103.	111.	105.	93.	107.	102.	90.
88.	82.	125.	136.	144.	153.	164.	156.	184.	166.
192.	201.	201.	203.	221.	202.	210.	243.	316.	334.
380.	458.	445.	430.	429.	389.	340.	295.	274.	245.
211.	171.	126.	115.	122.	111.	86.	82.	84.	94.
81.	87.	101.	99.	140.	162.	175.	163.	196.	191.
201.	190.	155.	170.	110.	140.	132.	120.	107.	117.
135.	128.	138.	148.	122.	119.	123.	136.	154.	159.
196.	189.	153.	161.	138.	132.	127.	99.	91.	102.
99.	85.	94.	120.	133.	127.	167.	167.	175.	179.
138.	170.	173.	153.	143.	178.	148.	194.	199.	195.
206.	216.	188.	178.	170.	157.	155.	167.	151.	152.
148.	166.	172.	189.	195.	218.	234.	225.	206.	203.
225.	190.	211.	168.	187.	150.	125.	124.	112.	92.
119.	97.	83.	125.	115.	109.	115.	112.	91.	114.
124.	137.	106.	118.	128.	139.	169.	158.	164.	158.
149.	136.	115.	108.	114.	97.	84.	106.	99.	100.
83.	75.	76.	108.	91.	95.	122.	106.	89.	95.
89.	90.	87.	64.	107.	74.	114.	86.	71.	68.
65.	64.	66.	69.	51.	59.	71.	68.	58.	56.
65.	61.	60.	79.	64.	74.	80.	79.	92.	101.
127.	161.	191.	195.	219.	224.	194.	164.	171.	136.
121.	126.	89.	83.	82.	70.	73.	80.	76.	84.
62.	81.	71.	85.	94.	93.	82.	98.	134.	110.
123.	114.	146.	146.	159.	175.	158.	150.	194.	212.
229.	207.	203.	177.	209.	196.	185.	175.	159.	129.
121.	123.	118.	131.	126.	119.	130.	142.	170.	198.
212.	195.	181.	194.	191.	163.	155.	163.	154.	150.
149.	168.	161.	175.	153.	164.	175.	148.	163.	191.
173.	131.	127.	135.	155.	154.	183.	222.	191.	222.
216.	224.	230.	207.	231.	229.	236.	256.	236.	216.

213.	178.	187.	177.	133.	147.	118.	104.	96.	100.
105.	114.	101.	117.	135.	156.	174.	182.	177.	156.
137.	159.	146.	119.	104.	118.	113.	111.	127.	137.
139.	145.	175.	156.	145.	121.	137.	119.	115.	120.
104.	109.	79.	72.	66.	82.	69.	76.	69.	78.
87.	91.	133.	135.	110.	106.	102.	107.	110.	100.
118.	104.	126.	128.	146.	186.	224.	227.	259.	224.
227.	206.	190.	187.	146.	142.	129.	101.	93.	86.
95.	62.	82.	76.	68.	85.	77.	82.	81.	71.
77.	97.	84.	76.	101.	102.	97.	111.	117.	120.
142.	157.	141.	162.	191.	200.	195.	216.	228.	208.
225.	219.	184.	212.	190.	199.	169.	218.	231.	224.
231.	213.	237.	268.	240.	230.	230.	222.	235.	227.
207.	230.	212.	194.	177.	164.	157.	165.	161.	160.
185.	213.	191.	176.	205.	173.	185.	175.	158.	152.
166.	152.	157.	127.	104.	91.	113.	101.	96.	113.
98.	95.	84.	82.	86.	97.	108.	100.	118.	122.
105.	128.	115.	140.	125.	133.	127.	112.	100.	107.
125.	95.	110.	98.	95.	91.	108.	94.	107.	102.
96.	87.	98.	94.	107.	118.	106.	115.	110.	127.
136.	159.	200.	206.	223.	262.	330.	403.	371.	339.
285.	252.	250.	262.	243.	214.	184.	152.	125.	112.
106.	96.	109.	108.	81.	114.	88.	121.	90.	103.
109.	101.	116.	122.	106.	111.	122.	116.	107.	121.
133.	128.	165.	193.	214.	245.	256.	254.	253.	235.
219.	203.	185.	247.	211.	182.	157.	134.	121.	115.
110.	130.	119.	150.	157.	166.	135.	124.	127.	114.
120.	122.	138.	116.	122.	115.	114.	118.	108.	128.
125.	147.	130.	105.	108.	134.	121.	107.	132.	114.
115.	129.	133.	128.	141.	167.	202.	209.	200.	191.
173.	157.	159.	165.	189.	168.	159.	158.	134.	128.
118.	123.	127.	136.	137.	143.	146.	166.	142.	129.
110.	120.	135.	116.	113.	105.	81.	105.	98.	78.
105.	97.	92.	105.	122.	111.	129.	140.	139.	142.
171.	139.	149.	105.	109.	107.	110.	131.	104.	96.
84.	113.	85.	103.	109.	113.	116.	142.	180.	206.
176.	173.	171.	162.	150.	137.	154.	147.	158.	148.
154.	133.	123.	121.	111.	116.	128.	144.	138.	140.
155.	165.	196.	164.	162.	130.	132.	134.	126.	145.
148.	129.	135.	108.	109.	108.	110.	99.	122.	122.
114.	124.	119.	98.	100.	98.	99.	95.	111.	123.
111.	137.	164.	127.	130.	98.	123.	99.	172.	130.
122.	115.	120.	122.	92.	100.	88.	89.	113.	89.
81.	105.	101.	89.	81.	66.	76.	81.	89.	59.
79.	70.	75.	70.	80.	68.	83.	97.	76.	89.
68.	81.	71.	83.	76.	86.	118.	95.	99.	111.
108.	122.	117.	117.	97.	86.	93.	106.	124.	103.
121.	100.	108.	88.	99.	95.	98.	110.	101.	88.
94.	124.	104.	102.	106.	101.	96.	130.	151.	181.
198.	188.	163.	160.	139.	116.	121.	163.	141.	168.
166.	180.	186.	147.	153.	148.	125.	113.	130.	115.
137.	139.	124.	103.	126.	116.	134.	162.	173.	162.
167.	145.	142.	123.	146.	158.	153.	173.	152.	181.
181.	209.	240.	234.	188.	179.	161.	126.	142.	160.
150.	145.	198.	161.	141.	125.	117.	106.	131.	130.
107.	144.	139.	154.	155.	129.	138.	146.	140.	157.
157.	154.	143.	138.	145.	133.	112.	120.	138.	125.
122.	131.	143.	150.	161.	130.	141.	135.	123.	106.
122.	133.	130.	157.	165.	123.	122.	141.	133.	106.
132.	138.	123.	125.	112.	108.	116.	91.	119.	121.
108.	88.	96.	100.	115.	116.	105.	95.	113.	95.
102.	113.	151.	130.	158.	176.	157.	186.	162.	160.
119.	119.	120.	95.	164.	131.	143.	122.	125.	107.
73.	85.	107.	92.	92.	80.	84.	94.	119.	110.
135.	147.	144.	132.	135.	102.	129.	139.	95.	119.
129.	116.	132.	111.	135.	114.	108.	106.	127.	106.
96.	98.	106.	81.	82.	96.	88.	92.	88.	89.
86.	77.	79.	68.	82.	90.	84.	79.	83.	74.
80.	86.	92.	87.	92.	79.	85.	89.	104.	84.

102.	94.	81.	83.	85.	94.	88.	78.	93.	87.
91.	106.	101.	86.	102.	102.	93.	64.	83.	78.
92.	105.	99.	126.	140.	154.	126.	180.	192.	162.
142.	155.	145.	149.	136.	138.	137.	157.	136.	120.
133.	109.	114.	105.	104.	104.	112.	106.	122.	118.
106.	118.	132.	135.	150.	154.	163.	179.	179.	175.
158.	168.	193.	165.	176.	183.	182.	151.	165.	164.
181.	209.	204.	217.	203.	177.	158.	155.	142.	129.
133.	144.	147.	146.	148.	150.	126.	138.	124.	110.
108.	106.	110.	124.	125.	86.	104.	103.	90.	92.
99.	91.	89.	94.	82.	98.	102.	110.	100.	89.
78.	92.	80.	92.	73.	81.	72.	94.	111.	80.
115.	100.	112.	110.	128.	120.	122.	134.	135.	171.
221.	193.	232.	241.	164.	157.	156.	127.	156.	140.
126.	152.	148.	165.	175.	151.	134.	126.	145.	102.
127.	102.	119.	133.	130.	143.	135.	173.	179.	168.
215.	168.	163.	144.	138.	133.	118.	138.	142.	145.
176.	173.	156.	158.	138.	122.	130.	120.	126.	120.
115.	141.	151.	165.	158.	171.	139.	150.	150.	158.
182.	181.	217.	179.	181.	207.	164.	157.	123.	143.
132.	147.	152.	161.	153.	147.	163.	148.	162.	150.
143.	140.	128.	113.	137.	134.	125.	116.	126.	133.
122.	108.	109.	108.	123.	159.	144.	185.	151.	164.
155.	175.	198.	184.	156.	159.	150.	139.	149.	169.
180.	142.	153.	162.	148.	144.	152.	151.	123.	119.
130.	122.	126.	107.	134.	152.	108.	112.	110.	127.
118.	99.	103.	117.	100.	92.	93.	101.	97.	112.
86.	108.	126.	129.	121.	119.	131.	115.	121.	121.
136.	139.	129.	111.	129.	129.	132.	123.	135.	147.
156.	190.	211.	245.	251.	250.	243.	203.	178.	186.
187.	155.	160.	147.	160.	160.	179.	174.	199.	208.
198.	193.	151.	169.	193.	187.	188.	170.	164.	173.
155.	205.	220.	257.	278.	289.	302.	272.	263.	247.
203.	206.	189.	166.	179.	146.	154.	168.	194.	197.
206.	218.	170.	183.	172.	149.	168.	163.	127.	131.
103.	131.	106.	117.	97.	111.	107.	88.	105.	131.
105.	98.	94.	107.	131.	104.	95.	106.	104.	107.
99.	100.	94.	99.	105.	107.	94.	100.	120.	117.
92.									

Appendix P-10: step-intensity data of the 90 wt% olivine mixture of Ol+Py

19.00 .05 139.00 90% olivine mixture

89.	94.	97.	74.	88.	93.	86.	79.	79.	77.
84.	91.	80.	106.	91.	89.	91.	94.	84.	92.
89.	105.	100.	102.	101.	89.	94.	79.	91.	101.
91.	95.	98.	100.	95.	108.	90.	86.	88.	77.
85.	83.	81.	67.	83.	84.	91.	81.	85.	76.
101.	74.	76.	80.	77.	70.	80.	70.	90.	91.
93.	82.	87.	86.	90.	95.	87.	102.	100.	107.
136.	161.	197.	287.	406.	601.	875.	1205.	1515.	1552.
1525.	1192.	883.	564.	338.	230.	170.	166.	118.	106.
124.	109.	133.	143.	188.	208.	339.	434.	505.	575.
575.	505.	391.	248.	191.	146.	125.	100.	90.	84.
89.	91.	82.	94.	99.	78.	92.	82.	83.	81.
89.	105.	112.	117.	138.	161.	259.	365.	546.	769.
864.	958.	870.	769.	649.	483.	382.	256.	198.	154.
107.	82.	88.	99.	83.	81.	86.	94.	76.	90.
87.	96.	94.	130.	120.	119.	127.	126.	103.	104.
97.	90.	83.	76.	71.	73.	87.	92.	86.	85.
105.	145.	167.	189.	186.	203.	186.	147.	127.	115.
89.	91.	74.	86.	71.	76.	67.	80.	75.	65.
87.	84.	82.	82.	77.	73.	81.	88.	77.	77.
68.	85.	88.	87.	87.	82.	84.	117.	119.	117.
177.	213.	251.	353.	451.	615.	710.	812.	959.	895.
804.	693.	587.	404.	298.	280.	254.	236.	259.	208.
209.	184.	154.	116.	125.	137.	167.	209.	199.	231.
223.	230.	200.	185.	131.	121.	102.	116.	83.	105.
90.	97.	98.	98.	107.	97.	111.	122.	151.	181.
194.	269.	371.	599.	1023.	1473.	1870.	2073.	2023.	1708.
1300.	837.	476.	277.	213.	171.	137.	102.	109.	122.
103.	118.	76.	82.	78.	84.	87.	101.	97.	85.
82.	81.	82.	68.	68.	76.	79.	90.	87.	66.
78.	66.	69.	87.	85.	86.	83.	95.	91.	111.
83.	99.	100.	131.	159.	169.	157.	182.	205.	235.
250.	263.	278.	287.	270.	319.	325.	353.	404.	566.
689.	1128.	1587.	2092.	2402.	2557.	2425.	2084.	1623.	1021.
713.	515.	389.	364.	397.	421.	567.	948.	1393.	2012.
2553.	2775.	2569.	2228.	1697.	1240.	814.	529.	368.	271.
200.	183.	140.	151.	116.	107.	116.	103.	103.	88.
107.	79.	112.	106.	123.	132.	129.	149.	171.	136.
148.	138.	166.	230.	308.	364.	428.	409.	431.	348.
230.	200.	154.	155.	172.	231.	303.	306.	374.	347.
361.	292.	242.	243.	222.	205.	218.	241.	276.	326.
403.	645.	855.	1016.	1214.	1138.	1163.	1012.	954.	945.
949.	1000.	1009.	872.	645.	490.	323.	217.	178.	128.
107.	122.	102.	117.	133.	123.	135.	156.	115.	117.
124.	134.	142.	122.	124.	123.	88.	116.	111.	105.
126.	134.	209.	285.	414.	504.	540.	535.	532.	402.
357.	250.	185.	145.	136.	148.	141.	140.	141.	156.
155.	139.	121.	127.	101.	104.	78.	110.	105.	92.
111.	112.	103.	115.	102.	99.	103.	135.	149.	131.
150.	152.	131.	137.	89.	90.	101.	85.	97.	77.
84.	70.	82.	84.	77.	104.	130.	153.	222.	249.
317.	306.	280.	230.	218.	171.	148.	133.	117.	126.
127.	150.	139.	109.	133.	144.	137.	100.	85.	91.
65.	78.	64.	76.	65.	60.	67.	62.	80.	71.
78.	73.	89.	99.	86.	97.	92.	116.	107.	117.
147.	150.	166.	179.	178.	166.	150.	133.	106.	95.
71.	84.	50.	74.	71.	60.	45.	57.	68.	47.
43.	45.	56.	48.	55.	55.	43.	52.	41.	70.
61.	60.	70.	83.	95.	108.	165.	194.	185.	204.
218.	182.	165.	146.	120.	99.	113.	106.	109.	110.
91.	114.	95.	87.	89.	79.	85.	72.	83.	88.
93.	83.	90.	107.	119.	141.	127.	119.	125.	109.
108.	106.	97.	110.	139.	159.	177.	191.	197.	189.
177.	142.	125.	134.	107.	143.	155.	175.	184.	195.

180.	148.	141.	120.	117.	114.	69.	75.	104.	83.
102.	113.	108.	119.	136.	150.	176.	190.	281.	320.
412.	627.	958.	1338.	1620.	1792.	1802.	1626.	1559.	1361.
1155.	1026.	896.	785.	572.	511.	415.	350.	306.	240.
204.	187.	164.	120.	106.	90.	98.	91.	82.	94.
74.	78.	71.	69.	79.	72.	64.	71.	63.	74.
57.	59.	74.	65.	70.	86.	64.	80.	68.	81.
100.	125.	123.	169.	187.	279.	307.	368.	391.	426.
354.	308.	239.	185.	149.	123.	107.	100.	116.	105.
98.	102.	97.	111.	123.	127.	121.	148.	194.	273.
381.	438.	539.	473.	461.	433.	340.	286.	288.	214.
241.	264.	320.	436.	514.	590.	591.	624.	534.	440.
407.	327.	249.	210.	200.	188.	146.	145.	170.	137.
188.	168.	175.	175.	141.	188.	188.	225.	230.	217.
181.	165.	145.	148.	136.	126.	113.	127.	158.	153.
207.	261.	253.	315.	325.	301.	268.	263.	236.	196.
185.	174.	129.	107.	119.	107.	106.	90.	87.	80.
87.	88.	88.	79.	78.	96.	85.	107.	93.	61.
71.	62.	78.	99.	89.	102.	120.	139.	121.	120.
123.	117.	103.	139.	134.	142.	141.	146.	178.	211.
239.	278.	282.	294.	319.	294.	323.	292.	280.	333.
327.	427.	376.	500.	546.	609.	689.	796.	839.	822.
799.	686.	621.	460.	385.	330.	298.	284.	317.	361.
502.	738.	858.	1000.	970.	1026.	935.	769.	592.	473.
349.	286.	234.	197.	184.	184.	164.	147.	156.	160.
134.	116.	108.	97.	96.	68.	79.	96.	55.	78.
80.	75.	82.	56.	78.	74.	89.	68.	76.	61.
83.	91.	100.	148.	154.	180.	163.	209.	174.	143.
124.	116.	93.	65.	75.	86.	68.	82.	81.	88.
104.	116.	131.	121.	122.	114.	146.	128.	127.	123.
105.	117.	100.	108.	107.	111.	127.	131.	144.	146.
175.	180.	202.	222.	263.	335.	386.	440.	535.	521.
478.	486.	429.	359.	366.	348.	312.	319.	312.	281.
207.	211.	188.	151.	178.	105.	96.	110.	117.	122.
98.	95.	109.	107.	104.	103.	93.	99.	109.	109.
86.	100.	108.	96.	111.	85.	78.	72.	91.	105.
123.	127.	115.	140.	163.	180.	253.	390.	419.	445.
499.	538.	499.	451.	420.	357.	308.	304.	203.	207.
132.	127.	111.	99.	65.	81.	81.	75.	61.	70.
90.	73.	85.	76.	83.	92.	76.	92.	111.	95.
118.	114.	119.	106.	120.	129.	141.	170.	238.	284.
290.	372.	332.	318.	338.	335.	302.	242.	205.	199.
182.	147.	114.	98.	86.	78.	85.	72.	74.	69.
59.	71.	74.	72.	83.	120.	148.	124.	154.	132.
151.	136.	138.	112.	115.	101.	95.	103.	71.	92.
74.	62.	64.	76.	84.	86.	68.	71.	87.	88.
100.	97.	96.	82.	84.	72.	79.	77.	82.	82.
93.	70.	88.	86.	106.	103.	115.	113.	114.	125.
116.	110.	124.	106.	104.	105.	93.	124.	142.	157.
134.	155.	142.	131.	142.	108.	132.	124.	100.	121.
128.	108.	115.	119.	133.	161.	149.	146.	137.	131.
157.	136.	154.	143.	120.	128.	95.	90.	104.	78.
91.	105.	98.	64.	70.	104.	103.	96.	92.	86.
88.	97.	86.	96.	106.	114.	123.	127.	117.	121.
118.	102.	84.	87.	87.	70.	65.	61.	64.	72.
70.	49.	50.	70.	63.	64.	50.	56.	54.	73.
62.	50.	64.	50.	52.	45.	56.	59.	48.	58.
62.	46.	51.	45.	48.	37.	55.	51.	38.	47.
46.	38.	43.	52.	40.	52.	51.	63.	74.	81.
108.	106.	128.	181.	166.	144.	125.	153.	113.	120.
97.	92.	82.	64.	69.	50.	57.	53.	67.	63.
56.	53.	59.	60.	77.	71.	65.	86.	96.	91.
84.	85.	107.	120.	123.	135.	112.	121.	153.	158.
170.	172.	193.	164.	163.	145.	122.	144.	117.	118.
128.	99.	123.	119.	80.	94.	101.	116.	143.	171.
163.	159.	157.	137.	134.	137.	134.	107.	112.	91.
121.	129.	149.	131.	134.	119.	121.	122.	115.	108.
88.	111.	120.	122.	116.	117.	139.	143.	167.	172.
171.	182.	170.	183.	192.	171.	194.	205.	197.	179.

161.	159.	126.	135.	103.	98.	97.	79.	72.	79.
72.	95.	97.	100.	123.	137.	130.	114.	127.	124.
120.	116.	117.	89.	99.	95.	88.	82.	86.	87.
99.	132.	118.	113.	112.	114.	120.	86.	79.	94.
79.	53.	59.	70.	63.	47.	61.	55.	58.	67.
71.	72.	66.	80.	82.	83.	78.	51.	82.	88.
90.	88.	89.	87.	125.	154.	154.	196.	174.	174.
148.	150.	123.	141.	145.	133.	103.	74.	78.	77.
74.	73.	57.	45.	73.	58.	58.	60.	49.	60.
67.	57.	64.	73.	96.	76.	85.	78.	102.	90.
127.	132.	110.	140.	130.	144.	156.	149.	140.	149.
150.	122.	155.	143.	133.	134.	136.	151.	155.	166.
170.	216.	157.	152.	136.	126.	119.	130.	120.	121.
106.	112.	96.	82.	90.	111.	92.	103.	121.	118.
137.	133.	126.	155.	127.	121.	128.	97.	111.	114.
93.	102.	76.	86.	69.	80.	84.	74.	60.	77.
89.	74.	87.	67.	81.	78.	87.	80.	55.	90.
78.	98.	90.	92.	88.	76.	76.	83.	60.	102.
79.	87.	54.	83.	65.	71.	59.	67.	56.	70.
58.	74.	70.	78.	57.	61.	85.	72.	77.	83.
96.	112.	132.	133.	172.	193.	244.	311.	288.	243.
242.	231.	185.	186.	199.	186.	163.	117.	104.	83.
66.	80.	68.	54.	74.	68.	75.	79.	84.	82.
76.	86.	79.	73.	64.	82.	88.	74.	85.	60.
97.	102.	112.	116.	178.	195.	247.	212.	182.	174.
144.	163.	151.	127.	141.	136.	110.	98.	85.	91.
92.	81.	80.	72.	104.	102.	87.	119.	85.	91.
64.	82.	88.	86.	89.	100.	75.	63.	64.	87.
99.	88.	86.	105.	89.	92.	71.	75.	73.	110.
85.	72.	92.	96.	92.	123.	148.	136.	146.	135.
129.	102.	129.	113.	121.	132.	122.	123.	88.	91.
93.	80.	85.	104.	115.	131.	143.	126.	119.	117.
88.	75.	95.	99.	95.	90.	81.	72.	64.	81.
55.	47.	68.	78.	60.	77.	73.	97.	89.	101.
114.	108.	98.	113.	95.	132.	100.	82.	99.	100.
75.	85.	79.	64.	88.	101.	103.	99.	150.	131.
136.	123.	108.	108.	129.	113.	129.	99.	82.	100.
83.	82.	90.	80.	92.	103.	76.	96.	91.	114.
123.	136.	173.	139.	143.	118.	106.	103.	112.	130.
134.	110.	121.	110.	107.	85.	85.	90.	79.	105.
76.	85.	69.	69.	75.	72.	54.	70.	94.	70.
83.	93.	110.	108.	116.	89.	86.	91.	86.	85.
83.	90.	84.	85.	76.	81.	73.	76.	69.	82.
72.	57.	62.	58.	58.	50.	62.	76.	59.	56.
62.	49.	56.	56.	53.	52.	72.	57.	73.	64.
55.	72.	46.	68.	87.	70.	74.	63.	73.	104.
105.	103.	75.	109.	79.	66.	83.	97.	88.	93.
80.	77.	72.	79.	69.	83.	78.	82.	58.	89.
58.	68.	82.	79.	73.	77.	111.	104.	113.	133.
160.	142.	109.	118.	106.	97.	95.	109.	121.	124.
112.	128.	155.	123.	125.	98.	101.	96.	89.	93.
108.	95.	82.	91.	98.	93.	88.	126.	127.	123.
131.	95.	97.	116.	116.	111.	116.	119.	112.	156.
137.	181.	149.	169.	172.	150.	121.	99.	103.	106.
126.	144.	114.	113.	106.	106.	91.	86.	67.	80.
93.	112.	85.	96.	94.	96.	97.	88.	110.	101.
127.	110.	95.	85.	85.	79.	83.	98.	95.	86.
94.	108.	100.	101.	90.	113.	83.	91.	89.	75.
105.	109.	112.	92.	110.	89.	69.	79.	76.	80.
84.	92.	124.	69.	89.	80.	75.	77.	76.	77.
111.	86.	94.	89.	63.	82.	72.	59.	80.	79.
101.	91.	103.	127.	112.	148.	172.	154.	116.	110.
80.	93.	85.	131.	111.	92.	109.	97.	85.	73.
98.	72.	66.	75.	72.	73.	79.	77.	82.	107.
111.	120.	106.	103.	90.	120.	118.	95.	81.	100.
105.	91.	84.	77.	72.	96.	76.	83.	96.	76.
89.	86.	69.	72.	64.	52.	57.	62.	74.	64.
64.	65.	63.	60.	47.	65.	53.	53.	52.	54.
47.	76.	52.	65.	67.	55.	60.	57.	70.	52.

77.	78.	54.	58.	55.	59.	64.	62.	58.	63.
77.	58.	63.	81.	60.	68.	66.	75.	62.	53.
68.	79.	74.	83.	104.	103.	133.	142.	148.	131.
132.	126.	121.	94.	109.	75.	97.	137.	112.	111.
91.	91.	76.	88.	67.	87.	78.	72.	71.	89.
80.	90.	98.	114.	115.	148.	119.	134.	128.	129.
107.	120.	149.	143.	125.	113.	137.	118.	123.	104.
135.	147.	168.	185.	161.	148.	133.	112.	102.	100.
100.	108.	139.	114.	139.	123.	96.	83.	87.	87.
73.	77.	78.	77.	60.	61.	54.	69.	73.	70.
67.	59.	57.	65.	72.	67.	78.	75.	65.	59.
69.	56.	69.	64.	64.	63.	76.	62.	79.	70.
69.	82.	95.	89.	97.	105.	82.	116.	94.	152.
143.	147.	167.	171.	112.	126.	116.	134.	112.	107.
124.	98.	124.	126.	127.	116.	108.	115.	84.	89.
91.	98.	93.	103.	104.	108.	106.	140.	146.	141.
137.	124.	104.	138.	93.	98.	97.	97.	110.	116.
112.	139.	121.	106.	120.	110.	88.	95.	103.	71.
71.	87.	109.	131.	111.	101.	112.	105.	123.	124.
137.	154.	127.	162.	148.	156.	154.	109.	112.	93.
112.	117.	116.	125.	122.	126.	122.	115.	126.	119.
98.	97.	107.	81.	80.	86.	116.	95.	97.	85.
97.	98.	85.	103.	105.	111.	93.	117.	121.	113.
125.	119.	156.	162.	144.	138.	101.	127.	109.	117.
104.	142.	111.	109.	130.	114.	122.	121.	103.	88.
83.	92.	101.	82.	92.	80.	91.	96.	106.	88.
74.	75.	102.	60.	76.	73.	76.	77.	77.	77.
96.	63.	80.	86.	89.	67.	94.	96.	96.	97.
78.	93.	91.	88.	81.	87.	92.	112.	100.	95.
110.	124.	124.	165.	204.	192.	190.	161.	128.	140.
106.	126.	115.	107.	129.	140.	112.	132.	174.	141.
148.	153.	139.	123.	123.	100.	109.	120.	124.	153.
147.	140.	177.	191.	214.	238.	236.	235.	207.	204.
187.	152.	146.	149.	139.	126.	144.	114.	131.	172.
178.	176.	149.	156.	133.	127.	121.	118.	112.	98.
108.	88.	88.	71.	82.	73.	81.	75.	69.	62.
65.	85.	84.	72.	77.	76.	78.	90.	62.	75.
81.	65.	82.	75.	57.	81.	69.	73.	70.	72.
84.									

Appendix P-11: step-intensity data of pure olivine

16.00	.10	136.00	pure olivine						
87.	96.	100.	97.	93.	96.	75.	89.	73.	95.
118.	171.	248.	640.	1011.	409.	170.	110.	98.	88.
95.	91.	90.	93.	97.	90.	77.	89.	72.	79.
87.	84.	93.	96.	86.	80.	80.	82.	76.	68.
94.	74.	76.	84.	100.	88.	115.	90.	83.	90.
81.	82.	70.	73.	89.	82.	63.	68.	83.	83.
70.	95.	82.	92.	117.	147.	264.	469.	1314.	2339.
1205.	419.	197.	125.	120.	100.	138.	211.	435.	732.
461.	167.	110.	105.	79.	87.	82.	78.	80.	95.
102.	124.	175.	289.	848.	1161.	869.	470.	186.	102.
98.	85.	75.	69.	80.	80.	79.	74.	76.	53.
62.	54.	58.	67.	79.	69.	68.	66.	73.	62.
64.	84.	66.	73.	59.	61.	56.	68.	73.	73.
72.	86.	61.	83.	105.	149.	293.	483.	721.	561.
257.	121.	97.	82.	73.	63.	62.	84.	82.	80.
67.	69.	75.	89.	74.	94.	93.	76.	101.	148.
242.	423.	1339.	3205.	1937.	582.	237.	151.	127.	96.
78.	84.	78.	78.	61.	65.	78.	78.	72.	82.
57.	81.	79.	107.	85.	85.	106.	153.	141.	129.
134.	144.	222.	248.	346.	649.	1973.	3222.	2082.	747.
402.	309.	386.	684.	1874.	3533.	2408.	924.	414.	232.
173.	129.	120.	100.	87.	97.	85.	116.	147.	115.
120.	191.	443.	630.	339.	152.	129.	173.	412.	413.
232.	123.	130.	154.	250.	448.	1292.	1509.	1005.	742.
1507.	1134.	450.	191.	121.	100.	91.	79.	76.	70.
82.	61.	78.	80.	88.	109.	183.	516.	678.	425.
143.	84.	78.	64.	72.	76.	53.	56.	68.	56.
65.	66.	73.	114.	136.	102.	83.	77.	84.	70.
63.	66.	78.	96.	142.	270.	231.	128.	89.	64.
60.	54.	54.	53.	49.	66.	49.	55.	56.	47.
56.	60.	69.	74.	104.	167.	167.	189.	155.	89.
60.	63.	53.	61.	44.	48.	59.	59.	58.	63.
48.	68.	93.	168.	328.	268.	124.	108.	100.	101.
70.	64.	58.	58.	66.	76.	75.	98.	79.	71.
77.	90.	121.	206.	175.	120.	98.	109.	155.	239.
208.	142.	79.	91.	98.	102.	103.	168.	180.	293.
475.	1083.	2357.	1843.	1324.	1110.	812.	489.	312.	265.
147.	122.	90.	76.	79.	69.	74.	63.	65.	57.
70.	64.	74.	64.	83.	103.	113.	198.	533.	447.
383.	185.	103.	76.	88.	71.	93.	111.	139.	236.
568.	612.	502.	253.	201.	189.	261.	530.	590.	495.
266.	169.	116.	140.	141.	167.	129.	152.	186.	269.
198.	147.	124.	96.	128.	258.	336.	328.	300.	195.
146.	105.	85.	76.	78.	71.	52.	66.	67.	67.
42.	84.	80.	122.	83.	92.	99.	83.	104.	133.
248.	300.	323.	246.	250.	371.	379.	553.	729.	1002.
698.	500.	325.	252.	314.	555.	1402.	1220.	1022.	630.
258.	160.	150.	157.	140.	132.	100.	81.	62.	66.
77.	75.	73.	69.	62.	63.	91.	179.	144.	124.
104.	66.	69.	57.	51.	63.	58.	53.	72.	59.
76.	52.	46.	76.	84.	120.	151.	217.	443.	661.
513.	397.	286.	349.	258.	226.	144.	111.	82.	85.
107.	82.	103.	97.	103.	85.	102.	90.	75.	97.
124.	123.	177.	295.	584.	499.	528.	402.	240.	174.
107.	82.	69.	59.	51.	59.	53.	63.	60.	75.
66.	76.	73.	131.	192.	363.	318.	326.	290.	237.
157.	97.	72.	63.	57.	70.	72.	90.	134.	188.
151.	149.	82.	65.	59.	43.	53.	39.	56.	67.
58.	46.	49.	57.	46.	72.	66.	103.	109.	121.
110.	101.	76.	85.	121.	166.	112.	133.	109.	115.
123.	114.	134.	107.	97.	123.	122.	89.	109.	91.
77.	92.	83.	61.	89.	90.	94.	85.	125.	128.
94.	92.	79.	73.	66.	50.	45.	58.	42.	36.
55.	58.	52.	57.	52.	51.	48.	60.	45.	37.
45.	47.	42.	53.	65.	78.	180.	144.	106.	132.

67.	63.	63.	56.	56.	58.	53.	50.	72.	84.
80.	118.	130.	113.	128.	214.	186.	142.	148.	131.
130.	107.	92.	99.	157.	196.	142.	161.	106.	106.
102.	124.	116.	109.	104.	92.	113.	93.	180.	195.
183.	166.	186.	210.	172.	128.	153.	105.	69.	63.
72.	80.	132.	156.	103.	132.	115.	73.	64.	78.
103.	142.	98.	113.	82.	75.	62.	61.	50.	57.
60.	69.	67.	67.	93.	70.	97.	105.	169.	183.
149.	155.	110.	82.	72.	51.	68.	59.	53.	53.
66.	64.	87.	89.	99.	100.	116.	110.	169.	144.
106.	134.	120.	130.	149.	193.	137.	113.	113.	77.
52.	64.	66.	67.	80.	89.	113.	83.	92.	105.
74.	57.	53.	52.	59.	70.	58.	61.	67.	79.
74.	69.	59.	65.	55.	60.	37.	48.	49.	47.
58.	64.	59.	72.	77.	85.	93.	159.	290.	374.
223.	188.	214.	139.	94.	67.	75.	53.	74.	67.
70.	73.	89.	93.	106.	86.	134.	169.	302.	206.
130.	164.	124.	99.	64.	64.	72.	76.	76.	76.
59.	90.	83.	86.	60.	82.	105.	85.	64.	88.
75.	92.	110.	119.	131.	82.	111.	97.	91.	103.
72.	68.	120.	143.	83.	84.	84.	75.	66.	60.
55.	43.	49.	76.	96.	126.	86.	67.	111.	74.
77.	62.	72.	83.	142.	149.	88.	106.	89.	92.
81.	96.	72.	82.	73.	127.	168.	121.	93.	114.
120.	104.	68.	85.	78.	83.	89.	62.	71.	69.
49.	62.	71.	72.	77.	66.	72.	52.	60.	68.
80.	74.	55.	65.	64.	54.	51.	56.	55.	59.
48.	52.	64.	79.	74.	95.	93.	69.	65.	94.
78.	82.	78.	71.	65.	72.	66.	67.	62.	93.
130.	119.	93.	84.	115.	136.	125.	97.	78.	73.
96.	104.	95.	106.	139.	111.	107.	103.	148.	120.
146.	199.	162.	105.	99.	129.	126.	94.	81.	66.
74.	63.	71.	81.	96.	106.	64.	53.	60.	81.
68.	101.	104.	77.	73.	67.	90.	97.	69.	69.
82.	96.	67.	76.	71.	105.	77.	68.	65.	91.
85.	98.	135.	159.	109.	87.	87.	98.	85.	85.
79.	70.	76.	73.	81.	113.	128.	86.	107.	78.
85.	90.	68.	72.	82.	76.	61.	51.	60.	47.
57.	57.	54.	56.	47.	55.	50.	59.	56.	63.
60.	71.	50.	55.	61.	60.	53.	65.	61.	69.
65.	54.	57.	134.	148.	105.	76.	90.	107.	95.
89.	74.	64.	67.	58.	76.	82.	89.	137.	111.
83.	131.	124.	119.	103.	116.	185.	145.	123.	107.
87.	118.	110.	96.	63.	61.	56.	54.	62.	43.
53.	55.	55.	57.	65.	74.	61.	57.	61.	70.
76.	64.	86.	90.	107.	127.	203.	137.	90.	81.
98.	107.	134.	91.	84.	84.	87.	109.	107.	119.
170.	100.	87.	89.	102.	128.	143.	101.	100.	84.
96.	110.	135.	120.	109.	173.	148.	179.	135.	100.
108.	118.	133.	121.	133.	100.	88.	107.	85.	86.
97.	87.	80.	106.	124.	138.	137.	142.	112.	89.
102.	106.	107.	108.	99.	91.	69.	83.	78.	59.
62.	67.	47.	65.	46.	70.	81.	70.	68.	88.
86.	70.	102.	62.	76.	102.	136.	210.	153.	123.
106.	124.	112.	112.	142.	130.	115.	118.	99.	123.
123.									

Appendix P-12: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.01° 2θ

19.00 .01 139.00 50%-olivine, 0.01 degree two-theta

92.	91.	94.	106.	98.	96.	94.	99.	98.	88.
78.	84.	82.	88.	94.	70.	80.	93.	77.	85.
86.	67.	96.	76.	87.	69.	78.	69.	73.	76.
89.	85.	96.	98.	83.	72.	91.	92.	88.	88.
83.	89.	78.	86.	77.	86.	83.	82.	91.	98.
87.	103.	89.	93.	92.	91.	90.	76.	92.	69.
101.	77.	97.	96.	84.	103.	69.	112.	90.	93.
91.	105.	92.	81.	77.	90.	98.	95.	110.	116.
105.	110.	120.	108.	102.	140.	118.	119.	126.	131.
152.	137.	149.	124.	152.	165.	128.	150.	137.	152.
178.	166.	170.	149.	176.	167.	161.	141.	135.	149.
110.	121.	128.	133.	107.	104.	121.	119.	121.	124.
107.	126.	120.	105.	109.	116.	99.	106.	98.	99.
100.	108.	96.	93.	112.	94.	104.	84.	70.	87.
102.	80.	94.	94.	80.	82.	83.	82.	96.	88.
69.	87.	79.	89.	94.	79.	82.	91.	85.	109.
85.	89.	76.	95.	101.	84.	89.	86.	93.	114.
91.	77.	89.	98.	102.	102.	84.	83.	64.	89.
85.	68.	85.	77.	72.	89.	90.	76.	73.	97.
77.	83.	88.	78.	94.	87.	85.	94.	58.	90.
70.	82.	82.	74.	86.	78.	68.	81.	76.	72.
75.	81.	76.	79.	86.	83.	79.	67.	75.	75.
74.	83.	74.	79.	58.	78.	86.	68.	59.	77.
76.	74.	83.	80.	81.	68.	71.	82.	74.	97.
81.	64.	100.	83.	60.	90.	72.	67.	67.	70.
71.	62.	70.	81.	66.	71.	86.	75.	72.	67.
81.	64.	89.	67.	64.	69.	89.	84.	69.	73.
65.	75.	71.	72.	70.	84.	61.	75.	80.	78.
61.	80.	91.	72.	82.	78.	61.	84.	73.	71.
84.	74.	95.	69.	64.	67.	82.	70.	69.	77.
85.	88.	75.	71.	85.	64.	70.	87.	73.	74.
72.	61.	98.	101.	78.	70.	101.	71.	71.	90.
97.	67.	83.	74.	70.	66.	67.	73.	92.	65.
76.	71.	76.	71.	85.	100.	84.	99.	77.	80.
103.	94.	87.	93.	97.	104.	89.	111.	115.	118.
99.	103.	146.	133.	121.	133.	141.	117.	137.	135.
134.	186.	131.	170.	182.	208.	218.	214.	220.	248.
261.	231.	293.	338.	356.	401.	433.	471.	516.	566.
627.	652.	707.	658.	800.	849.	907.	907.	959.	966.
990.	1049.	1078.	1066.	1024.	1035.	1064.	979.	920.	920.
892.	813.	802.	771.	686.	613.	545.	558.	443.	415.
379.	330.	306.	294.	255.	237.	209.	191.	186.	172.
192.	159.	143.	155.	145.	154.	124.	120.	102.	121.
112.	108.	114.	119.	112.	117.	97.	115.	102.	77.
94.	98.	96.	102.	88.	92.	92.	98.	98.	93.
78.	97.	103.	85.	99.	98.	99.	93.	102.	112.
86.	103.	95.	105.	117.	119.	103.	119.	124.	143.
137.	134.	138.	128.	160.	156.	155.	192.	214.	203.
196.	226.	247.	263.	281.	281.	348.	314.	346.	391.
402.	376.	379.	416.	415.	420.	375.	365.	374.	367.
369.	299.	309.	312.	309.	238.	261.	222.	230.	199.
209.	200.	158.	166.	141.	146.	135.	130.	116.	119.
124.	135.	130.	129.	131.	116.	129.	114.	126.	121.
135.	115.	147.	119.	145.	136.	147.	149.	148.	123.
136.	151.	121.	141.	135.	123.	141.	115.	126.	121.
102.	119.	105.	101.	97.	104.	102.	92.	92.	83.
96.	64.	81.	74.	78.	85.	79.	95.	88.	72.
81.	86.	93.	67.	88.	81.	70.	83.	81.	98.
66.	76.	91.	69.	78.	101.	84.	82.	64.	77.
55.	77.	89.	70.	71.	74.	96.	80.	90.	91.
74.	90.	69.	92.	103.	91.	93.	95.	83.	81.
102.	82.	85.	106.	99.	73.	113.	107.	99.	114.
116.	112.	137.	112.	139.	155.	151.	175.	170.	153.
202.	201.	225.	200.	219.	281.	265.	325.	331.	331.

361.	408.	437.	473.	471.	475.	495.	532.	555.	574.
570.	572.	570.	593.	578.	591.	555.	603.	553.	572.
568.	501.	508.	545.	495.	454.	463.	443.	396.	381.
341.	378.	321.	297.	253.	273.	273.	231.	227.	198.
220.	187.	161.	152.	146.	138.	130.	124.	114.	103.
113.	104.	95.	107.	111.	96.	83.	103.	83.	85.
72.	87.	81.	87.	93.	68.	89.	80.	80.	74.
80.	75.	90.	62.	79.	86.	84.	76.	80.	97.
86.	88.	68.	62.	84.	88.	92.	82.	84.	73.
76.	84.	87.	89.	82.	100.	92.	97.	85.	104.
82.	112.	93.	95.	121.	102.	109.	113.	120.	125.
104.	144.	140.	151.	131.	151.	165.	174.	167.	203.
201.	214.	233.	239.	255.	260.	292.	314.	291.	300.
341.	334.	332.	331.	338.	366.	348.	347.	339.	339.
289.	272.	291.	265.	271.	241.	209.	205.	232.	176.
156.	171.	174.	155.	147.	155.	126.	130.	121.	115.
105.	121.	110.	90.	99.	102.	82.	81.	102.	107.
90.	85.	103.	93.	115.	87.	86.	99.	97.	89.
98.	91.	98.	99.	102.	101.	102.	91.	94.	111.
117.	101.	92.	101.	114.	99.	116.	125.	138.	148.
144.	157.	152.	177.	164.	157.	193.	204.	203.	230.
265.	271.	303.	326.	333.	386.	404.	420.	532.	523.
513.	614.	606.	676.	663.	708.	750.	726.	723.	736.
708.	729.	757.	678.	691.	649.	625.	627.	571.	506.
494.	492.	435.	364.	340.	290.	285.	278.	262.	234.
218.	182.	188.	167.	152.	151.	125.	139.	121.	120.
103.	111.	90.	101.	88.	95.	79.	92.	107.	98.
89.	86.	97.	87.	91.	68.	101.	93.	84.	63.
67.	77.	84.	91.	69.	83.	95.	72.	87.	77.
75.	70.	78.	66.	58.	78.	74.	84.	78.	60.
76.	71.	70.	71.	74.	78.	70.	70.	83.	86.
92.	86.	79.	76.	87.	110.	101.	71.	77.	93.
108.	91.	66.	76.	73.	84.	106.	92.	78.	93.
55.	82.	79.	71.	84.	90.	78.	82.	95.	88.
57.	74.	83.	101.	81.	90.	76.	88.	89.	64.
94.	102.	86.	83.	88.	65.	90.	83.	75.	89.
89.	88.	90.	111.	71.	95.	104.	87.	96.	96.
83.	97.	87.	110.	115.	90.	111.	129.	104.	85.
111.	121.	114.	96.	98.	109.	117.	122.	116.	118.
135.	137.	128.	128.	164.	136.	148.	167.	155.	158.
146.	160.	191.	214.	190.	202.	211.	220.	244.	237.
257.	280.	293.	270.	311.	297.	315.	373.	351.	350.
391.	423.	403.	457.	455.	480.	528.	559.	580.	637.
665.	642.	701.	766.	834.	907.	1005.	1074.	1199.	1299.
1482.	1643.	1847.	1908.	2173.	2174.	2452.	2531.	2640.	2601.
2724.	2782.	2834.	2980.	2999.	3003.	2964.	3014.	2886.	2891.
2754.	2816.	2625.	2757.	2322.	2273.	2189.	2016.	1775.	1760.
1628.	1505.	1369.	1250.	1214.	1077.	1047.	901.	858.	845.
870.	767.	790.	744.	766.	728.	795.	801.	815.	816.
826.	847.	939.	941.	959.	920.	951.	1017.	973.	993.
1024.	927.	942.	892.	893.	834.	860.	795.	767.	669.
610.	607.	544.	461.	496.	475.	409.	369.	339.	341.
342.	323.	315.	301.	261.	220.	256.	255.	244.	266.
238.	235.	256.	269.	280.	303.	320.	327.	377.	361.
394.	413.	468.	469.	488.	593.	567.	593.	692.	692.
736.	847.	922.	886.	895.	955.	1016.	1000.	1016.	1070.
1066.	1122.	1002.	1017.	937.	936.	847.	856.	770.	723.
709.	621.	620.	554.	546.	477.	423.	398.	384.	327.
282.	311.	245.	230.	223.	241.	221.	187.	161.	169.
158.	141.	150.	134.	140.	135.	107.	129.	110.	114.
125.	115.	112.	120.	124.	112.	116.	98.	129.	98.
115.	99.	107.	128.	122.	114.	123.	105.	126.	129.
112.	124.	113.	121.	130.	136.	121.	117.	112.	109.
133.	111.	123.	129.	119.	122.	107.	112.	111.	110.
111.	123.	117.	88.	119.	119.	122.	107.	140.	115.
116.	136.	106.	121.	130.	121.	129.	130.	143.	140.
151.	152.	178.	164.	177.	191.	185.	199.	236.	219.
256.	265.	271.	314.	351.	365.	376.	448.	451.	534.
566.	629.	756.	757.	799.	858.	993.	982.	1064.	1094.

1192.	1194.	1256.	1320.	1335.	1359.	1301.	1312.	1281.	1214.
1149.	1086.	1082.	1007.	1014.	864.	789.	774.	702.	638.
561.	541.	499.	401.	395.	346.	314.	307.	293.	250.
224.	219.	184.	173.	183.	154.	159.	140.	131.	128.
132.	121.	115.	126.	120.	97.	107.	108.	123.	113.
92.	93.	102.	108.	108.	108.	108.	84.	95.	102.
88.	68.	76.	89.	80.	78.	86.	77.	87.	80.
67.	61.	78.	68.	96.	78.	71.	82.	72.	77.
80.	79.	67.	77.	73.	71.	81.	82.	70.	89.
90.	83.	82.	84.	67.	60.	56.	74.	73.	71.
76.	70.	58.	65.	58.	72.	63.	60.	61.	75.
62.	73.	53.	76.	65.	58.	56.	70.	76.	80.
67.	90.	57.	90.	79.	72.	72.	61.	56.	71.
76.	69.	65.	60.	68.	70.	82.	72.	81.	72.
62.	72.	62.	61.	67.	60.	86.	76.	73.	60.
70.	65.	65.	71.	68.	60.	83.	57.	77.	70.
71.	84.	66.	85.	80.	72.	72.	66.	73.	84.
82.	64.	71.	73.	76.	77.	92.	71.	100.	76.
67.	71.	77.	66.	77.	80.	59.	80.	76.	82.
92.	79.	68.	67.	79.	87.	93.	89.	93.	72.
67.	82.	84.	90.	90.	92.	92.	97.	90.	85.
77.	89.	91.	77.	89.	92.	94.	93.	95.	85.
102.	78.	112.	95.	116.	113.	100.	111.	110.	104.
116.	127.	111.	123.	131.	147.	130.	145.	147.	133.
160.	172.	181.	170.	179.	174.	174.	185.	210.	205.
194.	207.	201.	214.	218.	234.	255.	232.	278.	299.
337.	344.	368.	374.	417.	442.	456.	464.	500.	500.
576.	613.	596.	657.	674.	724.	737.	731.	751.	750.
772.	731.	757.	745.	723.	725.	688.	727.	652.	640.
647.	585.	559.	525.	550.	516.	521.	485.	481.	476.
465.	444.	478.	459.	540.	506.	550.	518.	524.	562.
642.	617.	700.	749.	780.	893.	942.	1008.	1056.	1077.
1203.	1358.	1380.	1515.	1688.	1743.	1932.	2007.	2082.	2276.
2388.	2507.	2606.	2621.	2675.	2693.	2814.	2821.	2873.	2893.
2833.	2971.	2892.	2967.	2891.	2876.	2825.	2785.	2697.	2653.
2560.	2476.	2399.	2278.	2217.	2187.	1957.	1826.	1695.	1570.
1520.	1388.	1295.	1197.	1106.	994.	924.	824.	758.	720.
681.	604.	518.	554.	456.	473.	395.	392.	345.	352.
369.	316.	365.	316.	312.	277.	271.	295.	264.	261.
312.	276.	325.	266.	307.	331.	333.	308.	308.	361.
378.	384.	441.	471.	465.	549.	545.	599.	693.	729.
846.	897.	957.	1014.	1090.	1176.	1269.	1316.	1421.	1533.
1587.	1675.	1698.	1797.	1741.	1769.	1810.	1702.	1737.	1675.
1677.	1582.	1498.	1529.	1429.	1359.	1268.	1195.	1149.	1065.
993.	923.	896.	797.	731.	638.	585.	548.	528.	486.
419.	396.	358.	334.	342.	266.	279.	268.	245.	232.
205.	196.	190.	175.	177.	153.	172.	161.	136.	157.
132.	159.	143.	133.	122.	115.	133.	138.	117.	127.
113.	119.	123.	126.	91.	94.	79.	98.	111.	112.
95.	107.	109.	93.	107.	82.	105.	97.	76.	88.
81.	82.	89.	85.	89.	77.	88.	63.	92.	90.
89.	73.	80.	75.	83.	100.	89.	104.	77.	107.
87.	90.	90.	83.	82.	93.	111.	107.	84.	100.
109.	97.	83.	101.	99.	113.	114.	123.	117.	134.
118.	117.	116.	166.	127.	129.	136.	140.	152.	146.
143.	136.	143.	131.	149.	159.	140.	129.	95.	147.
120.	138.	125.	132.	128.	123.	136.	122.	109.	106.
114.	121.	106.	100.	93.	115.	117.	117.	99.	101.
121.	139.	129.	124.	137.	168.	161.	181.	193.	205.
210.	224.	240.	215.	219.	253.	232.	286.	268.	270.
270.	289.	298.	260.	274.	289.	295.	278.	268.	241.
261.	238.	188.	210.	203.	177.	194.	174.	171.	162.
167.	149.	147.	139.	157.	118.	142.	111.	134.	121.
105.	111.	110.	98.	117.	125.	124.	122.	127.	119.
132.	133.	133.	168.	156.	151.	179.	168.	193.	217.
204.	231.	259.	263.	239.	266.	242.	297.	278.	288.
271.	308.	259.	297.	288.	283.	289.	274.	286.	295.
254.	299.	298.	302.	297.	276.	291.	293.	319.	341.
345.	355.	371.	370.	419.	432.	459.	502.	488.	506.

529.	539.	556.	534.	489.	517.	494.	495.	470.	518.
441.	484.	415.	386.	381.	379.	337.	348.	343.	290.
274.	309.	285.	316.	285.	306.	280.	269.	287.	296.
313.	328.	266.	374.	387.	407.	382.	427.	504.	535.
603.	590.	625.	681.	724.	666.	777.	698.	798.	726.
840.	805.	864.	863.	818.	851.	802.	797.	685.	737.
698.	674.	638.	633.	581.	596.	612.	594.	526.	565.
564.	540.	514.	545.	524.	565.	557.	512.	577.	623.
582.	614.	728.	662.	733.	692.	678.	669.	673.	627.
686.	610.	591.	600.	620.	551.	518.	502.	457.	402.
422.	446.	377.	332.	333.	295.	286.	264.	246.	227.
196.	190.	151.	151.	153.	140.	138.	148.	144.	129.
111.	121.	124.	107.	123.	134.	114.	113.	111.	116.
127.	133.	132.	133.	121.	133.	136.	148.	138.	173.
169.	184.	189.	211.	226.	228.	237.	252.	265.	280.
268.	311.	291.	305.	339.	319.	334.	338.	344.	380.
377.	332.	355.	382.	335.	326.	357.	353.	358.	327.
350.	306.	323.	335.	282.	302.	299.	325.	308.	280.
326.	316.	328.	304.	306.	311.	362.	353.	357.	365.
383.	355.	370.	356.	390.	363.	334.	343.	338.	333.
324.	321.	297.	270.	249.	243.	235.	222.	211.	216.
199.	183.	162.	164.	154.	133.	149.	139.	128.	124.
137.	115.	122.	112.	132.	124.	113.	111.	115.	127.
111.	106.	114.	113.	121.	113.	142.	148.	144.	150.
126.	151.	206.	156.	168.	226.	209.	216.	227.	248.
260.	317.	291.	322.	353.	363.	359.	395.	419.	396.
419.	435.	428.	447.	473.	482.	498.	492.	469.	506.
484.	461.	449.	483.	494.	477.	459.	475.	466.	429.
487.	433.	431.	442.	432.	416.	403.	385.	373.	377.
359.	342.	347.	335.	310.	314.	291.	305.	271.	290.
229.	274.	256.	227.	268.	233.	239.	252.	252.	301.
297.	324.	316.	371.	393.	384.	417.	421.	438.	469.
516.	508.	536.	506.	541.	586.	590.	599.	565.	561.
540.	531.	528.	510.	508.	478.	465.	464.	398.	393.
405.	374.	325.	326.	289.	288.	288.	263.	241.	224.
216.	200.	227.	201.	214.	172.	183.	171.	157.	170.
159.	171.	188.	167.	197.	180.	178.	216.	207.	231.
207.	225.	236.	229.	268.	268.	312.	263.	278.	263.
284.	308.	304.	270.	297.	259.	272.	294.	253.	231.
248.	241.	235.	214.	220.	201.	189.	205.	177.	162.
168.	163.	153.	145.	138.	145.	135.	147.	131.	113.
138.	128.	121.	118.	133.	123.	127.	137.	123.	109.
134.	127.	140.	131.	135.	131.	144.	142.	120.	127.
125.	130.	145.	114.	151.	113.	138.	111.	126.	127.
125.	103.	131.	118.	125.	116.	143.	121.	132.	122.
102.	107.	119.	126.	123.	105.	107.	98.	105.	91.
122.	102.	104.	106.	68.	94.	105.	87.	93.	101.
79.	86.	84.	81.	80.	105.	74.	83.	94.	73.
104.	84.	77.	100.	110.	82.	99.	107.	101.	99.
92.	108.	110.	109.	114.	106.	123.	106.	127.	141.
121.	148.	152.	157.	153.	162.	184.	177.	206.	204.
224.	254.	250.	287.	316.	343.	366.	382.	396.	443.
440.	445.	475.	564.	554.	600.	612.	687.	651.	646.
679.	707.	611.	669.	640.	654.	655.	591.	619.	538.
534.	499.	453.	458.	405.	446.	387.	385.	387.	344.
333.	298.	256.	279.	278.	242.	239.	209.	218.	197.
190.	225.	199.	209.	209.	196.	206.	227.	210.	269.
242.	268.	267.	284.	258.	324.	288.	341.	372.	356.
394.	377.	408.	392.	444.	448.	435.	444.	464.	452.
465.	443.	414.	433.	450.	420.	393.	435.	381.	421.
367.	418.	397.	395.	407.	369.	385.	312.	314.	290.
291.	281.	287.	246.	247.	231.	251.	223.	211.	166.
181.	166.	155.	177.	169.	135.	145.	114.	126.	103.
116.	107.	110.	103.	96.	112.	107.	104.	81.	97.
91.	72.	83.	73.	89.	76.	88.	77.	69.	67.
76.	68.	72.	89.	70.	94.	67.	88.	76.	72.
81.	89.	103.	63.	71.	105.	77.	98.	89.	86.
91.	92.	114.	76.	86.	97.	97.	115.	91.	97.
136.	115.	110.	112.	159.	165.	173.	187.	199.	187.

195.	225.	229.	228.	235.	267.	255.	284.	293.	251.
253.	273.	248.	234.	255.	234.	209.	215.	203.	211.
188.	178.	163.	178.	159.	143.	159.	132.	122.	141.
142.	128.	119.	109.	112.	112.	123.	133.	142.	121.
116.	142.	112.	117.	154.	140.	151.	118.	143.	136.
142.	134.	138.	137.	158.	147.	147.	140.	125.	146.
126.	156.	130.	129.	125.	116.	127.	124.	116.	109.
106.	111.	102.	103.	122.	95.	112.	72.	99.	88.
96.	88.	74.	71.	63.	78.	77.	62.	79.	68.
75.	69.	62.	55.	63.	77.	65.	66.	72.	64.
52.	41.	64.	58.	69.	60.	65.	72.	58.	71.
69.	56.	59.	61.	61.	68.	64.	55.	61.	55.
56.	62.	51.	57.	54.	55.	58.	53.	53.	46.
46.	57.	55.	53.	49.	57.	60.	62.	60.	64.
51.	62.	61.	63.	55.	57.	65.	63.	64.	64.
51.	55.	56.	58.	45.	57.	55.	56.	50.	57.
61.	65.	61.	71.	55.	65.	54.	45.	58.	62.
55.	49.	48.	61.	50.	58.	62.	61.	54.	51.
59.	52.	55.	56.	76.	61.	63.	63.	72.	65.
59.	54.	61.	73.	57.	74.	67.	58.	62.	67.
55.	69.	64.	78.	55.	68.	75.	70.	80.	78.
67.	83.	64.	60.	96.	79.	86.	86.	82.	88.
92.	109.	99.	111.	126.	134.	117.	116.	145.	137.
145.	172.	176.	175.	146.	184.	161.	179.	146.	158.
163.	160.	174.	159.	139.	130.	124.	134.	114.	139.
120.	106.	119.	107.	108.	101.	102.	108.	102.	103.
83.	93.	105.	92.	83.	77.	110.	77.	83.	105.
80.	83.	102.	89.	109.	98.	110.	100.	84.	106.
108.	83.	109.	102.	111.	127.	110.	109.	123.	116.
126.	115.	124.	130.	125.	121.	123.	107.	152.	134.
127.	120.	116.	118.	111.	137.	103.	100.	112.	107.
122.	87.	98.	97.	116.	96.	74.	78.	87.	67.
82.	79.	88.	78.	88.	69.	75.	67.	83.	85.
75.	74.	79.	93.	74.	85.	73.	100.	106.	111.
109.	94.	99.	104.	114.	110.	139.	117.	170.	167.
163.	164.	175.	184.	197.	188.	216.	225.	241.	256.
275.	259.	284.	291.	278.	265.	262.	285.	307.	330.
292.	282.	266.	331.	282.	261.	279.	251.	234.	243.
262.	269.	233.	227.	248.	199.	209.	200.	217.	217.
174.	195.	173.	156.	156.	133.	157.	133.	129.	136.
140.	119.	113.	109.	112.	114.	123.	112.	129.	130.
138.	138.	163.	167.	159.	148.	173.	155.	207.	175.
194.	192.	191.	185.	187.	200.	227.	220.	229.	200.
200.	208.	209.	200.	184.	205.	181.	162.	189.	141.
166.	151.	149.	160.	148.	120.	146.	147.	130.	134.
108.	115.	103.	103.	108.	105.	119.	103.	106.	104.
96.	102.	120.	111.	100.	89.	87.	123.	134.	101.
114.	127.	132.	123.	126.	139.	117.	125.	125.	154.
118.	124.	144.	139.	122.	141.	139.	155.	131.	139.
123.	152.	132.	117.	120.	120.	121.	146.	122.	112.
112.	98.	96.	94.	78.	86.	95.	100.	85.	82.
97.	83.	68.	82.	78.	71.	68.	78.	77.	70.
77.	83.	77.	71.	62.	77.	76.	63.	91.	79.
79.	68.	97.	81.	89.	89.	83.	110.	98.	89.
112.	93.	93.	95.	91.	107.	120.	110.	109.	87.
121.	95.	108.	117.	111.	137.	118.	131.	112.	99.
119.	126.	146.	103.	117.	97.	162.	144.	136.	140.
131.	160.	130.	162.	141.	159.	166.	161.	160.	176.
143.	192.	188.	215.	212.	208.	216.	257.	273.	263.
286.	300.	306.	354.	396.	387.	436.	450.	573.	590.
625.	699.	744.	767.	858.	940.	1003.	1060.	1101.	1171.
1200.	1200.	1311.	1352.	1354.	1430.	1437.	1462.	1382.	1345.
1410.	1316.	1301.	1317.	1240.	1215.	1219.	1117.	1087.	1123.
1062.	925.	1012.	974.	919.	898.	827.	818.	854.	800.
781.	780.	727.	710.	680.	638.	684.	656.	549.	529.
553.	530.	499.	464.	469.	457.	424.	392.	421.	389.
358.	359.	327.	320.	289.	320.	314.	288.	308.	250.
296.	250.	250.	249.	222.	229.	232.	232.	181.	221.
192.	181.	193.	197.	158.	181.	175.	140.	152.	162.

148.	129.	153.	149.	143.	132.	115.	130.	131.	119.
99.	92.	103.	111.	103.	94.	117.	124.	100.	107.
125.	101.	114.	102.	114.	112.	131.	117.	117.	120.
98.	124.	99.	115.	113.	117.	117.	109.	96.	107.
106.	105.	108.	105.	110.	110.	106.	107.	97.	95.
93.	99.	95.	103.	99.	75.	88.	96.	94.	84.
89.	86.	98.	81.	80.	63.	77.	76.	92.	87.
81.	57.	88.	83.	76.	85.	71.	82.	49.	70.
72.	75.	71.	63.	57.	56.	72.	67.	59.	66.
62.	73.	71.	61.	72.	60.	62.	58.	46.	60.
63.	65.	48.	66.	51.	60.	60.	46.	62.	51.
85.	73.	70.	76.	64.	49.	72.	60.	76.	46.
67.	66.	61.	76.	64.	74.	82.	75.	63.	59.
76.	66.	67.	87.	73.	54.	79.	78.	63.	71.
87.	84.	79.	100.	63.	109.	96.	86.	98.	96.
89.	85.	94.	111.	116.	110.	125.	108.	111.	117.
136.	140.	132.	144.	162.	147.	157.	166.	184.	156.
188.	215.	205.	162.	202.	245.	271.	245.	293.	298.
285.	297.	336.	339.	379.	329.	363.	361.	384.	362.
374.	400.	386.	376.	393.	422.	358.	342.	352.	344.
348.	372.	366.	329.	331.	335.	298.	310.	292.	261.
260.	270.	236.	240.	209.	227.	217.	175.	184.	178.
172.	189.	163.	170.	177.	151.	142.	170.	181.	169.
204.	205.	188.	210.	208.	199.	198.	227.	200.	207.
203.	193.	192.	203.	215.	187.	197.	172.	172.	204.
171.	174.	180.	175.	159.	152.	150.	170.	140.	146.
160.	151.	123.	140.	134.	135.	124.	113.	114.	128.
115.	99.	123.	97.	108.	118.	137.	129.	105.	120.
104.	114.	138.	132.	130.	117.	121.	117.	127.	128.
173.	151.	149.	149.	177.	220.	209.	244.	263.	257.
221.	220.	273.	304.	264.	306.	271.	313.	310.	320.
362.	324.	354.	337.	360.	357.	332.	316.	331.	343.
309.	326.	307.	288.	290.	329.	303.	264.	288.	301.
265.	271.	277.	261.	249.	258.	258.	254.	247.	239.
272.	274.	279.	305.	268.	274.	289.	290.	330.	324.
361.	354.	368.	387.	453.	484.	512.	533.	592.	617.
640.	691.	717.	758.	833.	857.	895.	913.	882.	936.
881.	918.	968.	964.	951.	940.	888.	881.	902.	914.
877.	874.	898.	882.	781.	846.	812.	765.	800.	702.
660.	639.	649.	629.	581.	535.	572.	513.	532.	484.
463.	510.	436.	397.	447.	401.	415.	390.	382.	346.
347.	307.	318.	302.	256.	277.	271.	262.	263.	248.
224.	212.	213.	206.	224.	194.	178.	183.	183.	161.
161.	169.	138.	158.	147.	142.	145.	156.	158.	132.
143.	123.	122.	135.	120.	140.	123.	142.	135.	149.
138.	124.	118.	155.	145.	130.	139.	124.	130.	136.
136.	144.	134.	153.	132.	125.	145.	126.	124.	131.
123.	126.	115.	110.	133.	131.	122.	135.	128.	146.
149.	139.	147.	163.	159.	150.	171.	149.	130.	146.
150.	144.	160.	141.	157.	155.	144.	140.	144.	151.
158.	159.	150.	145.	133.	120.	172.	135.	159.	144.
119.	142.	131.	159.	133.	146.	141.	139.	132.	130.
150.	151.	137.	144.	138.	127.	126.	135.	122.	135.
134.	135.	138.	120.	129.	136.	151.	118.	118.	128.
122.	120.	115.	123.	150.	141.	121.	135.	147.	130.
158.	171.	156.	172.	176.	178.	190.	186.	206.	173.
204.	229.	203.	213.	202.	212.	194.	223.	230.	212.
200.	222.	219.	182.	207.	184.	217.	204.	193.	220.
216.	190.	220.	198.	174.	199.	185.	161.	177.	165.
170.	175.	140.	168.	166.	160.	165.	154.	172.	157.
165.	150.	144.	126.	153.	157.	169.	141.	151.	155.
153.	155.	174.	167.	170.	181.	163.	159.	194.	150.
161.	189.	172.	161.	165.	160.	176.	161.	146.	153.
122.	148.	136.	131.	128.	125.	140.	126.	126.	134.
119.	113.	147.	125.	110.	113.	96.	95.	95.	105.
99.	97.	89.	117.	95.	117.	114.	117.	122.	127.
124.	118.	158.	141.	134.	132.	155.	154.	158.	164.
167.	157.	171.	178.	162.	147.	168.	190.	188.	197.
167.	177.	181.	181.	158.	166.	158.	133.	140.	162.

147.	135.	142.	129.	131.	149.	135.	125.	124.	120.
97.	113.	98.	100.	109.	92.	95.	84.	101.	94.
86.	90.	87.	99.	103.	90.	108.	99.	114.	95.
89.	95.	97.	122.	118.	117.	112.	116.	128.	104.
136.	128.	106.	119.	121.	127.	122.	130.	138.	133.
119.	130.	154.	157.	152.	166.	183.	158.	191.	162.
183.	170.	200.	194.	191.	239.	226.	194.	223.	218.
222.	229.	234.	233.	269.	229.	244.	269.	254.	259.
262.	264.	285.	278.	292.	321.	304.	307.	304.	319.
304.	314.	293.	314.	310.	295.	315.	278.	291.	291.
307.	307.	297.	306.	290.	295.	303.	315.	285.	284.
269.	281.	279.	280.	311.	298.	278.	273.	267.	276.
283.	271.	277.	260.	265.	229.	241.	256.	264.	229.
239.	246.	253.	229.	250.	251.	271.	242.	229.	262.
256.	228.	226.	232.	253.	258.	248.	238.	244.	250.
223.	268.	242.	259.	263.	245.	275.	270.	316.	282.
304.	350.	331.	333.	356.	352.	370.	421.	399.	446.
415.	460.	464.	474.	477.	497.	528.	518.	599.	592.
568.	584.	562.	603.	616.	579.	604.	626.	610.	609.
640.	584.	654.	700.	634.	638.	700.	655.	725.	736.
702.	687.	734.	661.	627.	621.	606.	570.	578.	543.
547.	572.	525.	519.	504.	484.	453.	441.	453.	422.
422.	402.	398.	375.	381.	336.	325.	342.	297.	288.
284.	304.	303.	337.	269.	279.	266.	251.	250.	241.
244.	233.	235.	233.	257.	253.	269.	283.	281.	307.
283.	288.	277.	278.	270.	299.	291.	337.	351.	351.
375.	398.	398.	431.	436.	511.	496.	501.	597.	621.
596.	643.	588.	716.	656.	679.	685.	741.	689.	696.
694.	723.	660.	737.	693.	702.	694.	641.	675.	646.
671.	615.	586.	527.	521.	489.	502.	461.	464.	467.
381.	403.	405.	413.	323.	336.	303.	258.	288.	290.
246.	236.	201.	191.	212.	174.	180.	190.	177.	155.
142.	171.	165.	163.	128.	145.	141.	122.	143.	152.
129.	133.	131.	139.	114.	128.	129.	132.	132.	119.
119.	134.	138.	119.	112.	138.	125.	145.	131.	136.
125.	122.	131.	115.	104.	134.	104.	130.	110.	111.
112.	112.	134.	101.	118.	102.	108.	111.	114.	98.
110.	99.	109.	112.	109.	109.	121.	111.	100.	131.
125.	108.	116.	124.	105.	115.	115.	105.	109.	97.
104.	111.	120.	86.	106.	100.	103.	105.	88.	97.
91.	84.	73.	79.	82.	97.	92.	96.	91.	80.
60.	84.	77.	81.	74.	68.	59.	76.	65.	80.
69.	75.	63.	82.	86.	81.	85.	93.	81.	63.
78.	71.	92.	84.	85.	81.	112.	124.	99.	95.
117.	91.	105.	102.	106.	138.	133.	129.	133.	124.
114.	129.	109.	127.	132.	129.	108.	121.	149.	117.
135.	110.	133.	123.	133.	143.	141.	129.	155.	136.
143.	145.	133.	159.	148.	144.	130.	138.	148.	161.
169.	178.	163.	158.	149.	156.	163.	164.	176.	160.
163.	167.	135.	158.	154.	163.	164.	140.	127.	153.
153.	134.	132.	123.	147.	119.	137.	115.	123.	105.
112.	106.	127.	92.	98.	118.	87.	107.	89.	93.
90.	101.	104.	99.	87.	110.	94.	105.	96.	98.
87.	102.	88.	111.	95.	99.	87.	104.	111.	128.
133.	116.	132.	128.	115.	127.	147.	152.	155.	152.
154.	171.	153.	178.	188.	201.	211.	212.	197.	243.
246.	251.	283.	290.	281.	304.	348.	361.	366.	394.
372.	416.	420.	500.	477.	525.	553.	532.	547.	539.
556.	533.	562.	497.	488.	532.	498.	493.	470.	481.
420.	423.	406.	395.	413.	395.	379.	370.	345.	365.
395.	379.	340.	342.	298.	289.	291.	267.	298.	277.
246.	231.	218.	183.	207.	194.	184.	184.	174.	177.
157.	177.	165.	186.	175.	153.	174.	154.	151.	170.
183.	181.	184.	200.	216.	204.	216.	227.	229.	220.
266.	263.	291.	313.	276.	317.	305.	324.	322.	377.
347.	334.	331.	333.	327.	345.	328.	329.	322.	346.
338.	331.	323.	330.	308.	325.	335.	328.	280.	265.
282.	282.	273.	264.	278.	263.	263.	267.	245.	244.
246.	269.	238.	283.	259.	278.	298.	279.	266.	259.

291.	294.	324.	325.	337.	364.	323.	374.	388.	369.
341.	377.	371.	340.	360.	374.	301.	340.	343.	348.
356.	353.	343.	324.	329.	323.	324.	311.	302.	290.
299.	282.	274.	278.	276.	248.	238.	263.	211.	235.
235.	268.	237.	223.	255.	231.	276.	272.	263.	264.
291.	312.	300.	342.	328.	283.	348.	326.	333.	327.
330.	277.	276.	254.	279.	231.	261.	247.	219.	230.
218.	260.	220.	196.	234.	224.	229.	200.	193.	184.
187.	152.	172.	148.	136.	175.	153.	138.	123.	125.
136.	99.	114.	97.	78.	97.	102.	99.	96.	115.
104.	75.	87.	92.	77.	80.	69.	92.	104.	94.
75.	99.	93.	97.	80.	99.	77.	97.	76.	94.
89.	87.	87.	96.	92.	113.	96.	94.	109.	113.
110.	124.	133.	109.	121.	132.	120.	106.	149.	108.
105.	125.	121.	142.	119.	120.	140.	132.	112.	132.
119.	119.	125.	125.	126.	115.	112.	106.	120.	111.
110.	121.	100.	99.	116.	104.	97.	115.	93.	106.
107.	90.	99.	92.	105.	93.	106.	92.	89.	88.
76.	91.	95.	73.	80.	74.	79.	70.	77.	62.
82.	83.	71.	60.	70.	75.	68.	87.	71.	79.
74.	69.	74.	81.	72.	86.	66.	77.	71.	75.
84.	74.	62.	73.	70.	84.	89.	78.	69.	83.
77.	81.	82.	87.	80.	79.	72.	78.	113.	85.
90.	117.	99.	95.	113.	92.	88.	112.	120.	96.
110.	123.	128.	116.	137.	135.	154.	142.	132.	158.
163.	201.	189.	209.	222.	224.	238.	276.	278.	283.
295.	274.	283.	300.	295.	322.	340.	352.	331.	297.
356.	319.	308.	322.	314.	311.	299.	328.	317.	289.
318.	301.	331.	287.	328.	321.	315.	334.	270.	288.
288.	263.	266.	285.	240.	221.	250.	233.	220.	204.
194.	189.	189.	184.	185.	198.	187.	174.	171.	156.
142.	165.	135.	183.	152.	168.	127.	149.	139.	128.
159.	126.	137.	114.	114.	131.	115.	111.	120.	138.
106.	90.	88.	111.	94.	99.	89.	113.	97.	95.
87.	95.	109.	90.	83.	76.	82.	86.	70.	96.
64.	87.	78.	80.	71.	85.	90.	68.	75.	75.
63.	75.	74.	93.	91.	78.	86.	76.	97.	80.
88.	99.	93.	105.	86.	100.	82.	95.	115.	92.
103.	96.	110.	104.	96.	131.	143.	140.	132.	116.
150.	142.	167.	186.	190.	184.	187.	182.	226.	190.
176.	193.	211.	235.	228.	196.	209.	245.	231.	213.
214.	256.	215.	224.	231.	223.	198.	227.	235.	212.
223.	243.	253.	238.	271.	243.	259.	270.	228.	264.
256.	259.	243.	251.	240.	226.	242.	234.	256.	242.
237.	212.	228.	222.	223.	212.	218.	225.	219.	205.
219.	212.	202.	228.	206.	191.	191.	218.	208.	199.
225.	228.	229.	198.	231.	247.	259.	249.	244.	229.
244.	233.	239.	272.	286.	297.	270.	269.	279.	308.
265.	304.	294.	304.	307.	293.	273.	314.	303.	286.
309.	280.	295.	264.	232.	285.	244.	261.	246.	204.
245.	247.	234.	228.	205.	232.	226.	222.	199.	190.
178.	194.	164.	168.	174.	173.	160.	143.	167.	139.
132.	144.	148.	118.	113.	108.	132.	117.	99.	108.
85.	82.	92.	94.	83.	88.	75.	99.	94.	84.
84.	79.	74.	68.	61.	69.	73.	68.	60.	73.
60.	57.	66.	69.	75.	64.	68.	56.	79.	63.
59.	56.	53.	77.	80.	67.	59.	55.	75.	68.
76.	60.	66.	49.	55.	68.	64.	77.	66.	68.
59.	74.	74.	68.	73.	92.	78.	66.	67.	68.
85.	94.	72.	80.	86.	90.	78.	93.	106.	110.
115.	93.	103.	102.	120.	115.	112.	112.	99.	116.
106.	110.	132.	131.	139.	107.	105.	119.	106.	121.
125.	117.	125.	126.	136.	113.	128.	116.	127.	141.
124.	114.	120.	119.	130.	98.	121.	135.	104.	123.
105.	112.	102.	95.	102.	97.	115.	114.	99.	101.
93.	111.	111.	109.	122.	108.	126.	108.	101.	142.
151.	126.	138.	136.	154.	154.	146.	150.	165.	157.
160.	161.	173.	154.	168.	191.	162.	172.	166.	164.
149.	181.	161.	186.	153.	160.	161.	173.	159.	156.

138.	185.	151.	166.	159.	149.	178.	156.	178.	158.
188.	185.	194.	178.	170.	197.	184.	181.	206.	176.
200.	219.	271.	222.	200.	250.	230.	233.	236.	215.
221.	229.	240.	256.	234.	217.	175.	215.	207.	238.
194.	229.	242.	228.	231.	201.	186.	197.	198.	184.
164.	196.	173.	181.	154.	182.	141.	146.	122.	140.
129.	128.	126.	116.	111.	133.	112.	114.	110.	98.
94.	98.	93.	79.	85.	93.	78.	71.	93.	90.
81.	72.	72.	88.	83.	76.	83.	76.	86.	77.
89.	105.	82.	81.	84.	76.	94.	97.	99.	87.
100.	119.	101.	90.	115.	94.	100.	128.	130.	106.
115.	105.	116.	122.	117.	122.	126.	145.	122.	123.
125.	126.	130.	131.	139.	153.	141.	143.	144.	119.
133.	169.	168.	142.	158.	148.	159.	151.	170.	150.
151.	180.	155.	161.	164.	172.	166.	175.	181.	194.
188.	175.	199.	186.	178.	200.	191.	181.	189.	213.
187.	186.	191.	171.	166.	178.	176.	174.	176.	188.
192.	158.	190.	213.	193.	159.	183.	171.	192.	170.
182.	169.	198.	163.	190.	163.	165.	172.	170.	143.
147.	145.	169.	151.	134.	138.	140.	136.	150.	140.
132.	134.	125.	128.	141.	131.	133.	123.	136.	144.
134.	116.	136.	124.	120.	128.	118.	128.	127.	107.
109.	105.	95.	93.	114.	103.	104.	103.	101.	115.
104.	118.	107.	121.	111.	107.	125.	113.	110.	115.
110.	122.	97.	117.	132.	125.	135.	133.	152.	160.
155.	158.	181.	176.	171.	188.	207.	186.	205.	218.
204.	231.	217.	236.	243.	230.	233.	228.	205.	223.
217.	198.	207.	204.	176.	206.	223.	202.	191.	166.
169.	195.	170.	198.	186.	175.	226.	177.	196.	172.
177.	181.	163.	167.	156.	156.	131.	142.	130.	132.
118.	134.	117.	119.	105.	106.	95.	96.	107.	82.
104.	97.	79.	94.	95.	87.	123.	88.	97.	103.
87.	84.	85.	100.	94.	78.	99.	69.	72.	73.
86.	76.	65.	68.	87.	70.	82.	88.	85.	85.
73.	93.	87.	78.	92.	77.	93.	94.	84.	92.
98.	80.	96.	105.	86.	90.	102.	86.	80.	77.
94.	85.	91.	92.	80.	108.	89.	74.	96.	103.
87.	86.	99.	80.	90.	84.	87.	87.	76.	87.
70.	88.	84.	90.	80.	83.	91.	97.	89.	76.
94.	73.	85.	79.	88.	79.	91.	73.	80.	101.
76.	77.	86.	76.	88.	94.	95.	86.	75.	105.
87.	113.	97.	83.	94.	111.	118.	110.	91.	111.
92.	109.	102.	104.	95.	113.	92.	114.	107.	98.
101.	115.	84.	95.	91.	100.	99.	100.	98.	89.
80.	93.	100.	80.	107.	80.	90.	96.	80.	75.
77.	94.	83.	84.	86.	76.	77.	79.	96.	93.
93.	84.	84.	62.	66.	76.	78.	70.	82.	79.
62.	95.	75.	71.	65.	80.	65.	88.	87.	78.
82.	84.	89.	81.	68.	83.	77.	84.	79.	59.
71.	82.	74.	98.	105.	57.	70.	78.	98.	97.
74.	88.	94.	101.	106.	103.	96.	104.	120.	105.
112.	94.	121.	117.	114.	111.	122.	100.	109.	105.
104.	107.	111.	90.	91.	100.	102.	102.	88.	91.
83.	90.	89.	94.	94.	93.	89.	94.	82.	92.
93.	102.	79.	88.	63.	75.	92.	78.	75.	86.
63.	69.	59.	65.	70.	60.	60.	60.	52.	53.
63.	60.	67.	63.	61.	54.	48.	61.	62.	45.
54.	46.	55.	51.	64.	46.	52.	41.	59.	45.
60.	49.	57.	49.	65.	62.	63.	48.	48.	61.
64.	65.	61.	54.	62.	62.	58.	60.	52.	57.
56.	65.	51.	61.	62.	57.	44.	41.	52.	54.
54.	52.	64.	47.	58.	47.	51.	62.	55.	49.
59.	66.	59.	55.	49.	41.	65.	60.	52.	39.
58.	53.	48.	47.	44.	57.	49.	48.	65.	64.
53.	43.	52.	65.	57.	56.	56.	72.	48.	45.
38.	62.	59.	61.	69.	57.	74.	55.	68.	61.
72.	60.	55.	66.	56.	76.	64.	78.	66.	74.
67.	71.	76.	64.	86.	70.	80.	81.	78.	71.
98.	95.	94.	98.	94.	104.	114.	113.	122.	102.

111.	132.	109.	132.	130.	128.	128.	118.	140.	135.
151.	131.	115.	121.	139.	110.	99.	95.	109.	103.
124.	118.	101.	98.	91.	82.	117.	96.	103.	80.
97.	100.	91.	90.	103.	72.	103.	96.	76.	72.
97.	71.	81.	73.	82.	87.	81.	70.	69.	62.
70.	64.	61.	61.	63.	61.	78.	65.	75.	70.
68.	80.	62.	66.	49.	66.	60.	62.	58.	57.
50.	69.	75.	48.	56.	49.	56.	51.	55.	47.
56.	45.	56.	64.	51.	58.	59.	59.	53.	58.
45.	58.	65.	55.	52.	65.	50.	51.	62.	70.
68.	69.	64.	57.	64.	71.	74.	59.	72.	76.
71.	66.	64.	89.	75.	87.	62.	72.	60.	78.
80.	83.	81.	81.	78.	58.	64.	71.	63.	93.
77.	89.	91.	83.	74.	84.	79.	83.	82.	76.
95.	77.	104.	88.	79.	102.	80.	84.	98.	91.
98.	102.	115.	102.	123.	104.	106.	120.	117.	119.
122.	121.	125.	136.	138.	129.	128.	118.	105.	112.
124.	128.	128.	113.	94.	121.	108.	115.	130.	131.
124.	102.	116.	116.	134.	133.	123.	151.	123.	128.
119.	141.	141.	151.	149.	133.	124.	156.	160.	153.
144.	125.	153.	114.	142.	116.	118.	121.	108.	105.
109.	131.	106.	98.	108.	112.	84.	91.	114.	81.
91.	97.	106.	94.	114.	88.	120.	88.	96.	108.
88.	77.	79.	84.	88.	66.	81.	81.	92.	69.
78.	77.	66.	73.	76.	81.	72.	61.	83.	55.
84.	74.	86.	59.	72.	68.	84.	69.	68.	63.
82.	64.	80.	73.	81.	81.	88.	74.	61.	84.
77.	74.	81.	83.	95.	92.	76.	93.	94.	95.
92.	112.	128.	98.	103.	93.	112.	127.	108.	127.
135.	115.	123.	110.	127.	102.	116.	120.	129.	103.
95.	117.	111.	141.	104.	80.	109.	92.	104.	102.
112.	102.	112.	111.	106.	90.	109.	98.	95.	118.
129.	90.	111.	115.	113.	104.	101.	108.	96.	105.
110.	111.	112.	110.	102.	94.	88.	105.	96.	130.
109.	120.	118.	97.	137.	120.	136.	117.	127.	118.
142.	122.	150.	113.	131.	144.	154.	139.	119.	151.
143.	144.	156.	160.	156.	157.	136.	139.	152.	138.
170.	154.	136.	152.	142.	157.	151.	174.	175.	159.
156.	132.	154.	149.	140.	140.	121.	134.	120.	139.
136.	127.	128.	120.	139.	131.	131.	130.	109.	108.
138.	112.	126.	119.	118.	107.	117.	91.	123.	107.
102.	98.	96.	99.	103.	116.	93.	107.	108.	121.
109.	113.	122.	130.	86.	108.	120.	103.	127.	138.
110.	128.	145.	138.	120.	133.	138.	143.	130.	118.
144.	118.	130.	129.	125.	125.	120.	127.	123.	112.
118.	111.	119.	93.	122.	125.	126.	130.	100.	105.
105.	123.	141.	119.	129.	128.	130.	119.	153.	120.
160.	140.	140.	147.	168.	134.	130.	147.	126.	149.
142.	111.	131.	121.	107.	108.	120.	110.	113.	117.
106.	99.	114.	130.	111.	118.	122.	103.	111.	92.
114.	115.	108.	103.	111.	92.	90.	106.	122.	78.
87.	116.	82.	87.	90.	109.	88.	80.	92.	73.
89.	80.	78.	77.	82.	83.	96.	78.	92.	81.
82.	84.	74.	81.	67.	74.	71.	71.	56.	80.
88.	67.	75.	63.	68.	67.	71.	82.	61.	69.
58.	70.	62.	84.	66.	87.	82.	70.	71.	88.
79.	84.	97.	115.	90.	94.	86.	89.	98.	95.
98.	104.	94.	97.	94.	90.	102.	93.	87.	91.
88.	71.	92.	72.	65.	90.	79.	94.	81.	89.
93.	89.	94.	92.	91.	85.	80.	91.	71.	69.
81.	69.	95.	78.	78.	84.	88.	75.	70.	79.
91.	76.	82.	79.	67.	72.	75.	75.	62.	72.
70.	63.	72.	78.	70.	58.	60.	75.	65.	84.
77.	65.	74.	59.	68.	73.	72.	76.	88.	70.
78.	70.	63.	70.	98.	96.	93.	92.	93.	94.
89.	94.	90.	96.	93.	82.	77.	102.	89.	80.
74.	89.	94.	80.	78.	75.	90.	82.	56.	78.
72.	66.	86.	86.	62.	70.	72.	71.	77.	79.
76.	78.	88.	77.	92.	91.	74.	95.	73.	69.

64.	82.	80.	64.	61.	67.	63.	58.	59.	73.
51.	67.	59.	70.	62.	59.	61.	66.	55.	66.
61.	43.	67.	68.	54.	52.	67.	52.	49.	59.
48.	64.	52.	53.	57.	59.	60.	64.	55.	62.
53.	50.	64.	59.	57.	56.	52.	72.	65.	60.
65.	65.	62.	69.	75.	91.	63.	79.	65.	87.
78.	106.	80.	82.	101.	82.	98.	90.	95.	101.
61.	95.	96.	76.	85.	77.	81.	101.	92.	66.
71.	87.	82.	84.	88.	74.	84.	87.	72.	75.
81.	80.	79.	78.	83.	75.	85.	70.	75.	82.
66.	73.	63.	71.	62.	69.	71.	80.	55.	78.
80.	73.	62.	59.	79.	70.	70.	76.	77.	85.
93.	92.	72.	111.	100.	102.	92.	95.	116.	113.
140.	105.	124.	118.	114.	150.	135.	152.	124.	125.
143.	138.	142.	119.	138.	125.	140.	123.	109.	103.
120.	91.	109.	107.	89.	107.	103.	103.	107.	99.
102.	104.	108.	107.	113.	106.	111.	111.	96.	95.
98.	93.	99.	87.	103.	76.	87.	98.	81.	84.
80.	72.	78.	88.	76.	70.	79.	77.	70.	66.
64.	76.	48.	66.	66.	64.	68.	48.	68.	66.
75.	59.	58.	70.	55.	57.	65.	64.	58.	57.
48.	42.	55.	61.	60.	47.	57.	41.	56.	50.
54.	44.	54.	57.	49.	54.	50.	54.	56.	43.
55.	49.	63.	55.	47.	55.	54.	38.	46.	53.
60.	66.	60.	48.	41.	56.	52.	53.	41.	53.
49.	74.	48.	68.	55.	58.	60.	57.	72.	85.
54.	55.	62.	61.	66.	72.	68.	63.	86.	75.
59.	68.	65.	75.	76.	60.	83.	76.	71.	71.
72.	59.	69.	81.	88.	74.	90.	78.	77.	72.
71.	59.	87.	74.	96.	83.	95.	96.	100.	115.
104.	91.	94.	76.	108.	89.	108.	123.	118.	101.
109.	144.	113.	125.	125.	114.	124.	114.	104.	94.
116.	117.	128.	126.	156.	135.	133.	130.	123.	136.
155.	164.	148.	140.	139.	130.	118.	133.	150.	163.
132.	131.	138.	141.	116.	125.	128.	130.	146.	126.
125.	121.	139.	155.	148.	119.	159.	137.	119.	139.
127.	132.	149.	113.	125.	135.	128.	123.	123.	123.
129.	105.	101.	114.	122.	108.	120.	131.	116.	129.
122.	140.	122.	120.	126.	115.	119.	135.	136.	128.
139.	137.	141.	163.	145.	142.	163.	192.	195.	198.
201.	195.	163.	205.	184.	192.	207.	229.	217.	219.
242.	227.	228.	243.	288.	240.	256.	264.	229.	261.
283.	263.	278.	248.	239.	237.	245.	238.	251.	211.
240.	251.	228.	191.	210.	206.	219.	231.	210.	231.
256.	243.	244.	221.	235.	215.	271.	248.	276.	268.
272.	263.	276.	260.	290.	267.	273.	292.	273.	294.
287.	280.	278.	253.	253.	251.	211.	210.	205.	189.
235.	182.	194.	190.	179.	192.	183.	180.	186.	197.
178.	189.	220.	200.	201.	189.	177.	190.	182.	167.
187.	222.	184.	170.	209.	197.	173.	165.	161.	175.
174.	165.	177.	179.	173.	193.	177.	185.	159.	198.
203.	197.	180.	205.	210.	215.	205.	181.	162.	213.
230.	242.	191.	201.	236.	177.	235.	201.	218.	205.
226.	166.	198.	202.	211.	195.	218.	191.	201.	181.
178.	168.	159.	165.	191.	164.	157.	166.	151.	164.
139.	140.	164.	148.	134.	151.	155.	155.	142.	165.
140.	120.	151.	141.	146.	157.	142.	131.	114.	115.
102.	116.	104.	115.	102.	96.	112.	85.	82.	92.
82.	110.	72.	85.	91.	100.	102.	93.	86.	86.
97.	98.	78.	104.	67.	95.	86.	72.	77.	70.
88.	79.	70.	87.	95.	85.	77.	74.	79.	76.
74.	84.	73.	70.	95.	81.	76.	76.	61.	93.
65.	68.	60.	69.	69.	86.	90.	69.	79.	85.
70.	63.	86.	94.	92.	82.	74.	103.	98.	94.
100.	84.	91.	85.	89.	97.	85.	97.	101.	101.
111.	89.	106.	102.	115.	97.	120.	116.	115.	115.
110.	91.	108.	95.	105.	117.	114.	116.	112.	117.
126.	147.	139.	110.	113.	113.	131.	134.	134.	126.
113.	131.	121.	129.	97.	119.	92.	102.	97.	129.

100.	95.	111.	92.	103.	87.	116.	112.	96.	104.
98.	119.	102.	102.	94.	94.	93.	89.	98.	118.
109.	116.	91.	97.	99.	82.	107.	99.	111.	94.
101.	97.	108.	92.	115.	109.	83.	101.	91.	100.
102.	86.	91.	110.	97.	107.	94.	92.	96.	82.
82.	108.	88.	105.	84.	95.	73.	94.	84.	114.
99.	81.	112.	91.	91.	95.	75.	86.	78.	89.
88.	87.	81.	94.	99.	91.	87.	106.	88.	93.
93.	106.	90.	105.	92.	90.	95.	92.	83.	77.
93.	101.	87.	113.	97.	90.	96.	95.	98.	105.
113.	109.	117.	96.	120.	120.	111.	118.	120.	129.
125.	116.	114.	113.	136.	116.	118.	125.	121.	126.
117.	127.	136.	136.	137.	122.	137.	131.	132.	123.
127.	132.	143.	142.	168.	138.	152.	154.	187.	193.
213.	185.	192.	237.	210.	225.	233.	217.	212.	240.
204.	230.	215.	204.	215.	188.	194.	185.	192.	172.
173.	164.	139.	156.	137.	142.	138.	149.	130.	105.
123.	143.	134.	140.	131.	148.	123.	113.	146.	148.
142.	145.	132.	118.	139.	113.	104.	122.	92.	94.
107.	100.	95.	97.	112.	91.	83.	102.	68.	78.
78.	82.	98.	76.	65.	62.	78.	84.	64.	72.
70.	78.	66.	62.	66.	74.	64.	51.	63.	69.
65.	66.	61.	70.	62.	57.	58.	74.	68.	61.
67.	57.	68.	61.	80.	76.	78.	70.	78.	61.
70.	71.	81.	64.	77.	64.	84.	67.	72.	82.
87.	93.	84.	105.	93.	96.	90.	82.	99.	103.
91.	102.	113.	94.	102.	100.	95.	80.	105.	76.
87.	86.	84.	89.	94.	79.	85.	80.	77.	93.
87.	76.	85.	79.	82.	85.	91.	89.	90.	72.
99.	88.	99.	82.	84.	92.	73.	90.	82.	91.
99.	87.	74.	69.	83.	88.	91.	61.	65.	86.
72.	74.	78.	74.	96.	71.	83.	90.	86.	85.
90.	109.	102.	88.	100.	114.	94.	99.	91.	120.
117.	124.	128.	124.	108.	138.	129.	153.	135.	149.
173.	121.	151.	165.	155.	150.	146.	136.	163.	144.
134.	146.	133.	129.	143.	145.	148.	125.	110.	137.
136.	133.	130.	114.	136.	130.	139.	125.	127.	116.
121.	125.	111.	120.	122.	139.	119.	126.	124.	131.
107.	118.	102.	110.	120.	111.	99.	90.	106.	87.
114.	100.	113.	91.	94.	93.	95.	89.	107.	100.
100.	94.	93.	101.	93.	93.	90.	97.	94.	104.
98.	85.	91.	97.	88.	71.	73.	87.	88.	80.
82.	85.	82.	81.	89.	92.	92.	93.	106.	115.
130.	97.	111.	124.	118.	110.	109.	127.	155.	122.
119.	121.	144.	106.	104.	116.	109.	139.	100.	105.
109.	74.	85.	87.	79.	100.	82.	79.	88.	89.
74.	93.	95.	81.	85.	75.	95.	91.	107.	81.
78.	95.	85.	97.	84.	103.	97.	102.	97.	74.
82.	79.	75.	88.	95.	99.	105.	80.	68.	61.
76.	72.	88.	80.	76.	90.	74.	92.	81.	73.
69.	77.	70.	67.	74.	94.	81.	76.	68.	82.
106.	104.	90.	102.	64.	102.	84.	94.	83.	102.
97.	88.	103.	84.	90.	90.	95.	96.	101.	89.
78.	76.	94.	78.	81.	93.	90.	87.	102.	87.
104.	96.	98.	85.	98.	83.	85.	109.	115.	95.
104.	99.	85.	104.	90.	101.	90.	94.	100.	87.
114.	92.	74.	88.	107.	93.	103.	91.	98.	108.
92.	97.	98.	112.	116.	86.	100.	101.	84.	103.
105.	107.	93.	107.	130.	105.	133.	101.	118.	126.
151.	129.	147.	130.	137.	157.	167.	154.	135.	141.
140.	163.	160.	139.	146.	128.	146.	126.	126.	118.
115.	119.	132.	127.	125.	128.	123.	131.	122.	141.
141.	144.	124.	123.	152.	130.	147.	143.	146.	147.
143.	133.	128.	123.	138.	147.	142.	114.	130.	140.
123.	127.	135.	104.	113.	114.	88.	103.	110.	111.
90.	90.	104.	83.	96.	94.	104.	91.	97.	106.
102.	105.	114.	91.	93.	89.	89.	100.	96.	85.
82.	97.	92.	85.	86.	82.	96.	90.	86.	63.
94.	80.	99.	88.	79.	90.	103.	83.	105.	99.

117.	109.	87.	92.	102.	84.	95.	110.	79.	112.
99.	85.	91.	96.	89.	85.	78.	90.	57.	65.
79.	63.	85.	68.	73.	73.	67.	82.	67.	91.
63.	77.	71.	79.	60.	74.	73.	75.	75.	72.
75.	75.	74.	73.	85.	72.	71.	64.	86.	69.
72.	79.	73.	70.	63.	68.	75.	67.	67.	64.
69.	69.	66.	76.	69.	66.	70.	70.	67.	60.
67.	60.	60.	65.	80.	72.	76.	60.	89.	71.
63.	79.	83.	86.	91.	74.	73.	84.	92.	96.
90.	101.	87.	110.	88.	90.	80.	91.	102.	98.
89.	102.	98.	100.	95.	98.	82.	88.	106.	107.
91.	99.	91.	97.	119.	100.	97.	111.	114.	111.
91.	123.	107.	95.	99.	114.	99.	103.	111.	100.
97.	87.	111.	80.	101.	73.	80.	92.	87.	86.
80.	98.	72.	79.	90.	76.	89.	84.	75.	80.
72.	85.	61.	76.	74.	71.	73.	73.	74.	79.
77.	74.	87.	80.	78.	85.	70.	77.	76.	70.
71.	65.	78.	76.	76.	82.	60.	81.	76.	78.
77.	78.	81.	69.	90.	66.	58.	69.	69.	82.
86.	79.	98.	81.	85.	100.	78.	84.	89.	75.
90.	96.	102.	110.	96.	83.	85.	114.	95.	120.
96.	126.	131.	88.	128.	107.	119.	111.	101.	99.
92.	100.	115.	100.	109.	116.	117.	104.	92.	86.
107.	94.	97.	106.	104.	94.	102.	95.	91.	108.
79.	104.	103.	101.	98.	114.	102.	105.	101.	113.
109.	101.	120.	116.	128.	114.	142.	125.	128.	142.
124.	118.	118.	142.	127.	137.	147.	155.	136.	119.
131.	147.	123.	117.	132.	104.	97.	113.	107.	83.
90.	106.	80.	101.	101.	108.	76.	88.	108.	117.
93.	111.	125.	98.	98.	98.	94.	100.	113.	112.
101.	94.	110.	106.	102.	108.	107.	92.	102.	106.
105.	104.	95.	91.	82.	92.	103.	76.	95.	83.
99.	108.	101.	113.	115.	116.	100.	106.	113.	106.
109.	109.	126.	132.	119.	123.	107.	108.	123.	107.
89.	86.	108.	103.	89.	76.	92.	101.	95.	88.
99.	82.	79.	88.	75.	83.	89.	86.	104.	87.
94.	81.	98.	90.	92.	83.	101.	81.	101.	79.
85.	97.	99.	95.	93.	80.	80.	95.	91.	92.
90.	100.	92.	99.	94.	94.	80.	88.	88.	94.
74.	69.	92.	95.	86.	92.	72.	75.	71.	98.
99.	104.	94.	94.	94.	90.	87.	81.	72.	106.
81.	67.	93.	85.	71.	79.	76.	73.	83.	79.
104.	85.	82.	85.	63.	89.	92.	87.	97.	99.
77.	80.	90.	88.	75.	88.	82.	77.	91.	98.
79.	111.	89.	81.	79.	87.	107.	99.	88.	88.
87.	85.	97.	75.	102.	89.	74.	80.	79.	88.
80.	120.	75.	93.	105.	105.	102.	90.	87.	129.
122.	127.	120.	107.	120.	122.	126.	130.	136.	134.
129.	127.	136.	138.	127.	119.	136.	140.	116.	120.
109.	115.	106.	111.	113.	107.	118.	93.	111.	102.
102.	110.	121.	99.	107.	123.	100.	109.	109.	113.
122.	131.	123.	138.	131.	139.	131.	108.	112.	121.
123.	122.	108.	118.	94.	102.	107.	108.	80.	100.
87.	101.	104.	90.	79.	105.	101.	87.	97.	84.
103.	90.	81.	89.	83.	90.	85.	79.	103.	88.
85.	94.	85.	93.	89.	70.	82.	79.	79.	87.
92.	70.	87.	71.	90.	79.	72.	74.	64.	71.
73.	86.	78.	74.	62.	57.	93.	67.	65.	83.
61.	57.	67.	64.	68.	67.	63.	67.	61.	65.
67.	51.	62.	65.	54.	53.	63.	65.	61.	65.
66.	58.	59.	69.	58.	58.	53.	77.	54.	41.
67.	64.	53.	56.	53.	66.	57.	55.	43.	54.
42.	53.	49.	55.	40.	54.	46.	63.	61.	59.
55.	47.	56.	43.	49.	49.	59.	58.	48.	44.
41.	48.	46.	49.	40.	40.	58.	51.	38.	49.
52.	55.	32.	41.	50.	50.	69.	55.	50.	63.
46.	67.	69.	38.	51.	51.	61.	46.	49.	62.
62.	62.	57.	50.	55.	56.	52.	55.	50.	45.
55.	44.	45.	44.	48.	52.	53.	65.	63.	57.

54.	50.	52.	51.	46.	52.	65.	67.	50.	57.
57.	52.	64.	71.	67.	73.	65.	50.	68.	68.
49.	55.	72.	66.	75.	76.	67.	64.	67.	68.
97.	84.	58.	74.	71.	68.	68.	73.	66.	70.
73.	76.	59.	85.	64.	60.	69.	69.	63.	81.
78.	70.	56.	60.	65.	62.	69.	69.	65.	54.
70.	67.	60.	72.	65.	63.	63.	72.	75.	81.
70.	51.	68.	59.	68.	74.	61.	65.	66.	57.
67.	66.	61.	75.	71.	78.	79.	73.	64.	75.
69.	67.	78.	62.	75.	74.	93.	74.	72.	66.
70.	87.	75.	80.	76.	75.	72.	79.	78.	68.
77.	95.	77.	69.	74.	93.	66.	65.	56.	58.
63.	53.	81.	67.	64.	75.	69.	61.	54.	58.
51.	47.	72.	70.	82.	76.	73.	61.	87.	75.
81.	88.	72.	76.	78.	77.	101.	77.	64.	87.
96.	76.	100.	75.	75.	84.	104.	88.	89.	77.
93.	89.	78.	91.	72.	76.	95.	101.	79.	78.
89.	98.	91.	94.	111.	108.	115.	104.	105.	113.
122.	133.	110.	133.	134.	158.	105.	106.	108.	123.
110.	119.	108.	105.	104.	121.	111.	114.	97.	94.
106.	115.	95.	101.	99.	97.	105.	120.	111.	104.
101.	92.	95.	87.	116.	95.	109.	99.	103.	91.
105.	98.	100.	109.	106.	101.	105.	100.	116.	92.
109.	104.	106.	109.	91.	128.	121.	108.	105.	118.
127.	116.	120.	107.	116.	140.	125.	114.	103.	124.
96.	104.	119.	101.	98.	94.	102.	87.	64.	92.
63.	91.	82.	73.	90.	95.	93.	63.	78.	77.
73.	81.	86.	86.	76.	82.	79.	76.	86.	83.
82.	90.	81.	101.	75.	74.	88.	72.	81.	87.
88.	82.	81.	97.	84.	91.	62.	75.	64.	81.
86.	80.	88.	79.	75.	85.	82.	74.	79.	86.
78.	65.	81.	98.	97.	88.	98.	91.	82.	84.
105.	95.	87.	112.	105.	96.	94.	101.	79.	83.
81.	86.	78.	87.	81.	79.	85.	74.	76.	67.
86.	69.	89.	71.	89.	75.	83.	73.	80.	81.
75.	84.	76.	85.	86.	89.	97.	74.	89.	78.
83.	96.	82.	99.	89.	107.	71.	88.	85.	88.
96.	100.	83.	89.	90.	80.	92.	93.	96.	122.
112.	104.	95.	93.	135.	115.	140.	112.	130.	128.
117.	129.	116.	137.	139.	137.	102.	154.	118.	136.
126.	141.	117.	113.	117.	104.	126.	109.	108.	94.
112.	96.	102.	80.	89.	91.	75.	97.	93.	93.
92.	108.	93.	95.	92.	95.	112.	97.	110.	102.
100.	105.	106.	104.	106.	107.	101.	127.	119.	89.
100.	92.	83.	104.	95.	108.	109.	107.	83.	90.
101.	89.	94.	91.	104.	98.	91.	93.	95.	90.
89.	94.	86.	93.	77.	81.	94.	80.	76.	92.
76.	87.	84.	88.	74.	84.	97.	99.	93.	73.
100.	96.	106.	83.	93.	91.	109.	104.	113.	125.
124.	119.	115.	124.	132.	131.	138.	143.	144.	127.
137.	141.	144.	139.	167.	137.	145.	151.	137.	127.
142.	138.	111.	141.	129.	129.	129.	129.	118.	128.
121.	133.	119.	120.	118.	126.	146.	137.	153.	125.
134.	135.	154.	141.	137.	134.	151.	157.	148.	134.
138.	138.	145.	137.	126.	139.	136.	139.	121.	122.
144.	130.	126.	149.	157.	132.	141.	113.	116.	131.
132.	120.	124.	126.	125.	124.	119.	128.	126.	129.
122.	86.	113.	127.	116.	104.	114.	100.	116.	98.
93.	108.	96.	112.	111.	119.	89.	95.	101.	114.
112.	116.	107.	111.	100.	112.	136.	131.	124.	140.
110.	138.	144.	108.	129.	141.	126.	124.	139.	140.
136.	140.	141.	133.	152.	151.	121.	134.	158.	150.
138.	158.	133.	164.	156.	145.	135.	132.	151.	144.
125.	140.	120.	143.	112.	127.	128.	138.	122.	135.
130.	124.	120.	116.	105.	140.	120.	120.	137.	119.
123.	122.	118.	106.	110.	117.	139.	116.	127.	121.
120.	122.	101.	124.	117.	125.	106.	126.	123.	114.
99.	99.	92.	98.	79.	106.	95.	73.	88.	92.
107.	90.	89.	88.	99.	104.	93.	101.	102.	114.

91.	98.	85.	86.	99.	117.	91.	81.	97.	85.
86.	90.	84.	81.	66.	91.	88.	90.	79.	84.
68.	78.	73.	69.	73.	66.	66.	78.	64.	72.
74.	79.	74.	69.	49.	74.	71.	78.	65.	91.
72.	68.	78.	78.	81.	69.	69.	61.	90.	78.
78.	64.	64.	76.	72.	68.	69.	74.	84.	64.
71.	84.	84.	74.	72.	55.	54.	84.	53.	86.
74.	64.	79.	73.	85.	68.	90.	80.	79.	68.
70.	82.	75.	81.	83.	79.	68.	76.	78.	77.
72.	70.	100.	77.	68.	75.	80.	78.	78.	79.
71.	92.	91.	94.	75.	88.	82.	86.	101.	90.
93.	102.	80.	94.	111.	96.	82.	125.	110.	119.
108.	122.	102.	99.	128.	114.	108.	105.	72.	101.
93.	88.	79.	100.	84.	104.	86.	75.	80.	82.
80.	64.	75.	86.	69.	82.	76.	83.	97.	68.
71.	86.	76.	76.	82.	72.	78.	82.	58.	97.
83.	82.	86.	75.	80.	86.	72.	71.	65.	100.
68.	65.	96.	61.	80.	61.	63.	65.	62.	53.
66.	74.	77.	56.	73.	49.	73.	53.	54.	57.
70.	67.	44.	68.	62.	64.	45.	43.	51.	46.
43.	46.	57.	58.	52.	50.	61.	61.	56.	59.
63.	58.	54.	55.	53.	60.	43.	55.	64.	46.
50.	50.	65.	75.	53.	53.	73.	67.	73.	78.
73.	49.	64.	84.	77.	74.	61.	87.	71.	84.
83.	79.	76.	84.	86.	74.	86.	95.	79.	82.
93.	91.	90.	88.	78.	85.	77.	72.	71.	87.
89.	73.	56.	80.	79.	76.	75.	75.	58.	69.
75.	85.	75.	71.	92.	86.	92.	80.	90.	79.
89.	83.	84.	77.	69.	79.	76.	85.	79.	77.
83.	94.	71.	69.	87.	69.	82.	78.	73.	74.
84.	63.	78.	79.	63.	65.	56.	72.	73.	74.
70.	75.	58.	69.	72.	65.	53.	83.	63.	62.
66.	78.	86.	89.	73.	72.	69.	65.	63.	79.
63.	68.	76.	46.	69.	89.	66.	83.	91.	59.
67.	51.	70.	77.	68.	63.	80.	68.	63.	72.
74.	64.	71.	58.	77.	72.	63.	65.	58.	73.
52.	48.	74.	54.	55.	65.	58.	67.	80.	71.
56.	55.	48.	57.	68.	63.	65.	71.	48.	57.
48.	46.	59.	66.	50.	58.	58.	56.	47.	69.
45.	52.	58.	61.	60.	58.	68.	63.	61.	65.
58.	55.	65.	52.	48.	60.	62.	54.	80.	56.
42.	64.	55.	60.	52.	55.	69.	66.	52.	67.
64.	68.	55.	54.	86.	68.	79.	67.	74.	65.
55.	71.	65.	66.	70.	68.	102.	68.	79.	77.
68.	84.	81.	87.	72.	70.	70.	82.	81.	72.
84.	64.	65.	76.	92.	75.	70.	62.	77.	69.
72.	70.	71.	58.	63.	69.	68.	75.	54.	75.
79.	78.	74.	57.	62.	82.	77.	76.	76.	68.
59.	81.	85.	68.	65.	79.	81.	86.	73.	85.
78.	92.	78.	94.	95.	80.	69.	77.	80.	74.
80.	77.	71.	62.	56.	71.	71.	68.	86.	69.
70.	82.	69.	76.	64.	72.	65.	64.	54.	58.
74.	73.	73.	59.	65.	66.	74.	58.	71.	78.
72.	80.	73.	81.	71.	67.	80.	85.	67.	73.
77.	86.	71.	82.	69.	70.	78.	76.	79.	68.
98.	81.	84.	82.	92.	88.	92.	84.	75.	102.
95.	98.	96.	87.	79.	103.	87.	76.	97.	87.
81.	83.	91.	69.	88.	60.	73.	82.	76.	81.
62.	72.	71.	71.	82.	59.	76.	87.	71.	81.
62.	64.	81.	65.	80.	89.	81.	83.	80.	71.
71.	100.	76.	82.	74.	75.	83.	76.	69.	92.
105.	72.	95.	103.	86.	77.	113.	98.	84.	95.
108.	100.	110.	97.	108.	83.	102.	124.	121.	107.
112.	100.	102.	103.	107.	106.	115.	98.	101.	94.
104.	91.	89.	84.	99.	85.	88.	100.	80.	113.
93.	102.	91.	82.	103.	93.	81.	75.	78.	78.
97.	74.	79.	85.	102.	100.	100.	91.	92.	111.
99.	107.	96.	97.	85.	85.	91.	84.	80.	93.
85.	102.	83.	93.	82.	96.	83.	89.	76.	90.

82.	86.	72.	93.	86.	73.	93.	79.	85.	94.
82.	83.	96.	80.	80.	72.	80.	74.	80.	84.
76.	92.	77.	87.	91.	84.	98.	91.	98.	80.
86.	92.	88.	91.	90.	79.	94.	72.	89.	74.
96.	96.	66.	90.	95.	89.	90.	102.	105.	114.
99.	102.	88.	84.	112.	93.	110.	97.	99.	95.
85.	94.	83.	99.	82.	90.	103.	97.	86.	110.
104.	94.	99.	111.	116.	114.	122.	126.	130.	140.
126.	143.	129.	121.	127.	123.	119.	115.	135.	120.
118.	130.	125.	133.	119.	125.	130.	129.	151.	126.
101.	136.	113.	126.	122.	117.	128.	108.	128.	134.
128.	115.	114.	115.	127.	116.	119.	109.	121.	120.
111.	112.	129.	106.	94.	116.	119.	117.	121.	123.
105.	91.	90.	101.	129.	117.	108.	119.	109.	87.
101.	107.	120.	112.	109.	112.	103.	103.	92.	108.
100.	98.	118.	125.	122.	122.	125.	122.	124.	140.
125.	122.	127.	148.	156.	138.	153.	121.	150.	138.
131.	158.	130.	127.	138.	111.	130.	124.	120.	116.
114.	105.	102.	115.	98.	102.	103.	113.	110.	134.
113.	97.	105.	127.	107.	111.	120.	120.	118.	105.
117.	103.	121.	103.	110.	129.	111.	107.	103.	108.
118.	127.	119.	124.	115.	102.	127.	124.	118.	94.
135.	103.	112.	116.	105.	102.	101.	86.	84.	103.
89.	108.	100.	101.	95.	85.	86.	96.	95.	92.
96.	102.	89.	96.	78.	93.	93.	106.	110.	109.
115.	109.	90.	88.	108.	97.	122.	95.	91.	103.
102.	76.	81.	99.	111.	88.	91.	87.	85.	89.
93.	94.	89.	109.	84.	76.	104.	97.	94.	102.
86.	101.	99.	93.	111.	93.	91.	87.	105.	89.
69.	91.	78.	97.	86.	92.	72.	94.	83.	76.
66.	72.	82.	66.	81.	63.	70.	81.	78.	79.
76.	74.	83.	92.	84.	77.	76.	75.	73.	78.
90.	71.	75.	58.	76.	62.	79.	69.	77.	94.
63.	77.	84.	80.	79.	86.	94.	84.	67.	92.
88.	68.	77.	71.	78.	89.	77.	76.	70.	71.
60.	70.	82.	56.	74.	65.	64.	71.	79.	54.
65.	69.	73.	61.	61.	53.	76.	67.	55.	66.
64.	59.	70.	58.	62.	59.	65.	68.	59.	54.
85.	64.	58.	61.	67.	63.	67.	68.	53.	64.
66.	63.	79.	80.	62.	57.	72.	72.	79.	79.
65.	67.	82.	64.	68.	91.	85.	66.	90.	83.
82.	90.	81.	85.	90.	89.	90.	101.	92.	101.
82.	103.	95.	89.	84.	83.	100.	107.	92.	107.
118.	83.	97.	91.	72.	87.	88.	95.	96.	98.
72.	95.	101.	98.	98.	105.	97.	116.	99.	118.
120.	120.	128.	117.	119.	115.	127.	132.	135.	146.
139.	130.	116.	139.	126.	127.	120.	117.	122.	97.
130.	96.	121.	131.	104.	142.	109.	97.	100.	109.
77.	82.	100.	97.	112.	96.	107.	93.	103.	93.
108.	90.	92.	84.	82.	91.	98.	91.	91.	88.
104.	89.	98.	98.	100.	86.	93.	86.	94.	94.
91.	89.	99.	95.	80.	101.	104.	108.	90.	105.
100.	85.	85.	102.	103.	92.	90.	79.	90.	94.
103.	66.	97.	88.	88.	76.	86.	70.	79.	78.
83.	79.	78.	85.	87.	76.	75.	73.	67.	75.
83.	86.	63.	73.	65.	89.	75.	85.	73.	72.
72.	77.	71.	76.	79.	68.	99.	95.	69.	76.
93.	80.	81.	74.	88.	86.	74.	85.	102.	79.
98.	95.	94.	76.	83.	103.	95.	87.	94.	108.
93.	99.	99.	98.	96.	100.	93.	105.	109.	91.
108.	97.	127.	115.	100.	104.	83.	97.	104.	90.
81.	86.	82.	93.	61.	83.	76.	79.	83.	90.
82.	83.	87.	79.	81.	71.	76.	81.	77.	73.
92.	85.	90.	69.	84.	89.	67.	89.	83.	74.
94.	73.	101.	77.	81.	99.	88.	77.	90.	93.
101.	78.	85.	78.	113.	108.	92.	104.	99.	97.
98.	110.	98.	88.	105.	102.	83.	95.	95.	83.
96.	82.	90.	87.	85.	79.	81.	81.	91.	78.
80.	63.	75.	72.	85.	62.	77.	75.	68.	80.

59.	78.	66.	71.	70.	83.	77.	60.	80.	75.
80.	81.	86.	82.	67.	76.	78.	76.	76.	70.
75.	61.	88.	75.	95.	81.	75.	87.	85.	91.
103.	77.	82.	85.	91.	99.	94.	90.	92.	82.
74.	95.	74.	100.	89.	72.	92.	81.	83.	72.
88.	87.	85.	104.	75.	90.	107.	111.	100.	94.
105.	95.	105.	105.	108.	88.	131.	97.	100.	119.
107.	101.	116.	102.	85.	117.	123.	102.	87.	92.
105.	105.	98.	99.	103.	113.	112.	92.	98.	108.
104.	89.	86.	87.	112.	97.	109.	99.	108.	101.
74.	89.	92.	68.	77.	90.	91.	98.	81.	110.
83.	98.	94.	104.	88.	92.	97.	107.	76.	93.
92.	92.	100.	114.	106.	95.	85.	90.	91.	94.
92.	112.	90.	98.	109.	105.	85.	82.	97.	87.
99.	92.	93.	95.	94.	82.	110.	93.	103.	93.
109.	89.	90.	106.	94.	104.	91.	101.	104.	100.
110.	100.	98.	89.	83.	75.	95.	97.	75.	108.
88.	80.	92.	88.	74.	97.	80.	79.	80.	68.
95.	73.	89.	79.	91.	71.	82.	79.	69.	82.
80.	68.	88.	86.	81.	69.	76.	71.	84.	78.
65.	84.	75.	82.	70.	85.	88.	86.	91.	78.
69.	92.	63.	84.	90.	80.	84.	79.	87.	86.
82.	71.	85.	88.	95.	89.	93.	86.	87.	72.
70.	76.	82.	79.	85.	87.	93.	90.	88.	90.
78.	76.	85.	88.	95.	102.	91.	122.	102.	88.
97.	105.	86.	114.	99.	106.	109.	99.	91.	103.
104.	117.	102.	119.	108.	95.	117.	114.	100.	108.
119.	113.	122.	114.	107.	125.	113.	113.	137.	101.
116.	129.	108.	110.	100.	107.	102.	107.	103.	93.
89.	103.	95.	102.	93.	84.	89.	91.	77.	80.
86.	104.	91.	89.	115.	99.	94.	96.	111.	114.
110.	86.	99.	111.	98.	115.	116.	92.	113.	116.
105.	90.	110.	111.	122.	108.	88.	116.	103.	118.
88.	120.	106.	113.	109.	103.	126.	94.	111.	138.
105.	97.	113.	103.	108.	119.	99.	87.	111.	116.
96.	81.	107.	76.	86.	105.	92.	87.	90.	88.
82.	84.	101.	94.	103.	93.	91.	81.	105.	91.
86.	87.	90.	84.	97.	101.	99.	98.	98.	110.
87.	91.	127.	87.	103.	93.	131.	115.	118.	101.
143.	124.	115.	101.	97.	95.	110.	89.	104.	114.
114.	113.	96.	90.	97.	107.	110.	111.	117.	90.
111.	98.	89.	89.	94.	92.	91.	104.	84.	101.
91.	92.	98.	74.	78.	64.	66.	68.	91.	89.
88.	90.	70.	79.	80.	67.	86.	90.	78.	88.
81.	97.	83.	82.	88.	96.	80.	99.	97.	90.
69.	82.	94.	95.	93.	105.	75.	88.	72.	85.
102.	87.	74.	113.	90.	79.	91.	94.	78.	97.
78.	85.	91.	84.	100.	88.	81.	88.	82.	74.
88.	92.	105.	85.	79.	77.	104.	107.	101.	109.
94.	71.	114.	100.	96.	93.	109.	92.	115.	96.
101.	103.	97.	118.	102.	105.	111.	98.	80.	99.
92.	98.	101.	99.	101.	96.	92.	95.	94.	96.
88.	96.	93.	89.	90.	96.	104.	93.	76.	82.
93.	85.	93.	71.	84.	89.	76.	90.	90.	80.
97.	72.	102.	84.	87.	98.	89.	86.	77.	92.
84.	103.	106.	106.	91.	87.	91.	81.	105.	95.
111.	120.	110.	101.	89.	111.	110.	124.	124.	116.
119.	123.	128.	116.	150.	133.	137.	115.	131.	136.
144.	159.	132.	164.	167.	135.	148.	160.	158.	174.
157.	150.	136.	155.	151.	118.	136.	158.	147.	113.
116.	136.	143.	128.	114.	130.	130.	116.	140.	125.
114.	130.	137.	126.	117.	120.	112.	133.	109.	127.
128.	121.	143.	120.	144.	132.	158.	128.	134.	134.
127.	130.	135.	125.	125.	133.	137.	140.	140.	140.
121.	109.	151.	124.	113.	130.	131.	147.	143.	116.
114.	152.	136.	123.	112.	127.	157.	142.	135.	140.
144.	135.	120.	119.	116.	141.	122.	123.	113.	116.
128.	106.	135.	122.	120.	129.	145.	125.	120.	118.
140.	140.	147.	126.	128.	135.	136.	127.	111.	140.

154.	126.	139.	147.	117.	147.	133.	140.	121.	115.
124.	112.	135.	135.	133.	114.	122.	127.	112.	115.
105.	110.	110.	138.	142.	119.	117.	131.	141.	119.
137.	126.	129.	119.	143.	125.	160.	134.	141.	143.
130.	160.	161.	153.	177.	180.	153.	155.	162.	149.
162.	167.	147.	183.	176.	176.	164.	182.	164.	177.
156.	142.	174.	158.	167.	158.	156.	150.	144.	130.
147.	153.	153.	139.	145.	128.	108.	101.	108.	112.
107.	129.	121.	120.	113.	98.	108.	112.	110.	112.
98.	94.	108.	119.	112.	114.	99.	95.	111.	95.
107.	105.	90.	117.	97.	106.	92.	110.	124.	117.
114.	137.	124.	128.	126.	114.	115.	126.	122.	119.
138.	134.	125.	138.	107.	122.	122.	103.	119.	113.
131.	130.	126.	126.	116.	111.	89.	123.	99.	112.
135.	112.	128.	114.	114.	115.	117.	121.	112.	105.
107.	112.	121.	96.	103.	88.	113.	118.	112.	92.
104.	96.	99.	93.	87.	108.	105.	103.	104.	91.
107.	81.	110.	87.	84.	93.	82.	91.	92.	71.
94.	85.	88.	83.	87.	74.	82.	90.	84.	79.
74.	87.	74.	77.	84.	71.	67.	78.	75.	83.
69.	79.	86.	79.	82.	79.	74.	83.	93.	82.
84.	72.	73.	74.	73.	77.	74.	68.	83.	68.
84.	87.	75.	77.	64.	71.	84.	88.	80.	85.
70.	84.	71.	75.	87.	79.	89.	73.	80.	74.
76.	80.	82.	91.	69.	79.	87.	84.	72.	83.
72.	88.	73.	81.	80.	77.	74.	96.	71.	66.
72.	73.	78.	91.	81.	80.	67.	82.	83.	84.
78.	75.	83.	81.	77.	73.	80.	62.	91.	74.
91.	72.	89.	88.	51.	84.	80.	72.	66.	76.
76.	79.	71.	71.	92.	68.	56.	63.	90.	84.
65.	72.	73.	80.	78.	90.	73.	72.	78.	77.
79.	76.	83.	81.	88.	78.	81.	92.	93.	83.
92.									

Appendix P-13: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.02° 2θ

19.00 .02 139.00 50%-olivine mixture of Ol+Py, step 0.02

94.	98.	98.	78.	75.	97.	96.	84.	72.	82.
69.	83.	92.	90.	81.	95.	96.	86.	80.	72.
83.	84.	89.	99.	73.	80.	80.	88.	72.	96.
67.	116.	82.	80.	99.	72.	96.	89.	96.	110.
107.	103.	109.	128.	147.	144.	158.	158.	176.	152.
169.	141.	132.	120.	138.	87.	100.	106.	113.	110.
115.	97.	83.	107.	94.	90.	82.	85.	77.	82.
87.	95.	78.	81.	91.	87.	85.	72.	98.	92.
93.	97.	101.	87.	70.	72.	104.	90.	90.	63.
71.	68.	67.	81.	73.	90.	85.	84.	85.	68.
60.	59.	67.	72.	81.	74.	69.	70.	68.	80.
68.	71.	68.	71.	71.	96.	86.	79.	89.	74.
70.	81.	65.	75.	65.	77.	65.	82.	77.	69.
82.	77.	64.	68.	82.	66.	65.	79.	74.	80.
77.	72.	65.	69.	80.	70.	76.	85.	64.	74.
63.	86.	81.	73.	86.	89.	85.	80.	84.	81.
77.	88.	88.	99.	79.	75.	87.	81.	83.	90.
83.	80.	108.	114.	115.	126.	123.	144.	152.	182.
189.	204.	214.	252.	283.	391.	386.	467.	572.	732.
864.	1026.	1077.	1174.	1141.	1113.	1053.	825.	712.	555.
433.	392.	293.	266.	231.	196.	153.	153.	115.	110.
109.	102.	112.	97.	93.	97.	83.	95.	98.	81.
87.	79.	75.	68.	83.	99.	77.	93.	125.	106.
98.	114.	134.	119.	136.	171.	161.	194.	221.	267.
318.	351.	380.	397.	385.	417.	365.	349.	298.	259.
209.	186.	159.	148.	133.	97.	109.	106.	107.	115.
106.	111.	104.	137.	98.	135.	135.	138.	133.	122.
118.	106.	110.	92.	99.	85.	90.	65.	65.	80.
85.	74.	64.	84.	77.	54.	73.	69.	74.	73.
79.	64.	81.	71.	65.	78.	80.	76.	85.	79.
84.	85.	80.	99.	101.	77.	101.	88.	100.	93.
113.	132.	144.	185.	210.	257.	281.	354.	441.	437.
538.	500.	537.	596.	591.	526.	492.	525.	435.	446.
393.	346.	290.	270.	241.	202.	171.	150.	132.	139.
102.	96.	86.	84.	93.	85.	82.	79.	66.	69.
74.	82.	86.	69.	76.	76.	82.	65.	73.	83.
84.	67.	77.	75.	86.	82.	77.	73.	90.	109.
101.	87.	98.	113.	121.	130.	161.	180.	199.	245.
311.	318.	339.	367.	360.	412.	316.	295.	268.	220.
154.	134.	138.	146.	123.	101.	96.	112.	91.	85.
103.	81.	82.	103.	83.	98.	75.	69.	65.	75.
101.	102.	95.	99.	106.	120.	107.	132.	137.	165.
166.	191.	205.	250.	318.	417.	478.	594.	655.	809.
835.	849.	901.	837.	766.	700.	572.	475.	408.	308.
266.	206.	173.	130.	145.	123.	102.	107.	104.	97.
87.	74.	89.	91.	76.	93.	66.	77.	83.	77.
76.	77.	68.	53.	68.	70.	76.	62.	76.	80.
81.	84.	75.	53.	84.	81.	79.	73.	80.	81.
80.	89.	75.	78.	76.	77.	86.	85.	78.	64.
88.	70.	87.	65.	69.	65.	73.	81.	87.	77.
81.	70.	85.	87.	120.	89.	92.	99.	107.	94.
120.	112.	105.	106.	126.	150.	143.	152.	161.	197.
160.	216.	218.	246.	279.	279.	330.	345.	390.	467.
489.	537.	624.	697.	745.	892.	1026.	1156.	1387.	1728.
2024.	2306.	2608.	2950.	3137.	3057.	3005.	2778.	2490.	2131.
1808.	1491.	1211.	1027.	794.	718.	657.	616.	633.	604.
619.	699.	825.	914.	1025.	1087.	1090.	1064.	979.	910.
704.	617.	551.	425.	347.	303.	283.	247.	234.	237.
235.	218.	223.	214.	259.	264.	311.	328.	372.	443.
537.	657.	799.	847.	1006.	1097.	1153.	1098.	1089.	889.
837.	631.	603.	446.	389.	305.	282.	231.	205.	161.
189.	159.	154.	119.	113.	133.	124.	100.	95.	89.
90.	93.	118.	93.	97.	119.	118.	133.	129.	128.
117.	120.	119.	117.	105.	98.	102.	114.	96.	117.

96.	121.	117.	102.	116.	126.	129.	143.	151.	169.
200.	214.	236.	236.	299.	309.	374.	496.	652.	752.
937.	1071.	1289.	1404.	1503.	1427.	1279.	1232.	1015.	808.
703.	537.	418.	342.	259.	223.	200.	160.	139.	134.
124.	113.	136.	100.	89.	100.	101.	103.	83.	108.
61.	80.	83.	71.	79.	76.	95.	74.	76.	86.
71.	63.	61.	74.	78.	72.	67.	63.	79.	56.
68.	76.	71.	63.	74.	64.	75.	63.	65.	64.
77.	74.	60.	64.	59.	52.	69.	68.	60.	69.
75.	61.	65.	70.	68.	58.	68.	62.	74.	63.
62.	68.	71.	63.	73.	63.	67.	73.	86.	72.
73.	67.	69.	66.	66.	77.	81.	71.	76.	92.
71.	72.	84.	96.	67.	82.	81.	74.	70.	97.
84.	100.	89.	102.	102.	104.	109.	126.	131.	113.
130.	153.	140.	136.	183.	195.	190.	183.	212.	220.
230.	259.	266.	306.	371.	464.	519.	585.	710.	732.
777.	837.	853.	795.	745.	691.	614.	544.	503.	472.
374.	376.	405.	400.	434.	462.	465.	570.	635.	760.
917.	1080.	1362.	1502.	1618.	1776.	1862.	2117.	2195.	2326.
2590.	2696.	2859.	2949.	2988.	2820.	2780.	2425.	2222.	2015.
1671.	1419.	1152.	955.	784.	642.	534.	457.	365.	360.
329.	301.	292.	278.	259.	291.	231.	224.	256.	293.
282.	290.	354.	369.	432.	504.	604.	722.	885.	1082.
1303.	1474.	1650.	1800.	1786.	1755.	1636.	1487.	1350.	1197.
1036.	782.	705.	550.	464.	361.	342.	302.	252.	267.
220.	183.	179.	162.	144.	137.	138.	112.	117.	107.
109.	102.	94.	80.	88.	84.	86.	92.	77.	88.
61.	82.	78.	68.	82.	71.	76.	98.	77.	73.
76.	94.	83.	92.	82.	91.	100.	102.	104.	119.
125.	112.	120.	131.	138.	140.	131.	131.	118.	141.
133.	132.	135.	103.	101.	92.	100.	99.	96.	111.
116.	94.	109.	123.	153.	143.	159.	197.	232.	245.
282.	275.	314.	323.	313.	331.	303.	260.	204.	176.
170.	165.	125.	126.	113.	115.	95.	116.	86.	116.
118.	105.	115.	127.	147.	179.	214.	198.	223.	266.
298.	287.	296.	285.	243.	255.	269.	248.	250.	274.
245.	291.	335.	387.	427.	487.	568.	561.	574.	507.
531.	545.	474.	413.	408.	298.	308.	259.	253.	253.
224.	244.	282.	261.	321.	339.	457.	544.	561.	690.
731.	719.	873.	800.	783.	697.	694.	630.	617.	522.
466.	415.	393.	395.	466.	466.	561.	539.	642.	689.
658.	671.	672.	633.	521.	491.	442.	364.	284.	268.
207.	186.	167.	132.	121.	131.	117.	122.	105.	112.
102.	126.	103.	134.	140.	124.	143.	148.	198.	200.
225.	270.	287.	330.	394.	383.	405.	410.	369.	368.
307.	329.	283.	269.	229.	251.	260.	250.	254.	309.
299.	323.	331.	354.	354.	291.	241.	271.	222.	197.
172.	156.	135.	143.	146.	135.	106.	100.	104.	88.
111.	98.	100.	110.	103.	127.	128.	135.	143.	185.
195.	257.	277.	308.	330.	361.	320.	406.	391.	426.
416.	406.	440.	446.	466.	450.	438.	427.	428.	466.
428.	359.	322.	301.	283.	254.	256.	232.	205.	227.
200.	237.	243.	270.	321.	370.	437.	482.	518.	596.
616.	566.	511.	502.	475.	419.	402.	367.	276.	287.
198.	203.	176.	167.	132.	163.	172.	146.	157.	180.
184.	220.	207.	258.	274.	290.	318.	355.	322.	286.
288.	263.	224.	208.	205.	168.	156.	125.	138.	142.
126.	113.	105.	103.	98.	136.	134.	132.	114.	130.
113.	134.	108.	141.	119.	111.	102.	122.	132.	129.
85.	120.	104.	114.	111.	105.	118.	105.	104.	95.
84.	80.	99.	80.	79.	86.	70.	89.	82.	74.
83.	109.	84.	94.	115.	93.	110.	119.	113.	139.
170.	186.	209.	228.	296.	314.	375.	406.	523.	539.
574.	595.	579.	629.	575.	521.	482.	397.	361.	342.
334.	255.	221.	237.	184.	204.	185.	178.	187.	196.
174.	190.	216.	272.	312.	331.	369.	397.	385.	387.
388.	376.	363.	421.	356.	352.	357.	332.	337.	317.
299.	277.	250.	231.	205.	198.	212.	138.	122.	120.
103.	100.	97.	108.	93.	77.	81.	76.	81.	72.

74.	79.	85.	67.	83.	65.	79.	84.	62.	85.
89.	83.	78.	100.	85.	77.	91.	110.	112.	134.
162.	182.	186.	214.	235.	211.	244.	237.	241.	194.
218.	185.	168.	158.	138.	133.	112.	105.	140.	117.
105.	128.	121.	124.	124.	130.	128.	146.	140.	138.
159.	117.	132.	119.	130.	112.	87.	110.	85.	91.
88.	69.	64.	90.	67.	61.	65.	64.	56.	65.
62.	46.	60.	50.	55.	58.	66.	53.	66.	68.
60.	49.	52.	56.	50.	56.	50.	48.	59.	61.
36.	58.	56.	60.	47.	56.	52.	59.	55.	67.
46.	49.	60.	39.	66.	53.	63.	64.	49.	60.
59.	69.	68.	63.	55.	53.	55.	61.	65.	80.
70.	64.	64.	55.	57.	57.	76.	68.	61.	68.
81.	69.	99.	102.	99.	125.	142.	148.	144.	183.
164.	154.	171.	127.	122.	147.	110.	112.	109.	95.
86.	95.	78.	85.	84.	70.	85.	84.	84.	94.
92.	88.	102.	98.	99.	116.	104.	105.	126.	140.
137.	121.	102.	108.	115.	113.	100.	89.	84.	96.
77.	90.	87.	87.	68.	86.	81.	79.	73.	90.
88.	89.	102.	94.	88.	108.	119.	141.	160.	211.
221.	238.	252.	330.	297.	274.	269.	287.	273.	282.
301.	273.	255.	228.	194.	201.	146.	141.	139.	121.
128.	135.	106.	100.	98.	109.	106.	118.	123.	142.
156.	166.	157.	209.	181.	208.	231.	207.	176.	182.
168.	154.	152.	131.	135.	127.	113.	105.	104.	99.
101.	101.	85.	89.	93.	90.	103.	119.	122.	121.
140.	145.	136.	134.	136.	136.	132.	111.	116.	108.
121.	104.	105.	98.	80.	60.	80.	72.	67.	76.
74.	89.	69.	45.	74.	70.	69.	79.	83.	77.
108.	92.	86.	95.	121.	98.	96.	115.	102.	112.
100.	117.	110.	116.	101.	110.	110.	133.	117.	121.
136.	179.	139.	177.	183.	202.	233.	282.	315.	371.
378.	406.	523.	640.	801.	960.	1167.	1255.	1363.	1455.
1475.	1494.	1401.	1336.	1230.	1155.	1085.	1038.	942.	915.
888.	807.	756.	661.	613.	549.	532.	505.	460.	381.
399.	379.	338.	333.	284.	239.	226.	225.	196.	199.
175.	187.	187.	160.	150.	155.	148.	136.	129.	106.
109.	102.	107.	78.	91.	106.	84.	92.	107.	119.
116.	91.	132.	128.	111.	103.	111.	115.	89.	98.
106.	89.	104.	87.	106.	85.	78.	73.	73.	70.
69.	80.	81.	58.	66.	55.	63.	60.	61.	63.
55.	49.	56.	57.	69.	56.	61.	58.	57.	57.
77.	71.	57.	76.	62.	66.	57.	70.	61.	70.
58.	68.	68.	85.	64.	73.	66.	68.	63.	75.
95.	95.	88.	111.	95.	113.	107.	112.	131.	149.
172.	173.	169.	168.	197.	180.	204.	253.	332.	344.
342.	402.	393.	378.	365.	412.	361.	352.	308.	275.
275.	234.	262.	204.	185.	177.	157.	170.	143.	140.
153.	138.	150.	165.	176.	190.	174.	201.	188.	186.
172.	157.	175.	164.	159.	131.	140.	157.	131.	120.
118.	119.	122.	99.	102.	115.	111.	105.	123.	93.
120.	114.	124.	144.	159.	168.	211.	215.	280.	286.
329.	338.	317.	367.	325.	327.	293.	272.	304.	273.
256.	261.	244.	236.	222.	229.	248.	236.	246.	262.
287.	275.	287.	341.	387.	477.	521.	600.	621.	708.
880.	888.	938.	884.	891.	884.	899.	815.	850.	758.
733.	706.	623.	576.	549.	470.	488.	412.	363.	381.
340.	337.	313.	281.	245.	263.	233.	214.	192.	175.
168.	163.	171.	109.	113.	122.	137.	120.	116.	110.
108.	141.	134.	129.	145.	138.	123.	122.	125.	120.
101.	108.	105.	133.	102.	117.	122.	118.	148.	118.
137.	156.	154.	149.	157.	143.	131.	124.	137.	114.
132.	110.	119.	125.	141.	123.	149.	141.	134.	126.
135.	122.	132.	121.	117.	121.	124.	141.	111.	120.
113.	128.	110.	156.	169.	196.	183.	186.	229.	204.
179.	199.	214.	176.	205.	183.	187.	189.	186.	218.
172.	160.	149.	172.	134.	125.	123.	118.	151.	142.
127.	142.	167.	142.	170.	172.	156.	197.	153.	176.
143.	145.	139.	155.	141.	122.	139.	131.	112.	97.

105.	88.	87.	87.	90.	104.	111.	131.	134.	142.
149.	188.	163.	168.	179.	146.	182.	152.	177.	146.
145.	141.	133.	119.	123.	131.	131.	94.	98.	87.
94.	97.	89.	82.	96.	105.	82.	100.	102.	103.
97.	98.	96.	111.	123.	115.	116.	123.	130.	131.
154.	167.	186.	193.	199.	203.	235.	218.	209.	240.
240.	237.	252.	261.	267.	296.	351.	314.	328.	305.
329.	360.	319.	282.	312.	273.	290.	297.	255.	262.
289.	298.	251.	244.	245.	252.	247.	238.	241.	218.
226.	204.	237.	200.	213.	198.	231.	229.	217.	277.
263.	283.	301.	273.	322.	350.	368.	413.	403.	477.
484.	499.	532.	589.	521.	545.	535.	560.	575.	593.
675.	635.	672.	641.	579.	549.	565.	463.	443.	414.
402.	386.	371.	378.	320.	273.	269.	248.	239.	242.
244.	239.	223.	215.	211.	230.	211.	259.	247.	298.
295.	331.	352.	390.	372.	439.	436.	540.	601.	649.
689.	716.	693.	667.	626.	530.	523.	493.	469.	524.
437.	419.	397.	310.	316.	271.	208.	195.	180.	158.
162.	139.	184.	142.	123.	142.	127.	119.	131.	115.
143.	128.	105.	126.	106.	113.	133.	118.	129.	123.
106.	108.	107.	106.	92.	94.	89.	104.	108.	85.
106.	106.	110.	85.	100.	111.	117.	108.	85.	101.
92.	105.	119.	83.	88.	66.	76.	68.	70.	72.
84.	77.	64.	61.	65.	66.	82.	85.	82.	74.
77.	88.	77.	85.	124.	115.	121.	131.	135.	115.
130.	115.	130.	98.	106.	114.	120.	122.	112.	106.
144.	150.	165.	167.	159.	158.	176.	161.	185.	139.
128.	109.	125.	113.	124.	137.	132.	114.	108.	95.
96.	101.	100.	75.	93.	80.	89.	98.	89.	107.
69.	102.	98.	104.	111.	124.	123.	166.	145.	176.
170.	186.	212.	218.	257.	301.	315.	394.	454.	502.
554.	558.	550.	490.	468.	452.	431.	424.	412.	390.
398.	319.	320.	317.	304.	259.	249.	206.	204.	181.
210.	183.	177.	166.	187.	147.	148.	163.	154.	147.
161.	214.	233.	278.	289.	299.	331.	338.	336.	313.
328.	308.	309.	331.	281.	292.	295.	293.	275.	250.
233.	229.	217.	204.	249.	246.	248.	301.	255.	273.
297.	315.	354.	350.	336.	350.	317.	321.	354.	289.
259.	325.	264.	260.	267.	228.	243.	233.	210.	218.
231.	243.	259.	270.	251.	286.	304.	236.	242.	233.
207.	196.	198.	220.	194.	180.	178.	156.	141.	146.
109.	129.	109.	92.	110.	81.	84.	81.	81.	74.
82.	87.	87.	70.	83.	78.	85.	86.	86.	88.
87.	111.	90.	103.	114.	118.	130.	123.	122.	113.
113.	120.	111.	91.	116.	105.	100.	85.	89.	89.
97.	101.	98.	98.	93.	77.	72.	70.	70.	70.
76.	65.	75.	55.	77.	70.	60.	69.	66.	52.
65.	67.	77.	61.	81.	86.	72.	83.	76.	101.
87.	80.	59.	95.	87.	81.	97.	95.	88.	94.
121.	117.	140.	150.	178.	231.	268.	268.	318.	306.
299.	295.	300.	257.	253.	278.	273.	266.	288.	289.
279.	289.	265.	292.	248.	194.	197.	172.	175.	153.
154.	174.	156.	168.	154.	119.	121.	108.	131.	134.
106.	91.	103.	101.	79.	83.	95.	90.	75.	80.
78.	107.	75.	76.	69.	89.	73.	73.	70.	70.
87.	76.	65.	95.	82.	82.	119.	95.	90.	105.
107.	122.	122.	144.	160.	155.	217.	194.	225.	207.
229.	215.	207.	177.	187.	188.	200.	219.	203.	248.
234.	246.	223.	270.	265.	234.	220.	229.	229.	205.
238.	201.	223.	197.	201.	198.	198.	181.	186.	208.
217.	237.	252.	249.	269.	251.	272.	255.	261.	263.
239.	279.	316.	251.	244.	249.	249.	195.	205.	206.
215.	191.	170.	174.	164.	139.	123.	130.	118.	98.
97.	108.	80.	87.	83.	64.	72.	69.	68.	66.
56.	69.	56.	69.	52.	60.	70.	59.	55.	54.
58.	67.	55.	67.	63.	62.	62.	52.	51.	54.
55.	56.	49.	90.	73.	97.	90.	93.	103.	91.
119.	128.	107.	153.	121.	131.	118.	128.	141.	112.
100.	121.	127.	112.	121.	95.	101.	104.	98.	89.

92.	96.	84.	93.	110.	97.	101.	119.	119.	119.
157.	151.	131.	146.	141.	159.	164.	142.	152.	125.
146.	125.	128.	155.	167.	115.	157.	148.	137.	156.
164.	175.	177.	211.	221.	255.	259.	257.	258.	251.
229.	213.	190.	209.	221.	195.	184.	190.	185.	177.
143.	155.	139.	100.	120.	95.	99.	97.	87.	97.
75.	66.	66.	70.	72.	83.	74.	94.	65.	89.
76.	82.	84.	86.	91.	86.	94.	95.	102.	124.
114.	123.	100.	126.	126.	148.	147.	150.	139.	152.
141.	155.	152.	165.	142.	183.	170.	162.	176.	154.
147.	149.	167.	171.	168.	191.	169.	178.	181.	164.
171.	162.	170.	158.	152.	152.	148.	157.	173.	151.
144.	146.	126.	117.	127.	117.	117.	103.	113.	105.
112.	110.	102.	118.	104.	79.	118.	95.	96.	117.
105.	111.	103.	111.	92.	101.	120.	133.	125.	163.
185.	189.	209.	216.	207.	225.	234.	227.	186.	178.
194.	194.	173.	168.	163.	181.	166.	155.	153.	156.
128.	134.	108.	102.	112.	102.	84.	85.	90.	80.
93.	104.	93.	81.	75.	59.	58.	81.	78.	73.
74.	73.	83.	75.	76.	65.	74.	83.	89.	82.
82.	92.	86.	74.	88.	70.	84.	65.	75.	83.
90.	73.	88.	79.	79.	54.	90.	92.	72.	88.
80.	68.	77.	60.	71.	80.	79.	83.	89.	98.
80.	95.	95.	110.	97.	102.	95.	87.	87.	76.
88.	81.	84.	84.	98.	85.	87.	100.	91.	89.
82.	64.	80.	64.	65.	88.	78.	77.	86.	65.
68.	84.	67.	69.	76.	93.	91.	82.	78.	84.
72.	82.	77.	103.	74.	99.	96.	119.	108.	103.
106.	86.	100.	105.	106.	88.	88.	96.	99.	82.
80.	86.	68.	96.	72.	76.	64.	62.	48.	58.
60.	55.	62.	58.	42.	56.	48.	40.	53.	45.
67.	54.	50.	45.	44.	47.	46.	64.	70.	52.
50.	62.	58.	58.	43.	53.	56.	55.	53.	44.
61.	44.	55.	47.	45.	56.	43.	50.	51.	45.
52.	55.	58.	52.	44.	43.	52.	57.	52.	53.
49.	54.	53.	52.	64.	64.	58.	45.	57.	64.
84.	74.	79.	94.	83.	86.	98.	98.	112.	105.
132.	110.	127.	100.	108.	101.	82.	86.	100.	105.
77.	94.	83.	94.	73.	72.	74.	64.	64.	75.
68.	78.	70.	57.	68.	45.	68.	51.	66.	51.
60.	56.	63.	40.	54.	46.	55.	46.	51.	59.
50.	46.	53.	57.	44.	39.	53.	57.	54.	59.
57.	61.	73.	70.	67.	55.	63.	72.	81.	54.
82.	62.	73.	81.	64.	70.	76.	74.	79.	84.
83.	98.	103.	96.	91.	101.	127.	111.	128.	121.
119.	128.	139.	129.	111.	106.	110.	96.	110.	113.
120.	120.	138.	126.	137.	145.	146.	154.	140.	125.
122.	122.	102.	80.	91.	77.	86.	108.	96.	85.
107.	87.	76.	84.	73.	78.	72.	91.	78.	67.
84.	94.	66.	81.	62.	62.	61.	70.	57.	79.
75.	79.	78.	91.	73.	102.	92.	81.	88.	99.
100.	110.	132.	121.	114.	96.	91.	108.	97.	89.
115.	84.	95.	97.	121.	112.	112.	109.	100.	84.
105.	80.	91.	83.	94.	69.	80.	95.	116.	101.
99.	138.	121.	125.	143.	139.	118.	108.	135.	111.
141.	120.	136.	132.	130.	145.	152.	134.	136.	137.
117.	115.	116.	117.	107.	117.	116.	101.	125.	97.
92.	104.	116.	99.	91.	93.	117.	125.	118.	128.
117.	115.	95.	118.	132.	110.	126.	115.	120.	116.
114.	115.	132.	121.	121.	105.	104.	118.	124.	124.
113.	106.	111.	123.	129.	136.	123.	123.	131.	120.
111.	97.	103.	83.	83.	102.	94.	101.	102.	118.
114.	90.	103.	98.	73.	80.	80.	73.	87.	68.
71.	75.	73.	75.	76.	91.	87.	86.	66.	70.
62.	63.	82.	76.	64.	95.	72.	72.	83.	93.
75.	98.	97.	79.	81.	81.	75.	87.	66.	74.
92.	83.	83.	81.	80.	89.	79.	86.	80.	91.
92.	69.	95.	65.	72.	68.	66.	63.	66.	65.
76.	61.	59.	61.	84.	75.	58.	65.	65.	80.

68.	79.	76.	97.	90.	84.	93.	91.	80.	77.
75.	63.	63.	70.	84.	74.	66.	83.	75.	74.
75.	78.	65.	68.	75.	60.	55.	71.	63.	58.
45.	57.	47.	46.	57.	67.	67.	45.	54.	51.
56.	65.	59.	63.	65.	49.	53.	65.	61.	69.
57.	74.	71.	86.	96.	81.	100.	88.	98.	61.
85.	71.	67.	61.	74.	70.	75.	61.	70.	79.
96.	69.	74.	75.	54.	66.	62.	60.	79.	73.
66.	79.	62.	65.	86.	94.	80.	118.	99.	130.
131.	127.	142.	122.	127.	121.	115.	108.	82.	98.
100.	87.	112.	86.	91.	100.	106.	107.	83.	87.
68.	77.	68.	63.	77.	68.	73.	63.	65.	79.
52.	43.	65.	52.	55.	61.	57.	50.	44.	63.
65.	44.	48.	44.	64.	48.	67.	63.	48.	56.
52.	53.	48.	50.	42.	39.	55.	36.	42.	53.
49.	45.	54.	64.	70.	76.	66.	69.	73.	75.
85.	60.	69.	69.	70.	74.	65.	83.	72.	66.
72.	77.	100.	88.	81.	92.	86.	108.	98.	124.
116.	113.	119.	115.	117.	132.	127.	131.	147.	171.
124.	144.	158.	125.	110.	134.	126.	111.	128.	125.
130.	124.	124.	133.	131.	118.	135.	134.	120.	116.
110.	131.	103.	107.	105.	110.	117.	114.	121.	112.
157.	154.	173.	188.	191.	171.	197.	184.	240.	208.
244.	243.	276.	257.	250.	267.	208.	238.	227.	192.
190.	218.	207.	212.	221.	219.	270.	286.	315.	332.
340.	357.	362.	330.	252.	253.	251.	214.	180.	179.
175.	201.	188.	179.	201.	228.	218.	184.	166.	181.
184.	169.	162.	153.	165.	187.	183.	202.	174.	166.
186.	181.	197.	199.	196.	189.	193.	188.	162.	155.
148.	191.	134.	140.	145.	163.	134.	147.	132.	132.
121.	130.	134.	125.	105.	112.	112.	106.	100.	100.
79.	92.	79.	87.	84.	76.	67.	74.	77.	70.
91.	69.	65.	91.	66.	72.	69.	75.	71.	72.
87.	45.	55.	54.	68.	67.	69.	65.	69.	90.
77.	85.	75.	68.	73.	86.	101.	93.	89.	94.
104.	110.	97.	84.	134.	97.	123.	121.	101.	96.
117.	119.	111.	106.	117.	105.	96.	91.	94.	86.
71.	87.	90.	93.	91.	104.	111.	99.	78.	96.
95.	78.	93.	77.	93.	92.	100.	93.	86.	102.
90.	87.	108.	75.	91.	92.	79.	96.	75.	79.
95.	65.	94.	75.	84.	67.	80.	90.	75.	102.
85.	103.	112.	90.	80.	99.	86.	86.	86.	92.
100.	95.	118.	130.	130.	141.	120.	121.	138.	139.
121.	125.	130.	104.	143.	142.	155.	166.	174.	190.
209.	207.	248.	237.	205.	173.	190.	165.	149.	122.
125.	135.	126.	114.	129.	139.	152.	130.	136.	154.
145.	120.	102.	102.	99.	84.	80.	91.	70.	62.
65.	60.	78.	63.	77.	58.	76.	65.	60.	55.
75.	67.	55.	66.	66.	74.	48.	58.	65.	74.
76.	77.	84.	79.	95.	82.	102.	77.	68.	88.
102.	104.	70.	82.	77.	87.	85.	86.	88.	59.
73.	94.	86.	72.	85.	74.	90.	78.	62.	98.
82.	73.	60.	70.	65.	76.	91.	73.	79.	83.
88.	108.	108.	110.	124.	123.	119.	158.	157.	148.
139.	147.	136.	100.	123.	119.	115.	113.	116.	123.
113.	90.	113.	112.	109.	145.	122.	127.	113.	126.
99.	106.	91.	88.	81.	101.	89.	88.	93.	91.
88.	101.	80.	82.	79.	85.	73.	75.	104.	76.
72.	91.	116.	102.	119.	116.	108.	127.	133.	127.
119.	112.	74.	80.	83.	100.	90.	98.	80.	94.
100.	79.	73.	95.	91.	94.	98.	83.	77.	77.
88.	69.	71.	71.	74.	89.	63.	76.	71.	60.
78.	79.	55.	75.	78.	77.	99.	81.	84.	78.
79.	82.	87.	73.	64.	77.	76.	72.	88.	69.
94.	89.	88.	104.	90.	92.	95.	87.	95.	93.
106.	95.	82.	86.	72.	93.	89.	87.	101.	107.
100.	103.	112.	133.	126.	126.	125.	130.	166.	134.
129.	103.	95.	112.	110.	112.	104.	111.	150.	116.
142.	144.	152.	139.	137.	153.	132.	112.	99.	104.

99.	103.	94.	91.	100.	100.	92.	94.	84.	75.
86.	71.	92.	64.	81.	84.	75.	76.	81.	82.
82.	87.	75.	87.	88.	82.	83.	86.	75.	78.
56.	74.	69.	58.	68.	78.	62.	80.	79.	64.
64.	78.	85.	77.	79.	62.	67.	69.	61.	70.
72.	63.	72.	69.	52.	67.	62.	59.	56.	71.
69.	63.	75.	81.	79.	76.	88.	95.	96.	95.
74.	96.	82.	74.	88.	97.	99.	77.	79.	79.
92.	94.	102.	108.	91.	97.	84.	94.	91.	65.
82.	71.	72.	83.	86.	75.	88.	89.	70.	90.
76.	69.	72.	79.	83.	56.	60.	81.	76.	72.
58.	68.	74.	77.	82.	53.	82.	74.	75.	62.
78.	98.	83.	92.	95.	85.	104.	81.	101.	104.
90.	100.	102.	125.	86.	80.	95.	97.	89.	90.
90.	96.	85.	85.	77.	90.	112.	103.	106.	114.
105.	114.	103.	109.	98.	115.	101.	97.	88.	100.
96.	84.	93.	73.	83.	86.	86.	80.	84.	85.
89.	99.	88.	96.	80.	92.	87.	91.	85.	78.
80.	77.	81.	85.	100.	85.	105.	113.	112.	104.
94.	103.	105.	109.	76.	83.	88.	79.	75.	81.
77.	75.	76.	107.	93.	73.	86.	98.	93.	103.
73.	89.	89.	91.	76.	106.	89.	84.	84.	82.
79.	88.	76.	96.	70.	79.	82.	59.	68.	74.
86.	72.	75.	91.	72.	77.	86.	92.	86.	80.
91.	85.	80.	81.	85.	86.	73.	87.	83.	80.
76.	77.	77.	102.	75.	104.	95.	109.	103.	139.
111.	121.	137.	134.	112.	107.	143.	108.	120.	126.
110.	102.	107.	92.	113.	92.	112.	121.	119.	139.
132.	116.	121.	107.	123.	97.	84.	92.	89.	83.
67.	75.	78.	81.	79.	71.	75.	86.	78.	65.
84.	77.	77.	84.	67.	66.	68.	54.	80.	64.
61.	64.	58.	52.	62.	56.	53.	66.	56.	58.
57.	51.	66.	49.	73.	60.	55.	53.	52.	55.
56.	43.	68.	47.	45.	51.	52.	54.	58.	52.
47.	45.	57.	49.	46.	54.	46.	53.	46.	55.
56.	47.	56.	55.	67.	47.	47.	52.	47.	52.
49.	44.	44.	33.	42.	42.	40.	53.	48.	46.
61.	43.	65.	56.	64.	57.	59.	59.	67.	69.
50.	49.	71.	67.	72.	63.	58.	82.	49.	78.
59.	80.	68.	75.	66.	69.	62.	55.	49.	68.
55.	66.	54.	58.	71.	60.	60.	54.	78.	70.
66.	59.	68.	67.	59.	65.	66.	74.	81.	65.
62.	71.	62.	68.	60.	66.	62.	69.	65.	63.
55.	65.	69.	74.	55.	63.	62.	65.	79.	66.
75.	84.	78.	69.	90.	82.	90.	66.	76.	71.
78.	90.	82.	79.	95.	104.	103.	97.	105.	111.
111.	133.	112.	111.	108.	105.	97.	78.	92.	99.
84.	84.	79.	81.	85.	86.	81.	93.	108.	99.
89.	103.	108.	107.	89.	99.	100.	116.	104.	103.
115.	97.	103.	93.	89.	88.	81.	71.	67.	85.
73.	70.	77.	59.	70.	75.	77.	82.	89.	73.
73.	84.	80.	77.	89.	79.	77.	75.	73.	76.
52.	78.	70.	68.	85.	88.	93.	82.	105.	87.
65.	94.	68.	80.	84.	66.	77.	82.	52.	75.
72.	72.	63.	78.	66.	78.	83.	76.	84.	81.
82.	80.	89.	80.	88.	82.	91.	94.	84.	93.
100.	109.	121.	135.	132.	126.	133.	124.	106.	114.
111.	95.	97.	88.	89.	79.	79.	65.	88.	84.
83.	87.	92.	97.	105.	102.	90.	110.	105.	119.
88.	90.	91.	89.	79.	79.	79.	78.	83.	67.
88.	77.	89.	90.	72.	85.	99.	91.	105.	94.
82.	107.	113.	112.	107.	112.	109.	141.	152.	138.
139.	132.	132.	125.	127.	113.	127.	107.	111.	126.
120.	118.	123.	124.	124.	146.	135.	129.	130.	105.
120.	121.	124.	122.	121.	125.	102.	124.	104.	102.
108.	101.	91.	103.	112.	125.	110.	93.	110.	104.
100.	115.	90.	99.	97.	97.	109.	112.	119.	137.
99.	115.	114.	122.	148.	142.	146.	142.	135.	124.
130.	139.	121.	115.	117.	122.	129.	112.	124.	105.

109.	124.	135.	110.	147.	116.	112.	120.	105.	118.
113.	116.	99.	85.	107.	90.	89.	89.	74.	84.
87.	109.	64.	109.	80.	96.	80.	90.	95.	73.
81.	72.	54.	76.	64.	64.	71.	47.	62.	67.
76.	66.	56.	60.	59.	71.	77.	67.	70.	68.
60.	83.	64.	59.	67.	73.	72.	68.	73.	75.
69.	75.	61.	60.	76.	82.	69.	58.	77.	71.
75.	63.	70.	59.	72.	88.	85.	90.	78.	105.
113.	81.	109.	105.	110.	94.	97.	84.	104.	99.
95.	85.	66.	73.	74.	83.	78.	61.	75.	82.
56.	71.	74.	70.	74.	74.	85.	92.	88.	68.
63.	79.	53.	70.	75.	53.	48.	53.	51.	70.
51.	52.	56.	45.	40.	52.	48.	54.	52.	46.
56.	51.	58.	50.	50.	62.	50.	53.	58.	64.
68.	61.	73.	63.	97.	90.	90.	70.	85.	86.
87.	74.	65.	69.	78.	83.	75.	60.	79.	75.
82.	68.	81.	51.	71.	65.	63.	78.	83.	71.
74.	77.	60.	68.	73.	47.	74.	50.	67.	68.
70.	68.	61.	60.	59.	58.	71.	62.	83.	68.
58.	53.	78.	67.	79.	68.	58.	56.	66.	69.
54.	52.	60.	63.	47.	59.	53.	47.	48.	57.
48.	45.	68.	63.	57.	58.	55.	66.	58.	52.
60.	49.	60.	50.	46.	55.	57.	55.	58.	52.
75.	63.	66.	66.	51.	56.	55.	56.	53.	52.
68.	68.	64.	69.	70.	75.	62.	72.	72.	82.
69.	75.	59.	91.	68.	44.	66.	48.	62.	73.
82.	67.	72.	73.	67.	73.	84.	83.	77.	91.
78.	75.	77.	69.	78.	63.	75.	59.	56.	65.
78.	65.	63.	56.	67.	63.	66.	65.	66.	56.
80.	77.	70.	72.	76.	74.	79.	82.	83.	76.
100.	106.	104.	103.	91.	83.	82.	68.	86.	69.
70.	61.	66.	73.	52.	71.	60.	64.	70.	68.
60.	82.	78.	78.	74.	80.	85.	76.	93.	85.
98.	79.	100.	94.	100.	110.	97.	90.	112.	112.
95.	99.	82.	85.	88.	85.	80.	77.	86.	108.
76.	77.	87.	83.	84.	76.	80.	70.	81.	72.
87.	90.	81.	84.	70.	80.	76.	66.	87.	56.
86.	86.	51.	60.	86.	88.	79.	85.	72.	75.
85.	65.	70.	75.	70.	86.	77.	79.	82.	96.
83.	90.	90.	86.	76.	85.	78.	81.	100.	91.
79.	102.	94.	96.	88.	114.	116.	105.	104.	101.
99.	115.	103.	98.	109.	108.	137.	91.	102.	108.
112.	126.	134.	122.	116.	92.	118.	113.	103.	100.
105.	99.	109.	105.	96.	90.	90.	86.	94.	99.
92.	93.	97.	98.	101.	101.	114.	111.	136.	113.
157.	140.	120.	131.	117.	127.	110.	115.	93.	86.
116.	93.	101.	90.	97.	104.	89.	98.	106.	87.
84.	122.	112.	102.	102.	108.	90.	89.	96.	104.
87.	96.	94.	97.	105.	87.	70.	93.	67.	88.
94.	92.	89.	107.	85.	94.	81.	91.	80.	76.
88.	65.	106.	73.	82.	75.	94.	85.	84.	91.
99.	83.	72.	79.	76.	72.	79.	84.	61.	66.
53.	67.	70.	71.	74.	62.	66.	87.	68.	63.
72.	74.	68.	72.	68.	73.	83.	67.	73.	69.
81.	62.	51.	67.	56.	56.	68.	62.	51.	65.
59.	36.	51.	62.	78.	55.	65.	45.	50.	45.
62.	67.	65.	63.	68.	60.	60.	65.	69.	65.
69.	79.	74.	66.	89.	91.	77.	80.	96.	92.
84.	80.	82.	77.	98.	86.	95.	77.	79.	92.
101.	83.	112.	115.	106.	116.	135.	132.	123.	153.
133.	117.	97.	95.	109.	104.	113.	112.	120.	110.
91.	99.	79.	70.	95.	98.	87.	86.	74.	90.
92.	82.	98.	86.	99.	100.	87.	104.	84.	100.
95.	95.	75.	71.	67.	93.	76.	66.	65.	67.
97.	82.	74.	76.	63.	83.	85.	52.	66.	52.
73.	59.	79.	65.	78.	76.	79.	80.	76.	92.
87.	97.	102.	89.	101.	94.	77.	89.	113.	87.
96.	82.	97.	89.	84.	84.	74.	87.	75.	80.
81.	83.	75.	65.	77.	79.	86.	80.	93.	78.

73.	83.	80.	87.	84.	97.	83.	100.	97.	76.
90.	78.	89.	84.	80.	72.	73.	62.	66.	67.
74.	68.	64.	66.	61.	75.	55.	62.	58.	74.
67.	76.	68.	80.	63.	83.	77.	76.	75.	69.
87.	73.	75.	75.	76.	75.	66.	94.	74.	71.
69.	96.	95.	93.	86.	91.	120.	84.	81.	115.
103.	110.	112.	97.	91.	86.	105.	102.	102.	79.
95.	110.	82.	70.	81.	89.	74.	89.	73.	87.
87.	95.	80.	75.	90.	85.	78.	94.	87.	89.
100.	85.	79.	85.	99.	83.	77.	86.	103.	103.
68.	111.	81.	102.	86.	95.	84.	83.	77.	83.
75.	86.	98.	77.	82.	73.	67.	64.	66.	76.
81.	79.	66.	91.	69.	72.	84.	55.	67.	90.
71.	86.	72.	92.	74.	80.	68.	77.	76.	69.
78.	85.	83.	75.	80.	85.	86.	90.	90.	81.
107.	99.	87.	95.	95.	85.	87.	101.	115.	113.
119.	125.	102.	111.	105.	109.	92.	94.	82.	99.
75.	91.	88.	84.	96.	84.	100.	99.	93.	96.
93.	122.	122.	99.	123.	113.	97.	89.	104.	99.
95.	86.	99.	105.	98.	109.	77.	92.	84.	95.
86.	96.	79.	92.	69.	98.	78.	72.	81.	86.
87.	76.	95.	109.	94.	89.	102.	96.	102.	89.
94.	101.	105.	102.	93.	93.	90.	88.	81.	90.
87.	81.	99.	88.	79.	87.	83.	57.	80.	76.
67.	80.	60.	88.	66.	83.	60.	88.	95.	82.
83.	83.	74.	74.	83.	88.	87.	83.	86.	66.
77.	81.	81.	71.	82.	70.	86.	71.	84.	91.
105.	90.	104.	95.	97.	87.	84.	112.	86.	86.
92.	91.	74.	100.	93.	93.	91.	94.	97.	84.
75.	68.	84.	81.	63.	89.	91.	96.	85.	89.
84.	87.	112.	81.	92.	90.	104.	100.	113.	111.
119.	124.	127.	112.	119.	153.	123.	138.	123.	125.
127.	109.	112.	112.	127.	119.	120.	107.	98.	118.
96.	124.	119.	108.	104.	118.	122.	107.	135.	108.
106.	105.	109.	122.	120.	106.	105.	98.	113.	135.
132.	131.	128.	139.	115.	126.	136.	110.	113.	123.
118.	124.	115.	112.	123.	134.	112.	135.	114.	132.
103.	119.	117.	124.	120.	121.	114.	108.	113.	116.
129.	114.	113.	137.	138.	134.	125.	138.	136.	133.
156.	151.	150.	164.	178.	150.	194.	172.	150.	170.
154.	140.	134.	126.	114.	102.	114.	107.	113.	109.
115.	112.	92.	92.	106.	112.	100.	98.	92.	123.
109.	121.	99.	91.	102.	101.	100.	106.	110.	121.
118.	114.	107.	113.	116.	112.	104.	107.	100.	94.
80.	101.	97.	115.	83.	97.	90.	106.	84.	86.
114.	76.	72.	89.	89.	69.	95.	75.	74.	85.
62.	69.	67.	74.	65.	62.	65.	64.	78.	68.
79.	69.	76.	77.	81.	69.	66.	79.	69.	61.
84.	72.	78.	68.	81.	68.	73.	63.	67.	59.
81.	70.	71.	72.	70.	68.	85.	78.	52.	71.
83.	76.	88.	83.	81.	63.	76.	72.	79.	74.
64.	53.	77.	66.	70.	67.	73.	61.	75.	77.
72.	70.	92.	71.	67.	60.	71.	76.	86.	90.
71.									

Appendix P-14: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.03° 2θ

19.00	.03	139.00	50%-olivine, 0.03 degree 2-the						
90.	100.	79.	85.	83.	76.	80.	67.	60.	76.
81.	74.	83.	82.	96.	80.	82.	84.	87.	93.
104.	93.	77.	83.	80.	90.	81.	95.	109.	128.
130.	169.	153.	182.	135.	150.	137.	146.	130.	116.
98.	89.	117.	113.	89.	91.	90.	86.	81.	74.
81.	80.	80.	84.	95.	94.	92.	84.	81.	89.
95.	76.	79.	74.	74.	82.	71.	83.	78.	72.
67.	58.	69.	63.	76.	75.	68.	80.	65.	71.
78.	74.	87.	79.	74.	75.	77.	61.	75.	75.
60.	67.	73.	72.	83.	78.	85.	87.	68.	72.
77.	82.	54.	71.	75.	74.	95.	69.	89.	92.
70.	80.	94.	92.	97.	80.	90.	121.	111.	141.
155.	152.	197.	221.	280.	371.	423.	603.	783.	929.
1008.	985.	947.	827.	714.	526.	405.	296.	227.	175.
138.	133.	116.	123.	86.	93.	101.	98.	95.	89.
90.	80.	80.	105.	114.	115.	114.	120.	150.	192.
223.	270.	342.	335.	385.	388.	342.	308.	256.	221.
171.	141.	129.	105.	117.	106.	113.	117.	139.	110.
118.	141.	117.	129.	98.	92.	80.	81.	73.	78.
77.	77.	84.	65.	60.	77.	89.	78.	88.	90.
59.	80.	83.	84.	87.	102.	94.	91.	102.	129.
163.	220.	333.	344.	413.	472.	569.	587.	534.	500.
510.	458.	441.	345.	283.	242.	197.	134.	118.	97.
91.	77.	83.	77.	93.	70.	76.	72.	82.	84.
74.	85.	96.	75.	77.	78.	98.	79.	92.	113.
121.	132.	155.	181.	211.	278.	308.	333.	346.	315.
293.	262.	242.	167.	160.	133.	101.	106.	101.	85.
82.	83.	91.	69.	80.	85.	82.	126.	100.	135.
150.	148.	212.	220.	297.	416.	513.	622.	722.	711.
736.	684.	642.	481.	379.	299.	259.	196.	167.	124.
100.	87.	77.	99.	73.	83.	87.	64.	79.	78.
87.	59.	86.	81.	75.	74.	94.	78.	76.	75.
72.	86.	84.	76.	85.	87.	92.	79.	89.	88.
68.	93.	82.	78.	62.	88.	83.	89.	95.	117.
75.	88.	103.	109.	103.	134.	156.	184.	211.	229.
287.	280.	322.	347.	428.	488.	565.	685.	909.	1062.
1263.	1631.	2023.	2478.	2955.	3054.	2876.	2693.	2319.	1750.
1352.	1012.	853.	719.	655.	690.	753.	883.	874.	933.
983.	862.	743.	645.	446.	378.	312.	243.	236.	223.
221.	259.	270.	323.	457.	564.	701.	838.	966.	1048.
1096.	1057.	862.	725.	568.	401.	317.	211.	173.	154.
124.	120.	95.	102.	106.	89.	105.	113.	111.	114.
103.	117.	96.	95.	125.	91.	118.	91.	99.	107.
102.	119.	123.	143.	138.	169.	231.	232.	309.	397.
571.	805.	1003.	1187.	1311.	1338.	1237.	1068.	845.	615.
476.	321.	259.	206.	166.	142.	110.	105.	87.	104.
102.	101.	91.	96.	73.	73.	83.	72.	65.	66.
73.	74.	72.	75.	59.	65.	58.	79.	71.	75.
67.	62.	79.	56.	61.	67.	75.	65.	61.	61.
71.	66.	70.	56.	59.	76.	75.	60.	69.	72.
70.	63.	60.	64.	70.	63.	63.	72.	71.	75.
63.	93.	61.	68.	95.	73.	84.	86.	111.	107.
110.	142.	152.	152.	172.	154.	174.	183.	218.	244.
305.	411.	471.	593.	724.	731.	749.	722.	676.	626.
550.	492.	427.	438.	414.	513.	548.	680.	826.	1074.
1247.	1508.	1754.	2144.	2513.	2731.	2943.	3027.	3111.	2849.
2689.	2275.	1867.	1415.	1073.	757.	553.	466.	414.	364.
295.	270.	248.	282.	270.	272.	357.	410.	531.	616.
920.	1144.	1402.	1563.	1726.	1713.	1675.	1402.	1185.	1070.
844.	611.	474.	361.	276.	252.	197.	178.	142.	134.
117.	119.	91.	113.	101.	101.	96.	93.	73.	79.
76.	83.	61.	68.	86.	75.	83.	74.	79.	84.
107.	113.	112.	119.	114.	126.	131.	143.	150.	137.
131.	123.	105.	112.	100.	100.	125.	104.	131.	167.

202.	268.	276.	307.	313.	255.	267.	213.	177.	171.
132.	108.	113.	108.	105.	100.	122.	135.	146.	196.
210.	232.	272.	253.	266.	260.	239.	251.	254.	340.
334.	409.	479.	521.	524.	534.	497.	431.	355.	330.
283.	248.	226.	261.	322.	434.	437.	599.	697.	780.
804.	784.	755.	681.	598.	505.	512.	475.	520.	573.
572.	671.	642.	661.	595.	474.	428.	360.	253.	210.
173.	141.	132.	133.	123.	130.	121.	127.	145.	137.
160.	192.	255.	237.	307.	309.	331.	365.	310.	298.
290.	261.	254.	238.	313.	321.	321.	323.	373.	302.
281.	281.	209.	169.	172.	123.	122.	124.	104.	114.
103.	132.	128.	149.	180.	213.	247.	293.	338.	333.
429.	441.	432.	464.	486.	454.	467.	431.	408.	370.
330.	280.	266.	228.	240.	204.	236.	274.	352.	412.
472.	560.	554.	576.	545.	496.	415.	354.	286.	238.
198.	183.	178.	181.	160.	217.	261.	255.	275.	315.
300.	295.	244.	273.	216.	170.	162.	140.	118.	111.
99.	111.	119.	101.	116.	109.	130.	116.	129.	131.
127.	127.	122.	118.	110.	108.	91.	86.	96.	91.
72.	66.	72.	93.	87.	94.	102.	105.	99.	134.
112.	187.	145.	217.	290.	333.	433.	503.	544.	590.
633.	553.	530.	519.	354.	338.	293.	239.	205.	181.
199.	182.	176.	202.	210.	268.	354.	327.	359.	374.
365.	397.	359.	352.	330.	310.	246.	251.	231.	167.
146.	142.	120.	92.	103.	85.	75.	59.	75.	74.
84.	70.	84.	79.	84.	78.	100.	73.	98.	88.
142.	136.	174.	177.	204.	218.	206.	228.	224.	188.
184.	127.	125.	114.	122.	125.	134.	143.	142.	153.
152.	141.	143.	121.	128.	105.	104.	98.	99.	76.
74.	83.	69.	68.	66.	54.	73.	51.	54.	55.
58.	59.	63.	46.	52.	55.	43.	46.	63.	50.
54.	61.	54.	43.	55.	63.	54.	43.	45.	52.
55.	53.	58.	54.	47.	67.	53.	67.	58.	77.
63.	59.	58.	77.	74.	67.	97.	91.	138.	134.
156.	126.	179.	128.	141.	122.	135.	122.	91.	97.
84.	90.	90.	66.	86.	96.	82.	106.	113.	114.
100.	128.	120.	106.	93.	96.	122.	93.	80.	70.
70.	65.	85.	66.	79.	88.	98.	95.	117.	164.
157.	205.	243.	280.	315.	287.	341.	319.	299.	289.
250.	222.	205.	182.	160.	143.	136.	111.	113.	117.
147.	135.	154.	203.	195.	221.	190.	185.	197.	166.
164.	116.	109.	101.	114.	93.	104.	94.	102.	129.
105.	115.	120.	155.	137.	143.	143.	105.	120.	127.
102.	90.	65.	77.	75.	97.	57.	73.	61.	79.
79.	105.	95.	98.	125.	110.	103.	116.	120.	113.
115.	111.	110.	142.	130.	151.	164.	189.	218.	226.
284.	374.	418.	519.	759.	899.	1146.	1355.	1459.	1437.
1439.	1271.	1163.	1088.	983.	911.	822.	695.	661.	577.
517.	468.	389.	368.	338.	267.	257.	236.	208.	197.
191.	170.	156.	139.	126.	119.	101.	97.	94.	109.
112.	109.	107.	98.	112.	102.	89.	92.	88.	100.
93.	75.	96.	94.	81.	72.	77.	64.	61.	66.
70.	53.	65.	69.	64.	74.	54.	45.	48.	66.
77.	76.	57.	68.	60.	64.	61.	70.	74.	57.
80.	103.	102.	108.	95.	120.	134.	126.	153.	166.
134.	212.	237.	312.	311.	341.	347.	418.	364.	384.
310.	303.	308.	263.	237.	162.	172.	151.	151.	169.
143.	205.	188.	187.	217.	182.	160.	161.	157.	135.
143.	126.	113.	102.	117.	114.	103.	131.	113.	117.
130.	161.	187.	247.	286.	360.	362.	311.	361.	303.
301.	299.	289.	257.	233.	229.	229.	231.	273.	305.
339.	387.	505.	609.	690.	792.	844.	871.	916.	896.
922.	863.	729.	672.	652.	517.	465.	427.	362.	337.
313.	288.	240.	187.	195.	178.	156.	157.	130.	134.
145.	120.	133.	128.	146.	127.	126.	130.	122.	106.
109.	117.	149.	116.	132.	143.	159.	158.	151.	141.
159.	145.	137.	119.	146.	149.	133.	112.	127.	129.
112.	107.	127.	146.	118.	113.	127.	146.	154.	173.
211.	180.	206.	180.	160.	183.	224.	192.	190.	165.

143.	155.	152.	152.	122.	144.	159.	159.	173.	157.
146.	142.	139.	140.	116.	121.	92.	111.	103.	72.
93.	81.	102.	104.	149.	160.	165.	189.	148.	146.
159.	135.	143.	125.	132.	114.	107.	97.	101.	87.
91.	96.	90.	88.	102.	88.	117.	109.	129.	118.
141.	148.	153.	169.	174.	200.	234.	221.	251.	264.
293.	257.	288.	302.	318.	301.	260.	264.	291.	289.
271.	292.	283.	232.	262.	237.	254.	209.	235.	216.
228.	252.	227.	220.	248.	255.	302.	336.	325.	400.
459.	564.	510.	530.	533.	526.	588.	610.	611.	684.
675.	633.	573.	583.	488.	487.	404.	374.	363.	326.
296.	268.	233.	252.	242.	261.	247.	273.	291.	338.
369.	426.	537.	625.	705.	650.	665.	665.	595.	557.
527.	503.	427.	399.	330.	283.	240.	225.	173.	152.
153.	146.	127.	106.	133.	128.	124.	115.	122.	131.
123.	109.	108.	121.	117.	96.	99.	118.	118.	102.
117.	85.	106.	100.	91.	99.	81.	66.	106.	79.
82.	80.	80.	66.	72.	66.	71.	72.	80.	83.
112.	96.	132.	130.	116.	141.	120.	110.	126.	135.
131.	149.	140.	372.	150.	162.	161.	152.	147.	130.
128.	144.	99.	93.	124.	104.	81.	104.	87.	106.
106.	97.	93.	114.	115.	128.	154.	163.	188.	223.
222.	280.	336.	380.	459.	438.	486.	474.	485.	434.
390.	407.	338.	332.	283.	238.	184.	201.	160.	176.
181.	140.	155.	172.	190.	218.	225.	276.	322.	314.
323.	302.	345.	300.	331.	292.	306.	322.	253.	250.
261.	242.	277.	293.	321.	317.	324.	371.	426.	322.
329.	323.	314.	288.	254.	237.	271.	213.	240.	225.
257.	251.	265.	277.	228.	228.	213.	189.	230.	199.
158.	127.	108.	109.	84.	86.	84.	92.	78.	79.
83.	87.	74.	104.	87.	84.	82.	111.	101.	121.
125.	133.	110.	123.	114.	115.	109.	88.	116.	109.
84.	84.	76.	87.	67.	68.	84.	74.	65.	78.
54.	66.	76.	53.	89.	73.	80.	78.	69.	100.
88.	76.	111.	89.	104.	134.	129.	165.	196.	250.
262.	283.	283.	301.	305.	304.	321.	303.	286.	276.
253.	250.	220.	184.	179.	188.	160.	144.	139.	125.
137.	142.	117.	106.	100.	88.	89.	79.	89.	61.
78.	84.	97.	87.	70.	88.	85.	94.	102.	76.
95.	120.	122.	130.	158.	175.	215.	208.	218.	206.
205.	222.	216.	244.	246.	252.	258.	251.	213.	232.
190.	228.	233.	220.	180.	206.	232.	201.	218.	237.
250.	269.	275.	250.	257.	289.	273.	250.	232.	221.
222.	217.	216.	209.	177.	129.	119.	133.	134.	99.
69.	93.	77.	91.	67.	54.	83.	75.	60.	55.
66.	52.	71.	70.	65.	54.	69.	67.	73.	66.
86.	78.	91.	99.	102.	123.	119.	111.	109.	125.
124.	128.	117.	130.	108.	134.	116.	105.	116.	96.
102.	103.	108.	140.	137.	144.	161.	139.	161.	168.
147.	144.	118.	123.	156.	136.	155.	127.	163.	200.
216.	208.	225.	250.	213.	222.	216.	193.	204.	185.
191.	171.	156.	107.	112.	96.	114.	82.	92.	71.
66.	65.	74.	74.	68.	75.	78.	94.	105.	93.
91.	104.	121.	119.	128.	114.	133.	158.	151.	137.
148.	147.	181.	179.	179.	171.	160.	177.	171.	184.
178.	173.	189.	175.	170.	162.	148.	149.	133.	146.
122.	125.	119.	128.	112.	105.	107.	103.	112.	126.
119.	93.	100.	97.	93.	144.	148.	152.	185.	226.
235.	235.	256.	233.	198.	175.	187.	168.	169.	166.
179.	158.	148.	122.	108.	110.	94.	104.	81.	85.
91.	86.	61.	76.	80.	73.	75.	72.	80.	90.
96.	90.	92.	80.	79.	102.	85.	79.	83.	78.
87.	78.	89.	84.	89.	65.	74.	80.	75.	103.
85.	105.	105.	96.	104.	85.	88.	90.	86.	93.
96.	86.	84.	81.	103.	81.	56.	77.	60.	80.
76.	71.	74.	71.	76.	80.	78.	80.	60.	93.
84.	83.	87.	104.	112.	76.	119.	86.	93.	94.
84.	84.	81.	93.	69.	69.	64.	69.	51.	73.
65.	53.	45.	58.	51.	40.	34.	49.	54.	50.

51.	50.	54.	54.	41.	60.	43.	50.	67.	53.
57.	60.	53.	63.	56.	37.	64.	51.	50.	52.
67.	65.	56.	56.	72.	58.	76.	68.	57.	68.
82.	97.	102.	91.	115.	103.	118.	105.	110.	106.
112.	88.	88.	99.	93.	81.	73.	67.	71.	63.
63.	57.	56.	64.	57.	47.	66.	58.	48.	64.
63.	52.	54.	65.	52.	46.	70.	56.	39.	58.
65.	65.	87.	90.	83.	81.	62.	82.	68.	89.
93.	72.	112.	97.	109.	111.	106.	131.	133.	111.
132.	135.	120.	112.	106.	126.	133.	163.	161.	152.
140.	107.	129.	92.	94.	94.	104.	115.	94.	92.
93.	92.	68.	80.	74.	68.	74.	73.	69.	63.
69.	78.	70.	76.	67.	67.	84.	103.	125.	103.
114.	105.	96.	108.	100.	89.	117.	105.	101.	94.
96.	81.	98.	111.	92.	107.	119.	109.	112.	124.
138.	135.	113.	106.	121.	116.	160.	122.	149.	140.
129.	138.	121.	134.	126.	119.	120.	114.	99.	95.
96.	98.	96.	103.	111.	107.	110.	139.	100.	127.
132.	111.	109.	103.	114.	105.	111.	111.	128.	109.
144.	120.	133.	117.	109.	92.	101.	93.	119.	92.
103.	101.	107.	91.	100.	89.	79.	61.	66.	65.
76.	62.	63.	68.	74.	77.	74.	65.	70.	74.
66.	88.	96.	87.	89.	84.	87.	100.	73.	92.
79.	82.	83.	88.	82.	73.	82.	71.	71.	86.
76.	79.	62.	65.	58.	73.	66.	63.	97.	88.
91.	95.	95.	93.	81.	74.	78.	73.	71.	92.
85.	79.	59.	78.	67.	56.	72.	56.	70.	66.
61.	49.	54.	74.	59.	52.	45.	51.	63.	71.
55.	73.	68.	100.	92.	91.	87.	108.	83.	78.
66.	70.	73.	75.	81.	82.	75.	74.	62.	62.
75.	71.	77.	67.	82.	87.	117.	129.	125.	133.
146.	137.	121.	126.	110.	113.	98.	110.	96.	104.
100.	90.	72.	74.	78.	66.	73.	69.	72.	59.
71.	60.	64.	39.	60.	55.	56.	63.	48.	52.
52.	60.	44.	50.	50.	44.	61.	51.	61.	71.
56.	52.	70.	56.	59.	66.	55.	70.	70.	84.
92.	82.	95.	83.	96.	123.	98.	99.	91.	108.
126.	119.	126.	153.	144.	152.	134.	128.	125.	134.
138.	145.	117.	124.	121.	140.	137.	133.	127.	96.
118.	135.	126.	133.	155.	135.	146.	169.	199.	220.
221.	235.	279.	272.	274.	251.	224.	243.	215.	212.
222.	227.	242.	280.	300.	271.	297.	276.	275.	239.
205.	191.	192.	185.	189.	217.	209.	196.	208.	192.
181.	182.	204.	196.	206.	212.	214.	215.	198.	185.
191.	169.	168.	174.	172.	142.	151.	139.	152.	146.
134.	115.	102.	115.	126.	98.	99.	91.	68.	75.
65.	82.	94.	64.	68.	78.	72.	68.	72.	91.
81.	67.	69.	72.	70.	74.	67.	81.	92.	78.
85.	98.	93.	110.	114.	113.	100.	101.	143.	117.
116.	113.	94.	87.	100.	86.	88.	95.	93.	102.
108.	99.	98.	101.	79.	76.	107.	112.	99.	93.
100.	90.	88.	79.	83.	70.	82.	91.	85.	75.
72.	89.	100.	85.	89.	101.	82.	102.	94.	112.
129.	118.	118.	114.	126.	114.	133.	129.	137.	154.
194.	209.	230.	226.	213.	198.	189.	143.	149.	136.
139.	141.	151.	147.	121.	116.	129.	104.	86.	85.
92.	74.	71.	72.	53.	49.	59.	70.	60.	67.
61.	73.	75.	71.	73.	77.	74.	102.	76.	79.
106.	98.	96.	95.	97.	97.	81.	74.	83.	81.
95.	83.	78.	102.	78.	93.	82.	68.	102.	78.
79.	77.	98.	114.	104.	120.	120.	142.	141.	146.
127.	133.	119.	108.	104.	111.	110.	122.	128.	115.
105.	111.	114.	112.	96.	96.	84.	75.	101.	74.
91.	84.	75.	80.	77.	103.	119.	105.	131.	130.
102.	118.	97.	108.	92.	89.	84.	87.	104.	104.
94.	88.	76.	78.	96.	86.	85.	97.	73.	76.
72.	86.	75.	84.	85.	87.	81.	82.	82.	77.
79.	73.	69.	83.	70.	99.	95.	98.	92.	107.
89.	84.	87.	84.	103.	92.	105.	100.	97.	122.

135.	124.	142.	152.	149.	117.	139.	112.	116.	115.
114.	133.	131.	146.	142.	133.	125.	117.	113.	112.
100.	97.	95.	78.	98.	90.	101.	91.	89.	77.
91.	96.	97.	86.	106.	99.	81.	71.	66.	60.
70.	75.	71.	63.	72.	68.	77.	63.	76.	79.
61.	67.	72.	64.	66.	54.	56.	77.	85.	73.
80.	71.	97.	90.	92.	97.	101.	93.	94.	79.
86.	107.	111.	105.	89.	119.	93.	97.	85.	79.
80.	72.	82.	75.	70.	76.	63.	80.	68.	76.
80.	80.	74.	74.	78.	79.	74.	80.	120.	106.
77.	83.	101.	113.	97.	105.	123.	116.	121.	117.
104.	134.	174.	94.	99.	97.	114.	107.	119.	135.
119.	118.	126.	114.	109.	103.	100.	102.	88.	85.
96.	90.	78.	81.	88.	111.	99.	86.	96.	86.
60.	80.	106.	110.	111.	96.	93.	96.	86.	103.
78.	81.	68.	73.	71.	63.	77.	89.	105.	86.
74.	94.	76.	85.	86.	79.	102.	91.	84.	79.
71.	61.	97.	89.	83.	81.	101.	82.	80.	85.
86.	96.	86.	88.	85.	74.	90.	84.	111.	112.
119.	122.	118.	123.	125.	116.	120.	123.	114.	107.
105.	165.	121.	111.	111.	120.	116.	96.	97.	91.
91.	119.	71.	91.	72.	72.	91.	73.	81.	91.
73.	79.	68.	76.	70.	61.	66.	67.	57.	65.
47.	70.	58.	65.	58.	61.	55.	55.	53.	63.
49.	55.	47.	47.	50.	56.	49.	38.	51.	48.
50.	54.	44.	48.	49.	64.	55.	63.	51.	44.
61.	54.	59.	57.	60.	50.	47.	59.	66.	65.
70.	54.	64.	66.	80.	71.	84.	72.	72.	61.
45.	60.	105.	68.	101.	65.	72.	69.	62.	67.
60.	62.	59.	63.	78.	70.	79.	72.	50.	71.
66.	78.	54.	77.	64.	66.	67.	76.	68.	66.
63.	77.	70.	88.	149.	69.	79.	84.	82.	80.
90.	95.	87.	116.	93.	132.	112.	114.	93.	104.
119.	104.	116.	85.	96.	111.	85.	95.	96.	109.
109.	123.	121.	125.	114.	116.	96.	93.	92.	72.
75.	72.	77.	84.	88.	76.	82.	96.	72.	99.
80.	70.	76.	67.	66.	63.	88.	93.	73.	105.
71.	119.	88.	98.	94.	89.	72.	69.	92.	76.
79.	76.	65.	96.	78.	90.	85.	93.	87.	181.
104.	87.	106.	138.	122.	139.	134.	105.	105.	102.
83.	103.	107.	84.	88.	95.	93.	108.	95.	108.
95.	103.	93.	108.	78.	87.	86.	107.	90.	75.
82.	106.	81.	94.	96.	101.	110.	120.	121.	124.
146.	128.	138.	135.	127.	126.	126.	118.	143.	143.
125.	135.	125.	129.	120.	125.	124.	120.	110.	104.
121.	118.	111.	128.	88.	113.	98.	109.	114.	100.
113.	105.	113.	128.	102.	119.	125.	141.	152.	161.
151.	142.	122.	121.	114.	118.	125.	131.	126.	127.
131.	115.	147.	98.	118.	128.	120.	109.	83.	87.
95.	88.	101.	94.	68.	77.	96.	109.	71.	84.
80.	60.	79.	70.	68.	68.	77.	71.	73.	83.
93.	74.	61.	60.	53.	75.	62.	71.	63.	73.
68.	66.	69.	74.	60.	70.	85.	99.	84.	85.
102.	94.	100.	108.	124.	91.	86.	84.	76.	90.
72.	66.	73.	62.	74.	62.	69.	75.	82.	83.
65.	78.	59.	56.	71.	48.	51.	57.	64.	48.
63.	59.	52.	73.	57.	47.	52.	72.	46.	61.
59.	56.	50.	65.	92.	97.	91.	85.	83.	73.
86.	68.	70.	89.	74.	77.	74.	75.	77.	96.
84.	99.	82.	68.	64.	77.	63.	75.	66.	70.
77.	72.	77.	59.	61.	66.	77.	65.	61.	64.
61.	49.	60.	72.	70.	72.	58.	61.	70.	49.
58.	64.	68.	76.	62.	45.	63.	57.	59.	60.
59.	52.	70.	60.	77.	52.	46.	71.	57.	64.
81.	97.	93.	80.	87.	75.	71.	83.	65.	68.
63.	59.	78.	80.	67.	93.	69.	80.	82.	75.
82.	66.	43.	66.	81.	73.	55.	72.	59.	55.
69.	62.	69.	65.	84.	74.	87.	78.	75.	86.
97.	82.	75.	73.	72.	67.	60.	71.	69.	63.

68.	60.	70.	79.	68.	84.	84.	88.	94.	92.
81.	90.	105.	105.	89.	111.	102.	93.	98.	83.
90.	75.	83.	86.	84.	91.	91.	83.	89.	96.
94.	95.	86.	85.	71.	75.	61.	90.	84.	84.
80.	71.	78.	85.	78.	81.	109.	111.	100.	92.
103.	104.	97.	114.	104.	92.	89.	103.	108.	144.
118.	122.	109.	110.	106.	119.	122.	125.	116.	124.
124.	113.	116.	104.	122.	109.	104.	117.	96.	84.
94.	109.	106.	97.	105.	118.	127.	117.	134.	132.
139.	123.	111.	121.	100.	103.	111.	111.	88.	107.
100.	117.	114.	90.	110.	112.	96.	116.	107.	104.
92.	91.	100.	92.	81.	94.	92.	92.	67.	103.
68.	83.	93.	74.	101.	87.	96.	89.	101.	100.
101.	63.	63.	76.	85.	55.	84.	78.	60.	69.
69.	77.	73.	70.	78.	88.	64.	60.	72.	60.
85.	61.	63.	73.	64.	70.	69.	57.	60.	68.
56.	67.	63.	78.	54.	69.	58.	78.	63.	89.
100.	78.	94.	84.	85.	83.	86.	85.	102.	87.
85.	80.	73.	96.	111.	111.	130.	144.	138.	117.
125.	100.	112.	111.	100.	85.	98.	77.	88.	93.
97.	89.	89.	113.	82.	120.	108.	82.	92.	84.
80.	100.	100.	80.	70.	74.	68.	70.	87.	64.
82.	74.	68.	89.	84.	62.	80.	94.	90.	83.
104.	121.	101.	103.	91.	100.	101.	91.	78.	80.
68.	82.	74.	76.	74.	74.	81.	71.	75.	74.
81.	85.	105.	94.	107.	95.	80.	98.	80.	92.
87.	73.	81.	67.	63.	79.	71.	86.	56.	64.
79.	105.	85.	95.	98.	85.	99.	86.	77.	75.
82.	84.	91.	98.	123.	104.	101.	104.	97.	90.
97.	97.	95.	90.	105.	100.	93.	81.	106.	84.
84.	93.	85.	89.	93.	100.	84.	81.	79.	235.
91.	102.	96.	93.	89.	86.	84.	104.	77.	108.
91.	92.	78.	96.	76.	74.	75.	72.	69.	77.
85.	87.	81.	87.	72.	77.	85.	84.	81.	88.
89.	64.	63.	85.	72.	94.	95.	86.	96.	103.
96.	98.	107.	119.	98.	106.	138.	115.	94.	92.
112.	115.	105.	94.	98.	113.	86.	104.	114.	100.
113.	108.	110.	96.	114.	101.	118.	128.	101.	94.
86.	101.	82.	98.	102.	84.	89.	88.	105.	91.
108.	114.	118.	130.	122.	112.	106.	100.	98.	95.
88.	87.	97.	91.	79.	85.	66.	60.	93.	73.
73.	75.	98.	93.	102.	91.	112.	79.	96.	70.
69.	84.	83.	71.	79.	64.	91.	85.	92.	93.
88.	101.	87.	89.	90.	67.	107.	84.	86.	82.
88.	101.	98.	77.	95.	83.	90.	92.	101.	90.
87.	137.	118.	111.	113.	127.	130.	147.	143.	152.
140.	136.	137.	120.	106.	133.	125.	138.	110.	126.
116.	129.	118.	132.	118.	130.	122.	141.	131.	127.
135.	119.	143.	125.	149.	129.	115.	131.	138.	148.
133.	158.	142.	139.	132.	112.	96.	127.	112.	112.
107.	136.	124.	103.	126.	159.	143.	165.	155.	169.
178.	150.	164.	164.	169.	160.	148.	130.	131.	107.
116.	108.	120.	111.	107.	90.	91.	118.	86.	116.
103.	111.	127.	105.	122.	113.	124.	115.	131.	119.
108.	98.	127.	108.	100.	123.	102.	105.	91.	109.
69.	79.	69.	77.	83.	74.	79.	76.	72.	62.
63.	54.	71.	103.	75.	67.	65.	70.	79.	86.
77.	63.	65.	81.	71.	64.	71.	75.	93.	84.
101.	82.	67.	93.	72.	85.	77.	67.	72.	77.
63.	83.	60.	76.	80.	64.	69.	59.	75.	88.
95.									

Appendix P-15: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.04° 2θ

19.000 0.040 139.00 50%-olivine mixture, 0.04 degree 2-theta

	98	84	84	87	77	62	94	73	90	66
	84	92	89	86	81	77	85	94	105	100
	120	119	149	162	150	155	117	114	109	102
	83	95	97	73	92	74	78	85	90	88
	82	98	71	64	67	88	80	78	59	90
	54	82	73	80	73	77	69	70	79	69
	67	85	74	73	69	58	74	66	70	71
	67	82	73	74	67	69	91	70	67	75
	83	96	65	84	88	96	106	113	125	155
	156	247	347	463	616	913	1089	1102	878	598
	379	288	220	148	134	107	81	80	98	98
	78	75	85	81	104	101	126	129	186	231
	303	386	429	348	284	194	146	129	104	99
	93	106	122	135	145	125	101	111	82	71
	68	80	74	61	69	78	67	72	70	72
	77	88	98	87	98	121	149	202	236	389
	475	545	592	513	469	386	288	230	190	109
	117	100	68	75	86	79	86	79	74	96
	85	80	68	95	74	98	114	134	155	193
	301	327	352	319	261	190	158	123	99	89
	85	96	85	79	86	86	87	109	107	131
	162	211	317	511	708	841	855	733	514	327
	215	163	135	101	94	74	76	81	68	82
	82	69	81	67	76	88	76	83	63	70
	80	69	69	86	82	82	71	80	69	84
	100	86	91	94	83	114	112	124	133	168
	185	239	255	298	399	484	630	788	1070	1473
	2034	2559	2973	2880	2336	1600	1102	767	631	563
	575	761	1029	1017	884	725	524	362	281	234
	221	222	254	290	384	571	803	956	1026	954
	786	514	388	269	192	144	133	108	95	107
	100	97	105	103	110	104	92	83	97	95
	116	100	119	113	154	169	208	303	406	614
	946	1328	1407	1305	999	634	399	242	190	156
	128	101	92	89	84	70	75	79	76	74
	85	79	69	60	72	71	67	70	56	66
	52	63	72	62	64	73	57	69	68	57
	64	71	63	79	64	60	77	69	57	81
	55	82	79	82	83	89	94	97	117	119
	140	168	169	189	208	205	271	387	521	632
	771	817	724	622	454	437	388	429	512	673
	928	1324	1683	1977	2254	2605	2938	2742	2615	2147
	1564	1052	730	488	396	297	275	284	249	273
	291	338	449	641	928	1302	1625	1826	1566	1301
	919	664	392	337	267	202	176	130	115	132
	115	99	86	85	80	71	70	79	87	83
	71	71	82	92	93	130	127	147	116	130
	138	126	107	107	97	121	112	129	183	264
	269	312	274	238	194	152	145	117	110	93
	131	127	142	170	224	279	293	303	248	253
1	255	351	466	517	562	443	418	360	276	249
	226	275	343	455	643	759	789	734	614	516
	471	395	424	551	649	668	678	519	419	316
	209	142	108	139	128	127	100	118	134	166
	247	295	363	344	354	324	294	245	267	224
	327	306	298	251	221	170	145	124	116	88
	110	116	111	135	148	182	267	338	400	422
	424	450	443	442	443	438	327	254	220	203
	230	223	326	450	547	616	547	458	377	301
	214	181	144	151	148	200	231	296	272	313
	268	234	184	141	134	128	104	119	106	117
	122	129	114	105	118	95	114	97	97	99
	69	71	73	77	90	110	89	90	114	150
	162	214	220	395	525	545	585	523	435	367

309	239	190	173	175	201	235	318	355	431
373	398	375	384	319	310	232	202	173	173
111	87	75	79	74	65	79	66	83	72
79	87	73	100	112	169	193	246	221	234
189	145	136	108	119	121	115	129	140	139
127	145	135	94	90	81	70	63	60	63
60	61	56	45	66	53	56	55	57	54
49	52	58	61	71	54	68	61	46	50
55	51	51	61	62	56	74	63	66	68
89	91	104	155	137	173	146	126	114	116
100	78	69	76	79	88	82	93	111	98
118	117	112	90	86	79	73	57	69	65
75	90	101	127	152	216	261	279	263	258
252	260	198	173	148	112	115	100	110	125
124	201	208	222	172	168	152	150	97	93
95	80	93	124	106	126	147	127	124	106
117	111	72	74	69	65	64	77	72	62
80	106	95	84	99	108	111	121	129	126
143	164	200	244	325	360	570	807	1128	1402
1489	1349	1201	1029	986	822	682	605	509	428
428	307	274	223	203	184	170	139	144	110
113	91	88	93	122	119	119	109	118	93
70	93	91	74	84	91	70	75	67	58
65	49	52	64	58	66	60	51	60	55
58	73	69	79	79	88	96	111	118	119
133	163	178	271	307	348	373	354	332	292
283	240	195	180	171	144	151	190	185	191
174	157	123	131	121	112	120	94	112	101
120	136	160	193	265	342	344	331	320	310
297	254	206	230	221	243	294	382	526	697
804	906	880	860	790	700	581	525	440	427
330	303	220	199	219	171	160	132	122	128
136	145	134	130	114	115	102	128	117	128
154	148	151	157	134	127	130	138	123	139
132	120	125	119	116	116	136	145	199	219
193	178	182	173	200	168	170	146	138	129
148	149	147	170	168	142	135	116	100	99
96	88	90	91	125	141	184	188	157	149
132	132	108	100	87	101	86	82	81	104
125	106	116	115	126	129	178	191	189	205
217	282	285	291	317	302	316	285	273	291
246	253	246	207	198	189	191	203	232	220
254	302	299	388	409	521	558	563	508	570
605	627	625	522	410	396	367	312	285	248
234	247	223	211	250	295	326	389	516	627
712	692	583	553	479	418	411	303	214	171
152	144	128	129	117	113	108	123	119	128
95	88	88	99	91	118	127	110	95	100
89	95	96	80	78	57	82	73	59	82
90	88	83	108	103	108	109	113	122	126
128	151	164	171	142	129	124	107	108	110
89	79	89	78	88	88	87	107	139	179
176	206	293	326	451	550	544	490	425	384
392	349	291	249	178	177	178	153	161	180
201	227	275	331	356	309	324	314	277	264
241	222	219	248	267	287	323	304	318	329
311	239	225	241	231	209	275	268	268	243
210	196	178	170	149	122	94	99	112	77
75	81	79	76	74	96	98	91	120	118
129	123	109	94	80	105	82	85	81	91
74	68	62	71	57	67	58	61	68	80
83	85	86	104	108	113	145	190	230	291
283	290	272	244	283	308	252	236	198	178
149	147	132	120	103	110	89	94	82	73
83	83	65	73	78	69	80	71	92	103
110	114	164	185	203	185	208	156	203	222
264	263	262	232	200	220	223	208	216	213
210	226	234	280	251	275	233	211	201	216
179	175	126	116	102	119	92	71	71	55

	70	62	67	60	68	59	63	55	66	63
	58	81	69	79	95	117	128	130	104	118
	93	118	105	118	104	95	95	104	99	134
	117	132	132	148	148	161	132	145	129	161
	172	216	216	259	248	209	193	177	197	165
	132	100	98	89	86	60	77	85	72	73
	82	97	103	92	106	121	134	117	179	140
	131	157	154	183	193	155	158	154	164	157
	152	155	179	172	142	144	136	100	104	101
	115	104	110	117	92	113	105	116	118	144
	174	206	221	214	195	211	165	170	154	177
	124	126	104	91	94	75	61	67	68	60
	66	76	71	83	85	100	99	94	92	73
	81	91	87	81	79	84	71	77	72	87
	117	106	119	102	92	81	103	85	92	77
	68	72	68	77	70	82	72	69	74	53
	78	94	91	97	112	107	116	106	83	100
	80	67	71	71	51	52	57	48	45	31
	50	52	54	48	54	54	57	41	48	62
	53	47	60	42	51	52	33	52	50	52
	53	56	48	65	62	66	64	96	97	112
	125	97	114	109	86	76	81	87	81	76
	67	67	66	55	62	57	56	57	63	42
	59	52	51	50	60	60	67	70	66	73
	80	71	80	80	72	74	90	104	98	137
	117	123	126	89	117	123	133	149	124	115
	109	87	94	112	88	81	85	97	74	63
	76	77	61	75	70	64	69	67	81	90
	130	121	121	80	98	93	91	112	80	96
	100	98	90	107	114	110	103	137	125	119
	123	133	145	129	145	98	113	138	116	104
	89	96	98	115	117	122	137	125	129	111
	102	100	112	97	119	108	103	125	127	118
	103	102	84	82	115	115	108	89	71	78
	75	62	59	73	59	67	62	56	102	80
	88	96	79	90	67	71	81	90	91	83
	75	72	73	60	59	62	74	55	69	65
	69	81	94	90	71	78	71	63	84	60
	89	66	59	54	64	56	55	46	44	66
	42	52	47	58	62	75	86	95	96	82
	85	67	77	72	57	48	60	73	65	56
	73	82	76	103	101	122	147	132	96	109
	74	79	91	92	92	84	68	84	68	70
	43	71	43	57	63	58	46	54	48	42
	47	54	51	43	56	52	58	71	68	80
	58	55	90	75	68	76	77	104	95	93
	83	103	130	126	156	158	114	119	128	118
	103	129	143	142	119	99	112	120	146	122
	121	168	162	211	200	250	266	282	247	192
1	191	205	223	251	274	351	352	279	181	185
	174	167	212	193	181	174	138	172	173	177
	187	182	195	164	169	124	167	137	142	126
	126	147	121	109	91	91	88	77	61	69
	69	70	73	75	69	79	55	58	63	71
	71	63	83	86	88	112	114	91	99	118
	106	95	101	99	92	79	94	99	108	92
	103	98	97	102	87	104	94	79	79	74
	81	85	79	86	89	77	90	74	75	89
	100	110	118	119	113	118	115	132	141	181
	210	225	213	189	145	124	103	129	127	143
	133	120	98	85	67	71	66	74	67	57
	58	50	60	61	74	79	74	93	90	80
	80	92	97	78	73	66	89	75	80	66
	57	71	75	82	83	94	106	133	141	152
	144	121	127	110	118	114	97	116	113	101
	125	104	85	104	85	74	70	86	90	86
	81	103	98	120	135	109	103	85	85	82
	92	81	90	104	86	80	80	84	68	87
	59	84	93	83	99	75	77	68	78	71

	91	97	107	91	83	83	90	88	100	98
	119	117	100	134	140	110	115	110	117	135
	140	146	147	139	108	92	100	86	79	88
	86	82	64	92	78	91	87	89	94	77
	79	79	59	61	58	70	84	68	67	62
	45	55	54	66	53	61	76	84	95	92
	91	83	75	98	93	90	104	109	104	90
	66	74	72	68	82	82	74	73	66	72
	68	59	69	68	73	78	74	94	93	91
	102	90	92	99	90	89	98	85	90	96
	126	108	113	120	97	97	80	84	91	91
	74	83	102	90	93	80	90	91	111	119
	83	92	92	99	76	90	83	85	105	97
	75	77	70	64	80	77	82	76	66	72
	85	89	85	71	69	73	73	73	72	82
	75	80	79	100	94	131	105	133	118	96
	103	111	113	113	125	120	119	107	104	86
	70	85	80	79	85	88	65	84	68	65
	65	57	61	52	57	55	54	74	39	50
	50	53	61	38	61	45	46	41	63	46
	50	52	41	54	46	37	47	46	48	52
	62	47	51	55	61	58	67	68	56	67
	72	65	57	62	62	65	63	73	60	62
	55	62	65	87	67	72	75	59	67	70
	63	76	61	70	83	71	77	70	83	55
	87	97	92	96	107	112	118	128	100	80
	98	97	88	87	91	99	106	118	96	119
	95	92	79	60	81	76	72	81	86	87
	85	72	86	73	67	72	69	78	88	88
	96	71	67	77	65	78	61	76	93	88
	85	86	87	82	84	83	117	131	137	96
	108	94	93	76	85	87	125	77	91	98
	84	91	66	75	74	77	81	79	93	98
	98	114	107	127	137	146	143	126	112	113
	126	124	148	141	125	108	133	124	115	115
	120	101	108	114	82	96	107	114	107	117
	114	140	146	136	134	136	127	115	96	97
	125	131	99	128	123	113	106	104	92	75
	71	98	84	76	79	70	62	66	71	76
	64	61	64	62	60	100	77	67	61	57
	71	66	64	88	77	77	86	87	83	87
	92	95	104	94	84	70	92	71	88	72
	63	65	88	78	77	78	67	61	46	46
	49	56	58	37	62	53	52	54	50	62
	64	81	68	83	91	63	52	85	73	64
	68	63	56	70	73	71	61	49	72	65
1	66	71	79	60	57	68	67	78	56	50
	66	59	55	56	51	52	64	54	61	57
	55	43	47	39	60	59	55	57	57	62
	61	59	60	81	69	74	77	74	74	49
	60	67	64	63	68	83	77	63	76	78
	71	54	58	70	72	68	76	60	75	98
	83	91	85	70	76	73	76	65	64	64
	65	79	75	87	87	74	98	104	101	107
	97	106	77	86	96	101	77	95	87	78
	76	98	84	90	70	92	75	83	83	82
	84	88	86	72	79	82	95	101	77	75
	79	92	93	108	112	115	110	105	118	111
	125	131	108	112	105	99	115	105	95	75
	101	104	116	128	118	137	138	125	113	78
	103	88	118	93	92	93	94	100	99	99
	81	86	94	85	89	83	105	89	79	75
	83	80	90	100	91	100	83	88	83	69
	82	62	65	71	64	59	70	60	79	77
	73	67	70	59	67	72	51	56	64	68
	67	52	58	79	69	78	81	88	86	89
	93	85	88	76	79	89	92	126	112	112
	121	112	122	104	105	90	109	90	104	84
	93	87	92	89	79	67	68	78	76	71

63	67	60	69	86	56	59	68	74	93
72	99	88	82	84	100	75	64	77	80
71	79	88	58	91	85	91	91	90	98
93	89	72	89	81	66	73	68	63	58
62	76	70	74	86	79	93	82	82	83
79	71	81	96	111	95	86	92	78	99
83	91	88	76	82	79	87	76	60	81
80	89	89	89	93	92	105	88	101	80
80	60	64	72	64	69	77	68	80	84
84	87	73	85	89	98	75	92	81	95
94	85	113	82	109	112	105	121	100	81
82	99	95	84	97	100	95	102	105	98
106	111	104	103	101	85	81	84	86	83
100	90	109	106	103	87	89	89	80	91
89	70	67	55	73	81	85	83	75	87
81	81	88	64	64	63	89	70	85	93
103	103	93	80	100	92	71	87	77	94
76	88	96	84	70	97	106	116	101	107
99	134	135	107	116	130	124	111	125	108
120	114	114	125	126	119	105	119	124	139
109	115	125	143	134	102	130	118	127	112
127	106	103	112	108	109	115	138	118	113
172	155	172	154	155	139	125	136	120	87
109	80	98	103	88	86	125	120	114	93
119	97	108	101	109	85	101	101	91	69
81	87	81	76	89	91	80	88	72	82
84	70	74	74	77	77	66	85	75	59
64	64	62	64	76	58	76	87	68	61
72	69	75	74	69	62	79	61	70	72
64									

Appendix P-16: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.05° 2θ

19.00 .05 139.00 50%-olivine, .05 degree 2-thet

87.	82.	78.	85.	89.	87.	83.	74.	72.	94.
73.	80.	93.	73.	95.	82.	111.	113.	161.	175.
167.	158.	157.	124.	112.	104.	104.	93.	95.	77.
83.	72.	86.	63.	94.	69.	82.	69.	86.	84.
76.	82.	68.	82.	66.	54.	83.	70.	74.	81.
70.	90.	86.	68.	98.	65.	73.	63.	68.	78.
78.	72.	88.	78.	66.	85.	76.	84.	94.	93.
102.	143.	147.	178.	233.	358.	528.	835.	1040.	1021.
841.	573.	306.	208.	165.	131.	123.	92.	101.	83.
104.	89.	102.	115.	120.	129.	220.	305.	367.	371.
329.	241.	182.	119.	129.	129.	128.	147.	138.	134.
129.	88.	91.	75.	90.	66.	71.	85.	81.	82.
74.	78.	82.	95.	104.	112.	174.	254.	365.	521.
506.	577.	498.	440.	361.	257.	166.	129.	93.	93.
87.	85.	72.	79.	79.	84.	81.	96.	96.	107.
101.	151.	200.	256.	272.	328.	319.	236.	171.	128.
88.	95.	100.	88.	102.	95.	108.	93.	135.	164.
248.	421.	590.	704.	730.	640.	483.	320.	173.	137.
94.	95.	99.	86.	64.	77.	77.	80.	80.	73.
81.	83.	84.	93.	93.	86.	78.	81.	74.	72.
74.	86.	92.	100.	95.	109.	109.	110.	170.	200.
252.	301.	399.	471.	631.	831.	1284.	1951.	2678.	3175.
2681.	2091.	1350.	900.	625.	666.	756.	926.	974.	841.
621.	406.	295.	244.	228.	304.	335.	553.	779.	1037.
1129.	1003.	688.	401.	246.	187.	150.	118.	116.	109.
98.	123.	121.	108.	115.	95.	106.	116.	115.	117.
136.	169.	237.	360.	544.	870.	1148.	1301.	1133.	823.
508.	258.	181.	139.	121.	99.	101.	84.	102.	54.
84.	65.	73.	65.	73.	77.	81.	67.	80.	67.
51.	74.	67.	77.	59.	75.	64.	66.	70.	66.
75.	64.	72.	81.	64.	65.	86.	89.	86.	90.
93.	123.	124.	133.	140.	164.	197.	237.	294.	457.
596.	667.	760.	652.	573.	462.	438.	445.	611.	949.
1232.	1670.	2185.	2753.	2935.	3021.	2547.	2047.	1308.	873.
541.	368.	282.	271.	285.	303.	366.	552.	847.	1284.
1549.	1725.	1520.	1141.	817.	484.	327.	276.	181.	176.
123.	111.	97.	96.	68.	84.	88.	86.	88.	80.
85.	92.	108.	103.	146.	134.	132.	143.	126.	112.
142.	96.	115.	131.	207.	261.	292.	270.	235.	170.
164.	113.	93.	105.	117.	175.	208.	241.	277.	256.
255.	287.	350.	480.	525.	532.	429.	346.	296.	247.
293.	391.	535.	680.	808.	762.	671.	558.	436.	484.
590.	671.	593.	521.	373.	265.	166.	130.	117.	118.
135.	131.	178.	241.	267.	327.	367.	341.	259.	274.
283.	322.	340.	314.	326.	260.	186.	147.	99.	100.
105.	105.	146.	204.	265.	355.	396.	455.	441.	445.
419.	388.	309.	286.	264.	234.	260.	363.	457.	562.
539.	506.	347.	250.	185.	193.	163.	197.	243.	307.
308.	262.	256.	171.	154.	145.	138.	122.	128.	125.
137.	106.	112.	112.	118.	111.	98.	75.	81.	71.
79.	100.	99.	120.	138.	155.	252.	333.	436.	515.
577.	522.	411.	302.	270.	213.	202.	194.	229.	297.
348.	373.	361.	400.	351.	334.	253.	208.	141.	122.
93.	93.	73.	78.	54.	82.	81.	82.	90.	103.
109.	157.	209.	243.	225.	204.	166.	133.	122.	129.
133.	119.	128.	128.	131.	117.	111.	107.	76.	77.
49.	64.	64.	60.	50.	49.	40.	50.	53.	45.
45.	51.	53.	46.	37.	60.	53.	47.	52.	62.
63.	49.	77.	82.	78.	77.	102.	114.	172.	140.
150.	144.	116.	94.	102.	74.	79.	76.	90.	95.
130.	110.	130.	103.	102.	77.	79.	82.	80.	87.
87.	128.	155.	213.	234.	304.	299.	308.	265.	202.
171.	141.	111.	116.	136.	165.	177.	215.	204.	184.
148.	117.	117.	83.	92.	93.	114.	105.	139.	151.

122.	102.	96.	146.	85.	66.	83.	72.	88.	88.
119.	109.	106.	111.	108.	129.	121.	150.	195.	223.
266.	420.	649.	1013.	1286.	1461.	1275.	1263.	990.	851.
763.	580.	550.	406.	328.	272.	212.	195.	187.	151.
118.	119.	111.	85.	110.	100.	89.	96.	94.	90.
92.	76.	77.	77.	79.	78.	63.	63.	73.	52.
54.	60.	64.	57.	58.	53.	92.	74.	83.	100.
118.	132.	123.	144.	185.	250.	283.	358.	382.	351.
371.	276.	240.	178.	176.	146.	192.	190.	195.	192.
154.	163.	127.	117.	100.	116.	111.	130.	138.	170.
253.	302.	325.	319.	295.	284.	258.	233.	247.	235.
367.	405.	636.	777.	936.	898.	870.	780.	668.	568.
433.	371.	323.	267.	200.	188.	161.	141.	108.	114.
124.	138.	118.	126.	260.	134.	146.	142.	172.	147.
145.	134.	130.	123.	121.	124.	122.	117.	123.	125.
155.	175.	213.	216.	181.	173.	154.	184.	163.	154.
140.	157.	172.	164.	135.	157.	167.	90.	121.	95.
99.	80.	127.	147.	146.	143.	147.	134.	148.	124.
93.	82.	88.	98.	88.	78.	116.	124.	131.	173.
182.	217.	239.	243.	284.	311.	282.	309.	296.	278.
249.	278.	247.	260.	226.	238.	247.	211.	243.	239.
310.	322.	400.	484.	489.	826.	599.	704.	640.	620.
534.	431.	393.	344.	303.	270.	228.	244.	255.	346.
392.	496.	673.	710.	642.	589.	521.	470.	346.	281.
206.	156.	161.	134.	136.	118.	110.	116.	113.	103.
99.	114.	96.	92.	98.	84.	99.	91.	96.	83.
80.	64.	81.	67.	78.	95.	101.	103.	104.	130.
120.	122.	131.	146.	138.	157.	155.	136.	114.	136.
92.	104.	101.	81.	82.	115.	112.	128.	158.	199.
247.	298.	436.	465.	488.	450.	391.	374.	307.	265.
224.	179.	169.	157.	167.	181.	295.	283.	340.	318.
344.	306.	268.	238.	231.	252.	296.	318.	363.	338.
330.	290.	271.	253.	220.	223.	231.	265.	269.	253.
197.	172.	155.	122.	93.	91.	73.	84.	77.	88.
82.	83.	109.	119.	106.	140.	112.	127.	107.	112.
96.	79.	84.	73.	79.	81.	61.	67.	93.	88.
90.	93.	92.	100.	107.	110.	164.	218.	276.	329.
284.	286.	286.	307.	241.	230.	187.	179.	168.	156.
142.	109.	106.	96.	79.	77.	77.	76.	77.	79.
82.	91.	115.	119.	132.	181.	195.	234.	215.	219.
224.	242.	249.	237.	240.	217.	226.	216.	214.	216.
241.	265.	270.	307.	248.	249.	200.	242.	180.	157.
127.	95.	86.	84.	72.	66.	64.	80.	64.	56.
68.	66.	77.	85.	65.	78.	95.	121.	114.	84.
116.	129.	122.	109.	92.	88.	105.	109.	128.	133.
140.	184.	160.	162.	156.	137.	129.	178.	199.	247.
239.	227.	211.	168.	188.	156.	133.	102.	74.	77.
63.	66.	83.	80.	98.	103.	109.	120.	134.	145.
151.	151.	167.	158.	167.	175.	170.	157.	193.	195.
172.	168.	149.	133.	128.	114.	151.	95.	107.	94.
113.	102.	99.	146.	140.	213.	221.	225.	211.	173.
163.	188.	166.	141.	134.	111.	88.	66.	86.	96.
62.	72.	70.	77.	108.	77.	97.	92.	77.	90.
77.	78.	87.	72.	66.	73.	89.	109.	104.	89.
101.	85.	91.	110.	93.	90.	57.	76.	76.	75.
84.	75.	67.	74.	84.	96.	101.	112.	114.	88.
97.	114.	98.	93.	63.	60.	46.	47.	52.	54.
43.	60.	50.	76.	47.	53.	46.	52.	50.	50.
47.	48.	34.	42.	55.	51.	76.	65.	63.	87.
88.	104.	109.	117.	133.	119.	104.	80.	82.	98.
91.	86.	70.	76.	57.	54.	60.	60.	56.	57.
50.	61.	57.	67.	65.	58.	89.	82.	76.	88.
75.	92.	102.	112.	112.	123.	117.	114.	130.	136.
115.	126.	128.	118.	100.	91.	71.	78.	78.	65.
98.	62.	67.	62.	60.	67.	72.	74.	96.	97.
93.	94.	94.	99.	110.	120.	98.	95.	86.	92.
111.	134.	149.	132.	139.	151.	124.	141.	140.	113.
124.	130.	113.	123.	106.	111.	111.	125.	108.	107.
120.	120.	108.	110.	126.	100.	107.	126.	123.	113.

106.	109.	120.	86.	81.	78.	80.	68.	67.	66.
57.	60.	83.	86.	88.	80.	107.	87.	78.	75.
93.	80.	78.	79.	64.	69.	67.	71.	71.	75.
70.	82.	95.	102.	81.	84.	73.	65.	83.	77.
77.	65.	57.	44.	61.	56.	53.	64.	57.	58.
65.	65.	78.	81.	80.	72.	74.	75.	78.	71.
70.	54.	60.	40.	74.	82.	128.	147.	137.	123.
104.	98.	93.	107.	91.	84.	95.	75.	58.	78.
63.	53.	46.	58.	58.	55.	50.	51.	48.	52.
52.	52.	64.	73.	66.	71.	91.	66.	78.	91.
87.	97.	134.	87.	112.	150.	156.	143.	154.	145.
138.	133.	133.	145.	136.	120.	123.	126.	149.	158.
172.	217.	225.	285.	276.	263.	216.	206.	212.	261.
318.	291.	308.	247.	202.	208.	179.	203.	198.	201.
171.	183.	217.	220.	209.	196.	191.	187.	158.	140.
146.	140.	142.	125.	102.	75.	87.	87.	85.	82.
79.	94.	63.	79.	73.	65.	64.	68.	74.	72.
109.	116.	98.	107.	83.	117.	111.	102.	91.	88.
72.	100.	104.	86.	96.	93.	94.	102.	83.	87.
85.	88.	78.	82.	77.	93.	100.	78.	102.	95.
121.	121.	127.	131.	128.	135.	169.	182.	222.	203.
179.	145.	131.	139.	144.	127.	115.	80.	74.	62.
64.	58.	68.	56.	60.	85.	68.	56.	83.	74.
78.	76.	94.	85.	87.	86.	82.	85.	88.	90.
78.	65.	87.	83.	88.	126.	153.	130.	132.	117.
118.	133.	133.	103.	122.	122.	110.	110.	91.	74.
96.	73.	88.	108.	95.	114.	114.	130.	87.	85.
86.	107.	79.	87.	69.	78.	87.	66.	86.	82.
101.	80.	100.	77.	95.	92.	100.	89.	85.	103.
91.	93.	116.	79.	87.	108.	111.	139.	114.	119.
108.	103.	148.	124.	153.	146.	118.	137.	106.	96.
89.	105.	87.	103.	85.	90.	112.	110.	77.	81.
62.	64.	58.	77.	58.	71.	76.	78.	74.	79.
61.	71.	51.	91.	90.	93.	78.	88.	94.	103.
104.	111.	91.	79.	89.	74.	87.	81.	49.	71.
58.	79.	57.	80.	83.	98.	82.	86.	119.	102.
102.	101.	96.	104.	86.	80.	91.	100.	110.	105.
110.	93.	96.	97.	90.	74.	90.	78.	93.	73.
92.	97.	112.	109.	108.	76.	70.	83.	106.	97.
94.	110.	83.	99.	87.	91.	78.	74.	70.	97.
70.	90.	90.	100.	93.	91.	83.	96.	84.	98.
122.	120.	133.	126.	120.	115.	121.	123.	107.	91.
95.	110.	99.	99.	64.	60.	77.	66.	91.	70.
78.	67.	64.	62.	56.	54.	62.	58.	45.	68.
56.	63.	60.	42.	50.	60.	51.	53.	54.	53.
60.	50.	50.	51.	44.	55.	63.	65.	81.	54.
71.	82.	71.	64.	59.	58.	56.	59.	66.	60.
63.	62.	53.	72.	75.	78.	71.	52.	64.	71.
78.	65.	80.	73.	73.	73.	84.	91.	82.	108.
104.	95.	117.	107.	108.	86.	90.	87.	95.	105.
110.	105.	115.	112.	88.	76.	84.	90.	91.	87.
83.	69.	79.	82.	65.	81.	74.	88.	97.	100.
89.	74.	81.	78.	83.	79.	94.	100.	99.	78.
83.	102.	108.	127.	129.	112.	97.	95.	92.	103.
101.	101.	91.	105.	74.	78.	70.	91.	90.	86.
99.	88.	113.	141.	172.	146.	134.	107.	120.	151.
121.	150.	154.	136.	128.	117.	114.	110.	127.	113.
123.	108.	103.	94.	113.	142.	142.	147.	159.	140.
119.	118.	129.	104.	116.	123.	139.	121.	109.	82.
80.	88.	88.	86.	87.	89.	90.	69.	80.	70.
82.	72.	86.	67.	59.	65.	79.	66.	78.	69.
60.	79.	67.	90.	103.	87.	89.	92.	111.	71.
77.	85.	69.	70.	81.	80.	63.	71.	65.	55.
75.	57.	46.	53.	51.	70.	52.	64.	52.	71.
80.	81.	96.	93.	62.	70.	62.	64.	86.	64.
80.	71.	65.	68.	65.	69.	87.	69.	71.	75.
65.	66.	68.	62.	52.	57.	65.	49.	74.	45.
63.	65.	64.	62.	54.	57.	55.	62.	49.	77.
70.	92.	108.	84.	64.	65.	83.	75.	89.	66.

79.	76.	84.	89.	71.	76.	72.	92.	65.	64.
67.	73.	84.	90.	86.	74.	63.	79.	80.	80.
77.	88.	77.	93.	81.	100.	93.	108.	106.	97.
91.	93.	85.	92.	90.	78.	75.	93.	98.	98.
67.	71.	102.	73.	86.	78.	83.	80.	86.	89.
111.	114.	102.	99.	105.	101.	128.	96.	112.	96.
126.	127.	116.	117.	123.	104.	101.	100.	92.	105.
79.	119.	117.	134.	141.	128.	113.	99.	97.	110.
103.	115.	113.	113.	128.	101.	105.	92.	109.	89.
109.	105.	95.	98.	85.	80.	97.	103.	81.	92.
98.	87.	74.	61.	72.	73.	76.	50.	65.	67.
62.	51.	66.	70.	66.	57.	70.	65.	72.	77.
85.	70.	82.	97.	75.	92.	86.	84.	94.	86.
124.	121.	135.	121.	120.	108.	113.	104.	91.	106.
95.	102.	103.	116.	94.	84.	73.	75.	77.	73.
79.	80.	76.	58.	77.	82.	94.	90.	86.	111.
86.	105.	90.	90.	72.	80.	81.	83.	82.	68.
92.	105.	98.	91.	81.	79.	76.	68.	75.	74.
82.	62.	78.	76.	91.	64.	76.	80.	96.	92.
105.	105.	102.	103.	106.	94.	118.	85.	79.	84.
73.	101.	101.	74.	71.	85.	94.	102.	96.	101.
96.	103.	83.	65.	93.	77.	83.	60.	71.	69.
82.	75.	76.	91.	82.	64.	78.	98.	89.	106.
104.	107.	130.	119.	116.	108.	98.	85.	86.	102.
87.	109.	104.	107.	112.	95.	96.	95.	86.	89.
80.	90.	75.	83.	109.	114.	109.	90.	136.	93.
86.	91.	79.	83.	93.	73.	83.	102.	110.	107.
76.	91.	78.	76.	77.	106.	68.	84.	98.	89.
92.	70.	76.	99.	81.	85.	84.	89.	103.	85.
96.	99.	109.	132.	132.	136.	129.	126.	138.	106.
118.	120.	101.	127.	131.	119.	119.	142.	115.	135.
117.	122.	128.	139.	107.	133.	145.	141.	112.	120.
116.	104.	118.	125.	160.	137.	141.	171.	175.	168.
145.	127.	117.	102.	95.	101.	105.	101.	104.	106.
132.	124.	109.	114.	123.	103.	96.	100.	89.	93.
91.	91.	77.	69.	68.	79.	60.	78.	77.	77.
77.	71.	77.	82.	95.	64.	59.	69.	85.	61.
82.	94.	68.	71.	56.	65.	83.	79.	70.	77.
86.									

Appendix P-17: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.06° 2θ

19.000 0.060 139.00 50%-olivine mixture, 0.06 degree 2-theta

80	95	88	82	87	70	75	68	100	91
73	111	102	95	131	162	167	159	135	112
103	88	92	90	89	87	97	87	87	85
77	66	71	63	88	78	80	74	83	67
90	63	77	64	81	72	71	79	65	93
86	92	75	73	100	92	88	108	128	179
207	306	506	869	1231	1081	691	354	196	141
115	111	95	95	93	108	122	120	172	228
342	452	394	263	165	126	110	126	152	144
120	89	88	64	94	80	74	78	96	86
91	95	119	136	192	249	462	591	595	555
411	273	155	125	100	92	58	93	81	83
79	70	94	87	142	158	249	350	347	291
177	109	116	93	92	104	92	103	120	134
179	332	556	876	896	654	358	217	134	129
77	99	73	87	77	84	87	74	83	81
88	89	88	82	94	72	95	94	92	100
120	139	176	218	266	316	447	593	916	1371
2291	3087	3054	2112	1109	800	603	755	1111	1151
757	405	283	258	228	330	440	797	1027	1184
857	455	234	180	162	106	116	119	116	110
118	112	108	94	104	134	183	234	301	607
1036	1553	1413	826	413	257	164	133	107	91
89	80	82	93	75	57	74	82	82	65
73	61	77	74	67	61	66	80	75	71
81	93	83	89	73	84	87	89	111	130
142	157	197	208	288	543	759	902	780	543
452	431	573	909	1449	1968	2575	3052	3017	2581
1670	932	531	376	337	282	238	362	531	818
1506	1821	1765	1114	689	376	256	204	152	131
104	124	77	97	104	87	91	78	99	113
121	164	139	111	129	104	109	127	139	202
300	339	256	191	140	103	122	142	163	223
313	303	288	298	336	551	622	498	360	258
252	316	512	777	849	725	556	433	472	648
728	649	434	273	193	134	109	135	118	188
246	406	464	355	293	245	307	343	345	260
216	152	100	94	106	114	177	242	366	411
424	468	463	463	361	267	229	258	352	571
671	540	382	274	156	167	176	235	324	314
292	237	158	123	122	140	132	137	140	123
132	128	87	96	84	85	99	83	116	142
165	254	412	603	581	556	385	301	198	183
197	285	386	421	427	375	345	273	225	147
118	111	72	82	66	77	98	70	91	131
201	253	241	216	183	120	116	134	155	140
131	141	117	99	85	72	68	60	62	60
51	57	48	58	56	64	56	73	62	64
62	45	73	66	57	59	81	103	122	169
171	149	131	104	89	71	86	104	124	136
144	114	101	91	80	78	87	106	125	165
251	305	302	302	231	183	150	116	86	141
149	187	238	215	145	139	89	105	95	110
139	155	162	118	83	77	77	79	85	75
105	103	120	115	112	150	147	167	222	272
427	790	1227	1528	1408	1072	1004	860	631	525
400	316	247	204	169	153	134	113	116	107
116	116	112	105	101	70	83	81	60	70
59	49	51	55	76	64	62	78	82	87
89	124	139	126	187	220	364	367	389	361
263	224	165	134	163	199	199	209	190	130
129	104	106	118	132	201	303	358	355	290
288	279	250	269	334	543	746	979	1057	931
774	626	481	417	339	227	226	175	143	143

133	148	133	107	153	117	153	174	177	138
122	144	145	147	124	134	102	130	167	209
202	195	213	189	177	152	168	170	190	202
155	126	135	88	108	105	132	178	218	188
158	133	132	96	101	95	96	115	120	148
183	219	231	232	277	316	346	311	302	306
294	291	248	218	244	251	237	276	329	427
565	588	572	663	659	590	494	389	345	282
264	254	264	344	397	508	627	741	623	541
419	367	239	191	161	141	146	134	116	120
120	103	103	120	91	106	113	110	73	95
83	71	79	80	104	101	123	129	102	149
140	179	164	158	128	117	98	99	99	94
89	126	113	192	221	308	455	578	477	406
421	354	265	197	178	180	158	240	300	318
340	320	328	295	234	229	295	387	395	328
333	261	268	248	284	309	260	201	198	164
145	119	101	87	77	95	91	98	110	117
128	128	116	97	93	92	85	73	88	72
79	84	99	93	80	96	116	130	199	281
280	282	298	339	301	250	197	163	169	122
115	105	82	105	92	73	78	95	80	115
110	133	215	238	220	229	246	279	247	254
216	223	190	225	258	279	273	287	291	226
217	159	168	119	100	88	60	53	54	64
57	75	70	63	85	82	104	125	132	122
119	121	138	123	117	107	151	152	166	155
182	154	169	176	245	304	267	274	231	179
178	122	105	86	79	92	71	100	93	100
141	136	159	125	154	206	184	165	204	190
178	185	155	171	132	131	121	98	125	129
114	114	132	176	209	253	214	193	209	200
141	113	91	93	86	66	70	70	87	97
101	98	77	77	92	82	88	89	83	83
113	105	101	90	114	103	96	95	76	87
83	61	88	82	92	109	92	131	111	105
100	93	80	57	47	55	55	45	48	53
53	63	51	57	48	56	58	63	53	43
56	56	53	65	77	107	118	122	114	106
121	111	78	63	64	75	66	69	57	51
54	72	70	72	64	69	82	87	88	95
115	130	105	167	123	130	132	144	130	130
120	106	92	78	85	92	73	80	71	67
98	77	82	112	114	109	103	99	119	122
102	100	108	126	140	159	150	127	145	120
124	143	104	119	124	108	111	124	127	124
135	117	126	121	150	159	149	108	106	106
127	120	84	78	90	62	59	78	89	75
75	104	89	103	88	113	98	87	87	66
67	56	76	99	88	111	96	76	59	87
77	85	66	69	49	73	67	57	66	61
60	102	93	100	80	74	82	88	76	61
86	63	101	140	133	116	105	114	108	101
90	74	88	68	54	60	48	62	58	70
65	68	51	58	70	67	80	90	75	84
117	91	108	112	126	130	163	160	151	139
145	132	130	114	121	126	130	180	197	222
280	290	253	207	206	257	352	381	269	206
192	226	251	208	178	187	204	189	178	181
204	156	168	140	139	116	113	87	87	72
83	85	84	73	77	70	63	85	93	106
102	105	109	111	109	109	95	113	94	79
98	101	90	96	94	79	96	82	110	93
114	84	94	101	131	148	130	110	123	189
224	276	187	156	152	158	143	112	97	80
77	64	58	57	58	70	67	92	83	98
99	106	84	67	108	91	83	62	92	93
103	126	136	173	146	126	117	123	131	131
112	87	119	103	98	63	103	95	126	113

102	98	96	87	87	101	81	87	71	66
83	92	94	101	96	80	74	90	104	95
105	98	95	122	131	134	164	124	135	96
185	154	156	124	109	110	94	94	107	78
77	102	126	71	89	72	70	78	87	79
62	70	62	69	98	90	98	94	91	95
104	111	95	98	83	77	76	82	76	77
59	75	69	104	101	85	96	123	121	102
116	102	101	116	127	135	121	90	103	102
103	89	90	87	96	113	89	124	87	96
67	97	105	100	105	94	69	82	72	86
94	102	81	82	86	94	79	95	87	112
126	128	126	108	111	136	131	150	139	100
106	82	97	71	85	71	71	63	63	64
55	63	76	57	56	51	50	42	48	54
48	65	55	56	42	55	59	50	64	67
76	69	62	67	52	64	69	63	62	70
79	71	79	79	66	83	67	55	71	78
86	66	71	98	75	95	99	120	118	101
83	74	102	105	104	133	117	112	86	89
75	70	81	87	83	100	84	64	89	103
109	89	98	82	87	74	89	92	96	94
93	129	125	122	95	97	95	106	82	107
91	104	70	90	71	97	86	133	123	141
150	148	134	131	141	164	141	143	152	131
131	128	113	105	100	130	130	124	148	148
158	136	120	124	105	119	130	135	97	76
92	123	77	93	66	62	92	79	84	87
80	70	50	83	82	88	75	76	72	113
129	130	128	103	89	76	80	68	74	101
79	53	66	57	53	62	60	68	63	57
79	84	81	91	78	71	67	83	87	90
77	78	77	78	65	90	75	87	76	73
45	59	70	49	67	63	72	56	64	55
64	50	58	70	81	71	83	65	67	62
57	91	84	83	85	69	93	78	72	70
85	81	97	85	105	105	83	83	90	57
82	93	86	102	107	105	111	91	102	94
94	109	92	97	94	104	71	70	77	75
83	72	95	110	96	89	100	127	113	122
102	119	130	132	122	128	119	101	126	108
102	116	112	133	128	149	128	121	119	96
91	101	142	109	91	107	82	109	90	89
94	103	107	98	84	85	94	77	64	87
92	71	86	76	71	73	62	43	71	88
56	60	65	79	65	88	92	78	87	92
104	124	137	148	138	122	93	77	91	88
74	104	98	92	79	84	75	73	67	81
88	85	93	86	99	88	93	107	86	90
90	91	84	82	93	95	99	94	97	83
69	71	82	79	92	89	85	101	71	81
103	100	106	113	97	101	112	85	126	84
87	103	106	97	93	110	97	104	99	78
90	74	83	78	83	84	80	78	89	90
103	80	111	104	103	100	122	121	100	105
110	125	108	102	105	109	98	102	102	95
111	83	109	89	94	121	111	117	113	76
82	91	88	83	72	94	99	85	95	74
86	90	97	97	106	126	95	94	85	100
78	77	94	113	116	115	127	136	137	117
151	156	134	127	136	120	138	138	111	125
138	112	127	120	134	133	143	123	114	142
121	123	122	162	155	170	173	141	130	125
101	95	99	86	111	128	122	117	123	91
138	109	107	93	106	83	96	106	68	61
70	80	82	68	83	81	64	72	79	95
72	81	88	65	71	86	70	82	84	90
70									

Appendix P-18: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.07° 2θ

19.00	.07	139.00	50%-olivine, .07 degree 2-thet						
99.	99.	85.	94.	86.	79.	87.	66.	73.	105.
103.	101.	106.	129.	185.	169.	132.	127.	103.	103.
98.	104.	102.	89.	98.	71.	81.	89.	80.	86.
86.	68.	106.	69.	67.	73.	85.	70.	87.	89.
92.	69.	84.	85.	78.	87.	87.	83.	92.	109.
130.	153.	192.	285.	481.	816.	1079.	980.	571.	289.
153.	148.	99.	100.	94.	85.	115.	133.	172.	258.
401.	431.	293.	195.	103.	109.	128.	172.	129.	113.
102.	84.	76.	63.	78.	71.	70.	97.	122.	139.
188.	284.	489.	606.	620.	508.	330.	181.	125.	99.
82.	84.	82.	87.	99.	99.	101.	125.	160.	228.
351.	367.	255.	162.	119.	107.	102.	97.	97.	126.
145.	213.	363.	672.	845.	787.	458.	224.	144.	116.
92.	64.	90.	68.	85.	85.	80.	95.	80.	100.
105.	84.	85.	92.	105.	79.	128.	127.	159.	183.
263.	365.	501.	655.	1117.	2018.	2897.	3006.	2007.	1100.
716.	779.	992.	1096.	787.	462.	255.	254.	294.	486.
867.	1195.	1105.	698.	370.	186.	144.	134.	115.	107.
151.	135.	127.	129.	127.	139.	171.	234.	372.	790.
1239.	1422.	1085.	477.	277.	160.	134.	103.	106.	92.
70.	83.	75.	58.	76.	81.	61.	85.	77.	84.
74.	75.	68.	71.	74.	67.	75.	89.	78.	97.
99.	96.	102.	146.	140.	197.	205.	286.	506.	739.
740.	668.	505.	447.	581.	974.	1529.	2200.	2937.	3311.
2804.	1827.	944.	540.	352.	304.	318.	382.	579.	1169.
1695.	1802.	1381.	782.	453.	273.	164.	141.	111.	107.
113.	70.	81.	86.	82.	95.	113.	131.	119.	130.
136.	134.	113.	131.	203.	301.	306.	267.	201.	163.
126.	127.	161.	238.	328.	282.	268.	351.	561.	579.
511.	356.	271.	339.	502.	778.	907.	769.	555.	525.
626.	689.	642.	353.	218.	158.	116.	131.	139.	190.
330.	348.	325.	305.	264.	313.	353.	355.	223.	180.
113.	98.	146.	181.	256.	376.	456.	535.	519.	460.
362.	287.	251.	275.	430.	618.	567.	456.	310.	205.
194.	208.	333.	340.	297.	232.	169.	123.	124.	161.
118.	122.	102.	116.	126.	95.	104.	95.	98.	111.
142.	191.	349.	506.	641.	623.	442.	287.	209.	186.
227.	299.	420.	425.	405.	350.	247.	190.	132.	120.
89.	97.	75.	88.	94.	95.	150.	224.	226.	225.
165.	170.	135.	138.	155.	167.	137.	120.	88.	79.
61.	67.	62.	55.	72.	65.	63.	52.	75.	62.
51.	52.	47.	55.	45.	61.	64.	61.	77.	122.
136.	170.	161.	135.	77.	90.	94.	105.	129.	161.
127.	106.	112.	76.	74.	85.	107.	184.	235.	316.
323.	303.	247.	192.	153.	128.	169.	181.	244.	209.
168.	149.	124.	115.	114.	129.	118.	133.	115.	99.
72.	82.	97.	105.	106.	118.	112.	134.	135.	166.
203.	269.	376.	710.	1219.	1543.	1403.	1093.	908.	742.
578.	400.	332.	189.	210.	164.	137.	128.	114.	103.
114.	116.	114.	89.	87.	99.	69.	69.	63.	59.
66.	70.	68.	77.	82.	72.	79.	116.	133.	156.
151.	308.	357.	448.	377.	350.	248.	186.	162.	211.
216.	187.	177.	162.	117.	99.	111.	166.	242.	382.
351.	384.	297.	276.	262.	293.	375.	612.	816.	972.
932.	835.	630.	460.	378.	278.	203.	171.	143.	132.
148.	139.	139.	135.	135.	169.	185.	152.	149.	119.
136.	135.	135.	129.	144.	192.	229.	209.	199.	221.
203.	184.	153.	165.	195.	178.	130.	115.	94.	111.
133.	203.	172.	164.	130.	143.	89.	107.	96.	109.
122.	147.	178.	229.	282.	285.	274.	318.	340.	307.
297.	316.	280.	272.	288.	258.	319.	298.	408.	512.
615.	629.	710.	754.	609.	485.	366.	285.	271.	264.
283.	355.	493.	723.	688.	679.	531.	424.	293.	226.
159.	141.	132.	127.	133.	111.	108.	112.	104.	114.

101.	99.	71.	84.	75.	71.	83.	115.	124.	133.
144.	148.	152.	150.	169.	145.	108.	113.	105.	90.
110.	111.	140.	194.	227.	352.	516.	550.	504.	417.
378.	280.	208.	170.	176.	214.	318.	391.	394.	355.
321.	243.	272.	312.	368.	375.	368.	320.	255.	258.
271.	324.	256.	211.	164.	143.	125.	93.	101.	97.
89.	114.	119.	131.	106.	122.	109.	97.	88.	87.
74.	59.	74.	99.	88.	98.	93.	101.	139.	204.
277.	327.	315.	311.	356.	241.	213.	171.	153.	121.
118.	93.	101.	87.	84.	82.	109.	111.	144.	169.
196.	238.	233.	277.	296.	306.	243.	255.	228.	245.
271.	297.	290.	301.	251.	206.	194.	134.	119.	89.
78.	82.	72.	67.	74.	75.	69.	81.	97.	132.
140.	129.	119.	111.	100.	115.	116.	152.	166.	171.
161.	142.	162.	169.	208.	258.	260.	238.	224.	188.
134.	89.	99.	88.	85.	83.	100.	117.	143.	145.
144.	148.	164.	219.	190.	166.	159.	195.	171.	138.
128.	130.	140.	101.	142.	103.	134.	145.	213.	302.
254.	219.	184.	182.	137.	87.	98.	94.	110.	61.
95.	100.	105.	88.	98.	86.	79.	71.	77.	83.
103.	102.	123.	100.	103.	96.	96.	90.	68.	89.
60.	76.	85.	95.	110.	97.	95.	86.	80.	79.
66.	59.	62.	59.	61.	56.	65.	47.	55.	58.
54.	58.	61.	55.	53.	71.	59.	76.	81.	110.
142.	151.	117.	137.	90.	109.	49.	85.	62.	42.
60.	64.	68.	60.	73.	70.	74.	71.	87.	93.
99.	107.	120.	139.	121.	132.	107.	163.	182.	131.
103.	105.	125.	93.	95.	71.	77.	67.	92.	79.
96.	129.	118.	117.	91.	110.	109.	104.	110.	115.
145.	140.	162.	158.	138.	107.	117.	144.	93.	88.
144.	135.	145.	140.	148.	120.	141.	126.	126.	116.
93.	105.	103.	96.	102.	66.	66.	68.	78.	93.
102.	98.	105.	81.	91.	95.	92.	78.	71.	67.
78.	80.	85.	99.	95.	70.	85.	88.	81.	82.
56.	69.	49.	60.	62.	77.	72.	92.	96.	82.
75.	77.	81.	80.	79.	74.	90.	129.	161.	131.
100.	119.	115.	102.	105.	84.	61.	69.	70.	54.
58.	44.	55.	50.	61.	72.	70.	92.	80.	78.
91.	108.	97.	118.	145.	148.	158.	147.	121.	142.
154.	153.	135.	145.	134.	160.	192.	248.	308.	291.
257.	239.	274.	318.	315.	298.	208.	206.	218.	186.
228.	202.	208.	227.	203.	185.	156.	152.	154.	154.
115.	91.	102.	110.	95.	71.	91.	64.	68.	93.
94.	106.	103.	122.	126.	126.	146.	121.	117.	126.
98.	115.	96.	97.	97.	107.	96.	80.	105.	94.
92.	79.	117.	133.	130.	132.	129.	164.	239.	215.
178.	135.	126.	154.	116.	120.	80.	101.	72.	60.
82.	73.	89.	88.	76.	96.	90.	81.	80.	73.
95.	79.	90.	93.	111.	149.	175.	142.	115.	135.
154.	148.	138.	103.	115.	94.	86.	98.	104.	130.
131.	112.	91.	93.	116.	98.	73.	78.	71.	70.
98.	95.	106.	94.	101.	116.	104.	103.	107.	111.
106.	140.	175.	151.	104.	126.	141.	143.	148.	124.
102.	114.	115.	79.	86.	110.	102.	74.	78.	81.
85.	73.	92.	61.	65.	71.	85.	70.	113.	101.
103.	100.	113.	147.	105.	90.	92.	95.	108.	78.
70.	75.	68.	89.	87.	93.	115.	119.	101.	121.
99.	129.	130.	148.	139.	101.	97.	96.	94.	127.
87.	126.	102.	103.	108.	81.	88.	93.	101.	99.
87.	90.	85.	82.	92.	95.	67.	99.	82.	78.
74.	88.	105.	121.	149.	137.	109.	131.	118.	100.
95.	122.	107.	96.	72.	87.	80.	63.	87.	54.
59.	50.	66.	58.	71.	47.	50.	57.	53.	62.
64.	67.	62.	53.	65.	54.	67.	72.	74.	72.
87.	79.	57.	78.	53.	67.	78.	82.	95.	68.
72.	69.	71.	76.	69.	95.	90.	95.	90.	98.
116.	119.	126.	117.	106.	88.	127.	125.	146.	140.
117.	80.	86.	90.	87.	94.	88.	69.	70.	86.
105.	107.	86.	76.	89.	84.	111.	117.	114.	126.

142.	151.	124.	106.	89.	89.	101.	106.	95.	96.
87.	84.	96.	108.	132.	150.	150.	154.	127.	122.
133.	129.	135.	135.	123.	126.	119.	112.	114.	131.
132.	151.	145.	144.	110.	123.	136.	113.	124.	129.
117.	108.	73.	122.	104.	83.	74.	70.	73.	68.
55.	85.	69.	89.	72.	80.	71.	83.	94.	108.
118.	105.	83.	71.	71.	86.	77.	86.	77.	80.
63.	67.	62.	71.	55.	58.	72.	95.	90.	79.
82.	92.	78.	89.	77.	86.	72.	80.	71.	96.
84.	82.	78.	60.	80.	71.	78.	54.	63.	59.
72.	64.	65.	75.	71.	91.	80.	97.	91.	71.
78.	79.	93.	98.	103.	71.	86.	76.	87.	90.
95.	66.	80.	77.	92.	72.	75.	64.	85.	105.
100.	101.	115.	106.	105.	84.	76.	94.	85.	84.
93.	77.	90.	75.	90.	84.	89.	111.	116.	75.
97.	116.	114.	158.	109.	96.	122.	136.	135.	110.
126.	113.	112.	118.	142.	141.	152.	124.	106.	115.
97.	102.	104.	103.	113.	96.	97.	116.	109.	85.
129.	109.	89.	79.	83.	91.	72.	84.	92.	73.
71.	80.	89.	72.	59.	70.	60.	61.	66.	95.
88.	96.	93.	103.	89.	91.	125.	135.	112.	139.
111.	118.	84.	102.	129.	114.	108.	96.	70.	77.
82.	65.	78.	95.	95.	100.	145.	104.	108.	96.
95.	85.	101.	81.	113.	107.	112.	103.	79.	86.
82.	86.	71.	83.	96.	95.	82.	91.	77.	116.
109.	97.	107.	133.	98.	112.	96.	87.	100.	84.
117.	97.	108.	100.	96.	99.	77.	90.	78.	92.
83.	90.	91.	96.	91.	112.	146.	107.	125.	120.
125.	123.	95.	100.	95.	135.	125.	125.	132.	106.
102.	76.	98.	104.	113.	133.	120.	98.	122.	108.
97.	118.	105.	74.	90.	97.	88.	111.	75.	98.
98.	97.	108.	105.	72.	90.	82.	93.	93.	92.
112.	116.	146.	161.	162.	150.	139.	116.	136.	150.
135.	121.	141.	146.	139.	128.	147.	138.	151.	153.
159.	126.	128.	120.	173.	180.	193.	170.	167.	146.
123.	106.	107.	127.	117.	123.	107.	144.	130.	120.
95.	114.	106.	91.	76.	79.	96.	82.	96.	69.
85.	83.	109.	76.	72.	100.	71.	83.	68.	64.
72.	86.	93.	86.	80.	88.				

Appendix P-19: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.08° 2θ

19.00 .08 139.00 50%-olivine, .08 degree 2-thet

80.	96.	95.	84.	78.	90.	71.	83.	86.	86.
104.	128.	160.	147.	121.	113.	90.	91.	67.	70.
99.	86.	90.	90.	80.	68.	82.	82.	87.	69.
76.	78.	73.	80.	74.	88.	72.	72.	95.	78.
79.	70.	95.	100.	107.	166.	231.	438.	788.	994.
868.	377.	167.	133.	99.	83.	86.	97.	108.	175.
251.	361.	393.	280.	169.	125.	127.	128.	140.	102.
80.	74.	75.	78.	76.	75.	79.	112.	131.	213.
351.	533.	542.	459.	265.	164.	105.	99.	78.	81.
77.	77.	83.	105.	103.	214.	302.	345.	254.	128.
99.	89.	96.	97.	106.	128.	222.	425.	773.	844.
493.	214.	129.	99.	76.	69.	85.	81.	84.	83.
82.	75.	69.	74.	76.	86.	96.	124.	104.	116.
160.	237.	326.	519.	723.	1413.	2451.	3148.	2104.	1066.
683.	789.	1041.	852.	466.	264.	244.	320.	575.	939.
1137.	825.	396.	196.	141.	106.	98.	102.	129.	119.
113.	129.	135.	174.	264.	597.	1144.	1381.	861.	419.
214.	113.	115.	100.	77.	91.	59.	69.	75.	76.
77.	61.	78.	76.	62.	62.	67.	63.	85.	61.
76.	92.	70.	101.	103.	134.	158.	178.	231.	409.
624.	748.	665.	468.	434.	657.	1185.	1894.	2575.	3080.
2667.	1532.	724.	389.	320.	303.	340.	630.	1274.	1822.
1461.	941.	436.	240.	164.	142.	114.	100.	92.	70.
91.	77.	116.	118.	142.	140.	137.	110.	121.	119.
206.	296.	256.	195.	165.	111.	127.	196.	275.	297.
284.	335.	467.	554.	442.	297.	262.	435.	723.	783.
703.	446.	580.	659.	594.	370.	178.	145.	137.	108.
165.	289.	375.	365.	272.	281.	344.	323.	260.	167.
127.	102.	139.	211.	318.	435.	516.	463.	436.	311.
243.	282.	417.	542.	533.	377.	193.	172.	207.	270.
339.	271.	204.	132.	134.	136.	134.	109.	120.	115.
91.	95.	100.	99.	106.	149.	224.	366.	523.	642.
471.	321.	219.	198.	258.	339.	378.	400.	340.	261.
173.	87.	88.	98.	88.	77.	84.	118.	164.	220.
248.	158.	136.	118.	118.	124.	148.	123.	109.	94.
74.	55.	61.	60.	52.	64.	54.	59.	62.	49.
50.	71.	67.	72.	82.	72.	81.	112.	177.	135.
103.	99.	81.	90.	115.	116.	138.	109.	88.	82.
90.	78.	140.	221.	284.	309.	288.	223.	163.	123.
125.	199.	217.	197.	161.	103.	83.	99.	155.	149.
120.	106.	72.	75.	69.	79.	102.	122.	120.	123.
135.	182.	235.	374.	798.	1337.	1504.	1194.	869.	670.
541.	352.	277.	199.	150.	129.	107.	114.	119.	123.
99.	84.	92.	71.	78.	51.	58.	67.	70.	77.
75.	62.	85.	85.	103.	142.	167.	250.	358.	385.
358.	292.	195.	159.	162.	195.	199.	159.	140.	122.
98.	123.	235.	331.	312.	332.	278.	256.	290.	387.
670.	948.	916.	825.	637.	448.	327.	255.	202.	170.
136.	127.	149.	124.	140.	138.	148.	153.	142.	105.
147.	143.	124.	118.	182.	232.	225.	199.	202.	161.
151.	163.	174.	140.	110.	110.	94.	103.	176.	166.
167.	177.	122.	104.	75.	97.	106.	133.	156.	210.
234.	261.	308.	302.	308.	282.	284.	289.	258.	237.
286.	304.	408.	509.	560.	626.	681.	605.	480.	394.
254.	251.	216.	276.	419.	664.	724.	600.	505.	344.
229.	177.	131.	140.	130.	126.	102.	119.	118.	117.
79.	90.	94.	66.	87.	65.	86.	140.	139.	126.
131.	172.	158.	167.	118.	123.	94.	94.	101.	118.
157.	203.	342.	500.	514.	426.	383.	289.	200.	172.
183.	263.	370.	375.	345.	305.	250.	280.	333.	363.
343.	294.	270.	243.	316.	250.	208.	173.	124.	93.
98.	90.	93.	80.	103.	114.	116.	101.	114.	97.
82.	73.	77.	77.	66.	86.	83.	99.	126.	176.
266.	305.	328.	268.	273.	183.	147.	160.	140.	115.

104.	92.	80.	89.	100.	117.	139.	191.	228.	223.
241.	272.	235.	250.	207.	193.	247.	303.	322.	256.
238.	203.	169.	123.	85.	87.	87.	67.	61.	66.
69.	73.	85.	121.	119.	118.	112.	130.	109.	90.
140.	174.	171.	147.	157.	183.	218.	249.	229.	194.
173.	127.	94.	96.	97.	87.	89.	112.	125.	111.
133.	162.	201.	183.	167.	177.	189.	184.	151.	126.
135.	104.	107.	121.	118.	145.	216.	257.	199.	169.
163.	107.	110.	91.	76.	82.	76.	94.	95.	81.
97.	90.	77.	84.	83.	89.	128.	98.	96.	87.
94.	70.	94.	94.	84.	80.	94.	104.	103.	107.
97.	85.	70.	73.	51.	55.	47.	54.	52.	57.
53.	43.	53.	44.	51.	50.	60.	69.	59.	94.
122.	138.	105.	100.	70.	81.	58.	63.	64.	64.
54.	59.	58.	60.	75.	63.	93.	80.	97.	108.
130.	134.	113.	152.	153.	128.	101.	92.	96.	96.
82.	76.	77.	74.	79.	102.	130.	99.	101.	121.
113.	94.	101.	136.	145.	134.	136.	139.	157.	139.
110.	103.	109.	115.	147.	121.	112.	123.	139.	130.
106.	99.	105.	113.	108.	91.	77.	77.	68.	83.
76.	75.	90.	96.	86.	87.	79.	65.	69.	70.
65.	101.	82.	81.	83.	83.	60.	75.	51.	56.
70.	60.	55.	69.	105.	81.	71.	80.	65.	85.
62.	71.	108.	139.	134.	106.	128.	109.	96.	70.
77.	77.	71.	49.	39.	54.	46.	61.	69.	58.
79.	74.	92.	94.	102.	136.	127.	143.	137.	126.
130.	128.	120.	106.	129.	142.	156.	177.	265.	270.
231.	224.	254.	330.	266.	193.	192.	218.	217.	210.
198.	177.	207.	183.	171.	162.	154.	133.	123.	93.
68.	84.	71.	85.	63.	90.	89.	85.	94.	108.
108.	126.	103.	91.	101.	95.	121.	100.	96.	103.
85.	102.	92.	89.	85.	99.	125.	122.	156.	128.
185.	188.	204.	146.	136.	160.	126.	89.	72.	73.
63.	61.	72.	67.	91.	90.	100.	94.	91.	90.
100.	78.	73.	99.	132.	140.	147.	118.	111.	113.
108.	96.	93.	92.	97.	81.	117.	124.	110.	91.
89.	92.	120.	81.	81.	77.	96.	112.	89.	85.
77.	105.	94.	89.	67.	91.	121.	167.	150.	122.
128.	151.	151.	114.	90.	91.	79.	85.	94.	101.
88.	77.	68.	79.	85.	78.	63.	49.	80.	79.
91.	116.	103.	115.	94.	82.	98.	82.	74.	80.
80.	81.	76.	99.	100.	103.	109.	94.	94.	99.
103.	145.	125.	98.	97.	93.	99.	103.	85.	74.
106.	98.	95.	80.	108.	102.	93.	94.	89.	82.
90.	82.	86.	91.	80.	98.	101.	95.	130.	126.
126.	124.	130.	126.	115.	95.	96.	83.	80.	71.
67.	62.	58.	64.	56.	66.	57.	64.	45.	40.
52.	64.	61.	37.	50.	59.	65.	66.	73.	83.
58.	71.	56.	64.	61.	81.	60.	67.	80.	76.
66.	51.	80.	85.	71.	74.	91.	90.	126.	105.
118.	97.	83.	100.	125.	105.	121.	94.	68.	75.
80.	76.	77.	92.	68.	108.	101.	67.	94.	95.
77.	104.	107.	136.	129.	110.	105.	91.	89.	105.
127.	101.	86.	88.	98.	113.	122.	125.	144.	123.
117.	126.	121.	137.	102.	127.	127.	118.	92.	127.
121.	131.	148.	141.	125.	125.	152.	142.	133.	100.
87.	96.	78.	86.	63.	62.	75.	83.	71.	73.
68.	74.	73.	74.	101.	97.	104.	103.	78.	72.
81.	89.	94.	66.	69.	58.	60.	51.	59.	58.
58.	74.	68.	76.	76.	73.	92.	72.	67.	81.
56.	82.	61.	82.	61.	82.	59.	56.	64.	53.
60.	68.	65.	73.	64.	69.	68.	82.	78.	72.
74.	81.	77.	80.	85.	66.	65.	69.	79.	92.
98.	91.	90.	73.	70.	79.	84.	83.	83.	90.
96.	98.	92.	92.	102.	83.	86.	94.	96.	87.
90.	69.	74.	91.	100.	91.	100.	117.	124.	114.
111.	119.	132.	123.	123.	92.	109.	109.	155.	134.
106.	99.	118.	117.	126.	114.	104.	113.	104.	74.
109.	89.	88.	102.	106.	80.	83.	59.	76.	85.

87.	74.	80.	80.	74.	61.	83.	71.	71.	87.
105.	92.	91.	104.	103.	145.	125.	144.	120.	89.
89.	101.	104.	89.	80.	76.	81.	90.	68.	78.
86.	96.	112.	112.	95.	81.	76.	79.	92.	83.
88.	94.	76.	69.	53.	71.	92.	88.	74.	77.
76.	97.	109.	86.	100.	96.	98.	111.	83.	100.
87.	95.	91.	92.	85.	113.	90.	84.	75.	95.
82.	82.	89.	97.	79.	106.	119.	117.	107.	100.
99.	86.	89.	113.	116.	122.	124.	108.	100.	79.
93.	105.	102.	123.	104.	99.	84.	85.	83.	75.
85.	87.	76.	99.	84.	72.	108.	98.	107.	96.
85.	107.	108.	114.	102.	103.	148.	183.	130.	120.
123.	111.	111.	134.	111.	129.	124.	139.	123.	131.
137.	137.	98.	109.	134.	138.	170.	169.	154.	152.
126.	112.	126.	108.	109.	128.	137.	101.	109.	114.
104.	102.	74.	76.	83.	78.	98.	70.	92.	80.
64.	80.	66.	110.	70.	78.	63.	74.	79.	69.
67.									

Appendix P-20: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.09° 2θ

19.000 0.090 139.00 50%-olivine mixture, 0.9 degree 2-theta

	95	82	88	88	96	82	80	100	103	115
	187	144	127	130	101	74	78	89	106	79
	79	74	72	77	68	80	69	77	88	71
	74	66	81	71	80	92	81	86	108	150
	212	382	846	1196	634	217	139	104	82	85
	94	132	144	297	437	305	160	102	109	137
	130	97	72	77	75	82	73	96	101	138
	302	511	608	417	281	142	110	94	78	72
	77	76	91	144	277	385	293	155	134	82
	83	92	105	148	310	820	913	480	194	102
	71	60	89	65	63	80	82	90	91	93
	97	100	97	103	135	176	253	370	583	1203
	2358	3274	2107	883	613	1009	1071	573	287	261
	345	614	1147	964	447	193	152	104	122	117
	135	99	105	119	166	279	610	1391	1368	590
	195	148	119	93	89	83	82	79	89	78
	59	67	70	48	66	65	90	83	82	81
	92	101	97	133	185	183	331	658	877	638
	413	469	830	1826	2565	3193	2451	1247	508	335
	278	270	498	1183	1918	1368	665	290	183	151
	122	111	75	66	83	86	99	148	140	122
	103	93	156	275	352	227	148	105	146	191
	361	288	252	427	581	442	281	273	527	847
	689	494	467	781	631	298	169	118	147	156
	264	425	362	280	312	363	276	150	105	112
	118	223	379	431	476	473	359	217	242	501
	635	480	248	181	173	267	351	241	137	136
	116	118	129	140	121	85	67	90	83	133
	190	352	589	588	404	207	194	223	399	430
	387	315	243	144	102	84	78	71	86	124
	193	253	233	155	129	128	156	145	91	88
	76	57	78	70	58	74	61	51	52	53
	58	66	82	76	78	88	165	166	113	100
	70	99	111	129	120	106	84	73	91	124
	251	328	295	195	156	114	147	209	229	186
	130	90	99	131	147	110	100	84	81	87
	95	111	121	125	146	186	317	570	1213	1548
	1236	914	615	425	274	230	185	125	125	97
	113	120	115	77	74	65	57	60	66	47
	58	55	75	90	104	136	186	276	410	418
	278	200	139	193	184	168	145	118	124	128
	191	334	383	308	269	253	342	665	949	979
	760	551	364	256	207	161	124	149	142	130
	116	126	182	153	152	129	114	134	134	175
	205	172	205	168	141	150	189	130	118	105
	111	169	208	183	153	97	97	114	120	135
	193	229	228	300	350	319	291	274	229	223
	248	250	392	458	605	618	739	525	406	286
	233	232	305	432	661	689	553	410	235	165
	151	133	133	123	105	111	127	102	115	75
1	75	97	91	121	124	126	115	187	180	143
	129	92	89	90	129	155	238	364	607	458
	385	281	221	161	179	262	336	301	324	242
	256	340	377	326	263	233	282	294	212	207
	141	96	79	94	85	113	121	112	105	96
	79	64	65	62	78	84	93	89	142	228
	312	286	341	254	161	153	122	116	89	84
	75	75	94	121	147	220	219	226	264	257
	256	217	225	273	301	322	240	192	131	108
	83	79	62	78	69	83	77	97	132	130
	111	109	116	107	119	153	160	147	158	186
	256	260	193	185	119	86	77	82	97	91
	104	141	135	182	184	189	197	179	178	161
	144	123	109	139	115	167	213	224	187	175

	173	98	96	90	86	84	97	65	91	89
	94	70	83	100	123	87	81	113	84	82
	57	76	99	101	119	110	95	83	92	52
	59	66	50	57	57	49	63	67	48	46
	62	70	65	96	107	140	93	85	79	65
	83	83	49	65	57	64	50	84	83	83
	93	117	131	137	89	147	124	132	89	102
	93	71	72	84	79	99	129	115	92	96
	88	93	124	124	121	155	145	130	106	121
	119	130	153	112	118	129	131	142	116	100
	113	102	81	64	67	61	90	107	82	92
	89	76	72	79	61	59	86	98	92	69
	75	78	56	48	68	54	55	88	78	89
	78	65	69	78	83	127	149	93	106	96
	87	87	62	59	57	56	56	54	45	63
	66	69	68	106	98	97	117	148	171	125
	153	150	112	130	137	155	218	262	251	208
	270	379	273	203	212	241	189	193	217	187
	147	157	129	142	90	86	92	76	84	77
	65	77	96	105	122	110	113	97	93	102
	101	88	103	98	80	91	82	84	97	132
	147	139	175	212	242	171	149	153	114	103
	83	80	68	55	88	86	89	117	94	84
	99	79	81	82	108	155	141	113	126	110
	99	105	87	87	100	108	115	88	93	97
	109	72	67	95	98	90	81	94	100	106
	107	93	112	122	141	127	131	173	149	108
	103	116	83	91	85	86	77	71	73	68
	65	65	79	81	96	104	96	90	108	73
	89	84	81	82	79	76	91	111	106	116
	95	106	121	113	98	72	86	90	98	93
	118	133	101	85	78	98	98	68	83	85
	89	96	89	78	92	87	112	146	111	79
	120	121	122	97	101	95	73	77	72	52
	56	59	55	59	39	53	53	61	53	61
	48	58	54	56	81	82	75	67	58	82
	64	71	68	76	73	64	60	70	82	85
	83	136	125	102	109	111	116	96	115	92
	91	82	86	92	79	66	87	100	88	70
	78	87	93	115	110	125	104	80	105	126
	89	94	90	80	102	128	125	168	127	143
	114	125	141	122	98	98	131	111	127	148
	144	132	131	114	103	113	103	107	80	79
	79	72	69	79	76	60	71	70	72	82
	126	132	103	80	60	106	96	73	74	58
	66	65	40	68	76	97	90	95	85	79
	73	80	72	92	79	61	66	61	51	53
	71	63	63	76	62	61	73	69	103	66
	68	72	98	60	84	68	76	63	82	102
	106	74	85	74	95	96	114	106	103	71
	104	89	95	86	86	69	74	69	90	109
	116	101	120	137	129	134	119	122	107	104
1	84	104	159	143	122	112	107	109	121	119
	97	91	101	79	105	100	101	101	81	89
	61	77	83	82	64	76	55	62	81	81
	94	85	85	100	84	134	117	109	102	96
	96	91	95	88	93	67	84	93	87	90
	92	113	84	78	81	79	97	98	91	89
	75	75	92	77	76	89	88	94	117	117
	117	88	87	83	105	82	84	95	100	98
	98	69	83	85	84	84	102	95	102	87
	108	119	125	116	95	104	113	125	114	100
	86	87	105	110	113	109	98	81	80	94
	82	79	89	105	97	97	95	105	102	94
	100	103	97	103	117	132	149	142	128	123
	118	144	124	110	135	138	147	128	155	127
	112	141	146	171	178	154	135	112	104	93
	113	145	122	97	84	100	87	81	81	66
	74	80	74	67	66	67	75	95	78	86

80	84	91	99	84

Appendix P-21: step-intensity data of the 50 wt% olivine mixture of Ol+Py, step size 0.10° 2θ

19.00 .10 139.00 50%-olivine, .1 degree 2-theta

101.	106.	81.	77.	91.	91.	105.	98.	104.	138.
162.	139.	110.	110.	85.	79.	100.	93.	74.	89.
79.	80.	88.	73.	80.	104.	83.	67.	87.	88.
84.	86.	79.	101.	91.	105.	150.	232.	554.	996.
966.	394.	172.	105.	113.	92.	117.	132.	234.	356.
371.	208.	122.	138.	137.	109.	89.	85.	70.	80.
102.	83.	124.	165.	340.	589.	582.	363.	167.	98.
85.	77.	85.	81.	103.	108.	209.	280.	311.	195.
107.	101.	98.	104.	159.	225.	552.	789.	538.	252.
129.	86.	99.	85.	75.	76.	81.	68.	91.	76.
93.	85.	93.	116.	177.	249.	372.	721.	1316.	2619.
3014.	1470.	717.	811.	1028.	661.	333.	220.	351.	768.
1198.	760.	302.	156.	119.	129.	135.	105.	109.	118.
137.	253.	550.	1251.	1255.	557.	187.	124.	101.	99.
86.	82.	81.	79.	84.	60.	66.	75.	70.	75.
78.	86.	71.	97.	69.	122.	134.	166.	196.	302.
615.	773.	616.	444.	602.	1215.	2339.	3136.	2901.	1573.
579.	333.	320.	401.	895.	1611.	1697.	925.	372.	197.
137.	133.	87.	104.	83.	89.	100.	156.	166.	109.
110.	107.	204.	297.	270.	145.	140.	117.	241.	277.
289.	335.	531.	495.	342.	289.	565.	830.	737.	486.
574.	642.	423.	174.	124.	145.	174.	298.	372.	309.
278.	394.	314.	162.	107.	130.	153.	289.	435.	487.
434.	348.	268.	295.	485.	641.	439.	183.	167.	237.
359.	271.	124.	123.	160.	125.	111.	108.	93.	95.
84.	111.	134.	241.	483.	621.	476.	287.	173.	231.
403.	376.	398.	245.	185.	101.	91.	69.	73.	89.
120.	204.	246.	177.	109.	143.	137.	146.	105.	97.
79.	63.	48.	56.	65.	54.	66.	46.	50.	57.
61.	68.	77.	94.	158.	165.	127.	90.	81.	94.
103.	123.	98.	86.	69.	102.	168.	306.	305.	264.
171.	123.	149.	211.	239.	177.	107.	104.	117.	142.
128.	113.	102.	78.	94.	118.	100.	134.	131.	209.
269.	646.	1309.	1454.	1083.	822.	573.	347.	260.	191.
144.	109.	128.	118.	99.	82.	70.	72.	63.	64.
53.	54.	72.	80.	96.	114.	130.	208.	266.	399.
410.	244.	179.	168.	206.	187.	143.	117.	109.	136.
310.	363.	338.	282.	235.	341.	622.	945.	946.	698.
479.	330.	224.	163.	139.	123.	129.	147.	143.	148.
160.	147.	148.	124.	129.	149.	197.	219.	199.	174.
148.	163.	159.	147.	106.	106.	135.	190.	171.	140.
110.	92.	92.	126.	121.	190.	234.	278.	331.	294.
294.	273.	247.	274.	268.	316.	462.	553.	641.	702.
575.	439.	307.	228.	271.	398.	660.	715.	586.	367.
227.	153.	146.	131.	133.	108.	102.	114.	80.	73.
80.	75.	85.	95.	136.	130.	150.	141.	147.	138.
129.	78.	102.	104.	181.	195.	422.	513.	412.	366.
211.	168.	193.	286.	299.	343.	318.	258.	307.	377.
352.	281.	244.	246.	269.	238.	182.	103.	72.	102.
96.	116.	135.	124.	121.	93.	85.	81.	62.	80.
92.	78.	103.	169.	296.	299.	317.	297.	198.	178.
138.	111.	75.	78.	75.	93.	103.	152.	224.	220.
244.	284.	243.	226.	228.	264.	322.	289.	247.	198.
135.	101.	63.	58.	73.	69.	55.	81.	105.	135.
119.	124.	118.	103.	135.	141.	184.	148.	185.	223.
232.	213.	194.	116.	115.	90.	66.	82.	135.	136.
161.	167.	198.	199.	206.	200.	157.	113.	120.	119.
113.	153.	150.	270.	236.	186.	190.	134.	89.	88.
71.	66.	82.	95.	98.	109.	101.	82.	92.	123.
103.	74.	83.	63.	73.	84.	72.	89.	84.	113.
101.	86.	71.	70.	51.	49.	61.	54.	57.	63.
52.	56.	68.	59.	54.	88.	138.	117.	104.	107.
83.	47.	52.	55.	60.	58.	45.	57.	79.	81.
96.	110.	125.	135.	120.	137.	123.	124.	108.	78.

75.	84.	81.	78.	103.	110.	92.	103.	117.	92.
118.	140.	150.	151.	140.	142.	116.	118.	112.	119.
126.	122.	121.	122.	123.	109.	108.	107.	82.	76.
71.	61.	74.	95.	94.	89.	91.	76.	58.	61.
77.	84.	82.	75.	78.	74.	54.	50.	58.	50.
58.	84.	88.	81.	85.	69.	84.	74.	126.	150.
122.	112.	102.	77.	75.	72.	49.	72.	52.	68.
68.	61.	96.	74.	88.	88.	101.	120.	150.	143.
118.	146.	117.	125.	159.	183.	222.	313.	234.	248.
347.	328.	224.	202.	196.	159.	179.	192.	204.	165.
192.	153.	119.	89.	69.	77.	76.	75.	84.	92.
109.	98.	115.	122.	125.	84.	92.	90.	108.	106.
77.	86.	95.	86.	89.	124.	136.	134.	218.	225.
174.	147.	151.	101.	88.	63.	69.	65.	62.	78.
97.	98.	99.	97.	102.	81.	96.	126.	147.	139.
117.	121.	125.	94.	119.	90.	86.	119.	135.	91.
84.	96.	82.	98.	87.	76.	96.	88.	91.	109.
85.	96.	112.	127.	137.	128.	137.	126.	141.	111.
98.	101.	97.	102.	101.	96.	73.	82.	66.	54.
68.	99.	91.	100.	78.	119.	88.	93.	72.	74.
72.	78.	76.	108.	104.	106.	104.	92.	83.	134.
133.	73.	67.	105.	89.	92.	132.	115.	77.	96.
102.	74.	95.	79.	91.	86.	81.	85.	82.	91.
109.	128.	135.	110.	144.	122.	91.	89.	89.	97.
83.	67.	61.	67.	62.	50.	51.	46.	52.	73.
54.	54.	51.	55.	67.	64.	82.	70.	59.	70.
71.	70.	81.	75.	68.	64.	75.	86.	72.	83.
125.	103.	99.	110.	97.	112.	114.	98.	78.	83.
85.	91.	71.	79.	108.	101.	92.	62.	81.	75.
93.	127.	129.	107.	109.	110.	105.	109.	87.	89.
97.	117.	152.	129.	134.	130.	156.	137.	111.	134.
145.	107.	133.	164.	156.	134.	133.	143.	118.	122.
92.	92.	108.	76.	64.	85.	56.	70.	65.	67.
66.	83.	100.	127.	85.	100.	84.	70.	76.	52.
63.	62.	67.	59.	80.	65.	78.	75.	88.	81.
83.	76.	80.	74.	92.	82.	74.	58.	60.	82.
84.	49.	81.	64.	73.	65.	82.	73.	68.	72.
85.	97.	69.	71.	72.	84.	94.	82.	80.	77.
71.	67.	89.	96.	124.	97.	103.	102.	100.	81.
83.	90.	93.	81.	81.	108.	131.	111.	119.	134.
133.	142.	121.	101.	102.	104.	130.	138.	118.	84.
109.	122.	127.	105.	78.	98.	94.	72.	94.	82.
82.	69.	71.	72.	86.	71.	73.	58.	64.	69.
62.	85.	99.	88.	92.	108.	142.	117.	103.	88.
100.	102.	113.	78.	81.	103.	75.	69.	89.	100.
102.	113.	74.	85.	76.	97.	97.	86.	74.	89.
71.	64.	108.	92.	86.	104.	109.	114.	111.	91.
105.	104.	97.	101.	108.	101.	96.	82.	76.	83.
98.	88.	98.	96.	109.	105.	123.	127.	104.	112.
101.	117.	11.	101.	105.	83.	76.	105.	104.	104.
113.	101.	93.	87.	80.	92.	89.	88.	92.	112.
102.	98.	96.	100.	96.	99.	129.	149.	181.	142.
137.	100.	118.	125.	142.	133.	133.	125.	141.	123.
120.	137.	169.	186.	178.	158.	117.	102.	105.	130.
132.	147.	123.	109.	108.	113.	108.	88.	78.	78.
96.	76.	82.	84.	76.	94.	86.	72.	92.	75.
69.									

Appendix P-22: step-intensity data of pure muscovite, transmission geometry

8.00	.02	116.00	pure muscovite						
433.	386.	408.	377.	411.	438.	415.	403.	420.	410.
390.	407.	381.	407.	396.	459.	469.	466.	463.	472.
490.	514.	524.	545.	523.	630.	586.	663.	692.	668.
738.	730.	865.	847.	972.	1035.	1149.	1284.	1424.	1542.
1788.	1859.	1552.	1325.	916.	729.	566.	456.	448.	391.
419.	355.	392.	358.	363.	314.	297.	351.	328.	337.
320.	348.	325.	303.	312.	330.	325.	330.	299.	284.
313.	307.	332.	309.	290.	302.	283.	289.	332.	334.
291.	293.	311.	312.	313.	282.	341.	304.	278.	283.
307.	290.	273.	285.	278.	308.	273.	279.	295.	254.
268.	288.	239.	247.	309.	303.	279.	305.	293.	276.
266.	274.	255.	251.	294.	248.	275.	277.	240.	276.
253.	282.	244.	262.	238.	241.	249.	240.	269.	267.
280.	270.	273.	244.	268.	244.	284.	248.	256.	247.
241.	247.	253.	251.	255.	209.	268.	215.	270.	250.
242.	227.	220.	244.	290.	246.	235.	236.	243.	232.
253.	254.	240.	224.	234.	241.	238.	239.	254.	238.
233.	211.	256.	245.	225.	263.	239.	247.	278.	206.
263.	258.	226.	230.	239.	239.	227.	245.	215.	248.
209.	221.	220.	218.	219.	218.	189.	200.	212.	244.
203.	266.	223.	202.	193.	242.	240.	222.	220.	234.
245.	232.	242.	216.	231.	217.	220.	205.	254.	189.
195.	207.	238.	241.	243.	220.	228.	242.	237.	208.
238.	211.	221.	254.	222.	228.	185.	231.	228.	197.
226.	215.	221.	200.	216.	210.	215.	204.	230.	181.
209.	203.	209.	187.	217.	195.	213.	191.	223.	214.
216.	184.	224.	205.	193.	212.	224.	259.	221.	226.
198.	201.	219.	253.	197.	229.	223.	233.	222.	200.
226.	242.	244.	239.	256.	226.	235.	233.	221.	217.
247.	227.	222.	230.	222.	217.	244.	223.	198.	212.
227.	225.	217.	190.	225.	240.	202.	211.	209.	192.
198.	184.	216.	226.	201.	215.	225.	208.	213.	183.
213.	179.	182.	207.	195.	198.	184.	203.	179.	220.
181.	182.	169.	206.	214.	193.	163.	209.	177.	195.
177.	189.	219.	200.	204.	169.	206.	179.	201.	205.
154.	186.	185.	179.	168.	201.	191.	178.	180.	213.
200.	204.	201.	184.	211.	171.	178.	169.	186.	175.
168.	184.	175.	189.	168.	156.	175.	175.	179.	191.
155.	179.	173.	158.	150.	186.	207.	187.	172.	180.
177.	198.	143.	152.	192.	151.	155.	173.	158.	165.
170.	182.	175.	179.	201.	166.	189.	166.	152.	168.
158.	205.	167.	165.	182.	160.	197.	179.	160.	191.
173.	176.	169.	168.	138.	163.	171.	178.	159.	151.
184.	182.	169.	188.	180.	139.	169.	188.	154.	177.
137.	182.	183.	165.	163.	186.	195.	190.	167.	207.
177.	142.	190.	168.	176.	165.	161.	185.	197.	189.
175.	153.	159.	148.	170.	163.	221.	200.	187.	181.
174.	203.	184.	219.	204.	204.	202.	238.	255.	312.
306.	349.	416.	443.	495.	587.	595.	572.	550.	425.
339.	242.	232.	221.	214.	158.	193.	174.	182.	169.
192.	149.	152.	191.	177.	160.	169.	154.	163.	165.
160.	178.	162.	147.	140.	168.	170.	162.	164.	160.
186.	162.	163.	126.	135.	174.	149.	129.	151.	157.
172.	107.	163.	147.	152.	161.	162.	182.	173.	164.
134.	148.	131.	165.	169.	161.	147.	176.	177.	153.
172.	131.	162.	163.	160.	163.	166.	162.	154.	153.
147.	171.	161.	179.	168.	175.	167.	167.	151.	159.
151.	196.	154.	168.	208.	193.	207.	172.	202.	274.
291.	284.	307.	379.	467.	539.	601.	658.	842.	948.
1132.	1374.	1492.	1602.	1784.	1956.	2033.	2077.	1968.	1697.
1329.	933.	698.	514.	496.	386.	378.	355.	397.	392.
428.	355.	451.	341.	334.	264.	316.	230.	224.	258.
226.	185.	201.	209.	232.	215.	262.	226.	270.	258.
340.	362.	401.	482.	495.	520.	475.	490.	439.	384.

347.	274.	258.	244.	234.	220.	188.	216.	189.	208.
161.	207.	213.	183.	194.	194.	171.	196.	197.	190.
191.	191.	203.	222.	192.	188.	189.	164.	194.	163.
184.	199.	199.	197.	224.	254.	271.	280.	300.	335.
403.	465.	458.	446.	408.	386.	343.	317.	235.	250.
232.	201.	189.	157.	192.	183.	183.	155.	181.	194.
183.	159.	131.	177.	167.	169.	181.	173.	179.	180.
172.	187.	191.	202.	167.	202.	223.	230.	186.	284.
264.	234.	330.	280.	298.	254.	260.	236.	220.	196.
207.	220.	230.	234.	228.	214.	253.	261.	287.	360.
396.	410.	488.	577.	641.	803.	906.	926.	878.	829.
682.	613.	469.	410.	329.	249.	243.	223.	211.	210.
193.	164.	198.	188.	161.	189.	178.	164.	177.	174.
196.	168.	184.	179.	183.	196.	175.	202.	242.	245.
243.	236.	263.	293.	342.	367.	383.	453.	528.	630.
726.	856.	904.	770.	824.	675.	579.	529.	397.	350.
286.	241.	229.	211.	207.	187.	201.	154.	190.	169.
135.	170.	139.	165.	136.	130.	133.	165.	145.	160.
162.	131.	146.	148.	156.	149.	138.	149.	140.	126.
168.	155.	134.	171.	135.	142.	164.	142.	157.	187.
137.	185.	163.	173.	183.	177.	190.	198.	190.	197.
193.	160.	177.	172.	175.	227.	196.	191.	202.	190.
214.	249.	239.	242.	292.	327.	326.	367.	437.	508.
569.	598.	707.	919.	1016.	1213.	1189.	1161.	1196.	1086.
878.	751.	663.	548.	445.	370.	299.	306.	294.	263.
242.	215.	240.	209.	243.	210.	190.	171.	173.	171.
196.	184.	203.	175.	163.	146.	200.	169.	214.	179.
202.	170.	203.	211.	216.	232.	215.	237.	248.	292.
310.	332.	363.	397.	390.	438.	566.	610.	786.	893.
1038.	1200.	1414.	1558.	1586.	1587.	1634.	1603.	1490.	1262.
983.	772.	579.	418.	377.	321.	265.	250.	249.	246.
214.	225.	186.	217.	195.	227.	193.	202.	169.	171.
162.	190.	153.	162.	163.	189.	184.	203.	169.	175.
178.	177.	156.	188.	159.	181.	221.	187.	208.	222.
238.	253.	287.	260.	264.	347.	413.	439.	508.	544.
667.	725.	819.	1000.	1003.	1024.	914.	906.	851.	602.
540.	403.	404.	340.	295.	277.	246.	186.	219.	217.
220.	229.	197.	185.	184.	144.	155.	167.	158.	169.
181.	157.	167.	165.	169.	183.	167.	181.	197.	217.
216.	228.	178.	188.	181.	166.	176.	174.	169.	166.
160.	159.	148.	160.	130.	151.	155.	139.	149.	139.
136.	131.	139.	132.	128.	154.	141.	141.	126.	133.
123.	126.	123.	147.	134.	151.	158.	130.	131.	147.
145.	166.	180.	168.	187.	196.	199.	218.	195.	202.
236.	267.	265.	271.	315.	312.	368.	431.	485.	589.
600.	794.	824.	1002.	1065.	1047.	862.	862.	683.	631.
538.	475.	347.	303.	287.	302.	232.	190.	174.	241.
212.	172.	129.	173.	143.	154.	136.	107.	132.	138.
146.	142.	134.	134.	123.	151.	132.	136.	123.	165.
128.	126.	131.	132.	114.	123.	115.	101.	134.	148.
148.	144.	101.	137.	152.	160.	141.	172.	170.	149.
196.	175.	225.	252.	245.	242.	317.	334.	431.	480.
527.	578.	610.	666.	679.	648.	589.	484.	435.	339.
342.	264.	269.	213.	220.	168.	199.	152.	153.	169.
124.	132.	193.	145.	163.	160.	156.	157.	130.	180.
161.	174.	187.	204.	243.	223.	276.	275.	359.	366.
378.	480.	506.	484.	524.	439.	452.	406.	373.	249.
259.	209.	201.	227.	209.	155.	166.	159.	152.	143.
130.	123.	141.	106.	98.	110.	117.	114.	111.	111.
83.	94.	84.	101.	128.	97.	118.	110.	100.	99.
83.	107.	71.	98.	93.	98.	99.	92.	93.	99.
87.	73.	93.	97.	88.	81.	92.	84.	88.	84.
93.	76.	82.	84.	77.	70.	103.	93.	100.	104.
89.	84.	98.	80.	82.	95.	100.	92.	94.	98.
101.	92.	98.	81.	82.	104.	97.	95.	81.	87.
95.	99.	95.	92.	88.	98.	92.	94.	95.	93.
87.	99.	98.	102.	107.	92.	74.	115.	102.	107.
101.	121.	94.	128.	147.	136.	141.	121.	159.	170.
172.	201.	191.	251.	232.	293.	364.	455.	480.	602.

737.	790.	793.	846.	828.	755.	768.	799.	754.	631.
711.	689.	673.	693.	694.	720.	816.	904.	1075.	1234.
1442.	1732.	1920.	2171.	2439.	2475.	2496.	2220.	1876.	1665.
1392.	1049.	828.	744.	576.	533.	407.	393.	331.	283.
304.	283.	255.	220.	216.	234.	168.	212.	178.	176.
173.	169.	180.	193.	226.	197.	187.	218.	226.	201.
231.	209.	233.	240.	246.	255.	262.	201.	228.	179.
180.	159.	134.	144.	163.	147.	168.	145.	125.	109.
146.	127.	141.	163.	146.	147.	174.	222.	203.	218.
217.	290.	354.	373.	405.	455.	482.	530.	543.	489.
434.	386.	374.	303.	243.	265.	251.	245.	257.	287.
238.	279.	290.	296.	245.	297.	275.	244.	236.	216.
187.	159.	157.	172.	107.	87.	125.	131.	133.	144.
150.	146.	121.	150.	170.	137.	164.	162.	165.	137.
157.	161.	189.	193.	179.	216.	234.	273.	270.	324.
313.	339.	378.	348.	386.	395.	413.	419.	443.	457.
477.	515.	534.	551.	422.	517.	416.	392.	351.	254.
249.	220.	195.	178.	163.	140.	149.	162.	133.	132.
122.	95.	113.	98.	106.	105.	78.	97.	75.	97.
77.	86.	90.	71.	82.	97.	86.	99.	84.	70.
72.	59.	84.	74.	66.	71.	77.	79.	90.	75.
66.	61.	62.	80.	78.	68.	64.	91.	78.	84.
93.	74.	76.	83.	75.	54.	88.	84.	69.	67.
65.	78.	86.	80.	64.	75.	78.	98.	88.	68.
77.	67.	78.	74.	68.	68.	81.	108.	76.	70.
91.	87.	77.	81.	69.	65.	95.	89.	88.	84.
58.	87.	75.	95.	84.	95.	96.	123.	103.	123.
127.	127.	164.	142.	194.	194.	250.	256.	263.	286.
320.	293.	288.	279.	276.	286.	274.	267.	270.	274.
229.	186.	215.	200.	202.	160.	173.	158.	154.	152.
163.	108.	104.	105.	110.	147.	132.	132.	120.	127.
114.	161.	162.	172.	200.	179.	222.	231.	233.	240.
278.	242.	252.	251.	299.	227.	225.	224.	191.	199.
168.	186.	186.	167.	150.	144.	164.	206.	191.	192.
190.	211.	207.	229.	223.	225.	196.	181.	150.	147.
157.	137.	145.	153.	131.	129.	141.	127.	111.	158.
111.	130.	143.	171.	158.	160.	199.	224.	188.	224.
261.	273.	292.	294.	318.	400.	403.	385.	400.	355.
329.	336.	355.	319.	322.	357.	352.	426.	422.	477.
496.	508.	604.	563.	610.	581.	589.	554.	566.	485.
373.	403.	350.	282.	233.	237.	232.	225.	189.	193.
182.	161.	185.	153.	155.	167.	158.	142.	162.	141.
153.	173.	154.	150.	136.	178.	157.	182.	180.	166.
180.	188.	197.	234.	245.	226.	266.	272.	286.	232.
212.	253.	231.	198.	197.	204.	200.	156.	145.	154.
155.	136.	134.	116.	144.	144.	137.	168.	164.	147.
169.	139.	138.	180.	146.	146.	135.	133.	156.	151.
161.	173.	167.	149.	176.	178.	191.	173.	216.	207.
177.	168.	155.	167.	125.	136.	152.	153.	145.	143.
145.	136.	115.	133.	106.	123.	103.	143.	137.	116.
123.	119.	129.	149.	93.	114.	105.	141.	112.	120.
103.	99.	117.	117.	92.	93.	100.	114.	112.	116.
106.	125.	136.	108.	150.	156.	139.	113.	178.	235.
217.	276.	282.	322.	375.	422.	451.	470.	472.	424.
427.	371.	278.	281.	229.	230.	193.	182.	138.	160.
142.	132.	152.	145.	136.	125.	152.	149.	127.	152.
127.	123.	168.	166.	172.	204.	199.	200.	205.	229.
243.	272.	277.	293.	336.	290.	254.	260.	248.	215.
198.	180.	172.	192.	135.	152.	137.	116.	119.	123.
134.	121.	135.	115.	138.	139.	134.	126.	130.	146.
179.	190.	178.	189.	134.	175.	164.	157.	157.	150.
129.	141.	132.	139.	123.	104.	111.	108.	104.	83.
82.	98.	90.	76.	74.	90.	77.	91.	67.	71.
51.	66.	51.	81.	81.	57.	62.	65.	66.	69.
86.	44.	60.	77.	49.	62.	78.	51.	59.	69.
57.	57.	80.	60.	67.	79.	55.	69.	62.	60.
64.	61.	75.	70.	60.	76.	46.	62.	63.	74.
79.	73.	60.	61.	68.	70.	81.	72.	90.	66.
68.	64.	78.	62.	76.	91.	68.	80.	67.	61.

53.	80.	98.	82.	79.	79.	94.	97.	96.	89.
109.	96.	103.	83.	90.	76.	106.	97.	95.	82.
62.	105.	88.	91.	82.	76.	83.	71.	79.	79.
58.	73.	68.	79.	51.	86.	84.	58.	67.	60.
68.	84.	82.	66.	54.	59.	76.	63.	72.	74.
74.	67.	75.	78.	64.	64.	76.	73.	71.	82.
55.	53.	66.	55.	54.	66.	49.	50.	78.	65.
57.	56.	60.	55.	58.	52.	71.	68.	60.	71.
64.	76.	69.	54.	61.	59.	61.	72.	68.	88.
70.	70.	69.	45.	69.	59.	49.	50.	48.	48.
48.	48.	60.	54.	74.	50.	65.	52.	54.	64.
45.	59.	70.	62.	60.	52.	61.	50.	48.	53.
56.	58.	59.	46.	74.	52.	56.	69.	52.	63.
61.	61.	44.	69.	52.	55.	69.	60.	59.	66.
50.	65.	53.	64.	64.	52.	67.	66.	60.	69.
59.	63.	53.	77.	74.	52.	76.	88.	75.	92.
66.	80.	85.	86.	82.	78.	82.	83.	91.	62.
66.	61.	95.	84.	59.	67.	73.	57.	50.	71.
74.	73.	70.	61.	62.	78.	65.	74.	90.	82.
63.	82.	81.	100.	88.	115.	115.	100.	114.	135.
136.	163.	164.	159.	132.	169.	181.	149.	166.	197.
163.	166.	200.	175.	165.	152.	154.	166.	177.	180.
189.	169.	178.	175.	164.	163.	196.	184.	166.	167.
157.	117.	127.	141.	146.	119.	122.	122.	117.	112.
104.	106.	92.	117.	115.	78.	73.	98.	85.	110.
90.	77.	106.	113.	109.	123.	151.	113.	101.	111.
98.	108.	114.	113.	86.	87.	101.	87.	80.	89.
86.	104.	114.	89.	105.	119.	125.	124.	136.	152.
148.	181.	162.	145.	147.	179.	148.	167.	171.	150.
119.	142.	151.	136.	149.	119.	122.	138.	127.	125.
111.	111.	146.	123.	112.	117.	131.	129.	128.	120.
132.	99.	123.	116.	151.	104.	170.	142.	170.	146.
171.	125.	154.	154.	145.	153.	157.	159.	175.	124.
175.	158.	166.	175.	189.	235.	159.	168.	182.	216.
231.	209.	268.	217.	193.	259.	240.	258.	240.	232.
195.	240.	239.	211.	201.	226.	236.	221.	263.	241.
263.	247.	292.	261.	288.	301.	320.	303.	331.	341.
383.	395.	372.	393.	401.	341.	342.	335.	321.	304.
307.	280.	275.	261.	292.	259.	288.	278.	265.	264.
242.	204.	215.	225.	196.	190.	169.	171.	190.	167.
176.	158.	159.	171.	167.	176.	190.	206.	200.	194.
196.	173.	195.	182.	203.	169.	182.	186.	170.	150.
167.	152.	142.	180.	174.	154.	193.	177.	184.	190.
186.	186.	203.	210.	206.	219.	179.	216.	187.	196.
191.	190.	193.	210.	150.	180.	198.	222.	205.	206.
209.	263.	241.	304.	273.	259.	308.	356.	293.	290.
307.	283.	304.	321.	303.	259.	236.	223.	231.	224.
197.	187.	187.	194.	183.	156.	132.	132.	126.	142.
154.	139.	146.	107.	88.	96.	84.	112.	121.	89.
93.	76.	97.	87.	84.	75.	65.	74.	63.	69.
89.	68.	98.	72.	77.	82.	50.	55.	77.	84.
86.	64.	73.	66.	77.	92.	87.	106.	103.	103.
103.	92.	117.	79.	96.	102.	81.	76.	94.	108.
83.	104.	87.	104.	105.	104.	100.	90.	108.	102.
122.	111.	133.	143.	119.	98.	130.	141.	142.	149.
145.	136.	141.	180.	177.	178.	180.	146.	165.	173.
176.	142.	157.	153.	102.	89.	132.	116.	109.	130.
127.	124.	131.	102.	105.	129.	105.	105.	105.	83.
131.	107.	105.	117.	96.	83.	87.	74.	107.	117.
182.	106.	108.	122.	100.	139.	130.	125.	139.	90.
151.	129.	157.	152.	126.	136.	155.	152.	134.	160.
171.	193.	225.	217.	158.	183.	191.	206.	218.	210.
214.	199.	160.	144.	215.	198.	164.	126.	177.	141.
164.	145.	125.	128.	139.	152.	131.	123.	152.	131.
143.	131.	123.	107.	126.	152.	122.	169.	131.	156.
186.	150.	163.	211.	165.	173.	187.	197.	202.	205.
206.	270.	203.	262.	287.	271.	296.	347.	346.	445.
459.	543.	571.	562.	667.	690.	766.	805.	772.	778.
721.	730.	700.	675.	640.	526.	465.	436.	354.	324.

303.	261.	275.	244.	208.	190.	195.	198.	155.	132.
154.	137.	136.	124.	126.	134.	157.	135.	149.	135.
131.	134.	126.	123.	121.	137.	141.	125.	130.	120.
119.	123.	118.	119.	115.	105.	119.	115.	116.	125.
104.	80.	117.	113.	106.	114.	122.	130.	113.	104.
129.	124.	93.	111.	109.	96.	97.	91.	103.	108.
82.	114.	57.	101.	93.	71.	84.	87.	100.	94.
128.	95.	93.	80.	84.	98.	92.	103.	87.	84.
96.	95.	84.	83.	98.	88.	123.	117.	128.	119.
122.	123.	136.	102.	85.	128.	94.	106.	92.	104.
101.	73.	90.	75.	80.	93.	73.	63.	91.	65.
68.	82.	54.	69.	80.	71.	72.	75.	72.	77.
80.	66.	74.	64.	72.	54.	69.	85.	73.	75.
88.	79.	70.	80.	78.	101.	74.	72.	71.	88.
88.	98.	78.	92.	88.	112.	110.	91.	110.	90.
98.	134.	94.	111.	91.	90.	108.	95.	107.	102.
115.	87.	89.	78.	86.	88.	73.	98.	65.	64.
78.	73.	80.	77.	66.	58.	56.	64.	55.	71.
72.	80.	70.	90.	85.	81.	92.	82.	72.	79.
74.	96.	78.	101.	60.	100.	84.	94.	81.	83.
110.	79.	101.	90.	83.	92.	93.	90.	84.	110.
95.	117.	99.	96.	94.	114.	105.	98.	96.	98.
103.	116.	54.	102.	89.	94.	87.	73.	83.	83.
89.	74.	85.	105.	88.	94.	62.	93.	80.	88.
97.	80.	91.	83.	86.	87.	86.	96.	85.	67.
83.	82.	88.	80.	82.	87.	95.	59.	89.	64.
88.	70.	72.	75.	80.	59.	57.	71.	61.	81.
57.	86.	68.	67.	87.	74.	81.	60.	89.	89.
91.	82.	82.	87.	79.	83.	99.	87.	89.	97.
99.	83.	93.	105.	115.	126.	117.	121.	140.	140.
163.	151.	159.	179.	155.	146.	133.	142.	128.	119.
134.	129.	119.	131.	90.	133.	114.	110.	103.	140.
104.	86.	94.	101.	117.	103.	113.	83.	113.	97.
86.	71.	98.	137.	96.	117.	106.	133.	112.	120.
98.	109.	129.	108.	149.	127.	120.	130.	108.	156.
145.	158.	188.	132.	198.	170.	210.	223.	214.	270.
237.	263.	261.	227.	228.	231.	206.	247.	215.	214.
202.	200.	190.	159.	178.	159.	162.	151.	151.	158.
158.	150.	114.	107.	106.	115.	129.	105.	123.	116.
146.	96.	110.	141.	139.	165.	190.	188.	146.	178.
194.	181.	214.	201.	202.	185.	173.	220.	183.	200.
180.	132.	150.	131.	130.	149.	144.	115.	138.	116.
121.	123.	130.	97.	119.	97.	99.	97.	81.	86.
85.	92.	102.	91.	97.	86.	87.	79.	96.	84.
102.	87.	80.	81.	120.	75.	92.	94.	73.	90.
124.	93.	89.	89.	126.	86.	80.	98.	78.	99.
80.	84.	82.	83.	81.	99.	74.	65.	69.	82.
78.	76.	80.	58.	68.	76.	77.	73.	66.	69.
62.	88.	72.	60.	74.	73.	76.	95.	85.	67.
60.	73.	73.	68.	77.	70.	72.	63.	64.	83.
70.	68.	75.	79.	79.	73.	77.	71.	73.	94.
77.	79.	102.	78.	70.	69.	69.	73.	106.	100.
114.	110.	101.	98.	103.	147.	129.	107.	125.	137.
153.	175.	160.	180.	187.	197.	209.	214.	246.	266.
254.	256.	266.	237.	274.	300.	256.	268.	286.	279.
270.	239.	284.	232.	242.	252.	249.	218.	195.	199.
219.	200.	224.	205.	213.	182.	180.	173.	157.	189.
147.	132.	156.	168.	159.	120.	146.	151.	128.	134.
106.	107.	110.	87.	131.	87.	99.	141.	106.	99.
110.	125.	119.	108.	122.	121.	134.	121.	99.	113.
115.	125.	140.	135.	128.	162.	148.	106.	128.	109.
130.	110.	134.	99.	118.	113.	121.	125.	122.	119.
100.	157.	147.	143.	164.	121.	162.	145.	131.	136.
114.	109.	108.	133.	109.	97.	90.	79.	104.	103.
85.	85.	85.	93.	84.	76.	79.	104.	102.	99.
101.	92.	99.	131.	97.	97.	93.	92.	64.	80.
93.	74.	99.	79.	74.	71.	75.	65.	102.	62.
90.	96.	94.	90.	89.	77.	84.	103.	59.	91.
101.	105.	87.	90.	109.	100.	72.	107.	117.	106.

94.	114.	88.	101.	135.	122.	127.	129.	163.	131.
136.	138.	171.	131.	166.	154.	198.	182.	153.	181.
176.	168.	213.	202.	166.	185.	180.	179.	190.	184.
159.	193.	167.	168.	186.	159.	139.	146.	153.	168.
168.	171.	168.	152.	173.	163.	181.	164.	191.	163.
175.	157.	162.	148.	134.	140.	123.	135.	129.	120.
124.	123.	125.	109.	105.	120.	112.	102.	95.	95.
95.	117.	91.	97.	110.	94.	99.	101.	95.	93.
103.	81.	85.	72.	78.	73.	70.	108.	64.	80.
77.	65.	77.	87.	85.	95.	77.	87.	87.	88.
82.	101.	92.	117.	115.	101.	120.	115.	103.	81.
117.	127.	132.	131.	107.	150.	120.	124.	148.	105.
126.	119.	139.	133.	96.	155.	115.	125.	141.	139.
118.	140.	115.	101.	127.	115.	122.	107.	129.	113.
99.	91.	95.	92.	72.	85.	95.	97.	84.	82.
85.	74.	68.	79.	100.	77.	59.	95.	108.	74.
82.	96.	85.	103.	88.	96.	101.	77.	79.	74.
99.	88.	83.	104.	92.	80.	83.	77.	95.	93.
118.	94.	80.	91.	116.	91.	101.	113.	93.	108.
84.	97.	97.	92.	119.	98.	93.	69.	82.	112.
102.	85.	108.	125.	82.	95.	85.	115.	83.	86.
93.	119.	96.	79.	87.	100.	100.	104.	69.	101.
86.	96.	102.	92.	102.	95.	83.	76.	118.	112.
97.	105.	95.	96.	85.	78.	122.	92.	105.	74.
89.	84.	90.	100.	88.	83.	107.	138.	107.	91.
121.	127.	94.	69.	94.	88.	119.	72.	84.	111.
84.	78.	83.	103.	111.	86.	83.	80.	70.	98.
96.	93.	92.	86.	113.	85.	97.	85.	123.	90.
98.	93.	100.	117.	96.	114.	82.	141.	93.	93.
117.	98.	97.	84.	105.	72.	79.	72.	85.	71.
59.	78.	49.	74.	71.	81.	71.	86.	83.	72.
79.	74.	95.	92.	63.	63.	41.	65.	68.	62.
51.	63.	52.	58.	59.	53.	65.	59.	62.	63.
51.	76.	63.	69.	76.	53.	68.	62.	44.	45.
46.	64.	69.	51.	60.	81.	44.	37.	54.	89.
67.	54.	62.	79.	77.	65.	59.	69.	57.	59.
59.	52.	53.	68.	68.	75.	59.	46.	55.	74.
47.	72.	69.	74.	85.	76.	57.	74.	74.	68.
54.	70.	57.	50.	72.	73.	74.	65.	87.	69.
48.	96.	62.	87.	65.	111.	69.	75.	74.	60.
65.	77.	80.	64.	64.	59.	87.	68.	68.	75.
54.	61.	73.	80.	58.	67.	69.	62.	74.	50.
68.	54.	61.	62.	63.	41.	66.	71.	41.	54.
54.	62.	45.	49.	74.	66.	52.	46.	47.	47.
52.	68.	47.	73.	54.	55.	49.	63.	53.	42.
56.	48.	43.	52.	54.	58.	70.	48.	47.	58.
61.	55.	73.	50.	56.	65.	56.	67.	54.	65.
51.	40.	67.	73.	54.	67.	59.	65.	58.	45.
62.	54.	57.	75.	67.	96.	62.	54.	58.	71.
66.	78.	69.	64.	72.	65.	84.	88.	90.	77.
84.	79.	107.	59.	78.	65.	91.	114.	86.	68.
70.	79.	88.	87.	82.	92.	67.	73.	82.	75.
85.	77.	63.	78.	72.	76.	50.	67.	64.	68.
74.	57.	65.	67.	63.	64.	68.	74.	71.	68.
80.	67.	69.	49.	75.	76.	58.	90.	64.	64.
73.	62.	69.	71.	91.	84.	89.	74.	67.	82.
108.	97.	77.	131.	70.	78.	76.	95.	93.	81.
95.	89.	100.	79.	133.	123.	106.	108.	117.	98.
102.	121.	98.	101.	112.	113.	97.	121.	100.	103.
113.	92.	88.	85.	73.	102.	70.	96.	83.	91.
83.	90.	72.	62.	67.	90.	92.	69.	52.	68.
55.	78.	62.	55.	64.	44.	82.	61.	52.	70.
68.	79.	77.	67.	81.	61.	69.	82.	48.	70.
75.	72.	83.	83.	105.	72.	111.	81.	86.	99.
84.	90.	89.	80.	97.	76.	94.	91.	84.	72.
68.	62.	56.	69.	81.	70.	53.	62.	54.	83.
69.	51.	82.	59.	67.	56.	48.	40.	47.	37.
73.	58.	54.	58.	58.	47.	38.	46.	58.	37.
76.	52.	51.	61.	46.	35.	46.	54.	63.	38.

34.	49.	59.	50.	60.	62.	52.	35.	52.	51.
60.	32.	39.	61.	63.	60.	35.	63.	41.	48.
53.	67.	62.	43.	60.	48.	46.	55.	75.	54.
52.	46.	48.	57.	40.	49.	48.	50.	66.	52.
66.	67.	57.	55.	80.	89.	70.	75.	59.	56.
54.	79.	58.	69.	78.	62.	67.	92.	61.	86.
65.	60.	79.	65.	64.	47.	77.	52.	65.	52.
78.	65.	44.	75.	75.	77.	56.	52.	54.	69.
57.	85.	50.	61.	57.	56.	60.	70.	48.	50.
66.	73.	69.	67.	58.	69.	70.	69.	79.	58.
66.	81.	62.	58.	57.	58.	59.	66.	63.	87.
65.	55.	63.	64.	52.	58.	59.	50.	66.	60.
82.	83.	43.	66.	53.	52.	66.	39.	52.	63.
53.	70.	56.	60.	47.	56.	70.	68.	54.	61.
78.	60.	65.	74.	66.	59.	95.	55.	76.	81.
61.	41.	55.	87.	67.	74.	95.	80.	100.	82.
77.	78.	81.	87.	64.	62.	69.	70.	81.	87.
78.	76.	70.	78.	73.	73.	62.	65.	60.	59.
66.	62.	67.	53.	69.	59.	65.	69.	88.	54.
60.	76.	47.	65.	67.	69.	63.	62.	68.	72.
70.	67.	66.	56.	55.	55.	60.	73.	49.	48.
62.	78.	78.	64.	73.	81.	69.	65.	69.	75.
74.	85.	78.	85.	73.	84.	109.	89.	69.	70.
86.	88.	82.	76.	77.	61.	81.	79.	77.	86.
61.	62.	64.	77.	59.	51.	68.	67.	59.	72.
68.	46.	42.	66.	66.	75.	65.	44.	59.	69.
65.	64.	58.	70.	66.	70.	63.	70.	68.	52.
48.	84.	51.	66.	75.	52.	55.	61.	80.	68.
58.	83.	50.	69.	102.	49.	64.	89.	61.	74.
61.	87.	66.	67.	66.	68.	69.	60.	89.	69.
78.	63.	67.	83.	58.	63.	63.	64.	57.	60.
53.	53.	54.	59.	74.	67.	73.	75.	51.	70.
68.	54.	63.	51.	60.	62.	64.	59.	64.	59.
51.	86.	61.	60.	63.	73.	56.	56.	60.	74.
77.	54.	52.	39.	62.	46.	52.	63.	60.	57.
45.	53.	61.	63.	35.	71.	62.	64.	72.	52.
70.	64.	52.	57.	52.	75.	71.	71.	66.	54.
63.	62.	73.	68.	48.	58.	57.	56.	41.	82.
40.	54.	70.	55.	62.	53.	58.	55.	72.	58.
58.	52.	63.	49.	63.	60.	66.	44.	61.	57.
59.	52.	57.	65.	57.	53.	61.	66.	44.	43.
55.	57.	69.	55.	53.	68.	50.	48.	75.	45.
66.	61.	64.	54.	60.	57.	59.	52.	62.	65.
55.	42.	67.	58.	66.	63.	45.	64.	44.	45.
63.	67.	44.	66.	57.	57.	66.	54.	80.	66.
57.	56.	65.	53.	63.	73.	58.	74.	58.	63.
81.	47.	76.	61.	65.	44.	71.	73.	78.	76.
78.	64.	81.	69.	78.	61.	78.	88.	67.	71.
74.	76.	75.	70.	103.	66.	90.	74.	83.	77.
99.	83.	76.	89.	92.	72.	82.	75.	98.	80.
95.	80.	65.	83.	91.	73.	82.	81.	84.	79.
73.	83.	73.	61.	49.	59.	82.	73.	87.	71.
72.	55.	59.	72.	56.	64.	59.	44.	56.	57.
72.	57.	61.	66.	83.	64.	68.	46.	44.	70.
61.	90.	62.	57.	67.	70.	69.	64.	89.	53.
72.	83.	85.	76.	78.	93.	89.	80.	88.	84.
92.	85.	86.	117.	87.	84.	74.	80.	110.	75.
73.	81.	80.	77.	85.	89.	77.	89.	87.	87.
83.	60.	64.	73.	90.	64.	86.	71.	74.	83.
63.	76.	76.	68.	65.	79.	68.	56.	78.	73.
77.	59.	85.	94.	71.	53.	91.	100.	80.	70.
99.	85.	67.	69.	75.	69.	93.	65.	76.	65.
73.	59.	65.	81.	52.	62.	80.	58.	50.	84.
70.	57.	39.	51.	67.	76.	48.	75.	69.	76.
80.	61.	53.	82.	90.	45.	53.	66.	82.	51.
70.	69.	53.	84.	60.	75.	67.	49.	85.	78.
72.	61.	66.	64.	70.	64.	78.	82.	67.	82.
84.	75.	75.	79.	93.	69.	92.	70.	68.	85.
95.	96.	66.	96.	79.	89.	76.	80.	104.	84.

87.	84.	110.	106.	99.	104.	107.	99.	94.	85.
130.	106.	78.	102.	85.	108.	118.	76.	84.	116.
108.	93.	100.	116.	156.	76.	93.	111.	81.	77.
100.	111.	86.	85.	82.	71.	66.	83.	77.	64.
94.	53.	77.	71.	61.	68.	60.	59.	51.	68.
62.	59.	72.	61.	56.	73.	59.	66.	61.	59.
62.	76.	76.	70.	64.	75.	63.	75.	67.	86.
68.	62.	69.	66.	90.	70.	81.	73.	89.	92.
98.	87.	63.	89.	97.	104.	101.	118.	92.	124.
96.	99.	112.	118.	117.	100.	103.	126.	93.	99.
111.	99.	111.	114.	95.	112.	104.	110.	125.	98.
131.	102.	92.	78.	102.	101.	96.	117.	116.	72.
102.	114.	103.	78.	104.	105.	88.	107.	79.	95.
72.	77.	88.	105.	76.	93.	98.	82.	93.	77.
96.	85.	90.	62.	94.	68.	59.	81.	73.	76.
87.	63.	97.	91.	81.	84.	115.	73.	94.	85.
105.	68.	114.	68.	86.	82.	102.	81.	89.	108.
100.	95.	113.	100.	105.	97.	90.	133.	98.	95.
84.	77.	116.	98.	91.	74.	72.	107.	85.	87.
94.	105.	88.	81.	84.	90.	78.	70.	97.	94.
74.	81.	90.	70.	95.	56.	78.	87.	78.	96.
64.	91.	91.	95.	85.	76.	85.	88.	93.	79.
74.	88.	83.	72.	87.	69.	77.	75.	78.	72.
60.	77.	81.	66.	70.	84.	64.	68.	73.	55.
92.	62.	52.	49.	56.	70.	67.	56.	52.	47.
72.	71.	58.	66.	57.	79.	47.	65.	39.	53.
56.	44.	42.	36.	56.	52.	72.	47.	45.	71.
81.	60.	44.	79.	54.	45.	30.	61.	58.	57.
61.	57.	52.	62.	59.	60.	70.	57.	38.	55.
43.	57.	56.	58.	44.	40.	56.	71.	43.	64.
58.	34.	54.	54.	69.	42.	50.	51.	68.	63.
46.	46.	51.	65.	63.	47.	36.	58.	51.	48.
50.	62.	50.	56.	62.	66.	48.	62.	71.	60.
62.	72.	53.	50.	48.	41.	58.	39.	45.	41.
48.	66.	47.	64.	51.	68.	69.	50.	81.	66.
63.	48.	64.	43.	100.	59.	62.	81.	52.	83.
67.	63.	73.	63.	75.	67.	63.	55.	54.	75.
67.	41.	75.	79.	67.	73.	52.	86.	57.	54.
68.	69.	80.	55.	53.	66.	56.	70.	59.	53.
67.	69.	61.	64.	67.	45.	55.	82.	64.	62.
82.	64.	55.	58.	58.	65.	39.	63.	61.	50.
62.	51.	53.	68.	51.	71.	59.	72.	62.	66.
74.	67.	65.	55.	44.	65.	78.	71.	66.	77.
71.	48.	54.	51.	60.	63.	71.	62.	65.	64.
63.	76.	68.	34.	56.	90.	78.	52.	77.	67.
50.	55.	58.	64.	77.	80.	67.	72.	57.	66.
70.	71.	59.	69.	64.	90.	47.	61.	56.	48.
69.	64.	45.	60.	51.	58.	61.	58.	43.	61.
45.	60.	54.	57.	75.	60.	57.	57.	55.	60.
71.	67.	89.	54.	79.	55.	62.	72.	59.	71.
53.	48.	48.	47.	50.	64.	52.	65.	60.	75.
75.	96.	74.	64.	59.	83.	61.	74.	70.	52.
55.	80.	73.	63.	77.	68.	54.	68.	59.	49.
51.	71.	53.	66.	63.	94.	78.	54.	48.	74.
74.	75.	59.	42.	50.	51.	53.	57.	51.	50.
49.	72.	49.	57.	72.	53.	77.	55.	56.	82.
48.	53.	73.	60.	49.	60.	69.	50.	44.	76.
55.	55.	76.	63.	69.	63.	55.	71.	66.	60.
63.	58.	60.	61.	55.	89.	62.	58.	69.	54.
69.	81.	68.	70.	52.	63.	62.	59.	83.	72.
56.	84.	65.	89.	86.	68.	59.	69.	61.	51.
81.	83.	73.	94.	88.	82.	64.	91.	77.	79.
75.	67.	97.	93.	84.	72.	66.	85.	77.	88.
89.	82.	91.	81.	97.					

Appendix P-23: step-intensity data of pure muscovite, reflection geometry

8.0000 .020 138.0000 muscovite on the Phillips

423.	463.	461.	471.	476.	520.	492.	528.	459.	567.
538.	573.	569.	594.	577.	606.	666.	624.	689.	763.
801.	814.	854.	898.	988.	1106.	1167.	1270.	1358.	1462.
1558.	1733.	1859.	1818.	1845.	1714.	1679.	1406.	1172.	1124.
913.	751.	659.	617.	526.	471.	461.	443.	428.	383.
356.	355.	375.	342.	380.	309.	336.	365.	340.	363.
332.	321.	344.	342.	310.	325.	347.	302.	342.	340.
306.	314.	324.	293.	265.	309.	298.	328.	302.	301.
309.	301.	299.	310.	317.	347.	283.	308.	300.	293.
297.	319.	271.	282.	292.	327.	277.	282.	297.	269.
324.	301.	284.	246.	292.	259.	296.	296.	286.	267.
286.	311.	308.	298.	308.	304.	293.	279.	279.	266.
266.	258.	316.	289.	274.	268.	279.	278.	277.	240.
269.	268.	262.	298.	268.	252.	216.	267.	261.	288.
283.	257.	274.	276.	265.	275.	286.	272.	285.	292.
277.	251.	251.	251.	279.	269.	305.	262.	271.	281.
231.	288.	248.	295.	255.	246.	288.	272.	253.	251.
235.	260.	273.	257.	269.	280.	273.	259.	282.	271.
255.	259.	238.	278.	252.	253.	242.	228.	242.	258.
250.	267.	261.	215.	268.	249.	224.	228.	254.	280.
257.	254.	209.	263.	251.	239.	263.	234.	255.	253.
216.	228.	251.	252.	264.	248.	253.	226.	250.	252.
247.	226.	257.	244.	285.	223.	240.	220.	250.	246.
274.	236.	217.	226.	230.	243.	223.	237.	249.	226.
239.	252.	212.	217.	250.	229.	245.	220.	249.	234.
217.	231.	219.	234.	231.	243.	283.	232.	234.	225.
227.	222.	260.	227.	220.	242.	226.	232.	225.	229.
221.	234.	223.	260.	218.	251.	237.	229.	251.	246.
187.	230.	201.	260.	246.	227.	237.	233.	212.	227.
227.	220.	191.	190.	202.	227.	200.	217.	234.	236.
228.	206.	248.	219.	240.	224.	198.	229.	224.	252.
225.	237.	209.	240.	231.	210.	235.	213.	209.	203.
244.	232.	198.	200.	205.	204.	204.	240.	206.	251.
209.	232.	233.	195.	218.	228.	192.	225.	228.	219.
218.	241.	192.	200.	220.	219.	218.	188.	244.	217.
241.	219.	235.	206.	205.	208.	207.	222.	229.	219.
234.	225.	195.	229.	224.	218.	189.	220.	213.	226.
230.	213.	201.	209.	214.	196.	193.	216.	205.	204.
202.	224.	236.	213.	226.	200.	227.	226.	231.	198.
213.	206.	227.	215.	203.	214.	201.	189.	212.	191.
181.	208.	198.	203.	220.	223.	187.	199.	216.	223.
199.	226.	199.	212.	201.	207.	226.	181.	220.	184.
199.	202.	246.	238.	218.	215.	191.	208.	218.	198.
198.	226.	222.	214.	214.	193.	214.	198.	216.	217.
224.	209.	175.	233.	232.	205.	216.	219.	225.	229.
216.	203.	258.	232.	233.	264.	265.	269.	286.	251.
271.	321.	309.	320.	338.	364.	376.	426.	463.	518.
559.	634.	692.	793.	792.	855.	955.	1007.	984.	989.
887.	817.	687.	619.	570.	470.	445.	335.	371.	309.
304.	270.	273.	228.	241.	234.	227.	248.	232.	219.
211.	223.	210.	208.	201.	209.	192.	239.	210.	242.
214.	202.	204.	236.	204.	210.	199.	212.	194.	172.
216.	191.	194.	217.	206.	209.	204.	211.	191.	201.
200.	204.	194.	230.	177.	202.	221.	223.	215.	215.
187.	237.	207.	216.	216.	222.	219.	243.	219.	231.
209.	217.	249.	220.	217.	252.	238.	256.	232.	261.
278.	298.	292.	308.	344.	372.	374.	388.	488.	529.
580.	638.	733.	822.	876.	1047.	1140.	1389.	1479.	1709.
1811.	1990.	2072.	2319.	2451.	2624.	2718.	2583.	2680.	2623.
2533.	2371.	2036.	1876.	1641.	1398.	1206.	999.	926.	810.
774.	680.	697.	648.	636.	577.	522.	486.	521.	465.
451.	395.	397.	405.	424.	404.	416.	460.	507.	531.
569.	559.	617.	686.	682.	731.	719.	739.	685.	646.
649.	586.	573.	501.	465.	407.	358.	371.	354.	317.
304.	298.	271.	231.	291.	275.	279.	241.	256.	237.

239.	261.	257.	202.	230.	259.	320.	312.	304.	309.
304.	322.	309.	346.	370.	369.	446.	410.	530.	525.
556.	601.	682.	636.	635.	615.	558.	531.	515.	463.
444.	389.	397.	405.	339.	329.	289.	290.	283.	316.
275.	260.	250.	298.	254.	280.	287.	265.	278.	279.
309.	299.	333.	322.	346.	317.	328.	364.	390.	375.
408.	417.	447.	448.	444.	466.	467.	472.	467.	393.
435.	468.	520.	459.	511.	546.	550.	662.	586.	692.
797.	835.	947.	982.	1073.	1181.	1158.	1251.	1285.	1320.
1290.	1251.	1180.	1076.	998.	882.	845.	673.	645.	561.
518.	437.	425.	391.	401.	353.	374.	353.	375.	348.
397.	361.	326.	345.	358.	396.	376.	443.	411.	487.
527.	521.	538.	633.	669.	789.	842.	921.	955.	1077.
1122.	1188.	1245.	1296.	1250.	1276.	1194.	1081.	1039.	993.
875.	766.	688.	607.	532.	500.	462.	395.	344.	326.
342.	305.	288.	263.	287.	282.	295.	235.	286.	284.
294.	270.	260.	280.	268.	278.	258.	265.	249.	278.
292.	272.	249.	276.	279.	261.	277.	274.	280.	301.
307.	341.	326.	346.	317.	343.	306.	348.	370.	341.
359.	384.	386.	363.	391.	392.	375.	438.	399.	498.
517.	527.	562.	643.	638.	733.	799.	880.	1001.	1024.
1181.	1209.	1455.	1554.	1680.	1864.	1934.	1972.	2075.	2029.
1969.	1840.	1707.	1562.	1488.	1343.	1125.	987.	902.	749.
774.	615.	585.	555.	508.	465.	448.	440.	400.	427.
399.	403.	362.	375.	397.	416.	415.	384.	390.	401.
409.	477.	437.	466.	477.	578.	546.	579.	625.	685.
747.	816.	897.	964.	1097.	1229.	1351.	1506.	1579.	1777.
2060.	2198.	2516.	2660.	2761.	2964.	3019.	3011.	3171.	2969.
2791.	2636.	2300.	2034.	1777.	1584.	1267.	1057.	953.	756.
696.	611.	598.	490.	510.	469.	438.	402.	376.	373.
399.	372.	385.	359.	400.	333.	333.	365.	345.	385.
363.	388.	409.	387.	391.	414.	464.	442.	526.	539.
576.	631.	622.	661.	694.	790.	902.	1019.	1047.	1164.
1260.	1364.	1476.	1525.	1610.	1689.	1695.	1753.	1583.	1628.
1456.	1314.	1121.	1032.	992.	836.	758.	663.	590.	528.
504.	488.	393.	406.	379.	389.	404.	311.	344.	381.
314.	331.	306.	324.	325.	337.	344.	322.	347.	358.
349.	390.	362.	345.	381.	352.	338.	359.	308.	317.
280.	298.	273.	263.	269.	272.	268.	233.	256.	256.
253.	252.	239.	223.	252.	263.	236.	243.	305.	243.
234.	271.	266.	270.	297.	259.	296.	272.	281.	317.
355.	372.	310.	376.	364.	402.	416.	442.	416.	497.
573.	536.	645.	729.	747.	824.	861.	948.	1036.	1186.
1271.	1390.	1501.	1561.	1606.	1585.	1659.	1742.	1651.	1521.
1455.	1307.	1184.	1122.	980.	848.	739.	662.	612.	584.
486.	432.	421.	436.	380.	357.	350.	320.	308.	324.
287.	265.	277.	278.	273.	287.	286.	284.	247.	242.
248.	247.	300.	270.	253.	263.	278.	288.	295.	292.
308.	287.	296.	314.	340.	369.	362.	373.	408.	449.
432.	521.	495.	576.	618.	649.	684.	777.	835.	897.
991.	1063.	1170.	1153.	1215.	1248.	1189.	1234.	1071.	1081.
933.	876.	779.	751.	716.	642.	556.	517.	460.	440.
434.	417.	413.	368.	374.	425.	381.	393.	461.	436.
448.	447.	440.	495.	513.	580.	641.	664.	696.	792.
822.	841.	917.	930.	977.	970.	951.	877.	876.	784.
768.	664.	645.	590.	504.	470.	392.	404.	346.	331.
304.	289.	294.	238.	245.	258.	219.	253.	202.	210.
209.	207.	207.	212.	209.	189.	204.	184.	186.	171.
156.	178.	164.	184.	184.	164.	167.	165.	170.	170.
179.	162.	173.	169.	171.	161.	172.	164.	177.	172.
177.	179.	193.	163.	188.	158.	164.	188.	176.	181.
159.	169.	185.	185.	172.	175.	195.	163.	175.	175.
176.	219.	163.	184.	183.	168.	179.	155.	173.	186.
166.	181.	174.	196.	191.	186.	196.	170.	207.	198.
181.	219.	207.	227.	206.	212.	226.	222.	254.	261.
260.	226.	293.	268.	281.	342.	316.	358.	383.	387.
421.	476.	579.	600.	667.	669.	828.	880.	981.	1016.
1197.	1234.	1320.	1455.	1555.	1554.	1613.	1592.	1636.	1712.
1665.	1728.	1784.	1806.	1896.	1908.	2039.	2143.	2240.	2508.

2638.	2760.	3026.	3208.	3331.	3425.	3475.	3478.	3509.	3378.
3092.	2841.	2660.	2411.	2094.	1827.	1574.	1448.	1245.	1121.
965.	841.	705.	690.	612.	597.	539.	507.	489.	426.
457.	417.	454.	415.	412.	454.	443.	429.	479.	454.
484.	481.	486.	522.	542.	502.	519.	522.	502.	550.
478.	463.	432.	414.	396.	353.	347.	361.	334.	318.
362.	354.	362.	336.	351.	396.	421.	431.	487.	493.
532.	598.	608.	630.	718.	688.	730.	823.	748.	798.
803.	792.	727.	757.	732.	715.	635.	667.	674.	602.
552.	556.	570.	539.	596.	585.	501.	515.	491.	474.
462.	410.	376.	366.	385.	345.	349.	317.	318.	320.
317.	328.	326.	327.	340.	341.	339.	367.	373.	390.
383.	420.	415.	448.	497.	467.	481.	558.	604.	641.
673.	705.	708.	748.	749.	771.	817.	903.	874.	932.
952.	971.	924.	960.	951.	961.	883.	867.	765.	757.
697.	612.	585.	537.	493.	405.	415.	357.	348.	339.
289.	297.	237.	251.	250.	253.	247.	232.	192.	221.
246.	230.	248.	241.	211.	245.	209.	191.	171.	165.
164.	165.	150.	149.	165.	138.	148.	162.	152.	145.
146.	132.	161.	154.	142.	153.	137.	130.	151.	136.
158.	164.	143.	162.	151.	144.	151.	115.	140.	127.
148.	151.	140.	146.	142.	151.	152.	132.	143.	145.
146.	157.	151.	131.	144.	172.	146.	156.	154.	159.
157.	139.	143.	154.	152.	164.	176.	148.	167.	178.
181.	170.	177.	218.	197.	205.	217.	220.	245.	287.
263.	276.	280.	335.	343.	403.	357.	429.	449.	445.
458.	531.	505.	482.	519.	502.	479.	503.	491.	470.
492.	462.	441.	446.	397.	381.	400.	338.	335.	333.
333.	301.	334.	307.	313.	258.	304.	283.	313.	318.
304.	333.	317.	334.	346.	343.	387.	403.	463.	435.
455.	469.	474.	481.	493.	463.	473.	474.	429.	408.
430.	387.	416.	389.	360.	370.	366.	359.	329.	362.
388.	370.	384.	369.	359.	409.	366.	356.	330.	332.
334.	345.	315.	322.	291.	305.	287.	270.	278.	272.
300.	341.	341.	356.	354.	389.	390.	407.	448.	497.
507.	557.	555.	560.	652.	643.	671.	717.	755.	807.
787.	766.	776.	772.	777.	746.	781.	853.	834.	862.
889.	903.	940.	975.	949.	980.	974.	1000.	931.	852.
831.	854.	766.	752.	717.	607.	561.	553.	490.	473.
437.	390.	378.	398.	325.	359.	347.	354.	355.	346.
333.	301.	364.	393.	357.	394.	401.	408.	428.	431.
455.	493.	499.	480.	537.	534.	560.	589.	581.	630.
538.	563.	566.	562.	535.	520.	507.	471.	433.	416.
444.	386.	388.	353.	394.	349.	384.	364.	345.	412.
346.	350.	332.	330.	333.	383.	281.	351.	353.	330.
292.	347.	320.	306.	322.	282.	289.	347.	353.	354.
318.	344.	311.	297.	323.	281.	292.	319.	282.	277.
248.	280.	251.	214.	228.	204.	235.	226.	240.	242.
250.	293.	312.	278.	370.	357.	372.	300.	316.	330.
337.	292.	289.	293.	275.	278.	268.	253.	302.	301.
323.	331.	339.	345.	375.	427.	440.	473.	470.	574.
528.	646.	654.	705.	768.	873.	889.	908.	914.	973.
961.	1027.	969.	882.	784.	755.	685.	608.	635.	535.
455.	405.	412.	389.	386.	350.	355.	348.	338.	368.
313.	356.	382.	374.	377.	410.	419.	439.	457.	479.
490.	460.	528.	508.	516.	526.	534.	490.	521.	488.
493.	431.	402.	426.	371.	412.	365.	315.	324.	317.
322.	299.	305.	262.	297.	307.	292.	332.	317.	301.
332.	303.	307.	361.	332.	326.	375.	310.	271.	297.
294.	283.	268.	259.	257.	221.	238.	225.	234.	206.
204.	210.	200.	169.	176.	183.	147.	143.	147.	132.
141.	142.	161.	125.	136.	132.	128.	126.	133.	114.
127.	148.	126.	116.	134.	122.	119.	152.	109.	116.
141.	137.	118.	112.	118.	120.	121.	118.	131.	127.
130.	119.	144.	122.	116.	138.	129.	132.	148.	147.
146.	149.	141.	162.	149.	142.	160.	159.	156.	160.
150.	165.	160.	147.	177.	150.	184.	154.	150.	173.
157.	177.	158.	159.	174.	163.	176.	161.	166.	161.
191.	182.	185.	175.	184.	178.	194.	191.	177.	198.

185.	207.	189.	191.	179.	179.	175.	190.	159.	164.
162.	154.	130.	160.	132.	140.	143.	129.	109.	128.
135.	130.	127.	127.	137.	131.	132.	164.	152.	146.
138.	150.	126.	154.	149.	139.	114.	114.	122.	129.
146.	132.	145.	121.	141.	124.	134.	126.	140.	138.
131.	124.	126.	127.	129.	123.	135.	130.	138.	136.
125.	128.	121.	122.	132.	147.	146.	120.	140.	141.
144.	128.	123.	107.	128.	127.	115.	108.	107.	108.
112.	105.	102.	109.	112.	116.	115.	107.	98.	106.
109.	113.	105.	103.	115.	106.	110.	106.	109.	100.
132.	116.	120.	96.	109.	114.	114.	104.	107.	111.
123.	138.	107.	102.	145.	131.	105.	121.	102.	107.
102.	128.	128.	134.	110.	121.	113.	123.	114.	115.
107.	130.	134.	128.	141.	117.	133.	133.	136.	135.
140.	151.	126.	133.	131.	144.	136.	152.	142.	150.
138.	181.	163.	159.	138.	160.	122.	176.	171.	162.
162.	184.	162.	175.	206.	183.	188.	200.	205.	191.
230.	216.	233.	214.	233.	251.	277.	253.	267.	315.
305.	311.	340.	347.	348.	365.	363.	428.	381.	431.
394.	398.	394.	420.	421.	434.	425.	384.	420.	403.
447.	386.	371.	383.	354.	422.	391.	384.	384.	346.
377.	395.	326.	326.	311.	304.	268.	314.	254.	261.
248.	244.	263.	241.	237.	228.	242.	197.	221.	230.
226.	232.	205.	228.	227.	232.	229.	225.	231.	264.
245.	247.	253.	253.	220.	243.	235.	221.	230.	242.
220.	241.	228.	227.	237.	253.	257.	265.	253.	286.
284.	320.	283.	297.	305.	271.	314.	276.	313.	309.
277.	308.	314.	251.	272.	275.	261.	287.	277.	286.
258.	262.	253.	269.	248.	230.	244.	261.	256.	280.
286.	294.	261.	269.	264.	299.	286.	282.	289.	313.
342.	331.	341.	341.	333.	323.	370.	362.	333.	346.
373.	363.	414.	381.	399.	419.	416.	416.	427.	428.
433.	509.	481.	506.	462.	491.	489.	519.	524.	513.
504.	496.	554.	498.	530.	575.	539.	531.	560.	593.
605.	597.	599.	592.	612.	668.	666.	713.	689.	733.
737.	764.	794.	738.	780.	755.	764.	725.	755.	714.
672.	709.	614.	652.	668.	607.	635.	563.	545.	546.
536.	548.	548.	508.	476.	465.	457.	464.	404.	386.
374.	410.	387.	371.	385.	368.	389.	378.	376.	358.
395.	361.	392.	379.	374.	394.	389.	382.	375.	335.
364.	394.	395.	398.	395.	394.	408.	361.	415.	388.
408.	420.	385.	385.	435.	453.	479.	475.	478.	441.
443.	490.	505.	468.	466.	456.	429.	528.	506.	550.
525.	569.	571.	620.	659.	619.	653.	593.	665.	603.
656.	660.	629.	595.	571.	565.	583.	603.	590.	524.
484.	495.	472.	446.	415.	402.	390.	393.	349.	322.
327.	345.	330.	270.	277.	247.	247.	233.	211.	249.
207.	213.	210.	207.	218.	193.	192.	172.	211.	172.
162.	184.	154.	183.	171.	162.	184.	186.	174.	160.
177.	171.	181.	174.	204.	177.	190.	196.	173.	203.
192.	176.	160.	216.	205.	212.	206.	190.	208.	204.
200.	219.	202.	209.	247.	222.	221.	215.	258.	240.
260.	271.	276.	243.	294.	270.	268.	269.	281.	320.
303.	336.	314.	309.	338.	313.	354.	330.	358.	315.
323.	299.	330.	308.	302.	287.	290.	281.	312.	251.
276.	263.	264.	262.	227.	244.	239.	211.	217.	249.
228.	254.	261.	227.	225.	226.	261.	187.	232.	221.
223.	220.	262.	226.	232.	248.	271.	261.	284.	285.
271.	280.	279.	307.	303.	287.	312.	330.	308.	334.
367.	385.	346.	381.	416.	401.	431.	436.	449.	437.
452.	403.	456.	444.	443.	440.	414.	397.	373.	369.
396.	403.	330.	349.	370.	366.	345.	362.	334.	332.
313.	297.	314.	346.	337.	348.	355.	382.	351.	366.
385.	413.	400.	396.	452.	442.	430.	463.	527.	492.
550.	530.	550.	629.	621.	697.	641.	737.	742.	778.
864.	896.	994.	988.	999.	1072.	1108.	1164.	1161.	1197.
1221.	1182.	1104.	1092.	1116.	1059.	1021.	945.	913.	835.
852.	755.	722.	650.	608.	557.	496.	509.	428.	408.
385.	340.	325.	305.	355.	329.	312.	309.	302.	281.

291.	257.	270.	254.	267.	274.	276.	271.	248.	266.
262.	267.	231.	258.	233.	275.	247.	239.	248.	240.
272.	235.	233.	243.	243.	234.	257.	208.	240.	218.
251.	226.	236.	233.	224.	222.	233.	246.	232.	234.
211.	214.	231.	216.	175.	238.	186.	189.	176.	191.
188.	204.	195.	206.	193.	180.	181.	196.	193.	201.
232.	218.	193.	222.	220.	209.	224.	225.	240.	252.
232.	295.	237.	241.	216.	260.	228.	248.	218.	189.
242.	197.	193.	188.	200.	186.	150.	165.	186.	170.
166.	170.	148.	169.	151.	149.	163.	157.	167.	152.
147.	162.	149.	165.	166.	160.	170.	164.	164.	156.
150.	175.	167.	170.	184.	179.	171.	181.	171.	187.
186.	222.	243.	265.	253.	320.	311.	271.	245.	245.
250.	266.	257.	293.	271.	276.	257.	250.	253.	240.
231.	239.	242.	224.	205.	193.	197.	206.	184.	175.
176.	189.	182.	172.	181.	170.	167.	172.	161.	174.
162.	185.	180.	172.	186.	198.	187.	176.	181.	182.
209.	202.	196.	209.	218.	220.	204.	197.	195.	228.
203.	222.	224.	222.	202.	196.	217.	203.	203.	219.
217.	242.	217.	234.	230.	246.	221.	234.	233.	237.
226.	218.	249.	241.	243.	235.	202.	205.	209.	218.
198.	217.	208.	191.	193.	223.	197.	184.	195.	173.
215.	181.	219.	170.	199.	172.	192.	159.	191.	184.
182.	186.	170.	181.	173.	212.	172.	156.	188.	173.
178.	171.	160.	187.	163.	183.	194.	186.	155.	161.
159.	141.	183.	181.	187.	198.	172.	182.	199.	209.
206.	204.	211.	196.	235.	219.	205.	228.	254.	279.
244.	233.	257.	277.	241.	265.	262.	282.	310.	305.
288.	320.	343.	327.	343.	294.	301.	324.	308.	317.
341.	258.	284.	301.	279.	270.	300.	231.	271.	247.
248.	265.	251.	258.	258.	227.	224.	248.	209.	238.
232.	211.	242.	237.	265.	245.	245.	263.	267.	267.
288.	235.	288.	277.	271.	304.	289.	291.	345.	341.
352.	325.	389.	363.	406.	379.	438.	429.	468.	480.
460.	487.	491.	523.	502.	499.	497.	513.	514.	479.
460.	479.	440.	432.	409.	385.	418.	383.	390.	338.
357.	329.	324.	343.	314.	310.	320.	298.	323.	300.
321.	325.	317.	318.	338.	394.	344.	338.	352.	371.
343.	381.	397.	382.	396.	403.	358.	384.	393.	367.
365.	411.	354.	356.	359.	295.	305.	303.	266.	304.
289.	274.	262.	256.	239.	222.	210.	243.	226.	208.
183.	195.	183.	187.	219.	182.	204.	204.	204.	207.
193.	160.	207.	203.	204.	235.	177.	200.	184.	190.
168.	194.	189.	172.	206.	192.	212.	203.	174.	194.
203.	223.	180.	206.	166.	182.	188.	152.	161.	153.
174.	173.	160.	151.	137.	171.	147.	145.	137.	145.
151.	125.	144.	165.	153.	143.	164.	145.	150.	159.
150.	149.	134.	138.	145.	164.	149.	150.	152.	148.
161.	124.	149.	172.	177.	155.	194.	168.	153.	137.
165.	169.	173.	176.	175.	193.	185.	198.	182.	221.
199.	218.	226.	238.	233.	250.	260.	265.	316.	316.
281.	301.	315.	329.	358.	377.	401.	417.	354.	396.
427.	458.	463.	457.	455.	490.	481.	501.	510.	511.
460.	509.	471.	477.	465.	423.	458.	474.	467.	418.
432.	444.	401.	365.	398.	415.	390.	341.	340.	374.
347.	350.	345.	313.	317.	312.	303.	301.	300.	282.
310.	285.	280.	248.	265.	239.	238.	223.	249.	265.
221.	251.	223.	255.	262.	230.	275.	253.	282.	217.
245.	265.	268.	259.	269.	263.	275.	271.	273.	222.
250.	279.	270.	247.	263.	248.	254.	269.	244.	273.
254.	245.	246.	263.	248.	240.	238.	275.	270.	260.
255.	220.	235.	229.	192.	218.	201.	221.	227.	211.
238.	208.	191.	178.	192.	199.	182.	210.	207.	199.
203.	184.	184.	190.	189.	179.	195.	187.	168.	194.
182.	203.	199.	174.	171.	145.	170.	155.	159.	173.
177.	170.	168.	192.	165.	158.	179.	166.	167.	205.
198.	184.	191.	207.	206.	217.	183.	228.	210.	208.
200.	230.	234.	240.	251.	227.	261.	270.	238.	280.
271.	300.	293.	284.	325.	304.	298.	332.	327.	340.

331.	337.	315.	355.	355.	331.	301.	324.	343.	333.
344.	325.	339.	315.	346.	359.	344.	323.	338.	350.
362.	339.	333.	322.	360.	330.	314.	337.	327.	344.
338.	285.	296.	329.	310.	289.	278.	274.	272.	268.
278.	300.	238.	259.	243.	234.	215.	241.	234.	231.
203.	196.	201.	183.	197.	185.	192.	193.	182.	201.
195.	176.	170.	186.	146.	184.	167.	170.	179.	145.
189.	182.	171.	175.	193.	184.	192.	173.	184.	173.
200.	191.	189.	211.	216.	178.	222.	225.	210.	215.
251.	259.	272.	299.	293.	270.	277.	283.	243.	259.
260.	249.	254.	253.	263.	281.	262.	269.	272.	289.
263.	210.	248.	257.	241.	229.	236.	235.	232.	206.
190.	193.	221.	226.	209.	186.	169.	181.	199.	188.
178.	176.	217.	166.	170.	166.	175.	158.	170.	168.
173.	155.	190.	170.	164.	170.	149.	180.	195.	184.
190.	149.	173.	175.	202.	176.	182.	204.	183.	208.
187.	194.	187.	187.	177.	190.	212.	197.	179.	187.
193.	200.	190.	186.	211.	191.	219.	186.	202.	192.
203.	200.	180.	188.	201.	209.	195.	191.	182.	168.
175.	194.	190.	206.	168.	190.	192.	178.	183.	191.
199.	198.	201.	169.	159.	180.	210.	214.	192.	177.
215.	188.	177.	199.	190.	192.	168.	180.	177.	191.
207.	190.	201.	186.	203.	216.	189.	186.	215.	172.
204.	187.	184.	205.	200.	187.	215.	172.	214.	169.
206.	201.	185.	176.	224.	161.	196.	180.	205.	194.
205.	181.	184.	202.	164.	176.	191.	202.	211.	173.
212.	201.	178.	175.	191.	168.	190.	197.	165.	163.
165.	184.	188.	165.	168.	186.	165.	159.	160.	166.
159.	138.	142.	161.	154.	142.	120.	138.	133.	123.
137.	148.	136.	125.	127.	130.	116.	117.	126.	123.
133.	127.	128.	126.	119.	125.	108.	99.	119.	110.
122.	99.	103.	113.	102.	104.	111.	123.	111.	103.
106.	108.	113.	114.	121.	106.	122.	128.	120.	123.
124.	120.	121.	112.	127.	112.	118.	122.	128.	124.
114.	129.	127.	136.	127.	127.	127.	115.	148.	134.
140.	110.	138.	144.	126.	140.	132.	109.	140.	115.
119.	138.	115.	140.	131.	120.	135.	134.	145.	148.
135.	148.	135.	140.	126.	130.	161.	148.	147.	148.
157.	107.	148.	141.	136.	141.	141.	139.	131.	124.
136.	151.	120.	113.	148.	140.	139.	106.	123.	141.
128.	149.	138.	129.	115.	94.	128.	111.	125.	117.
134.	99.	128.	104.	108.	125.	116.	100.	100.	96.
102.	111.	104.	117.	87.	110.	113.	95.	99.	93.
92.	110.	131.	101.	100.	98.	118.	92.	110.	91.
105.	93.	117.	102.	103.	77.	122.	109.	119.	104.
102.	115.	109.	73.	92.	116.	113.	103.	112.	118.
112.	111.	117.	129.	127.	134.	136.	108.	136.	121.
109.	130.	149.	133.	125.	135.	116.	156.	158.	139.
142.	131.	143.	135.	165.	152.	143.	172.	173.	160.
153.	163.	139.	167.	124.	131.	162.	152.	152.	153.
159.	150.	166.	151.	139.	123.	128.	141.	136.	132.
147.	129.	147.	141.	124.	163.	121.	138.	111.	136.
141.	118.	125.	129.	122.	143.	146.	124.	130.	152.
120.	157.	128.	130.	152.	128.	152.	163.	169.	136.
140.	146.	148.	153.	140.	159.	154.	172.	185.	175.
167.	182.	159.	182.	169.	161.	207.	207.	184.	214.
207.	188.	204.	209.	195.	224.	196.	158.	165.	185.
198.	202.	172.	165.	187.	190.	175.	184.	195.	156.
175.	187.	173.	165.	157.	146.	147.	152.	153.	127.
138.	117.	144.	126.	153.	129.	134.	139.	162.	126.
130.	137.	152.	138.	130.	128.	150.	150.	148.	135.
115.	134.	134.	181.	171.	148.	150.	158.	145.	135.
135.	155.	140.	149.	161.	158.	160.	161.	157.	142.
161.	172.	147.	151.	144.	131.	138.	138.	132.	103.
139.	144.	147.	116.	130.	148.	133.	126.	120.	141.
102.	102.	97.	112.	108.	90.	99.	92.	117.	103.
95.	87.	103.	117.	95.	118.	89.	106.	111.	87.
94.	108.	95.	105.	95.	82.	101.	101.	90.	105.
99.	108.	100.	94.	92.	93.	87.	112.	114.	100.

106.	101.	104.	76.	97.	97.	100.	80.	107.	88.
105.	108.	104.	111.	108.	121.	102.	115.	117.	130.
107.	136.	137.	113.	107.	124.	133.	112.	127.	119.
124.	136.	137.	151.	130.	117.	143.	143.	125.	131.
137.	132.	137.	137.	143.	128.	145.	135.	139.	122.
125.	123.	124.	122.	125.	132.	130.	116.	119.	128.
116.	147.	119.	130.	129.	127.	141.	121.	123.	137.
113.	124.	133.	126.	137.	136.	123.	98.	134.	131.
127.	129.	124.	143.	125.	131.	127.	105.	117.	139.
143.	116.	137.	116.	137.	111.	133.	121.	120.	109.
127.	119.	112.	106.	101.	127.	111.	115.	108.	122.
104.	112.	102.	116.	121.	114.	121.	131.	124.	127.
121.	113.	105.	107.	123.	137.	112.	131.	114.	134.
130.	124.	149.	141.	145.	137.	131.	150.	117.	123.
131.	142.	117.	139.	134.	155.	123.	135.	147.	152.
139.	155.	123.	126.	156.	139.	134.	140.	125.	143.
126.	139.	138.	134.	127.	128.	137.	132.	135.	122.
125.	123.	118.	123.	115.	127.	121.	122.	127.	122.
110.	144.	134.	117.	125.	117.	139.	131.	125.	126.
121.	125.	143.	118.	128.	130.	114.	151.	124.	146.
120.	145.	134.	150.	125.	147.	141.	140.	145.	154.
152.	153.	159.	149.	148.	139.	135.	120.	161.	139.
150.	150.	148.	138.	138.	163.	175.	130.	148.	138.
131.	139.	137.	140.	124.	122.	141.	128.	132.	144.
143.	126.	127.	125.	152.	122.	139.	136.	145.	144.
140.	154.	139.	135.	145.	135.	153.	152.	139.	144.
137.	146.	129.	136.	134.	148.	131.	162.	170.	134.
156.	129.	167.	139.	162.	125.	133.	141.	138.	136.
143.	117.	128.	138.	131.	121.	127.	115.	132.	130.
111.	139.	112.	137.	120.	110.	122.	89.	84.	97.
131.	121.	109.	99.	112.	101.	109.	133.	100.	111.
91.	106.	114.	81.	120.	102.	113.	104.	104.	111.
104.	94.	114.	100.	119.	103.	77.	87.	116.	107.
101.	105.	108.	107.	96.	94.	96.	90.	105.	97.
104.	109.	111.	104.	92.	107.	105.	113.	99.	95.
106.	104.	130.	91.	93.	111.	97.	85.	137.	108.
101.	98.	108.	98.	107.	114.	100.	104.	99.	101.
121.	86.	119.	119.	100.	95.	91.	102.	96.	86.
102.	106.	85.	100.	98.	102.	81.	88.	84.	99.
106.	100.	93.	87.	100.	85.	93.	93.	100.	95.
104.	72.	105.	91.	99.	120.	105.	97.	107.	93.
119.	112.	87.	90.	86.	114.	93.	87.	92.	95.
96.	109.	112.	95.	99.	106.	101.	119.	81.	115.
93.	129.	112.	127.	90.	115.	106.	113.	112.	105.
130.	123.	110.	104.	117.	119.	113.	136.	133.	141.
113.	131.	137.	139.	122.	134.	118.	119.	137.	127.
129.	141.	136.	134.	166.	118.	149.	141.	145.	140.
159.	151.	154.	154.	145.	167.	149.	161.	154.	143.
132.	156.	154.	144.	144.	139.	134.	166.	137.	146.
128.	129.	163.	132.	132.	146.	129.	137.	142.	127.
127.	148.	146.	132.	145.	106.	134.	123.	121.	126.
131.	123.	128.	128.	129.	139.	144.	149.	142.	124.
123.	154.	120.	139.	125.	139.	159.	126.	132.	153.
140.	149.	154.	148.	146.	156.	179.	142.	154.	145.
174.	153.	183.	171.	166.	165.	181.	165.	173.	186.
169.	159.	169.	174.	168.	171.	155.	142.	149.	152.
178.	151.	173.	139.	151.	142.	164.	162.	186.	169.
151.	136.	160.	133.	151.	149.	161.	160.	137.	154.
148.	160.	154.	139.	162.	160.	163.	147.	167.	141.
140.	151.	169.	148.	152.	134.	138.	139.	141.	150.
149.	138.	146.	138.	131.	134.	131.	140.	123.	132.
121.	118.	129.	125.	107.	114.	121.	116.	135.	132.
118.	94.	114.	130.	119.	120.	137.	110.	109.	120.
124.	122.	128.	132.	133.	129.	119.	119.	120.	133.
132.	129.	133.	151.	124.	154.	131.	134.	146.	132.
148.	130.	145.	119.	128.	146.	142.	122.	161.	154.
160.	148.	146.	136.	152.	182.	152.	167.	183.	183.
183.	177.	161.	149.	181.	171.	199.	176.	168.	174.
212.	200.	161.	200.	182.	183.	173.	181.	187.	151.

203.	192.	157.	192.	166.	160.	189.	134.	179.	164.
173.	163.	151.	175.	159.	145.	142.	162.	154.	158.
155.	147.	138.	143.	147.	110.	151.	159.	146.	122.
120.	154.	146.	128.	126.	127.	131.	132.	142.	136.
117.	138.	115.	133.	139.	132.	124.	149.	121.	118.
133.	125.	141.	130.	130.	140.	118.	139.	133.	153.
134.	167.	178.	131.	155.	154.	165.	145.	172.	157.
176.	162.	199.	168.	192.	164.	185.	177.	190.	167.
183.	182.	188.	185.	171.	190.	182.	185.	181.	177.
198.	184.	193.	203.	186.	212.	186.	182.	185.	162.
171.	173.	206.	168.	182.	195.	164.	180.	177.	160.
183.	172.	155.	160.	174.	161.	167.	167.	175.	179.
139.	184.	147.	145.	153.	141.	153.	162.	175.	165.
180.	139.	166.	153.	151.	156.	167.	163.	185.	141.
148.	149.	148.	163.	179.	170.	192.	181.	165.	170.
183.	178.	148.	173.	169.	179.	163.	174.	187.	175.
162.	161.	178.	172.	167.	191.	175.	186.	177.	175.
185.	172.	189.	149.	169.	156.	172.	166.	180.	179.
156.	146.	176.	169.	185.	162.	169.	192.	145.	159.
161.	159.	172.	157.	158.	150.	162.	151.	151.	142.
151.	144.	147.	152.	160.	139.	141.	148.	160.	124.
128.	143.	143.	136.	136.	139.	136.	126.	119.	130.
140.	136.	124.	125.	115.	121.	115.	132.	97.	96.
105.	126.	95.	116.	118.	106.	98.	92.	96.	104.
95.	102.	101.	101.	104.	114.	94.	120.	96.	95.
107.	102.	99.	99.	81.	95.	98.	93.	100.	108.
99.	97.	102.	86.	98.	86.	93.	106.	92.	85.
89.	94.	92.	90.	91.	110.	103.	108.	90.	81.
94.	83.	96.	105.	106.	100.	115.	82.	93.	83.
111.	101.	101.	82.	83.	93.	96.	93.	95.	77.
87.	87.	106.	88.	97.	111.	104.	94.	97.	87.
106.	92.	96.	111.	95.	101.	84.	118.	96.	92.
109.	95.	95.	107.	104.	97.	97.	117.	103.	115.
117.	112.	106.	108.	100.	113.	125.	117.	99.	126.
121.	119.	92.	109.	110.	112.	110.	96.	133.	120.
107.	121.	95.	116.	116.	110.	100.	113.	107.	112.
146.	109.	110.	112.	117.	106.	119.	110.	120.	126.
132.	94.	133.	103.	103.	101.	101.	138.	119.	125.
97.	118.	104.	113.	117.	105.	108.	99.	119.	108.
109.	100.	105.	102.	100.	103.	101.	118.	122.	112.
82.	111.	114.	122.	115.	129.	107.	112.	100.	98.
106.	99.	107.	110.	117.	111.	97.	104.	111.	119.
119.	97.	115.	127.	118.	122.	121.	110.	135.	117.
117.	98.	115.	117.	106.	115.	114.	134.	118.	125.
120.	122.	119.	117.	87.	119.	116.	120.	121.	109.
116.	112.	122.	124.	114.	105.	99.	113.	105.	117.
116.	117.	119.	110.	104.	117.	95.	115.	119.	130.
95.	118.	119.	107.	123.	104.	107.	117.	100.	113.
117.	102.	114.	113.	111.	102.	101.	103.	108.	82.
99.	102.	101.	114.	116.	124.	102.	118.	101.	111.
119.	121.	97.	124.	103.	130.	106.	100.	103.	120.
104.	97.	98.	101.	118.	119.	105.	103.	132.	132.
149.	120.	113.	117.	125.	102.	100.	120.	107.	108.
112.	108.	100.	104.	113.	104.	106.	120.	114.	104.
101.	104.	115.	119.	109.	108.	110.	98.	111.	100.
100.	104.	104.	102.	110.	122.	139.	122.	89.	118.
106.	117.	110.	117.	123.	119.	106.	107.	114.	122.
100.	114.	114.	104.	130.	118.	114.	129.	106.	97.
126.	103.	122.	107.	129.	128.	116.	132.	105.	152.
135.	135.	128.	146.	130.	137.	118.	124.	114.	139.
144.	138.	153.	140.	182.	156.	161.	156.	159.	163.
146.	168.	138.	135.	136.	144.	144.	140.	173.	166.
150.	155.	148.	136.	149.	150.	171.	148.	156.	162.
168.	188.	163.	168.	177.	164.	153.	159.	176.	147.
139.	154.	137.	149.	173.	129.	125.	142.	147.	146.
143.	129.	160.	141.	138.	153.	162.	135.	125.	140.
132.	130.	130.	122.	123.	166.	126.	126.	119.	127.
146.	142.	141.	134.	112.	133.	100.	118.	134.	118.
131.	131.	132.	134.	144.	125.	124.	103.	137.	111.

109.	124.	122.	131.	138.	125.	143.	132.	132.	115.
153.	143.	139.	134.	145.	147.	150.	155.	152.	135.
154.	143.	154.	140.	137.	153.	118.	154.	160.	149.
168.	152.	150.	162.	151.	161.	151.	166.	196.	171.
181.	156.	187.	169.	169.	170.	176.	175.	170.	185.
204.	166.	160.	205.	192.	179.	151.	179.	178.	183.
202.	171.	198.	200.	178.	177.	169.	180.	177.	191.
180.	201.	175.	167.	171.	171.	173.	174.	183.	160.
197.	204.	189.	169.	170.	178.	196.	180.	166.	176.
178.	206.	171.	175.	166.	177.	176.	180.	155.	182.
164.	174.	181.	161.	173.	176.	177.	169.	170.	153.
158.	146.	155.	186.	164.	175.	156.	141.	187.	158.
172.	170.	149.	156.	175.	183.	165.	173.	171.	180.
180.	158.	169.	170.	179.	196.	181.	188.	178.	159.
173.	170.	176.	181.	193.	163.	170.	161.	149.	180.
146.	153.	183.	149.	149.	138.	151.	146.	171.	169.
161.	146.	144.	153.	149.	146.	155.	156.	169.	156.
162.	143.	173.	127.	115.	159.	142.	162.	149.	140.
139.	151.	138.	146.	142.	136.	126.	132.	158.	129.
116.	147.	137.	124.	138.	153.	143.	126.	138.	143.
151.	136.	138.	146.	148.	138.	125.	138.	133.	133.
168.	111.	122.	141.	142.	161.	162.	141.	110.	125.
138.	130.	132.	146.	146.	137.	149.	128.	144.	142.
147.	140.	135.	128.	132.	104.	122.	120.	121.	151.
150.	163.	128.	117.	125.	134.	135.	142.	131.	129.
131.	131.	120.	120.	137.	133.	120.	129.	143.	105.
106.	136.	148.	126.	139.	137.	138.	130.	126.	132.
126.	139.	145.	120.	124.	130.	119.	128.	146.	135.
149.	149.	141.	130.	124.	136.	148.	144.	150.	158.
146.	137.	152.	157.	143.	159.	183.	148.	139.	139.
146.	142.	164.	157.	146.	165.	171.	165.	173.	151.
166.	155.	120.	159.	155.	157.	151.	144.	129.	165.
167.	146.	136.	135.	156.	151.	149.	173.	163.	144.
155.	163.	146.	144.	156.	150.	142.	143.	152.	174.
131.	172.	179.	158.	151.	166.	137.	139.	165.	139.
163.	147.	161.	180.	166.	147.	128.	169.	159.	144.
143.	188.	152.	161.	151.	159.	170.	145.	149.	153.
159.	159.	153.	134.	150.	131.	151.	138.	170.	179.
160.	153.	159.	171.	183.	174.	165.	168.	170.	180.
163.	166.	161.	150.	182.	180.	163.	191.	191.	147.
159.	156.	166.	183.	179.	197.	217.	198.	202.	177.
177.	183.	163.	172.	204.	213.	176.	175.	203.	190.
186.	196.	169.	194.	186.	183.	188.	185.	180.	170.
187.	182.	186.	212.	177.	188.	195.	189.	191.	177.
154.	176.	191.	166.	148.	202.	181.	176.	154.	168.
165.	169.	142.	162.	156.	185.	176.	151.	162.	150.
162.	169.	153.	155.	144.	159.	173.	158.	162.	173.
161.	150.	163.	143.	145.	146.	150.	154.	158.	143.
152.	165.	148.	167.	169.	162.	165.	148.	147.	140.
134.	164.	137.	176.	171.	162.	161.	150.	189.	173.
141.	150.	162.	157.	127.	152.	154.	147.	147.	152.
163.	158.	151.	156.	164.	159.	140.	144.	135.	167.
147.	132.	165.	151.	168.	143.	149.	160.	147.	154.
149.	161.	138.	128.	160.	136.	153.	151.	171.	152.
191.	158.	152.	127.	137.	165.	144.	143.	140.	152.
151.	148.	144.	149.	167.	153.	155.	165.	147.	154.
159.	143.	143.	123.	155.	139.	156.	161.	141.	145.
152.	135.	158.	142.	150.	126.	201.	160.	158.	163.
147.	157.	145.	139.	150.	165.	162.	159.	164.	142.
133.	159.	143.	153.	145.	125.	160.	150.	151.	144.
160.	154.	171.	175.	147.	176.	148.	138.	153.	153.
153.	178.	183.	163.	148.	152.	166.	138.	151.	174.
152.	146.	170.	159.	160.	177.	173.	169.	171.	149.
145.	163.	168.	185.	158.	171.	165.	151.	187.	152.
171.	185.	161.	151.	172.	173.	165.	149.	157.	157.
155.	160.	184.	170.	165.	163.	179.	170.	126.	160.
180.	164.	188.	181.	165.	163.	162.	155.	157.	174.
179.	167.	163.	160.	185.	177.	148.	150.	165.	170.
159.	178.	165.	163.	164.	182.	146.	171.	136.	161.

138.	169.	149.	182.	139.	167.	161.	153.	155.	149.
155.	164.	143.	145.	181.	141.	160.	170.	139.	183.
148.	146.	174.	147.	154.	140.	174.	156.	165.	156.
154.	156.	150.	178.	130.	178.	171.	170.	170.	164.
142.	156.	164.	169.	166.	154.	155.	145.	177.	149.
142.	160.	160.	185.	160.	156.	144.	152.	126.	163.
174.	159.	159.	170.	137.	157.	154.	157.	154.	163.
180.	148.	155.	160.	142.	129.	172.	166.	171.	189.
180.	175.	161.	159.	163.	178.	162.	156.	169.	178.
173.	160.	157.	171.	185.	185.	168.	179.	165.	174.
193.	170.	193.	167.	183.	177.	190.	171.	176.	188.
186.	162.	162.	195.	169.	191.	181.	181.	203.	192.
180.	196.	204.	172.	179.	186.	183.	165.	193.	209.
181.	205.	188.	199.	195.	194.	176.	189.	225.	182.
213.	189.	188.	176.	219.	185.	203.	213.	188.	195.
215.	199.	212.	197.	198.	208.	192.	205.	236.	214.
215.	215.	217.	200.	208.	220.	197.	203.	201.	216.
212.	175.	220.	198.	212.	216.	205.	208.	220.	200.
201.	220.	227.	208.	202.	212.	209.	209.	185.	202.
203.	196.	223.	229.	176.	222.	251.	212.	221.	193.
218.	221.	196.	205.	205.	223.	209.	213.	238.	209.
219.	237.	240.	198.	234.	200.	208.	194.	219.	228.
197.	199.	221.	201.	202.	207.	189.	229.	210.	244.
220.	207.	213.	233.	207.	209.	218.	213.	224.	200.
202.	209.	194.	201.	217.	185.	191.	205.	215.	198.
182.	201.	207.	196.	210.	184.	192.	208.	192.	186.
174.	198.	196.	190.	196.	248.	192.	206.	199.	173.
191.	164.	183.	178.	174.	165.	191.	174.	193.	157.
199.	198.	194.	197.	202.	168.	197.	179.	196.	197.
191.	196.	197.	177.	210.	203.	197.	177.	206.	190.
182.	194.	197.	189.	176.	170.	180.	192.	194.	188.
196.	189.	188.	148.	165.	183.	184.	188.	172.	171.
195.	185.	178.	163.	192.	178.	191.	176.	162.	176.
187.									

Appendix P-24: step-intensity data of fluoro-phlogopite

8.00	.02	128.00	Pure phlogopite						
233.	234.	228.	237.	229.	264.	239.	221.	227.	242.
232.	234.	245.	256.	253.	239.	224.	220.	244.	275.
225.	262.	268.	265.	282.	274.	306.	343.	351.	343.
421.	490.	463.	473.	555.	615.	692.	743.	837.	1012.
1176.	1351.	1421.	1233.	1033.	609.	396.	275.	260.	268.
220.	211.	219.	204.	208.	169.	216.	205.	216.	184.
196.	187.	180.	188.	214.	174.	198.	211.	179.	192.
172.	158.	175.	179.	201.	182.	167.	166.	164.	191.
166.	197.	185.	161.	160.	167.	198.	176.	153.	165.
157.	196.	142.	149.	174.	159.	165.	156.	163.	165.
182.	192.	162.	162.	159.	177.	164.	163.	167.	168.
165.	171.	203.	181.	187.	172.	148.	208.	181.	160.
192.	214.	203.	210.	169.	178.	172.	162.	145.	152.
151.	172.	165.	162.	133.	154.	158.	179.	160.	161.
162.	154.	174.	146.	133.	143.	110.	148.	151.	147.
132.	128.	156.	149.	153.	144.	138.	144.	148.	159.
139.	128.	119.	134.	168.	142.	174.	152.	136.	163.
125.	136.	134.	128.	163.	126.	132.	152.	113.	169.
140.	132.	118.	150.	136.	139.	127.	143.	137.	148.
134.	140.	154.	139.	119.	135.	127.	132.	135.	136.
122.	108.	132.	130.	122.	111.	134.	118.	126.	139.
126.	119.	181.	133.	131.	161.	148.	109.	125.	162.
132.	104.	140.	127.	134.	122.	114.	123.	138.	138.
144.	133.	136.	133.	123.	116.	126.	146.	136.	125.
134.	171.	130.	131.	121.	123.	132.	136.	110.	106.
131.	109.	127.	128.	134.	130.	141.	112.	124.	127.
114.	122.	131.	133.	135.	129.	129.	112.	113.	124.
131.	141.	134.	126.	126.	144.	125.	143.	106.	135.
121.	118.	115.	123.	100.	124.	109.	128.	113.	135.
106.	138.	137.	156.	153.	122.	128.	150.	138.	126.
139.	126.	139.	102.	126.	93.	106.	118.	107.	136.
150.	109.	107.	116.	128.	100.	98.	117.	102.	99.
109.	119.	113.	102.	113.	127.	115.	128.	116.	128.
121.	106.	122.	95.	141.	126.	133.	92.	123.	111.
106.	114.	136.	107.	95.	107.	97.	95.	104.	113.
117.	89.	95.	108.	98.	102.	124.	99.	99.	98.
94.	116.	105.	134.	97.	92.	115.	80.	103.	115.
100.	102.	112.	84.	112.	112.	117.	110.	106.	111.
102.	94.	107.	107.	108.	94.	106.	107.	93.	94.
101.	103.	113.	108.	108.	91.	116.	99.	97.	93.
80.	111.	93.	98.	96.	83.	118.	95.	96.	97.
82.	98.	72.	101.	121.	110.	104.	96.	120.	120.
93.	90.	104.	114.	94.	114.	106.	127.	90.	113.
79.	91.	119.	75.	123.	104.	81.	84.	97.	95.
103.	83.	83.	106.	94.	106.	91.	91.	85.	98.
107.	86.	86.	107.	101.	86.	90.	105.	113.	90.
93.	91.	127.	109.	101.	105.	76.	87.	116.	85.
93.	96.	93.	96.	95.	105.	96.	104.	84.	85.
87.	110.	92.	105.	126.	105.	140.	133.	147.	121.
121.	117.	96.	85.	116.	97.	91.	114.	82.	113.
77.	90.	87.	108.	98.	89.	108.	93.	87.	107.
77.	95.	92.	105.	76.	100.	93.	107.	85.	82.
94.	72.	101.	70.	90.	83.	96.	110.	95.	69.
72.	69.	106.	97.	83.	69.	76.	98.	88.	75.
74.	90.	90.	90.	94.	92.	88.	83.	86.	93.
98.	89.	89.	102.	102.	126.	101.	119.	141.	154.
179.	215.	272.	320.	421.	416.	379.	355.	313.	280.
254.	294.	266.	299.	310.	384.	411.	367.	322.	217.
189.	135.	166.	157.	129.	139.	128.	153.	124.	169.
165.	114.	104.	112.	116.	119.	138.	116.	114.	91.
107.	104.	106.	114.	117.	119.	122.	119.	120.	148.
144.	158.	117.	99.	101.	91.	79.	82.	88.	95.
91.	79.	90.	91.	84.	92.	96.	87.	98.	98.
82.	88.	91.	68.	62.	84.	84.	104.	83.	87.
86.	86.	102.	90.	97.	97.	96.	107.	83.	101.

130.	97.	128.	85.	106.	90.	127.	103.	117.	100.
109.	107.	111.	92.	110.	87.	118.	93.	105.	78.
106.	103.	91.	97.	94.	88.	87.	109.	84.	95.
89.	82.	102.	87.	79.	77.	77.	80.	135.	113.
98.	88.	104.	110.	74.	104.	95.	92.	94.	82.
98.	66.	110.	66.	97.	101.	66.	81.	110.	109.
111.	92.	116.	80.	117.	90.	102.	86.	109.	83.
78.	107.	76.	86.	99.	87.	101.	127.	116.	148.
129.	183.	180.	225.	213.	228.	195.	162.	149.	131.
137.	122.	97.	110.	119.	100.	129.	118.	119.	107.
117.	97.	100.	93.	79.	84.	79.	87.	97.	92.
82.	83.	104.	87.	80.	87.	91.	102.	88.	112.
86.	87.	86.	113.	96.	85.	100.	104.	106.	107.
85.	96.	108.	101.	87.	86.	102.	92.	95.	83.
102.	83.	83.	82.	106.	90.	92.	89.	97.	80.
70.	86.	104.	100.	94.	112.	94.	114.	128.	126.
115.	144.	165.	186.	244.	254.	307.	364.	444.	417.
392.	370.	337.	246.	226.	166.	196.	165.	122.	98.
90.	122.	82.	114.	100.	103.	101.	84.	95.	99.
125.	87.	111.	122.	96.	81.	95.	95.	110.	118.
94.	96.	126.	134.	108.	103.	129.	107.	122.	135.
142.	145.	143.	136.	137.	149.	154.	168.	154.	164.
182.	168.	173.	195.	244.	238.	279.	291.	304.	343.
303.	301.	286.	253.	219.	189.	179.	167.	159.	145.
135.	116.	145.	131.	104.	122.	135.	127.	115.	117.
122.	157.	121.	141.	139.	113.	147.	156.	188.	232.
219.	284.	341.	338.	410.	499.	617.	678.	610.	542.
442.	366.	282.	219.	228.	192.	196.	165.	191.	147.
170.	239.	233.	266.	375.	448.	565.	760.	892.	1069.
990.	747.	505.	294.	195.	185.	138.	122.	148.	130.
111.	104.	128.	110.	138.	150.	196.	144.	158.	110.
132.	105.	95.	131.	148.	134.	151.	111.	137.	128.
124.	133.	119.	118.	95.	134.	102.	127.	98.	84.
100.	104.	101.	113.	75.	110.	100.	102.	104.	82.
102.	84.	92.	85.	101.	88.	89.	114.	98.	97.
106.	79.	105.	97.	103.	117.	123.	123.	167.	170.
165.	179.	148.	166.	135.	164.	212.	197.	208.	222.
255.	319.	399.	442.	441.	477.	477.	452.	318.	273.
227.	195.	186.	134.	128.	124.	106.	88.	116.	110.
90.	107.	117.	79.	114.	93.	73.	86.	76.	94.
91.	92.	100.	83.	102.	86.	108.	87.	83.	97.
73.	107.	87.	92.	85.	84.	100.	61.	95.	93.
93.	75.	79.	79.	99.	83.	107.	97.	91.	100.
109.	99.	100.	109.	105.	77.	103.	100.	82.	91.
80.	92.	81.	89.	91.	93.	66.	72.	49.	77.
78.	99.	66.	70.	86.	82.	82.	78.	82.	100.
92.	96.	105.	123.	122.	122.	99.	112.	87.	73.
97.	105.	91.	100.	84.	76.	97.	116.	104.	118.
113.	142.	152.	145.	186.	207.	238.	266.	325.	318.
351.	316.	256.	194.	180.	145.	150.	111.	98.	99.
81.	85.	80.	69.	84.	85.	62.	53.	60.	60.
85.	81.	72.	65.	45.	68.	70.	64.	67.	53.
68.	79.	67.	52.	56.	81.	69.	69.	63.	96.
165.	140.	102.	81.	69.	48.	75.	87.	59.	53.
83.	78.	81.	67.	79.	75.	58.	53.	54.	62.
73.	93.	77.	58.	65.	77.	60.	71.	65.	60.
57.	61.	72.	64.	79.	67.	82.	63.	72.	63.
68.	97.	92.	85.	92.	91.	112.	91.	112.	87.
91.	79.	55.	55.	69.	67.	79.	68.	62.	61.
69.	62.	64.	69.	68.	61.	79.	52.	59.	81.
77.	71.	84.	113.	118.	137.	196.	190.	210.	192.
201.	193.	170.	161.	154.	121.	120.	95.	94.	83.
69.	61.	69.	72.	65.	78.	77.	55.	74.	48.
56.	75.	86.	92.	83.	123.	139.	158.	174.	235.
282.	388.	529.	610.	671.	683.	554.	479.	394.	312.
254.	213.	226.	211.	224.	242.	260.	333.	430.	537.
659.	961.	1224.	1589.	1613.	1777.	1538.	1204.	980.	654.
506.	392.	305.	259.	179.	166.	152.	110.	126.	125.
110.	98.	122.	121.	131.	125.	160.	108.	94.	99.

126.	85.	112.	104.	115.	105.	105.	120.	137.	169.
138.	172.	239.	224.	259.	284.	318.	340.	347.	381.
398.	344.	264.	242.	245.	223.	224.	198.	183.	151.
134.	127.	116.	121.	117.	72.	113.	104.	88.	75.
89.	88.	95.	110.	80.	94.	123.	150.	148.	180.
171.	215.	231.	277.	226.	262.	209.	172.	163.	174.
155.	124.	94.	68.	81.	65.	84.	53.	54.	69.
58.	43.	56.	71.	45.	82.	69.	65.	51.	74.
61.	81.	48.	89.	63.	52.	77.	89.	79.	58.
80.	83.	82.	83.	86.	96.	105.	110.	120.	109.
145.	149.	157.	210.	289.	337.	398.	436.	578.	721.
821.	900.	855.	767.	700.	530.	433.	356.	216.	218.
165.	139.	132.	117.	127.	103.	111.	98.	76.	69.
89.	69.	69.	93.	100.	96.	107.	90.	101.	105.
107.	112.	93.	114.	122.	150.	134.	138.	178.	169.
167.	148.	156.	132.	116.	131.	85.	119.	53.	98.
79.	79.	53.	78.	70.	75.	66.	60.	68.	68.
68.	67.	74.	69.	99.	102.	84.	101.	94.	94.
93.	77.	55.	74.	52.	50.	48.	46.	51.	29.
46.	33.	44.	48.	39.	40.	37.	42.	47.	54.
44.	51.	38.	37.	54.	50.	48.	50.	47.	34.
46.	75.	68.	102.	76.	116.	127.	133.	175.	215.
227.	247.	230.	227.	248.	219.	224.	192.	176.	154.
149.	130.	126.	120.	85.	100.	108.	78.	101.	126.
121.	120.	127.	181.	124.	128.	112.	101.	83.	88.
78.	94.	78.	119.	87.	108.	109.	107.	106.	115.
110.	101.	105.	129.	106.	110.	99.	100.	142.	99.
104.	128.	112.	121.	100.	82.	77.	75.	81.	67.
72.	66.	45.	64.	50.	57.	67.	53.	48.	73.
66.	79.	55.	48.	56.	53.	64.	66.	48.	62.
47.	57.	60.	79.	65.	50.	69.	80.	72.	75.
97.	86.	82.	116.	124.	106.	84.	86.	74.	62.
68.	81.	90.	77.	80.	78.	98.	78.	85.	92.
86.	104.	128.	140.	123.	157.	190.	220.	246.	273.
339.	352.	391.	521.	512.	589.	521.	540.	485.	428.
348.	264.	228.	181.	163.	132.	126.	121.	130.	121.
102.	92.	99.	144.	116.	104.	112.	105.	89.	80.
104.	66.	77.	61.	93.	64.	68.	82.	83.	56.
78.	67.	66.	80.	83.	78.	95.	80.	59.	49.
78.	78.	77.	76.	74.	53.	84.	70.	90.	81.
74.	64.	80.	87.	75.	85.	100.	108.	102.	83.
96.	105.	124.	130.	132.	126.	147.	147.	135.	157.
185.	192.	236.	243.	259.	320.	324.	301.	300.	347.
355.	293.	296.	240.	253.	196.	185.	177.	166.	139.
147.	122.	116.	120.	93.	95.	102.	93.	86.	79.
70.	71.	68.	69.	68.	57.	75.	50.	60.	65.
63.	56.	51.	43.	63.	49.	58.	52.	81.	57.
74.	79.	76.	72.	78.	78.	93.	100.	70.	106.
97.	72.	81.	63.	56.	67.	66.	54.	68.	83.
66.	57.	79.	76.	66.	64.	71.	55.	54.	46.
61.	52.	44.	56.	62.	56.	44.	49.	35.	45.
52.	40.	48.	59.	50.	47.	47.	55.	61.	50.
66.	47.	99.	99.	105.	105.	150.	141.	213.	283.
265.	272.	266.	226.	210.	170.	156.	134.	136.	136.
152.	174.	160.	186.	167.	170.	144.	134.	130.	91.
100.	93.	67.	56.	61.	65.	49.	79.	56.	43.
33.	40.	45.	33.	54.	49.	36.	36.	52.	55.
43.	47.	41.	34.	41.	45.	39.	44.	29.	42.
44.	64.	50.	38.	41.	41.	32.	42.	41.	42.
47.	67.	46.	51.	42.	47.	45.	56.	54.	54.
58.	37.	55.	39.	49.	40.	46.	41.	30.	37.
45.	51.	44.	46.	31.	38.	51.	36.	27.	47.
32.	25.	38.	35.	26.	42.	42.	42.	39.	42.
57.	34.	49.	42.	42.	32.	41.	36.	46.	46.
47.	57.	43.	44.	43.	40.	48.	83.	61.	58.
90.	100.	81.	68.	54.	87.	63.	86.	62.	52.
70.	62.	39.	54.	41.	45.	37.	34.	45.	31.
34.	42.	32.	32.	28.	32.	44.	20.	44.	28.
32.	29.	41.	35.	18.	31.	39.	29.	32.	19.

26.	21.	32.	36.	38.	28.	33.	30.	33.	31.
32.	24.	34.	26.	33.	36.	35.	42.	33.	35.
43.	34.	38.	24.	33.	24.	37.	32.	25.	21.
39.	32.	33.	30.	35.	30.	21.	44.	26.	36.
34.	28.	30.	24.	36.	49.	27.	28.	31.	38.
26.	16.	22.	32.	31.	30.	32.	37.	30.	34.
20.	38.	32.	41.	23.	54.	39.	39.	32.	40.
40.	35.	38.	26.	33.	49.	42.	38.	24.	27.
37.	31.	27.	36.	27.	22.	46.	25.	44.	27.
28.	25.	39.	22.	30.	17.	34.	18.	31.	43.
26.	18.	33.	46.	26.	27.	39.	40.	30.	39.
36.	37.	31.	43.	39.	21.	32.	38.	21.	36.
35.	36.	30.	28.	31.	25.	35.	30.	34.	36.
22.	37.	33.	31.	38.	28.	39.	19.	29.	44.
33.	26.	38.	37.	49.	34.	45.	50.	24.	38.
35.	30.	46.	28.	43.	39.	36.	44.	36.	50.
44.	52.	31.	46.	43.	40.	59.	51.	44.	46.
46.	62.	37.	58.	58.	58.	67.	62.	58.	51.
58.	63.	77.	69.	88.	71.	73.	82.	88.	102.
101.	125.	118.	158.	158.	140.	200.	173.	184.	201.
193.	181.	203.	188.	196.	150.	135.	134.	112.	113.
84.	81.	100.	67.	82.	65.	65.	58.	70.	68.
80.	62.	47.	42.	55.	61.	41.	55.	42.	66.
54.	39.	38.	44.	36.	37.	34.	38.	39.	46.
35.	36.	46.	31.	52.	37.	49.	32.	43.	45.
44.	43.	42.	50.	44.	34.	48.	48.	42.	34.
62.	39.	45.	43.	38.	28.	48.	33.	48.	38.
45.	45.	49.	65.	51.	65.	56.	68.	64.	61.
50.	68.	43.	36.	59.	43.	40.	58.	54.	50.
73.	67.	58.	58.	72.	65.	54.	72.	91.	74.
81.	58.	71.	77.	88.	85.	72.	71.	98.	100.
101.	120.	110.	117.	169.	146.	180.	159.	241.	252.
248.	284.	310.	333.	398.	374.	370.	379.	353.	365.
329.	265.	236.	229.	210.	161.	168.	147.	154.	128.
156.	121.	117.	117.	101.	75.	84.	90.	57.	82.
64.	65.	70.	69.	57.	61.	66.	61.	74.	55.
74.	109.	74.	79.	92.	100.	83.	94.	111.	119.
112.	101.	129.	115.	103.	92.	84.	88.	81.	81.
57.	63.	69.	91.	66.	48.	57.	54.	50.	40.
51.	56.	50.	57.	80.	55.	71.	60.	65.	73.
63.	75.	62.	51.	74.	68.	71.	60.	62.	70.
75.	64.	78.	64.	64.	81.	87.	77.	90.	100.
89.	99.	123.	118.	123.	150.	149.	172.	192.	177.
156.	130.	187.	170.	146.	152.	184.	169.	176.	219.
198.	200.	211.	235.	247.	267.	288.	250.	248.	282.
216.	198.	153.	185.	194.	169.	140.	159.	150.	105.
140.	105.	108.	108.	90.	102.	89.	82.	120.	83.
123.	84.	82.	79.	85.	75.	73.	88.	68.	66.
75.	69.	56.	74.	63.	57.	64.	75.	98.	76.
79.	99.	78.	103.	93.	100.	105.	115.	88.	105.
83.	85.	61.	76.	70.	63.	48.	55.	63.	61.
45.	49.	34.	36.	52.	48.	36.	36.	47.	39.
49.	49.	44.	64.	63.	74.	85.	58.	50.	48.
46.	55.	50.	50.	49.	44.	45.	40.	56.	56.
50.	71.	35.	51.	41.	52.	46.	49.	48.	44.
51.	49.	52.	71.	50.	45.	69.	58.	77.	50.
54.	79.	75.	59.	53.	77.	70.	105.	104.	67.
70.	94.	111.	132.	131.	118.	171.	151.	191.	219.
280.	314.	415.	427.	553.	713.	800.	926.	887.	887.
873.	752.	608.	543.	519.	450.	390.	338.	283.	255.
224.	161.	179.	148.	129.	134.	123.	113.	109.	80.
111.	83.	80.	92.	72.	86.	82.	107.	93.	96.
120.	142.	148.	181.	197.	190.	235.	231.	205.	206.
212.	211.	162.	126.	120.	131.	122.	103.	115.	86.
95.	71.	71.	69.	79.	48.	72.	59.	61.	62.
45.	54.	65.	64.	54.	41.	57.	56.	52.	57.
54.	48.	35.	47.	55.	53.	51.	45.	38.	44.
44.	56.	26.	29.	43.	39.	33.	49.	26.	35.
39.	52.	45.	62.	26.	45.	27.	49.	29.	32.

31.	40.	37.	28.	30.	27.	39.	26.	22.	41.
35.	41.	29.	24.	26.	32.	44.	17.	31.	38.
34.	36.	23.	42.	44.	57.	39.	34.	41.	31.
29.	46.	46.	37.	45.	33.	38.	42.	39.	39.
57.	35.	45.	47.	63.	56.	54.	68.	56.	71.
59.	38.	45.	53.	37.	40.	50.	43.	40.	53.
33.	30.	46.	40.	37.	21.	51.	26.	38.	43.
31.	39.	32.	55.	31.	32.	32.	30.	43.	46.
33.	38.	40.	51.	65.	74.	42.	43.	42.	37.
49.	41.	45.	31.	37.	44.	35.	48.	45.	32.
46.	39.	35.	44.	37.	42.	34.	34.	37.	29.
32.	40.	31.	48.	30.	45.	37.	39.	30.	48.
42.	42.	40.	49.	36.	41.	35.	50.	44.	45.
36.	46.	32.	51.	46.	29.	39.	29.	39.	49.
28.	29.	51.	36.	32.	39.	46.	66.	45.	50.
50.	57.	46.	41.	62.	55.	44.	46.	40.	39.
49.	44.	43.	34.	47.	45.	29.	44.	32.	42.
34.	43.	41.	28.	55.	38.	41.	42.	52.	41.
41.	39.	44.	47.	38.	49.	51.	46.	50.	50.
52.	55.	55.	47.	61.	59.	70.	79.	76.	69.
71.	82.	112.	84.	90.	111.	112.	90.	99.	99.
86.	80.	89.	91.	73.	81.	86.	75.	70.	68.
48.	62.	78.	68.	59.	58.	63.	70.	69.	62.
52.	71.	57.	68.	58.	59.	58.	49.	59.	85.
70.	62.	68.	46.	58.	57.	72.	64.	43.	45.
45.	58.	53.	52.	55.	49.	46.	53.	68.	57.
42.	57.	50.	56.	47.	42.	70.	64.	67.	78.
62.	83.	58.	78.	74.	86.	81.	65.	95.	109.
121.	90.	97.	109.	113.	112.	106.	118.	128.	115.
180.	159.	159.	158.	174.	139.	150.	129.	123.	128.
107.	86.	93.	85.	76.	83.	93.	86.	88.	80.
72.	72.	86.	92.	74.	70.	70.	92.	57.	67.
79.	60.	60.	77.	70.	92.	85.	83.	79.	82.
83.	97.	83.	93.	78.	97.	93.	119.	83.	152.
149.	155.	176.	144.	176.	182.	174.	184.	163.	163.
116.	118.	90.	118.	108.	82.	99.	81.	67.	51.
82.	72.	85.	74.	69.	75.	68.	53.	63.	61.
50.	48.	39.	58.	64.	23.	37.	44.	56.	36.
52.	51.	27.	52.	53.	27.	43.	46.	40.	51.
47.	31.	32.	36.	45.	67.	33.	40.	50.	48.
42.	51.	52.	55.	37.	50.	36.	47.	51.	53.
67.	46.	53.	44.	54.	52.	35.	32.	43.	50.
52.	52.	73.	84.	90.	105.	101.	94.	118.	131.
154.	173.	154.	157.	159.	179.	168.	191.	190.	160.
196.	209.	176.	214.	211.	191.	206.	203.	161.	173.
122.	110.	125.	112.	86.	82.	51.	63.	64.	70.
54.	65.	57.	58.	62.	45.	46.	42.	54.	59.
51.	39.	40.	56.	49.	52.	47.	51.	58.	57.
52.	56.	66.	73.	76.	67.	57.	79.	94.	103.
94.	105.	125.	108.	125.	123.	142.	112.	121.	107.
119.	105.	115.	105.	112.	78.	79.	83.	68.	86.
84.	69.	58.	96.	82.	77.	72.	107.	69.	84.
89.	99.	97.	93.	118.	129.	138.	143.	117.	149.
110.	121.	114.	100.	82.	68.	75.	54.	63.	61.
61.	68.	61.	60.	57.	61.	49.	51.	50.	68.
44.	47.	34.	36.	37.	34.	32.	30.	28.	35.
26.	30.	27.	29.	24.	54.	26.	45.	44.	38.
31.	32.	28.	20.	38.	25.	31.	30.	36.	40.
29.	34.	27.	32.	35.	43.	33.	39.	31.	30.
47.	45.	34.	63.	39.	45.	46.	58.	44.	52.
57.	48.	53.	55.	48.	49.	45.	50.	78.	48.
44.	50.	50.	58.	46.	57.	86.	70.	65.	66.
81.	81.	85.	86.	73.	88.	61.	64.	60.	59.
44.	57.	42.	50.	49.	41.	30.	56.	49.	28.
37.	35.	33.	28.	28.	49.	33.	47.	30.	35.
31.	37.	45.	32.	36.	44.	34.	36.	38.	51.
42.	32.	44.	32.	59.	30.	60.	44.	44.	65.
54.	57.	48.	41.	48.	40.	52.	46.	50.	48.
58.	55.	51.	39.	45.	59.	43.	73.	50.	68.

63.	64.	57.	90.	57.	62.	63.	59.	65.	69.
53.	48.	61.	42.	58.	45.	52.	34.	59.	33.
53.	51.	48.	69.	60.	59.	55.	49.	65.	75.
62.	71.	58.	48.	73.	78.	99.	71.	72.	107.
65.	91.	79.	67.	70.	74.	76.	65.	71.	72.
83.	78.	82.	65.	67.	73.	67.	63.	83.	52.
52.	64.	62.	52.	35.	67.	50.	57.	49.	47.
67.	52.	53.	27.	48.	39.	55.	38.	49.	45.
47.	38.	70.	61.	49.	51.	52.	42.	47.	50.
52.	44.	67.	43.	53.	41.	48.	58.	71.	77.
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50.	63.	38.	44.	47.	43.	52.	66.	51.	67.
56.	69.	56.	67.	68.	79.	70.	50.	74.	75.
76.	59.	65.	59.	65.	52.	67.	59.	42.	47.
39.	44.	38.	30.	59.	61.	64.	38.	42.	45.
54.	48.	38.	42.	49.	38.	44.	51.	49.	43.
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31.	20.	18.	35.	23.	32.	22.	28.	33.	33.
39.	33.	31.	31.	33.	28.	31.	30.	35.	41.
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27.	28.	30.	26.	21.	26.	31.	22.	26.	26.
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26.	41.	25.	27.	18.	34.	27.	28.	28.	24.
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26.	34.	29.	37.	32.	36.	38.	39.	26.	39.
25.	31.	29.	36.	34.	37.	43.	20.	25.	18.
31.	37.	27.	46.	29.	36.	26.	26.	28.	31.
29.	28.	28.	24.	21.	27.	31.	23.	28.	29.
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29.	27.	29.	30.	22.	35.	25.	27.	41.	53.
32.	34.	39.	43.	43.	39.	35.	39.	50.	35.
31.	43.	46.	30.	25.	39.	55.	42.	31.	43.
35.	38.	47.	58.	41.	57.	46.	56.	63.	54.
54.	56.	63.	47.	56.	50.	59.	49.	62.	75.
55.	66.	89.	83.	76.	92.	94.	100.	88.	86.
90.	89.	97.	73.	59.	102.	90.	69.	87.	73.
62.	64.	58.	67.	59.	67.	64.	39.	55.	45.
62.	49.	48.	45.	43.	40.	31.	39.	27.	33.
31.	50.	27.	40.	34.	30.	35.	32.	37.	27.
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29.	26.	31.	29.	27.	23.	22.	30.	21.	19.
28.	26.	33.	25.	24.	24.	24.	21.	32.	24.
25.	23.	24.	23.	27.	22.	43.	19.	20.	21.
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44.	31.	35.	44.	31.	33.	37.	53.	46.	39.
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28.	38.	49.	45.	35.	21.	32.	41.	30.	40.
32.	33.	33.	37.	34.	27.	27.	30.	24.	29.
36.	43.	23.	36.	45.	36.	32.	24.	32.	32.
33.	30.	38.	21.	30.	29.	33.	21.	31.	42.

24.	30.	34.	19.	38.	36.	22.	29.	25.	24.
53.	31.	35.	33.	41.	31.	35.	49.	22.	32.
38.	41.	34.	40.	43.	42.	40.	53.	51.	77.
61.	66.	64.	63.	80.	65.	79.	89.	66.	57.
62.	53.	72.	59.	74.	65.	65.	68.	55.	42.
52.	50.	55.	40.	76.	48.	68.	44.	51.	37.
53.	53.	54.	47.	44.	52.	31.	54.	59.	47.
39.	33.	28.	33.	27.	34.	39.	26.	33.	34.
26.	48.	21.	39.	37.	23.	34.	42.	30.	34.
35.	25.	33.	23.	26.	33.	33.	36.	33.	42.
20.	29.	34.	31.	23.	28.	39.	27.	31.	35.
25.	29.	32.	31.	34.	35.	18.	33.	17.	26.
23.	16.	26.	28.	21.	30.	34.	20.	24.	30.
28.	24.	28.	25.	20.	24.	21.	24.	27.	33.
31.	26.	20.	24.	25.	36.	22.	21.	26.	33.
47.	31.	30.	24.	31.	28.	37.	29.	16.	26.
32.	26.	34.	39.	28.	27.	45.	33.	38.	31.
39.	47.	29.	39.	48.	45.	32.	38.	43.	47.
42.	35.	47.	61.	42.	43.	50.	33.	36.	38.
48.	61.	49.	58.	53.	51.	43.	58.	47.	54.
39.	42.	32.	48.	47.	25.	32.	37.	34.	35.
36.	30.	27.	36.	36.	43.	26.	26.	28.	37.
35.	36.	44.	26.	39.	29.	34.	36.	26.	43.
38.	48.	38.	43.	33.	41.	28.	41.	34.	34.
40.	52.	38.	66.	57.	59.	71.	86.	57.	72.
64.	78.	68.	65.	69.	87.	79.	78.	88.	77.
99.	81.	72.	77.	68.	67.	75.	64.	66.	72.
57.	49.	72.	75.	46.	58.	50.	65.	37.	37.
53.	51.	47.	67.	51.	40.	29.	42.	36.	56.
43.	45.	47.	35.	47.	47.	39.	30.	32.	31.
50.	37.	41.	34.	34.	35.	26.	36.	40.	25.
33.	37.	32.	59.	40.	34.	36.	36.	28.	50.
31.	38.	47.	37.	29.	28.	45.	40.	30.	44.
55.	39.	42.	33.	46.	30.	31.	30.	30.	37.
40.	31.	44.	49.	26.	19.	37.	20.	48.	30.
30.	31.	21.	36.	40.	23.	29.	30.	27.	29.
22.	31.	33.	32.	22.	33.	33.	29.	26.	22.
34.	37.	32.	33.	46.	21.	30.	35.	34.	44.
37.	30.	42.	41.	31.	42.	35.	46.	45.	30.
30.	25.	49.	37.	33.	39.	39.	37.	41.	40.
44.	24.	28.	38.	36.	36.	39.	29.	27.	43.
18.	34.	46.	41.	32.	36.	33.	41.	36.	31.
44.	45.	48.	56.	40.	34.	49.	45.	47.	50.
42.	56.	51.	36.	62.	41.	43.	47.	49.	55.
34.	34.	42.	52.	41.	52.	51.	72.	43.	41.
42.	36.	38.	44.	49.	39.	36.	29.	27.	19.
39.	38.	44.	23.	37.	22.	32.	35.	33.	48.
18.	32.	22.	33.	40.	41.	25.	22.	43.	33.
21.	42.	30.	32.	39.	32.	29.	34.	24.	33.
30.	40.	26.	34.	21.	33.	24.	43.	25.	40.
33.	36.	53.	36.	47.	38.	38.	32.	47.	46.
62.	44.	67.	49.	77.	59.	61.	63.	72.	66.
81.	87.	67.	73.	82.	69.	79.	78.	89.	70.
76.	91.	68.	89.	82.	64.	71.	72.	79.	71.
67.	61.	55.	69.	61.	54.	72.	55.	57.	54.
65.	53.	50.	50.	62.	59.	61.	56.	69.	58.
52.	58.	51.	46.	57.	63.	49.	56.	45.	45.
51.	46.	48.	33.	51.	48.	50.	53.	50.	43.
49.	42.	52.	44.	52.	59.	51.	68.	49.	63.
62.	62.	74.	73.	73.	47.	78.	96.	76.	93.
86.	83.	82.	85.	94.	96.	108.	96.	105.	123.
104.	100.	121.	103.	94.	97.	88.	84.	81.	88.
62.	59.	46.	59.	56.	53.	71.	62.	77.	46.
49.	25.	36.	51.	37.	29.	46.	41.	30.	38.
49.	31.	35.	47.	33.	35.	34.	37.	29.	30.
24.	36.	30.	28.	28.	46.	59.	38.	42.	49.
36.	54.	31.	36.	52.	35.	35.	49.	27.	27.
37.	21.	55.	37.	41.	39.	37.	55.	32.	21.
20.	43.	37.	34.	25.	34.	43.	40.	42.	35.

26.	44.	40.	57.	43.	34.	33.	31.	28.	46.
40.	32.	35.	57.	43.	33.	42.	34.	39.	49.
37.	40.	44.	31.	41.	49.	50.	33.	32.	39.
42.	33.	37.	38.	31.	31.	19.	32.	39.	35.
37.	35.	32.	30.	40.	28.	38.	40.	39.	38.
25.	30.	39.	47.	33.	41.	32.	51.	48.	32.
38.	46.	55.	40.	44.	45.	50.	53.	66.	50.
45.	53.	34.	36.	59.	62.	53.	51.	50.	60.
57.	57.	66.	66.	75.	50.	50.	35.	59.	65.
48.	47.	45.	61.	40.	43.	25.	36.	51.	46.
41.	52.	53.	39.	33.	36.	38.	38.	43.	46.
13.	37.	39.	42.	32.	35.	26.	30.	40.	39.
28.	22.	34.	30.	27.	25.	35.	45.	17.	38.
22.	35.	26.	27.	41.	28.	40.	38.	23.	28.
32.	46.	32.	22.	30.	20.	29.	31.	27.	27.
32.	17.	21.	24.	48.	34.	33.	24.	30.	27.
32.	32.	30.	24.	22.	33.	27.	29.	21.	34.
24.	30.	13.	39.	25.	23.	21.	26.	30.	28.
24.	25.	28.	16.	28.	27.	29.	15.	24.	33.
35.	31.	24.	38.	22.	16.	25.	32.	26.	23.
30.	38.	27.	30.	40.	54.	41.	34.	37.	39.
53.	50.	40.	38.	30.	43.	37.	48.	38.	30.
40.	55.	36.	37.	38.	42.	32.	32.	46.	32.
31.	41.	33.	32.	15.	34.	39.	21.	33.	38.
44.	22.	37.	27.	20.	40.	32.	28.	25.	32.
26.	13.	28.	25.	22.	37.	25.	30.	46.	29.
22.	27.	28.	24.	21.	25.	25.	28.	32.	32.
29.	33.	34.	30.	27.	24.	29.	17.	34.	25.
30.	28.	26.	28.	26.	28.	38.	29.	23.	21.
17.	31.	28.	41.	26.	26.	45.	28.	25.	23.
22.	32.	17.	38.	34.	32.	31.	25.	21.	35.
34.	31.	17.	34.	33.	28.	30.	23.	31.	26.
17.	33.	29.	31.	24.	30.	29.	21.	22.	42.
17.	39.	37.	26.	22.	23.	36.	27.	25.	26.
21.	37.	30.	34.	42.	39.	32.	18.	43.	19.
36.	32.	25.	18.	45.	35.	36.	25.	26.	30.
48.	25.	45.	34.	28.	40.	36.	35.	33.	31.
45.	26.	27.	32.	32.	36.	20.	36.	40.	33.
37.	35.	22.	38.	46.	29.	31.	26.	20.	31.
34.	32.	43.	43.	31.	25.	26.	42.	35.	40.
47.	36.	33.	36.	41.	42.	38.	41.	34.	26.
44.	48.	28.	31.	26.	43.	36.	31.	35.	27.
38.	30.	35.	26.	35.	41.	37.	23.	35.	38.
40.	28.	32.	26.	32.	35.	28.	27.	25.	30.
31.	39.	27.	25.	33.	42.	18.	25.	28.	27.
30.	37.	29.	30.	30.	29.	31.	22.	26.	40.
25.	25.	27.	36.	36.	40.	31.	28.	29.	34.
39.	37.	33.	22.	23.	29.	26.	36.	24.	37.
28.	19.	35.	33.	33.	19.	30.	33.	18.	35.
26.	25.	37.	24.	19.	29.	34.	39.	34.	22.
25.	41.	28.	17.	45.	19.	41.	43.	45.	32.
31.	42.	36.	28.	23.	20.	22.	37.	40.	31.
53.	32.	30.	30.	46.	40.	41.	48.	26.	28.
18.	45.	28.	39.	35.	51.	46.	37.	32.	38.
37.	33.	25.	25.	35.	34.	38.	41.	44.	32.
41.	42.	40.	45.	40.	38.	34.	48.	34.	37.
47.	43.	45.	52.	52.	48.	40.	54.	50.	49.
37.	34.	48.	61.	59.	60.	45.	74.	47.	46.
65.	66.	56.	57.	79.	70.	63.	73.	69.	82.
66.	92.	83.	74.	63.	97.	108.	89.	75.	105.
96.	101.	115.	117.	88.	128.	139.	146.	142.	132.
124.	131.	168.	141.	141.	117.	142.	142.	121.	122.
128.	110.	109.	114.	123.	105.	126.	105.	99.	84.
71.	84.	104.	88.	79.	97.	69.	89.	81.	77.
72.	63.	86.	47.	69.	81.	53.	67.	47.	69.
72.	53.	53.	37.	61.	67.	46.	55.	50.	53.
42.	45.	46.	43.	44.	48.	40.	63.	41.	40.
56.	38.	46.	54.	49.	25.	45.	37.	47.	37.
47.	58.	45.	52.	43.	44.	42.	48.	39.	48.

36.	43.	43.	37.	47.	53.	50.	35.	49.	47.
48.	57.	56.	48.	57.	46.	46.	42.	42.	48.
45.	55.	28.	38.	55.	46.	55.	50.	40.	34.
48.	42.	46.	40.	62.	45.	34.	39.	41.	47.
36.	41.	31.	38.	45.	39.	49.	33.	37.	40.
51.	34.	32.	39.	33.	36.	33.	42.	43.	37.
27.	34.	40.	41.	42.	44.	28.	38.	30.	34.
30.	38.	47.	40.	40.	30.	34.	29.	62.	41.
41.	28.	36.	29.	30.	54.	34.	40.	36.	36.
30.	30.	40.	35.	38.	42.	39.	30.	36.	34.
27.	27.	29.	29.	32.	39.	34.	42.	35.	36.
43.	40.	39.	39.	38.	28.	26.	35.	34.	20.
37.	34.	26.	32.	25.	40.	37.	28.	37.	29.
41.	29.	42.	44.	36.	38.	32.	43.	46.	46.
28.	60.	42.	60.	50.	32.	49.	48.	43.	45.
55.	61.	65.	54.	68.	65.	62.	63.	74.	74.
76.	87.	62.	82.	86.	84.	103.	94.	98.	107.
99.	59.	102.	93.	107.	109.	102.	116.	117.	76.
100.	98.	79.	78.	81.	104.	93.	88.	61.	53.
70.	64.	56.	67.	68.	78.	55.	53.	67.	58.
57.	65.	79.	78.	53.	55.	48.	63.	54.	67.
68.	65.	79.	57.	50.	75.	61.	52.	54.	53.
49.	70.	39.	59.	54.	51.	56.	56.	67.	48.
54.	46.	48.	46.	35.	38.	45.	43.	43.	46.
43.	43.	35.	31.	38.	51.	36.	49.	46.	39.
38.	53.	42.	38.	47.	35.	31.	51.	43.	39.
24.	35.	42.	41.	37.	42.	48.	37.	46.	42.
21.	41.	46.	50.	44.	47.	31.	34.	42.	42.
18.	33.	32.	30.	47.	51.	28.	46.	50.	36.
49.	49.	18.	35.	40.	41.	43.	50.	46.	40.
45.	37.	29.	50.	37.	38.	38.	30.	47.	37.
38.	34.	38.	44.	23.	32.	31.	42.	40.	39.
47.	40.	53.	45.	46.	32.	42.	41.	40.	36.
55.	54.	45.	42.	37.	34.	50.	40.	48.	38.
60.	41.	27.	45.	37.	40.	58.	40.	29.	30.
51.	47.	33.	40.	32.	48.	31.	44.	41.	46.
57.	28.	46.	44.	47.	33.	46.	46.	41.	35.
48.	37.	35.	33.	43.	30.	42.	41.	40.	47.
31.	39.	47.	39.	35.	48.	40.	31.	48.	49.
31.	47.	41.	30.	58.	36.	38.	36.	49.	41.
34.	42.	39.	40.	29.	36.	35.	44.	55.	29.
20.	26.	31.	37.	31.	39.	45.	40.	35.	35.
39.	29.	44.	34.	32.	50.	28.	35.	41.	43.
37.	34.	38.	34.	35.	44.	49.	41.	54.	40.
39.	38.	34.	26.	42.	52.	51.	53.	55.	49.
29.	35.	43.	46.	54.	35.	44.	39.	44.	40.
36.	51.	44.	48.	34.	26.	40.	31.	33.	47.
37.	32.	36.	36.	51.	51.	68.	42.	43.	35.
63.	52.	62.	46.	56.	43.	47.	59.	43.	50.
42.	46.	57.	55.	50.	65.	58.	59.	39.	58.
50.	45.	62.	71.	44.	51.	67.	52.	48.	70.
51.	47.	37.	70.	46.	50.	46.	47.	36.	44.
51.									

Appendix P-25: step-intensity data of chabazite

10.0000 .020 120.0000 Chabazite with Al2O3 impurity

165.	182.	183.	190.	164.	184.	177.	141.	166.	153.
152.	161.	168.	178.	182.	175.	160.	159.	144.	157.
170.	156.	168.	167.	187.	153.	172.	138.	158.	152.
154.	159.	166.	154.	171.	135.	175.	169.	161.	169.
114.	130.	141.	166.	151.	162.	144.	187.	130.	177.
195.	191.	193.	228.	214.	285.	266.	211.	208.	177.
151.	144.	174.	145.	152.	143.	144.	147.	152.	162.
171.	140.	167.	143.	163.	146.	144.	157.	165.	126.
135.	138.	159.	120.	140.	163.	147.	131.	152.	161.
132.	152.	143.	147.	155.	160.	160.	134.	134.	149.
132.	141.	120.	131.	106.	139.	123.	143.	155.	154.
143.	146.	124.	138.	119.	119.	156.	131.	153.	136.
134.	169.	144.	157.	140.	150.	159.	163.	146.	148.
168.	184.	179.	174.	204.	205.	271.	305.	365.	455.
539.	492.	373.	273.	218.	183.	203.	160.	178.	164.
153.	172.	127.	138.	134.	156.	162.	146.	108.	135.
156.	151.	177.	169.	175.	139.	139.	133.	180.	143.
128.	157.	128.	125.	152.	142.	147.	182.	137.	159.
147.	166.	145.	145.	162.	166.	169.	194.	181.	188.
215.	223.	235.	283.	286.	294.	343.	257.	224.	178.
193.	184.	174.	180.	189.	167.	190.	169.	163.	185.
147.	153.	187.	146.	161.	136.	163.	137.	137.	111.
175.	124.	131.	126.	124.	114.	122.	138.	123.	140.
150.	137.	146.	119.	127.	127.	139.	114.	124.	129.
146.	168.	143.	144.	132.	124.	118.	139.	105.	126.
110.	133.	127.	129.	113.	117.	104.	132.	105.	128.
123.	112.	122.	124.	110.	112.	137.	113.	128.	147.
139.	126.	120.	102.	120.	141.	101.	149.	121.	140.
127.	132.	147.	132.	126.	116.	148.	178.	158.	173.
219.	281.	262.	388.	536.	631.	795.	868.	747.	549.
325.	226.	178.	146.	144.	117.	125.	124.	123.	122.
130.	135.	136.	132.	125.	120.	118.	122.	139.	116.
122.	133.	120.	114.	114.	115.	115.	127.	137.	124.
146.	122.	122.	115.	114.	148.	130.	143.	152.	146.
168.	148.	156.	125.	146.	136.	118.	120.	120.	128.
151.	130.	137.	140.	120.	111.	180.	121.	159.	148.
156.	143.	163.	163.	215.	264.	204.	190.	155.	144.
182.	163.	175.	167.	158.	147.	161.	177.	184.	198.
281.	308.	406.	596.	826.	952.	842.	489.	257.	173.
135.	113.	113.	108.	142.	95.	119.	131.	108.	116.
96.	111.	97.	117.	119.	127.	90.	120.	88.	136.
93.	139.	102.	91.	119.	141.	129.	89.	114.	137.
118.	119.	111.	131.	112.	101.	131.	112.	114.	110.
112.	116.	112.	111.	122.	124.	103.	106.	115.	112.
117.	117.	146.	130.	124.	168.	180.	215.	216.	245.
230.	212.	174.	149.	192.	145.	127.	128.	118.	115.
101.	111.	105.	110.	85.	98.	119.	85.	100.	104.
113.	101.	88.	114.	114.	99.	88.	91.	115.	100.
118.	98.	93.	97.	96.	80.	86.	110.	84.	91.
100.	108.	99.	106.	107.	108.	92.	101.	104.	107.
69.	87.	100.	96.	84.	122.	100.	109.	100.	94.
151.	189.	153.	129.	188.	155.	196.	213.	271.	296.
399.	564.	771.	1054.	1644.	2276.	2564.	2175.	1255.	554.
278.	219.	178.	142.	113.	107.	123.	138.	101.	185.
109.	111.	133.	130.	117.	114.	119.	109.	114.	132.
109.	96.	116.	110.	123.	123.	111.	135.	112.	117.
107.	129.	113.	110.	85.	97.	103.	87.	104.	100.
105.	91.	101.	95.	119.	95.	102.	80.	91.	84.
87.	91.	94.	83.	99.	104.	97.	63.	119.	119.
80.	103.	107.	90.	134.	131.	126.	137.	136.	105.
86.	104.	102.	122.	96.	98.	114.	87.	135.	120.
157.	167.	193.	245.	308.	332.	327.	389.	293.	200.
168.	194.	165.	131.	130.	117.	110.	105.	129.	110.
130.	124.	120.	121.	116.	112.	135.	135.	142.	131.
124.	177.	201.	169.	237.	317.	369.	484.	594.	500.

430.	306.	172.	132.	119.	112.	100.	100.	99.	90.
89.	103.	118.	72.	104.	90.	65.	84.	81.	89.
85.	79.	77.	77.	75.	102.	105.	71.	74.	87.
98.	72.	74.	65.	83.	90.	101.	99.	91.	69.
83.	89.	98.	95.	72.	103.	86.	101.	128.	94.
88.	79.	84.	91.	85.	69.	84.	72.	69.	65.
72.	93.	92.	80.	84.	63.	79.	96.	98.	74.
95.	96.	95.	89.	85.	85.	73.	81.	92.	91.
82.	117.	87.	118.	106.	179.	183.	233.	356.	438.
549.	790.	931.	926.	705.	497.	326.	221.	156.	140.
112.	86.	116.	116.	106.	87.	106.	146.	105.	135.
136.	136.	152.	141.	168.	155.	170.	167.	240.	233.
276.	292.	348.	396.	430.	454.	440.	498.	470.	496.
379.	346.	327.	272.	310.	243.	267.	259.	368.	490.
521.	541.	496.	340.	265.	214.	205.	176.	195.	165.
119.	115.	112.	110.	130.	75.	113.	141.	168.	135.
121.	97.	116.	98.	77.	83.	75.	81.	85.	86.
75.	80.	77.	73.	101.	96.	106.	104.	82.	96.
101.	108.	105.	80.	88.	88.	87.	65.	101.	122.
102.	91.	99.	97.	84.	80.	100.	98.	89.	83.
76.	80.	74.	77.	82.	76.	77.	96.	99.	90.
79.	81.	65.	79.	69.	79.	78.	115.	67.	83.
84.	78.	91.	127.	127.	156.	188.	176.	174.	171.
138.	90.	101.	64.	79.	71.	69.	62.	71.	83.
76.	92.	92.	90.	86.	91.	101.	119.	133.	151.
229.	248.	349.	348.	300.	249.	167.	153.	135.	85.
91.	64.	80.	103.	126.	115.	118.	85.	62.	85.
82.	96.	88.	86.	87.	117.	100.	107.	123.	121.
99.	106.	70.	71.	71.	99.	68.	79.	87.	63.
57.	62.	77.	68.	71.	88.	62.	97.	111.	119.
98.	98.	91.	75.	74.	76.	63.	69.	84.	73.
70.	73.	77.	63.	93.	100.	81.	78.	69.	92.
83.	80.	78.	70.	76.	68.	77.	93.	75.	64.
70.	81.	81.	78.	84.	71.	77.	88.	86.	103.
104.	101.	80.	77.	99.	100.	105.	125.	163.	124.
156.	164.	201.	137.	194.	155.	134.	162.	152.	219.
228.	151.	133.	109.	117.	133.	119.	164.	207.	256.
349.	535.	917.	1269.	1945.	2191.	1922.	1165.	676.	348.
242.	214.	294.	321.	453.	412.	366.	276.	194.	141.
140.	147.	166.	202.	259.	369.	596.	877.	1016.	841.
697.	494.	321.	169.	123.	87.	95.	75.	84.	60.
67.	72.	75.	92.	74.	74.	71.	82.	80.	79.
83.	104.	140.	140.	173.	129.	142.	117.	88.	86.
87.	82.	68.	66.	56.	59.	87.	73.	94.	156.
104.	146.	164.	139.	130.	155.	104.	125.	83.	96.
105.	81.	84.	77.	60.	68.	72.	94.	93.	89.
126.	163.	129.	144.	119.	87.	73.	86.	47.	76.
45.	68.	76.	76.	81.	67.	77.	64.	79.	85.
83.	75.	65.	86.	68.	89.	97.	59.	74.	62.
99.	111.	99.	74.	72.	64.	56.	74.	72.	69.
77.	81.	77.	67.	73.	67.	66.	86.	94.	100.
128.	144.	104.	100.	104.	95.	128.	136.	154.	214.
226.	193.	160.	99.	92.	91.	70.	74.	90.	66.
87.	53.	59.	62.	77.	66.	65.	62.	82.	70.
58.	67.	71.	65.	78.	64.	76.	68.	63.	61.
72.	85.	59.	78.	72.	75.	68.	73.	74.	76.
64.	89.	108.	111.	172.	199.	256.	399.	485.	613.
564.	384.	239.	163.	138.	110.	101.	105.	95.	102.
121.	101.	120.	131.	108.	122.	132.	209.	175.	200.
213.	246.	275.	256.	274.	258.	309.	319.	320.	378.
425.	449.	471.	552.	682.	655.	616.	612.	553.	445.
397.	360.	284.	253.	277.	236.	208.	194.	175.	145.
150.	110.	134.	132.	117.	140.	125.	134.	116.	89.
88.	88.	90.	104.	115.	99.	70.	93.	114.	130.
159.	174.	277.	341.	774.	753.	485.	348.	313.	188.
140.	118.	114.	106.	82.	67.	67.	64.	59.	84.
51.	43.	55.	67.	61.	62.	90.	83.	89.	67.
70.	88.	61.	76.	72.	62.	85.	61.	76.	82.
67.	73.	79.	65.	62.	85.	63.	58.	74.	63.

101.	70.	78.	78.	91.	84.	77.	76.	85.	92.
72.	86.	71.	94.	82.	67.	84.	74.	77.	97.
79.	83.	63.	62.	80.	73.	66.	85.	99.	70.
100.	90.	115.	101.	118.	118.	141.	155.	177.	150.
178.	215.	242.	266.	218.	285.	329.	330.	310.	264.
240.	235.	178.	180.	175.	167.	148.	127.	115.	141.
121.	129.	108.	103.	123.	92.	114.	105.	97.	122.
108.	106.	126.	143.	119.	115.	106.	82.	84.	66.
75.	65.	57.	78.	66.	61.	86.	66.	58.	58.
57.	50.	61.	69.	67.	55.	66.	70.	66.	64.
68.	77.	48.	58.	90.	90.	104.	110.	91.	91.
100.	93.	74.	97.	73.	126.	148.	147.	174.	203.
166.	92.	103.	78.	55.	62.	49.	61.	51.	71.
57.	67.	72.	74.	65.	54.	79.	93.	105.	69.
93.	107.	72.	114.	71.	67.	55.	52.	48.	79.
55.	66.	50.	53.	50.	64.	48.	68.	63.	48.
59.	56.	56.	45.	53.	49.	59.	51.	49.	70.
63.	64.	67.	53.	59.	56.	52.	73.	92.	67.
82.	70.	76.	61.	54.	52.	52.	55.	73.	61.
60.	54.	57.	52.	65.	61.	39.	93.	63.	64.
66.	67.	58.	59.	60.	56.	76.	56.	67.	55.
51.	43.	64.	46.	52.	49.	48.	46.	44.	41.
52.	47.	45.	48.	62.	50.	62.	45.	66.	64.
51.	67.	60.	61.	58.	56.	61.	53.	66.	41.
60.	66.	67.	68.	70.	73.	64.	65.	91.	93.
79.	81.	61.	74.	61.	67.	50.	67.	68.	73.
79.	74.	54.	60.	62.	64.	84.	56.	76.	64.
57.	78.	75.	83.	70.	71.	82.	60.	75.	68.
77.	83.	68.	94.	108.	124.	122.	124.	133.	113.
119.	135.	100.	97.	121.	98.	132.	136.	104.	118.
118.	147.	124.	144.	144.	140.	177.	171.	175.	183.
181.	231.	218.	272.	272.	320.	275.	372.	411.	451.
466.	560.	663.	731.	786.	780.	765.	688.	639.	556.
484.	401.	379.	300.	284.	236.	246.	214.	197.	178.
170.	164.	164.	156.	125.	130.	147.	129.	97.	125.
130.	97.	129.	114.	112.	115.	108.	87.	93.	86.
89.	58.	75.	62.	70.	63.	52.	60.	52.	61.
59.	56.	69.	66.	52.	53.	71.	72.	77.	59.
62.	70.	55.	60.	69.	60.	61.	90.	64.	54.
59.	55.	43.	57.	77.	79.	89.	116.	108.	70.
82.	89.	71.	80.	68.	73.	56.	75.	91.	69.
65.	74.	88.	70.	69.	57.	60.	47.	49.	53.
61.	60.	50.	40.	47.	45.	44.	46.	34.	53.
54.	50.	22.	55.	44.	54.	51.	52.	50.	49.
60.	62.	68.	49.	56.	44.	53.	65.	38.	53.
64.	64.	57.	60.	56.	64.	53.	63.	40.	52.
55.	59.	61.	52.	64.	51.	49.	64.	74.	73.
51.	47.	62.	78.	66.	64.	58.	57.	63.	55.
45.	39.	50.	49.	47.	43.	55.	54.	40.	54.
67.	58.	66.	61.	55.	52.	55.	47.	49.	52.
59.	81.	77.	67.	64.	92.	65.	72.	48.	60.
50.	36.	32.	41.	75.	56.	59.	53.	42.	47.
64.	44.	62.	36.	47.	43.	52.	49.	38.	40.
42.	64.	66.	108.	90.	99.	114.	92.	77.	56.
50.	48.	52.	35.	53.	48.	31.	46.	41.	41.
38.	66.	53.	56.	47.	34.	31.	32.	53.	43.
35.	49.	49.	43.	45.	43.	39.	44.	45.	57.
45.	35.	26.	52.	51.	42.	35.	47.	41.	41.
38.	51.	44.	37.	36.	59.	43.	52.	51.	80.
87.	90.	109.	162.	189.	207.	167.	119.	110.	87.
60.	47.	53.	39.	45.	36.	58.	47.	52.	60.
50.	67.	64.	88.	81.	107.	112.	131.	99.	80.
71.	41.	49.	53.	46.	50.	42.	41.	46.	38.
45.	37.	29.	45.	44.	66.	58.	40.	37.	35.
62.	57.	43.	37.	34.	40.	39.	52.	37.	41.
42.	50.	50.	47.	45.	20.	50.	46.	39.	41.
42.	53.	80.	54.	43.	48.	48.	41.	50.	48.
46.	51.	50.	45.	56.	56.	46.	76.	96.	122.
129.	157.	183.	240.	242.	284.	276.	303.	332.	273.

231.	196.	152.	119.	94.	79.	75.	64.	56.	49.
34.	36.	48.	41.	67.	69.	43.	51.	43.	65.
68.	71.	51.	64.	78.	93.	55.	69.	69.	67.
48.	44.	66.	45.	58.	63.	49.	55.	51.	37.
35.	47.	63.	71.	57.	92.	94.	68.	92.	84.
127.	117.	83.	100.	65.	82.	72.	68.	67.	72.
71.	61.	52.	66.	66.	60.	68.	67.	98.	82.
84.	74.	79.	66.	90.	95.	105.	99.	99.	100.
108.	97.	114.	151.	115.	148.	146.	151.	191.	194.
221.	211.	222.	236.	234.	248.	258.	241.	235.	209.
190.	183.	154.	153.	148.	113.	128.	153.	156.	142.
177.	162.	148.	123.	123.	141.	104.	127.	116.	134.
152.	186.	214.	212.	259.	282.	246.	196.	144.	124.
109.	79.	65.	64.	37.	49.	56.	59.	63.	38.
43.	56.	64.	40.	59.	40.	54.	41.	51.	58.
51.	57.	32.	56.	46.	50.	46.	39.	35.	44.
47.	49.	44.	46.	42.	54.	46.	62.	57.	52.
60.	70.	91.	71.	102.	95.	94.	105.	99.	109.
104.	104.	70.	63.	38.	34.	51.	58.	48.	33.
45.	30.	50.	46.	45.	34.	29.	39.	44.	55.
33.	36.	32.	48.	48.	25.	35.	42.	56.	50.
40.	40.	49.	48.	67.	45.	84.	54.	66.	78.
102.	108.	127.	154.	152.	120.	85.	53.	57.	41.
33.	29.	32.	41.	36.	36.	56.	40.	44.	27.
38.	55.	45.	65.	39.	39.	41.	45.	49.	58.
48.	49.	37.	52.	78.	81.	77.	125.	143.	136.
161.	156.	169.	124.	106.	59.	84.	93.	83.	64.
84.	106.	71.	73.	98.	106.	106.	85.	94.	74.
74.	78.	59.	58.	40.	56.	66.	59.	63.	42.
56.	56.	61.	56.	49.	51.	66.	63.	66.	46.
74.	63.	81.	68.	64.	92.	89.	84.	86.	99.
106.	112.	92.	92.	101.	94.	113.	117.	118.	117.
157.	134.	143.	163.	182.	162.	191.	187.	185.	215.
246.	238.	284.	255.	301.	335.	346.	361.	401.	437.
431.	454.	493.	493.	454.	448.	382.	376.	326.	304.
272.	242.	222.	213.	187.	188.	164.	168.	162.	177.
135.	158.	130.	124.	121.	108.	95.	110.	112.	107.
138.	101.	120.	97.	74.	76.	74.	97.	74.	79.
64.	69.	62.	61.	57.	70.	57.	61.	56.	47.
52.	39.	50.	55.	42.	34.	64.	45.	51.	58.
41.	41.	49.	41.	44.	35.	48.	55.	44.	51.
45.	46.	50.	33.	32.	53.	44.	41.	44.	47.
41.	39.	41.	36.	55.	51.	49.	51.	57.	85.
73.	80.	128.	164.	173.	188.	190.	153.	158.	131.
98.	87.	79.	76.	62.	58.	67.	56.	56.	44.
49.	45.	50.	51.	36.	65.	65.	49.	43.	51.
49.	40.	59.	54.	41.	50.	35.	50.	52.	34.
31.	53.	40.	53.	50.	32.	66.	57.	42.	59.
74.	47.	49.	52.	49.	43.	37.	43.	38.	49.
49.	39.	48.	36.	50.	39.	37.	54.	44.	43.
31.	52.	40.	45.	54.	50.	58.	75.	82.	95.
92.	120.	129.	91.	123.	92.	95.	77.	97.	76.
55.	99.	95.	108.	103.	134.	125.	119.	133.	114.
96.	78.	100.	89.	87.	71.	58.	80.	70.	67.
66.	74.	78.	49.	62.	49.	62.	51.	52.	57.
60.	55.	51.	61.	49.	43.	57.	45.	48.	55.
42.	58.	47.	53.	44.	51.	32.	43.	46.	40.
55.	43.	36.	36.	43.	42.	43.	38.	30.	51.
28.	46.	49.	59.	48.	55.	72.	58.	66.	65.
90.	93.	93.	87.	77.	56.	98.	95.	97.	64.
68.	56.	50.	55.	56.	45.	44.	51.	33.	53.
46.	33.	46.	40.	40.	44.	39.	44.	48.	47.
42.	44.	53.	31.	31.	44.	34.	34.	43.	34.
32.	38.	36.	38.	36.	30.	45.	39.	32.	47.
51.	55.	40.	32.	77.	49.	53.	54.	41.	54.
34.	25.	48.	34.	36.	44.	32.	49.	40.	49.
45.	55.	32.	47.	55.	41.	57.	52.	45.	67.
48.	58.	49.	74.	71.	72.	48.	74.	60.	82.
72.	67.	58.	55.	73.	64.	59.	58.	50.	37.

48.	51.	44.	47.	32.	35.	47.	36.	37.	67.
67.	56.	65.	52.	41.	69.	48.	34.	53.	48.
56.	44.	52.	52.	53.	52.	47.	51.	51.	51.
61.	62.	47.	55.	44.	56.	49.	41.	45.	41.
49.	48.	60.	55.	29.	38.	51.	49.	58.	61.
72.	66.	73.	53.	62.	57.	73.	91.	67.	65.
55.	57.	61.	96.	96.	90.	72.	84.	72.	96.
99.	117.	136.	110.	117.	141.	130.	115.	125.	124.
104.	110.	102.	82.	109.	104.	80.	100.	93.	89.
107.	104.	110.	144.	135.	122.	145.	181.	200.	209.
213.	186.	254.	253.	289.	243.	247.	263.	267.	237.
224.	182.	153.	143.	129.	119.	114.	99.	88.	95.
102.	84.	72.	96.	71.	72.	83.	68.	66.	63.
61.	64.	59.	73.	76.	63.	67.	67.	94.	83.
83.	81.	78.	89.	76.	82.	88.	75.	77.	68.
71.	87.	64.	82.	84.	93.	87.	100.	94.	98.
97.	120.	111.	97.	106.	88.	93.	100.	105.	131.
96.	113.	125.	149.	165.	162.	177.	176.	193.	181.
211.	194.	260.	243.	247.	280.	260.	263.	281.	285.
291.	227.	226.	203.	191.	172.	202.	161.	146.	137.
138.	129.	110.	112.	100.	94.	132.	106.	90.	94.
73.	80.	89.	90.	84.	83.	91.	92.	92.	81.
106.	130.	115.	109.	104.	104.	98.	114.	112.	102.
101.	73.	75.	70.	78.	46.	64.	37.	58.	57.
62.	56.	40.	53.	54.	55.	60.	51.	42.	40.
69.	53.	30.	52.	57.	60.	50.	52.	84.	60.
63.	63.	88.	67.	58.	48.	59.	49.	56.	64.
37.	40.	47.	41.	41.	39.	59.	55.	68.	62.
45.	78.	93.	88.	82.	94.	111.	117.	117.	129.
98.	112.	110.	97.	73.	77.	91.	108.	78.	78.
82.	81.	81.	79.	44.	63.	45.	42.	46.	51.
48.	53.	39.	26.	47.	38.	61.	32.	63.	49.
57.	70.	84.	94.	92.	114.	137.	121.	143.	131.
170.	111.	143.	105.	89.	77.	71.	62.	65.	65.
50.	54.	45.	66.	55.	54.	57.	41.	49.	42.
50.	19.	27.	35.	45.	44.	47.	38.	46.	41.
47.	53.	58.	36.	85.	44.	39.	38.	50.	48.
37.	31.	65.	56.	37.	50.	55.	58.	54.	71.
66.	84.	68.	67.	66.	122.	62.	60.	61.	56.
48.	57.	62.	67.	46.	61.	41.	54.	52.	56.
37.	55.	49.	53.	29.	63.	59.	50.	38.	41.
41.	48.	48.	50.	37.	50.	40.	41.	41.	51.
36.	42.	42.	52.	40.	20.	37.	26.	27.	43.
37.	37.	32.	38.	21.	39.	35.	37.	35.	38.
49.	28.	24.	30.	38.	31.	30.	40.	36.	34.
42.	38.	42.	36.	42.	49.	32.	38.	33.	46.
46.	33.	43.	45.	42.	41.	79.	87.	77.	99.
113.	99.	87.	84.	102.	81.	65.	56.	68.	60.
44.	45.	73.	53.	67.	50.	50.	40.	60.	49.
63.	47.	61.	56.	44.	38.	46.	31.	37.	49.
26.	59.	34.	49.	48.	53.	33.	51.	54.	54.
58.	41.	66.	71.	67.	43.	57.	59.	50.	70.
63.	63.	72.	66.	58.	85.	53.	115.	58.	70.
81.	70.	71.	77.	74.	54.	74.	51.	49.	57.
47.	42.	43.	59.	47.	38.	55.	56.	53.	51.
49.	51.	30.	43.	56.	37.	47.	51.	50.	38.
50.	51.	53.	55.	31.	60.	53.	50.	46.	54.
46.	54.	46.	51.	39.	46.	36.	69.	55.	46.
51.	35.	46.	52.	55.	52.	65.	67.	84.	95.
148.	160.	109.	85.	66.	59.	61.	54.	62.	58.
53.	76.	65.	82.	94.	67.	73.	70.	72.	101.
92.	81.	110.	88.	115.	114.	139.	136.	156.	125.
148.	147.	132.	127.	96.	127.	133.	93.	96.	93.
103.	85.	97.	88.	77.	75.	62.	95.	90.	93.
97.	71.	71.	78.	69.	64.	59.	71.	63.	66.
56.	54.	58.	64.	58.	57.	50.	45.	50.	51.
68.	73.	56.	56.	72.	63.	52.	57.	86.	80.
95.	106.	77.	85.	65.	73.	62.	78.	63.	63.
46.	48.	54.	39.	51.	51.	54.	49.	44.	53.

39.	51.	60.	60.	51.	43.	47.	52.	38.	53.
47.	27.	44.	21.	43.	53.	36.	43.	30.	38.
48.	37.	71.	40.	36.	26.	39.	42.	37.	31.
27.	50.	47.	29.	35.	42.	38.	29.	34.	60.
38.	34.	30.	37.	48.	45.	63.	67.	56.	45.
49.	54.	51.	40.	50.	37.	55.	62.	43.	47.
35.	41.	47.	23.	38.	41.	35.	33.	41.	44.
31.	43.	34.	33.	34.	39.	50.	57.	52.	44.
42.	57.	55.	84.	51.	57.	75.	89.	86.	90.
73.	90.	87.	76.	87.	99.	80.	54.	63.	63.
63.	75.	46.	58.	43.	50.	64.	45.	43.	51.
58.	49.	51.	51.	76.	59.	72.	57.	61.	80.
63.	83.	49.	48.	95.	51.	48.	55.	55.	52.
55.	44.	59.	58.	74.	62.	88.	48.	64.	56.
46.	61.	54.	53.	54.	50.	53.	64.	48.	38.
35.	34.	50.	33.	49.	39.	36.	34.	27.	46.
34.	29.	37.	30.	32.	35.	35.	42.	36.	21.
28.	28.	53.	27.	23.	46.	35.	34.	28.	37.
37.	45.	35.	32.	34.	31.	37.	31.	45.	31.
35.	42.	49.	39.	52.	45.	37.	39.	42.	44.
47.	47.	44.	49.	47.	32.	31.	44.	41.	32.
33.	38.	41.	29.	40.	33.	39.	52.	37.	35.
33.	49.	38.	44.	31.	30.	30.	22.	26.	38.
21.	41.	36.	36.	32.	32.	34.	33.	49.	32.
36.	35.	32.	33.	33.	39.	46.	37.	42.	28.
36.	29.	28.	29.	39.	29.	31.	39.	27.	38.
47.	50.	47.	21.	45.	37.	36.	43.	56.	47.
53.	47.	53.	55.	76.	54.	54.	58.	50.	46.
44.	50.	45.	43.	45.	130.	62.	52.	48.	44.
52.	46.	43.	45.	37.	40.	36.	37.	45.	44.
38.	31.	50.	55.	45.	36.	48.	42.	30.	43.
54.	39.	36.	40.	46.	29.	43.	43.	30.	25.
39.	34.	44.	38.	35.	34.	31.	30.	28.	34.
20.	37.	38.	34.	38.	36.	36.	31.	40.	35.
27.	30.	37.	27.	38.	26.	47.	29.	24.	59.
29.	19.	40.	49.	35.	26.	32.	36.	37.	36.
50.	27.	34.	24.	37.	37.	22.	43.	28.	34.
34.	35.	35.	28.	36.	46.	33.	36.	36.	41.
45.	36.	54.	31.	30.	34.	39.	45.	38.	60.
49.	43.	44.	42.	39.	40.	45.	43.	34.	54.
43.	56.	52.	51.	64.	54.	59.	66.	61.	83.
55.	49.	66.	74.	44.	60.	60.	69.	69.	58.
43.	47.	58.	40.	34.	36.	51.	30.	45.	47.
41.	23.	47.	36.	43.	44.	54.	38.	51.	40.
48.	53.	35.	43.	33.	37.	31.	25.	36.	37.
29.	39.	34.	38.	41.	37.	29.	42.	34.	25.
33.	26.	33.	30.	35.	34.	44.	36.	35.	38.
35.	49.	17.	34.	35.	34.	44.	41.	37.	36.
41.	34.	42.	35.	38.	32.	30.	44.	69.	31.
33.	47.	46.	40.	36.	27.	24.	36.	46.	28.
42.	33.	32.	43.	43.	36.	34.	29.	36.	29.
41.	43.	36.	47.	44.	41.	47.	46.	53.	46.
33.	44.	31.	42.	36.	52.	37.	33.	47.	56.
50.	46.	43.	47.	57.	65.	49.	79.	63.	50.
44.	55.	51.	45.	41.	34.	34.	42.	43.	39.
33.	41.	61.	50.	48.	41.	40.	48.	44.	45.
41.	45.	40.	51.	35.	33.	49.	41.	47.	50.
35.	37.	40.	45.	44.	22.	36.	31.	48.	50.
38.	52.	40.	45.	34.	50.	36.	51.	28.	28.
41.	39.	34.	27.	36.	33.	34.	30.	30.	34.
29.	35.	29.	41.	36.	43.	36.	39.	32.	22.
24.	47.	48.	64.	34.	34.	45.	50.	29.	40.
38.	49.	52.	52.	54.	46.	51.	30.	53.	51.
59.	53.	50.	44.	51.	61.	39.	59.	43.	57.
55.	61.	56.	60.	73.	50.	55.	49.	66.	56.
40.	55.	47.	51.	63.	37.	34.	45.	39.	37.
45.	40.	52.	31.	42.	51.	40.	45.	38.	43.
40.	45.	33.	34.	25.	42.	34.	32.	30.	44.
38.	41.	55.	39.	35.	53.	43.	40.	47.	54.

50.	45.	55.	48.	65.	63.	51.	50.	38.	42.
48.	26.	31.	33.	43.	39.	28.	44.	27.	54.
30.	29.	25.	36.	28.	35.	32.	15.	34.	35.
36.	18.	26.	18.	36.	24.	21.	35.	36.	34.
34.	36.	36.	32.	27.	32.	36.	39.	40.	29.
30.	41.	23.	46.	38.	31.	47.	32.	30.	34.
35.	29.	37.	44.	31.	30.	53.	49.	53.	46.
54.	25.	74.	63.	48.	52.	47.	66.	69.	39.
60.	32.	44.	48.	35.	26.	30.	54.	44.	28.
33.	42.	43.	41.	30.	35.	41.	44.	39.	39.
28.	45.	35.	53.	40.	43.	54.	51.	58.	59.
54.	49.	47.	34.	71.	53.	44.	35.	45.	50.
48.	36.	36.	39.	34.	45.	65.	41.	56.	55.
54.	60.	50.	52.	51.	51.	45.	37.	42.	59.
53.	56.	57.	72.	70.	61.	63.	73.	67.	73.
68.	99.	98.	115.	95.	112.	85.	97.	86.	91.
91.	73.	76.	112.	91.	64.	88.	67.	60.	80.
78.	72.	62.	64.	63.	59.	59.	55.	57.	61.
45.	63.	49.	54.	51.	56.	68.	73.	54.	70.
56.	51.	68.	65.	78.	68.	44.	50.	51.	46.
45.	40.	41.	51.	43.	45.	35.	36.	43.	40.
38.	42.	45.	28.	33.	63.	34.	48.	53.	48.
51.	46.	49.	61.	64.	57.	48.	58.	54.	25.
46.	36.	49.	41.	33.	33.	38.	40.	38.	49.
36.	38.	32.	30.	48.	29.	45.	31.	35.	34.
41.	45.	29.	29.	29.	25.	23.	42.	31.	38.
38.	37.	43.	33.	25.	30.	37.	27.	32.	30.
15.	33.	26.	30.	37.	40.	31.	39.	36.	33.
31.	32.	33.	31.	21.	40.	47.	37.	30.	38.
27.	39.	30.	27.	52.	40.	39.	33.	32.	22.
39.	44.	40.	36.	42.	39.	37.	45.	25.	45.
34.	47.	44.	40.	40.	27.	53.	45.	32.	43.
45.	40.	46.	39.	39.	45.	49.	34.	44.	30.
34.	33.	49.	36.	27.	36.	32.	35.	44.	23.
32.	32.	33.	42.	29.	35.	41.	29.	35.	35.
43.	31.	28.	43.	31.	26.	36.	23.	27.	37.
20.	43.	35.	47.	34.	42.	27.	31.	46.	42.
45.	45.	52.	38.	48.	47.	51.	55.	47.	59.
40.	41.	40.	48.	29.	43.	29.	37.	44.	34.
28.	35.	49.	35.	45.	35.	51.	41.	31.	29.
35.	23.	35.	30.	48.	33.	29.	33.	39.	31.
51.	38.	25.	39.	41.	50.	35.	45.	42.	42.
44.	53.	38.	53.	52.	40.	54.	58.	35.	45.
43.	43.	53.	60.	64.	65.	71.	48.	49.	52.
55.	63.	68.	71.	78.	81.	77.	88.	69.	90.
79.	98.	77.	89.	99.	103.	75.	71.	61.	68.
58.	50.	64.	68.	78.	55.	44.	56.	42.	60.
39.	48.	47.	47.	53.	53.	45.	39.	48.	45.
51.	33.	49.	45.	40.	47.	28.	38.	36.	36.
33.	28.	42.	31.	25.	51.	45.	41.	45.	30.
31.	33.	38.	36.	32.	28.	51.	42.	24.	21.
32.	29.	40.	36.	37.	42.	28.	44.	33.	28.
35.	36.	26.	49.	29.	34.	29.	36.	32.	30.
39.	32.	21.	29.	21.	24.	21.	42.	39.	31.
30.	22.	48.	31.	35.	31.	35.	38.	19.	41.
54.	33.	33.	36.	36.	28.	35.	37.	33.	37.
36.	44.	40.	38.	25.	41.	30.	22.	47.	23.
41.	37.	37.	57.	45.	33.	24.	32.	29.	45.
39.	22.	30.	32.	37.	34.	35.	32.	48.	67.
48.	34.	31.	61.	74.	44.	67.	55.	46.	42.
52.	39.	30.	29.	48.	46.	36.	25.	48.	29.
26.	31.	19.	38.	34.	32.	22.	33.	37.	45.
26.	33.	31.	38.	28.	36.	29.	38.	23.	25.
31.	33.	25.	23.	23.	22.	23.	41.	27.	36.
67.	23.	20.	23.	27.	19.	21.	30.	40.	24.
40.	42.	33.	46.	38.	45.	44.	35.	45.	37.
35.	56.	54.	33.	42.	50.	37.	39.	41.	52.
40.	57.	47.	48.	44.	32.	38.	29.	49.	29.
36.	31.	26.	26.	30.	34.	29.	40.	31.	33.

24.	41.	38.	34.	36.	28.	34.	23.	26.	30.
28.	23.	38.	34.	26.	29.	28.	22.	34.	28.
44.	23.	22.	30.	34.	34.	24.	23.	23.	36.
31.	36.	26.	23.	24.	34.	66.	28.	29.	42.
33.	39.	48.	29.	37.	40.	36.	31.	33.	24.
33.	31.	33.	33.	35.	23.	35.	36.	24.	22.
38.	37.	36.	27.	32.	39.	28.	32.	34.	34.
24.	31.	30.	24.	32.	38.	34.	19.	28.	29.
42.	41.	24.	31.	16.	27.	34.	30.	19.	23.
27.	19.	20.	31.	29.	42.	35.	43.	22.	36.
27.	29.	55.	38.	26.	24.	38.	42.	17.	35.
31.	31.	31.	30.	36.	50.	41.	30.	28.	22.
18.	36.	29.	23.	25.	34.	29.	20.	25.	26.
28.	37.	35.	28.	34.	28.	21.	24.	37.	28.
33.	19.	30.	42.	26.	28.	34.	31.	35.	39.
25.	26.	62.	30.	41.	33.	35.	36.	40.	33.
43.	54.	43.	35.	35.	37.	39.	46.	46.	29.
26.	35.	31.	24.	28.	32.	29.	36.	21.	32.
25.	29.	33.	32.	33.	46.	34.	43.	31.	26.
33.	23.	29.	28.	34.	37.	29.	37.	41.	33.
43.	34.	36.	54.	40.	38.	31.	42.	32.	55.
40.	38.	36.	41.	43.	52.	23.	44.	34.	24.
36.	41.	22.	32.	34.	26.	39.	31.	30.	32.
38.	32.	22.	28.	38.	32.	35.	37.	51.	37.
31.	43.	30.	43.	42.	32.	31.	40.	35.	26.
38.	40.	29.	31.	42.	58.	43.	34.	34.	52.
39.	38.	37.	49.	51.	45.	45.	42.	55.	45.
43.	47.	44.	57.	39.	47.	45.	47.	40.	48.
29.	40.	45.	32.	42.	34.	50.	48.	40.	34.
44.	33.	38.	46.	40.	34.	32.	30.	32.	23.
25.	39.	27.	28.	29.	61.	33.	27.	29.	32.
39.	27.	29.	39.	35.	33.	44.	40.	29.	32.
52.	34.	34.	53.	27.	25.	24.	27.	39.	19.
35.	28.	26.	38.	42.	29.	41.	30.	42.	34.
40.	36.	23.	40.	37.	59.	44.	28.	53.	37.
41.	44.	45.	43.	39.	42.	40.	33.	54.	42.
37.	53.	40.	42.	54.	46.	39.	47.	48.	37.
29.	33.	41.	43.	40.	45.	34.	27.	51.	53.
51.	37.	34.	38.	34.	38.	50.	46.	40.	53.
40.	54.	40.	45.	49.	36.	38.	47.	49.	26.
49.	56.	47.	50.	45.	43.	36.	62.	43.	48.
35.	48.	64.	45.	43.	40.	45.	42.	39.	49.
52.	51.	47.	48.	42.	41.	58.	53.	53.	69.
43.	47.	47.	53.	40.	44.	49.	41.	44.	45.
42.	38.	56.	42.	37.	43.	22.	40.	38.	39.
48.	45.	41.	35.	33.	40.	40.	40.	48.	49.
33.	53.	45.	37.	51.	40.	37.	30.	42.	48.
44.	44.	53.	37.	44.	45.	47.	50.	43.	59.
36.	75.	44.	57.	58.	65.	68.	69.	80.	65.
65.	50.	66.	55.	54.	75.	78.	65.	59.	81.
59.	45.	59.	101.	93.	68.	64.	81.	77.	79.
70.	79.	74.	89.	80.	66.	78.	77.	71.	65.
71.	62.	67.	60.	57.	78.	65.	71.	63.	68.
99.	70.	80.	55.	90.	79.	56.	78.	50.	58.
55.	63.	51.	51.	64.	54.	58.	82.	56.	52.
61.	44.	52.	46.	53.	41.	55.	57.	60.	49.
55.	49.	47.	50.	58.	56.	54.	55.	43.	80.
46.	49.	63.	62.	41.	58.	51.	42.	51.	63.
54.	59.	56.	46.	70.	54.	75.	55.	61.	52.
112.	94.	79.	61.	62.	47.	60.	61.	64.	81.
50.	57.	54.	40.	45.	92.	53.	45.	53.	53.
48.	52.	51.	45.	48.	57.	56.	40.	45.	42.
38.	61.	41.	43.	46.	36.	43.	53.	42.	46.
26.	35.	32.	39.	39.	38.	36.	27.	30.	38.
38.	49.	36.	34.	57.	31.	50.	36.	40.	34.
38.	51.	37.	36.	35.	35.	46.	38.	44.	46.
34.	40.	52.	30.	43.	22.	43.	41.	47.	47.
57.	45.	39.	40.	52.	39.	79.	32.	48.	62.
57.	52.	56.	55.	46.	48.	51.	52.	51.	42.

38.	47.	47.	45.	34.	49.	72.	37.	43.	35.
60.	40.	50.	44.	54.	49.	43.	53.	59.	45.
43.	50.	66.	48.	47.	59.	54.	66.	45.	51.
38.	63.	51.	54.	73.	57.	44.	43.	37.	50.
41.	58.	49.	46.	30.	49.	35.	45.	56.	36.
53.	44.	40.	41.	27.	47.	47.	44.	26.	47.
41.	33.								

Appendix P-26: step-intensity (of neutron diffraction) data of muscovite

4.00	.05	117.00	pure muscovite						
5360.	5409.	5320.	5258.	5368.	5480.	5424.	5302.	5274.	5326.
5423.	5429.	5422.	5368.	5373.	5226.	5205.	5178.	5233.	5169.
5084.	5149.	5152.	5126.	5254.	5140.	5009.	5057.	5043.	4944.
4984.	5013.	4956.	4987.	5041.	4983.	4882.	4881.	4842.	4865.
4947.	5104.	5012.	4851.	4756.	4761.	4856.	4867.	4777.	4868.
4940.	4854.	4800.	4869.	4919.	4833.	4829.	4736.	4796.	4764.
4656.	4589.	4561.	4626.	4642.	4675.	4699.	4575.	4672.	4599.
4639.	4509.	4538.	4764.	4679.	4539.	4716.	4693.	4758.	4545.
4470.	4605.	4567.	4569.	4513.	4594.	4704.	4566.	4696.	4748.
4743.	4862.	4894.	4920.	4889.	5054.	5051.	5000.	5062.	4995.
4788.	4656.	4728.	4503.	4506.	4458.	4418.	4481.	4466.	4520.
4590.	4460.	4515.	4408.	4333.	4407.	4409.	4431.	4374.	4439.
4425.	4208.	4329.	4407.	4369.	4395.	4411.	4370.	4478.	4422.
4431.	4455.	4444.	4332.	4387.	4417.	4436.	4359.	4364.	4305.
4435.	4312.	4280.	4379.	4437.	4281.	4180.	4228.	4203.	4374.
4417.	4471.	4522.	4344.	4418.	4388.	4306.	4324.	4271.	4323.
4329.	4344.	4373.	4314.	4370.	4273.	4184.	4256.	4276.	4274.
4303.	4320.	4428.	4422.	4370.	4372.	4316.	4355.	4343.	4195.
4234.	4236.	4293.	4289.	4308.	4323.	4357.	4280.	4231.	4246.
4271.	4322.	4286.	4289.	4318.	4285.	4239.	4240.	4265.	4208.
4239.	4251.	4147.	4227.	4280.	4176.	4226.	4253.	4188.	4240.
4237.	4285.	4274.	4188.	4240.	4297.	4374.	4507.	4555.	4257.
4016.	4178.	4271.	4235.	4278.	4260.	4144.	4168.	4261.	4146.
4013.	4095.	4156.	4141.	4113.	4068.	3966.	4011.	4236.	4238.
4179.	4214.	4272.	4202.	4181.	4101.	4152.	4179.	4233.	4231.
4166.	4183.	4147.	4288.	4337.	4174.	4131.	4032.	4030.	4080.
3899.	3979.	4129.	4097.	4114.	4107.	3968.	4009.	4285.	4472.
4612.	4648.	4631.	4520.	4572.	4330.	4254.	4186.	4114.	3992.
4161.	4106.	4089.	4180.	4051.	4012.	3986.	4091.	4075.	4038.
4032.	4026.	4169.	4175.	4134.	4057.	4092.	4074.	4034.	4134.
4026.	4130.	4049.	4163.	4218.	4306.	4297.	4400.	4571.	4872.
5590.	6345.	6627.	7114.	7234.	6987.	6555.	6009.	5522.	5045.
5055.	4917.	4652.	4514.	4139.	4170.	4223.	4235.	4248.	4299.
4205.	4079.	4087.	4093.	4083.	4038.	4218.	4104.	4108.	4103.
4135.	4065.	4072.	4242.	4213.	4135.	4254.	4347.	4393.	4388.
4291.	4259.	4176.	4085.	3568.	3477.	3581.	3552.	3997.	4138.
3993.	3983.	4069.	4101.	4030.	3982.	4098.	4043.	4089.	4095.
4230.	4469.	4503.	4473.	4462.	4277.	4314.	4254.	4225.	4088.
3990.	4129.	4083.	3989.	3955.	4011.	4137.	4204.	4156.	4120.
4358.	4468.	4579.	4477.	4212.	4135.	4108.	4060.	3910.	3825.
3925.	3920.	3851.	3852.	3909.	3881.	3921.	4005.	4002.	3945.
3930.	3951.	4049.	4095.	4154.	4144.	4102.	4095.	4049.	4084.
4224.	4316.	4420.	4510.	4548.	4487.	4420.	4345.	4299.	4207.
4027.	3940.	3953.	4030.	3997.	3962.	3909.	3840.	3976.	4085.
4153.	4262.	4392.	4616.	4768.	4969.	5236.	5302.	5404.	5539.
5322.	5031.	4766.	4438.	4293.	4156.	4088.	4062.	4006.	3851.
3807.	3836.	3809.	3741.	3770.	3912.	3898.	3955.	4005.	4235.
4160.	3943.	3978.	4107.	4160.	4172.	4068.	4008.	3924.	3800.
3813.	3830.	3895.	3880.	3794.	3749.	3711.	3742.	3676.	3793.
3908.	3762.	3924.	3981.	3957.	3916.	4026.	3964.	3986.	3821.
3873.	4044.	4031.	3884.	3905.	3946.	3978.	4078.	4120.	4120.
4141.	4252.	4096.	4055.	4133.	4021.	3957.	3885.	3927.	3812.
3913.	3885.	4005.	3924.	3837.	3771.	3927.	3947.	3985.	4009.
3949.	3858.	3949.	3871.	3807.	3879.	3925.	3831.	3665.	3937.
3903.	3702.	3641.	3697.	3622.	3898.	3855.	3810.	3816.	3943.
4099.	3907.	3930.	4222.	4023.	4074.	4063.	3789.	3767.	3718.
3679.	3686.	3855.	3590.	3619.	3727.	3746.	3791.	3773.	3857.
3912.	3777.	3781.	3808.	3800.	3765.	3834.	3892.	3814.	3726.
3838.	3919.	3842.	3749.	3753.	3607.	3550.	3675.	3696.	3772.
3796.	3932.	3981.	3823.	3728.	3809.	3769.	3786.	3915.	3943.
3924.	4141.	4113.	4231.	4217.	4359.	4446.	4282.	4338.	4494.
4623.	4523.	4320.	4299.	4226.	3959.	3876.	3926.	3781.	3631.
3629.	3756.	3801.	3892.	4029.	4045.	3913.	3901.	3955.	3932.
3929.	4011.	4129.	4313.	4677.	4942.	5332.	5922.	6498.	6667.
6645.	6420.	6070.	5857.	5667.	5439.	5206.	4942.	4754.	4491.

4237.	4095.	4014.	3953.	3935.	3901.	3926.	3833.	3698.	3623.
3685.	3765.	3805.	3882.	3929.	3949.	3921.	3852.	3714.	3751.
3874.	3764.	3701.	3744.	3798.	3812.	3759.	3751.	3729.	3795.
3873.	3769.	3729.	3849.	3846.	3827.	3758.	3826.	3890.	3850.
3804.	3718.	3579.	3638.	3820.	3928.	3898.	3797.	3701.	3695.
3695.	3703.	3679.	3735.	3768.	3841.	3904.	4050.	4183.	4330.
4638.	4804.	4867.	4965.	4887.	4667.	4459.	4258.	4276.	4203.
3884.	3937.	4016.	4252.	4381.	4579.	4497.	4598.	4706.	4598.
4541.	4385.	4424.	4374.	4267.	4278.	4181.	4183.	4219.	4128.
4102.	3980.	3776.	3992.	4041.	4203.	4411.	4705.	4618.	4759.
5119.	5156.	5165.	5343.	5662.	5820.	5536.	5342.	5473.	5077.
4661.	4421.	4453.	4335.	4274.	4260.	4471.	4488.	4401.	4573.
4750.	4751.	4716.	4627.	4519.	4369.	4185.	4190.	4234.	4260.
4508.	4360.	4080.	4081.	4015.	3973.	3850.	3865.	3966.	3940.
3902.	3949.	3845.	3847.	3929.	3896.	3826.	3847.	3785.	3837.
3918.	3890.	3948.	4046.	3920.	3948.	4029.	4151.	4290.	4508.
4785.	5053.	5259.	5182.	5052.	4761.	4365.	4168.	4047.	4053.
3997.	3941.	3986.	4058.	3962.	3961.	3994.	3987.	3948.	3916.
3861.	3837.	3818.	3825.	3801.	3880.	3863.	3864.	3903.	3940.
3778.	3744.	3739.	3754.	3705.	3704.	3729.	3723.	3714.	3693.
3720.	3808.	3889.	3920.	3785.	3718.	3698.	3711.	3715.	3749.
3814.	3894.	3930.	3989.	4109.	4205.	4168.	4202.	4253.	4282.
4276.	4283.	4346.	4375.	4389.	4415.	4380.	4316.	4289.	4308.
4303.	4241.	4131.	4037.	3946.	3869.	3883.	3852.	3853.	3947.
3984.	4007.	4047.	4043.	4017.	3964.	3881.	3812.	3819.	3826.
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3596.	3677.	3640.	3566.	3589.	3636.	3662.	3561.	3531.	3646.
3608.	3577.	3695.	3801.	3842.	3802.	3837.	3846.	3755.	3727.
3691.	3700.	3697.	3642.	3751.	3760.	3820.	3832.	3871.	3926.
3951.	3926.	3929.	3909.	3889.	3901.	3892.	3994.	4010.	4015.
3947.	3821.	3783.	3774.	3719.	3675.	3526.	3442.	3569.	3689.
3671.	3848.	3776.	3854.	3827.	3932.	3967.	3938.	4015.	4309.
4393.	4024.	4054.	4165.	4122.	4054.	4022.	3926.	3783.	4045.
4082.	3995.	4116.	4267.	4333.	4189.	4178.	4173.	4185.	4241.
4224.	4055.	4088.	4226.	4044.	3893.	3910.	3996.	3825.	3990.
3977.	3868.	4004.	3993.	4107.	4214.	4291.	4223.	4355.	4515.
4571.	4568.	4412.	4429.	4322.	4365.	4253.	4061.	3985.	3983.
4028.	3990.	3997.	3940.	3898.	4031.	4054.	3952.	4007.	4065.
4070.	4085.	4078.	4092.	4115.	4125.	4106.	4139.	4257.	4053.
4027.	4024.	3957.	3934.	3928.	3854.	3770.	3774.	3724.	3643.
3700.	3696.	3695.	3668.	3660.	3724.	3720.	3737.	3716.	3616.
3647.	3712.	3730.	3712.	3744.	3721.	3700.	3656.	3636.	3650.
3640.	3725.	3846.	3834.	3751.	3673.	3642.	3711.	3733.	3718.
3723.	3785.	3760.	3766.	3745.	3679.	3611.	3620.	3650.	3648.
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3967.	4111.	4178.	4103.	4041.	3934.	3834.	3863.	3942.	4111.
4283.	4288.	4208.	4118.	4075.	4024.	4063.	4238.	4517.	4822.
5137.	5505.	5796.	6008.	6026.	5857.	5437.	5030.	4689.	4478.
4257.	4108.	4029.	3970.	3967.	3955.	3989.	4123.	4253.	4057.
3907.	3914.	3955.	3921.	3928.	3846.	3779.	3888.	3864.	3829.
3741.	3704.	3719.	3685.	3573.	3544.	3554.	3518.	3597.	3586.
3560.	3536.	3635.	3679.	3809.	3886.	3804.	3810.	3736.	3714.
3565.	3568.	3598.	3592.	3513.	3498.	3480.	3498.	3526.	3654.
3625.	3577.	3479.	3505.	3532.	3625.	3690.	3703.	3581.	3670.
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3571.	3537.	3558.	3478.	3515.	3405.	3444.	3429.	3411.	3401.
3346.	3477.	3386.	3494.	3538.	3593.	3637.	3683.	3628.	3617.
3530.	3407.	3437.	3470.	3571.	3504.	3552.	3542.	3585.	3589.
3560.	3674.	3756.	3786.	3952.	3842.	3866.	3794.	3673.	3664.
3539.	3546.	3628.	3643.	3624.	3591.	3576.	3521.	3550.	3635.
3637.	3684.	3721.	3825.	3952.	4025.	4142.	4367.	4497.	4779.
4885.	4970.	4987.	4876.	4643.	4362.	4203.	4022.	3932.	3889.
3886.	3945.	3939.	3971.	4039.	4171.	4291.	4356.	4386.	4260.
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3583.	3545.	3606.	3633.	3624.	3637.	3661.	3702.	3691.	3658.
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3709.	3710.	3813.	3908.	3989.	4116.	4214.	4213.	4355.	4424.
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3485.	3654.	3690.	3631.	3626.	3741.	3661.	3666.	3734.	3789.
3749.	3665.	3675.	3714.	3615.	3644.	3614.	3600.	3545.	3508.
3585.	3615.	3608.	3492.	3556.	3651.	3569.	3527.	3556.	3477.
3489.	3533.	3552.	3514.	3523.	3573.	3636.	3710.	3861.	3904.
4087.	4305.	4462.	4521.	4632.	4611.	4613.	4524.	4447.	4201.
4123.	4222.	4220.	4112.	4375.	4350.	4569.	4481.	4461.	4353.
4268.	4178.	3954.	3808.	3806.	3938.	4011.	3942.	3962.	4006.
4038.	3939.	3970.	3937.	3996.	3905.	4017.	4093.	4147.	4299.
4297.	4406.	4394.	4297.	4401.	4611.	4602.	4558.	4531.	4273.
3986.	3963.	3770.	3699.	3671.	3662.	3664.	3602.	3588.	3649.
3680.	3740.	3872.	4025.	4047.	4109.	4178.	4242.	4245.	4305.
4320.	4106.	4202.	4124.	4126.	4058.	3936.	3779.	3729.	3721.
3716.	3746.	3744.	3847.	3908.	3890.	3807.	3939.	3913.	3888.
3890.	3924.	3890.	3874.	3762.	3727.	3668.	3699.	3731.	3633.
3599.	3657.	3722.	3737.	3814.	3983.	4010.	3915.	3936.	4040.
4042.	3914.	3839.	3827.	3810.	3696.	3631.	3590.	3580.	3603.
3611.	3686.	3708.	3683.	3654.	3641.	3640.	3626.	3729.	3952.
4102.	4303.	4479.	4218.	4012.	4063.	4092.	3908.	3743.	3804.
3811.	3802.	3831.	3807.	3746.	3806.	3967.	3935.	3876.	3835.
3722.	3773.	3762.	3775.	3885.	3786.	3679.	3634.	3593.	3541.
3464.	3475.	3522.	3513.	3441.	3400.	3476.	3389.	3278.	3315.
3335.	3310.	3323.	3308.	3350.	3364.	3345.	3345.	3393.	3370.
3276.	3273.	3309.	3366.	3428.	3485.	3448.	3394.	3404.	3434.
3499.	3572.	3627.	3500.	3453.	3489.	3448.	3450.	3425.	3384.
3382.	3420.	3455.	3511.	3660.	3591.	3545.	3570.	3483.	3425.
3598.	3613.	3537.	3425.	3384.	3464.	3590.	3660.	3617.	3624.
3661.	3678.	3647.	3740.	3790.	3862.	3840.	3704.	3487.	3494.
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3146.	3276.	3299.	3366.	3245.	3351.	3131.	3049.	3165.	3288.
3243.	3243.	3341.	3450.	3184.	3201.	3390.	3391.	3236.	3273.
3354.	3332.	3388.	3368.	3386.	3214.	3377.	3548.	3462.	3520.
3298.	3313.	3451.	3452.	3583.	3578.	3364.	3357.	3494.	3354.
3491.	3528.	3506.	3514.	3467.	3473.	3493.	3380.	3390.	3342.
3332.	3399.	3247.	3188.	3254.	3352.	3344.	3343.	3308.	3293.
3041.	3553.	3623.	3585.	3505.	3478.	3505.	3491.	3442.	3458.
3592.	3592.	3373.	3334.	3294.	3294.	3275.	3165.	3144.	3167.
3231.	3195.	3166.	3115.	3174.	3253.	3230.	3206.	3253.	3361.
3313.	3243.	3228.	3182.	3234.	3321.	3185.	3115.	3197.	3153.
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3293.	3324.	3334.	3318.	3353.	3391.	3311.	3272.	3232.	3172.
3168.	3187.	3172.	3144.	3193.	3218.	3263.	3345.	3310.	3313.
3348.	3368.	3347.	3256.	3294.	3395.	3424.	3480.	3503.	3498.
3324.	3107.	3180.	3282.	3286.	3278.	3331.	3243.	3197.	3332.
3338.	3236.	3276.	3207.	3222.	3112.	3190.	3225.	3190.	3173.
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3227.	3062.	3094.	3024.	3056.	3158.	3159.	3050.	3129.	3337.
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3192.	3129.	3202.	3247.	3216.	3225.	3192.	3121.	3082.	3189.
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3518.	3436.	3442.	3473.	3457.	3370.	3309.	3357.	3400.	3337.
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3370.	3209.	3056.	3161.	3249.	3290.	3340.	3330.	3370.	3342.
3274.	3238.	3202.	3256.	3283.	3298.	3314.	3180.	3063.	3155.

3166.	3143.	3075.	3010.	2988.	3035.	3051.	3031.	3061.	3081.
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2781.	2722.	3094.	3196.	2922.	2994.	3159.	3351.	3155.	3156.
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3005.	2999.	3045.	3048.	3040.	3008.	3093.	3091.	3096.	3100.
2935.	3001.	3034.	2948.	2916.	2979.	3160.	3100.	3092.	3089.
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3473.	3394.	3463.	3526.	3435.	3373.	3423.	3461.	3459.	3409.
3320.	3300.	3299.	3337.	3374.	3400.	3380.	3286.	3373.	3396.
3287.	3311.	3381.	3344.	3283.	3330.	3415.	3460.	3368.	3249.
3234.	3266.	3284.	3291.	3294.	3289.	3270.	3231.	3163.	3142.
3145.	3166.	3159.	3061.	3086.	3151.	3131.	3066.	3129.	3165.
3131.	3173.	3230.	3214.	3228.	3301.	3206.	3193.	3234.	3277.
3277.	3202.	3148.	3175.	3272.	3282.	3256.	3096.	3106.	3009.
3078.	3226.	3171.	3171.	3163.	3181.	3181.	3187.	3237.	3213.
3321.	3248.	3256.	3276.	3175.	2955.	3022.	3287.	3243.	2904.
2904.	3243.	3212.	3289.	3239.	3367.	3262.	3368.	3274.	3336.
3182.	3070.	3137.	3314.	3245.	3344.	3239.	3214.	3151.	3261.
3283.	3162.	3165.	3152.	3249.	3176.	3155.	3169.	3341.	3091.

Appendix P-27: step-intensity data of B-muscovite

8.00	.02	122.00							
363.	381.	341.	321.	334.	334.	321.	350.	373.	360.
373.	371.	353.	412.	390.	407.	400.	367.	395.	358.
411.	399.	406.	396.	420.	487.	461.	444.	518.	589.
555.	569.	646.	665.	702.	880.	812.	834.	990.	1072.
1175.	1259.	1433.	1699.	1822.	1994.	2132.	2000.	1711.	1348.
1055.	760.	527.	451.	387.	402.	369.	316.	314.	334.
270.	295.	269.	251.	286.	280.	296.	271.	255.	246.
286.	231.	274.	254.	261.	276.	271.	279.	247.	269.
238.	256.	265.	243.	258.	236.	212.	256.	269.	252.
234.	232.	263.	272.	224.	252.	231.	245.	239.	232.
216.	249.	211.	228.	234.	236.	251.	219.	257.	227.
229.	239.	205.	248.	233.	206.	232.	203.	230.	209.
207.	185.	214.	224.	221.	210.	224.	203.	253.	219.
216.	221.	185.	217.	227.	220.	221.	212.	192.	209.
198.	228.	226.	201.	243.	247.	239.	219.	203.	214.
190.	211.	224.	221.	217.	201.	248.	181.	185.	203.
196.	212.	205.	194.	216.	202.	210.	212.	205.	214.
211.	209.	177.	197.	198.	193.	216.	174.	209.	205.
186.	191.	194.	175.	182.	181.	185.	184.	180.	190.
199.	163.	182.	188.	213.	195.	197.	167.	201.	181.
201.	200.	196.	198.	174.	176.	185.	183.	194.	210.
170.	199.	198.	217.	213.	203.	192.	202.	161.	178.
185.	180.	211.	195.	190.	194.	172.	165.	167.	167.
184.	170.	182.	179.	183.	216.	186.	185.	192.	152.
157.	189.	180.	177.	174.	163.	171.	171.	149.	170.
175.	189.	164.	162.	155.	191.	178.	187.	188.	179.
194.	174.	187.	155.	171.	207.	143.	190.	164.	186.
182.	200.	189.	153.	201.	203.	191.	192.	222.	202.
184.	165.	179.	180.	192.	207.	204.	178.	182.	168.
188.	192.	205.	212.	173.	182.	165.	195.	180.	222.
182.	186.	180.	218.	240.	175.	210.	172.	161.	190.
176.	202.	158.	174.	176.	173.	144.	211.	163.	167.
162.	154.	172.	141.	169.	186.	151.	158.	168.	172.
187.	164.	179.	163.	153.	159.	140.	133.	158.	168.
181.	155.	158.	186.	173.	148.	154.	150.	146.	171.
139.	170.	178.	164.	136.	126.	168.	159.	108.	160.
172.	153.	153.	126.	149.	166.	171.	133.	173.	152.
156.	162.	135.	133.	163.	119.	139.	170.	139.	130.
139.	135.	164.	152.	127.	144.	154.	131.	145.	121.
144.	134.	155.	158.	149.	149.	171.	124.	150.	158.
162.	139.	195.	137.	140.	132.	160.	132.	131.	149.
128.	142.	152.	195.	134.	140.	136.	143.	136.	167.
125.	137.	122.	152.	133.	124.	172.	152.	171.	143.
182.	161.	151.	149.	160.	140.	127.	158.	127.	126.
140.	148.	158.	163.	171.	132.	157.	141.	147.	150.
172.	149.	151.	142.	149.	162.	169.	134.	144.	117.
138.	151.	126.	166.	181.	148.	196.	150.	176.	177.
166.	177.	165.	145.	158.	190.	128.	164.	165.	193.
178.	160.	180.	179.	198.	184.	198.	201.	237.	237.
251.	306.	346.	388.	430.	445.	422.	434.	509.	454.
406.	347.	228.	239.	211.	203.	174.	162.	151.	140.
166.	194.	136.	150.	121.	147.	122.	134.	144.	145.
138.	144.	150.	144.	148.	151.	135.	137.	149.	154.
170.	136.	140.	150.	122.	134.	140.	147.	121.	136.
127.	129.	152.	119.	155.	140.	143.	143.	132.	143.
114.	134.	160.	133.	114.	154.	135.	128.	135.	141.
127.	136.	139.	127.	134.	128.	133.	150.	172.	135.
163.	138.	156.	181.	159.	196.	216.	201.	187.	197.
234.	234.	245.	238.	297.	332.	332.	423.	398.	391.
394.	397.	369.	364.	360.	397.	394.	452.	542.	573.
620.	738.	822.	964.	1124.	1184.	1315.	1402.	1530.	1616.
1666.	1667.	1720.	1561.	1432.	1343.	1259.	1194.	1043.	964.
805.	769.	629.	567.	506.	529.	508.	464.	453.	479.
439.	425.	397.	402.	413.	387.	377.	414.	385.	359.
369.	409.	383.	422.	407.	440.	403.	465.	423.	385.

460.	406.	414.	414.	427.	410.	366.	370.	362.	361.
349.	338.	291.	296.	304.	250.	280.	278.	238.	260.
223.	234.	244.	245.	256.	251.	247.	233.	258.	194.
229.	230.	236.	178.	241.	197.	231.	227.	237.	245.
247.	271.	276.	313.	300.	316.	304.	335.	354.	348.
347.	375.	351.	355.	329.	337.	306.	285.	297.	267.
238.	239.	198.	220.	240.	220.	219.	181.	236.	217.
209.	219.	209.	200.	217.	252.	217.	206.	186.	182.
238.	216.	234.	237.	254.	240.	270.	255.	280.	275.
270.	253.	288.	242.	264.	253.	234.	253.	264.	211.
249.	282.	252.	284.	266.	309.	271.	294.	349.	359.
393.	424.	467.	485.	507.	501.	571.	498.	489.	446.
460.	449.	431.	374.	380.	363.	310.	312.	265.	248.
278.	262.	225.	252.	261.	247.	224.	252.	227.	246.
234.	232.	256.	243.	218.	235.	281.	268.	279.	283.
272.	345.	322.	365.	373.	396.	411.	492.	526.	520.
540.	540.	584.	594.	569.	568.	527.	504.	473.	421.
389.	411.	298.	337.	297.	330.	296.	255.	243.	293.
312.	365.	331.	381.	313.	410.	439.	387.	457.	384.
440.	441.	374.	366.	393.	418.	368.	332.	326.	264.
310.	296.	267.	265.	237.	219.	277.	274.	272.	247.
259.	249.	243.	269.	242.	268.	243.	256.	265.	261.
235.	258.	260.	279.	254.	286.	265.	298.	345.	334.
333.	314.	335.	328.	318.	351.	426.	431.	417.	493.
531.	471.	582.	574.	563.	540.	565.	641.	596.	598.
533.	517.	500.	477.	481.	436.	350.	364.	361.	315.
276.	289.	276.	270.	240.	241.	256.	273.	231.	238.
246.	209.	249.	234.	246.	272.	238.	224.	258.	252.
292.	281.	298.	291.	257.	274.	301.	321.	324.	360.
341.	398.	373.	491.	559.	663.	779.	812.	899.	1103.
1008.	1176.	1147.	1239.	1185.	1206.	1195.	1089.	1013.	871.
745.	616.	563.	463.	450.	361.	365.	335.	303.	285.
271.	262.	273.	295.	255.	231.	200.	218.	235.	220.
211.	233.	201.	205.	224.	210.	217.	196.	207.	217.
239.	201.	204.	195.	270.	207.	213.	246.	263.	264.
273.	283.	334.	317.	372.	345.	383.	402.	492.	461.
521.	568.	561.	545.	543.	541.	514.	503.	519.	516.
502.	477.	445.	348.	396.	331.	293.	275.	269.	246.
250.	244.	234.	238.	233.	227.	194.	225.	250.	199.
197.	218.	209.	175.	243.	251.	192.	207.	208.	232.
231.	260.	223.	222.	235.	238.	244.	253.	233.	270.
230.	269.	240.	249.	243.	291.	240.	267.	276.	279.
304.	363.	368.	352.	334.	379.	403.	381.	388.	384.
301.	364.	312.	328.	323.	257.	286.	270.	271.	246.
263.	222.	225.	220.	243.	222.	227.	220.	242.	236.
231.	240.	274.	274.	294.	342.	393.	351.	416.	456.
449.	490.	511.	515.	518.	533.	571.	547.	514.	545.
489.	471.	530.	462.	456.	410.	386.	332.	326.	295.
285.	279.	231.	218.	202.	201.	186.	228.	200.	196.
217.	223.	205.	199.	189.	245.	214.	220.	186.	213.
207.	195.	203.	206.	203.	235.	214.	206.	237.	181.
198.	211.	228.	212.	223.	209.	198.	209.	225.	211.
231.	188.	236.	238.	259.	272.	301.	311.	343.	318.
328.	342.	329.	378.	364.	341.	314.	330.	363.	350.
312.	334.	292.	300.	276.	237.	250.	222.	183.	202.
231.	194.	187.	189.	177.	196.	194.	188.	195.	175.
199.	160.	187.	196.	206.	178.	254.	213.	235.	254.
281.	252.	299.	277.	308.	268.	276.	287.	301.	296.
294.	283.	267.	268.	269.	239.	256.	238.	192.	222.
165.	173.	212.	212.	199.	185.	171.	142.	122.	140.
140.	136.	90.	118.	114.	109.	111.	115.	122.	110.
110.	143.	121.	113.	123.	93.	101.	122.	115.	86.
93.	114.	109.	118.	117.	122.	103.	112.	93.	125.
121.	126.	114.	113.	111.	128.	150.	152.	134.	137.
136.	163.	156.	167.	140.	160.	173.	193.	156.	187.
177.	189.	176.	153.	134.	137.	155.	137.	120.	125.
139.	101.	134.	155.	105.	122.	121.	119.	119.	147.
169.	99.	138.	142.	129.	144.	153.	161.	145.	168.
180.	168.	153.	224.	200.	154.	189.	185.	244.	173.

221.	187.	197.	224.	230.	228.	201.	225.	243.	299.
292.	312.	344.	407.	422.	478.	493.	491.	598.	592.
648.	679.	754.	744.	831.	852.	901.	897.	979.	995.
1015.	1094.	1089.	1041.	1051.	1028.	1144.	1163.	1153.	1126.
1233.	1232.	1306.	1361.	1391.	1404.	1456.	1502.	1419.	1456.
1478.	1395.	1315.	1220.	1144.	997.	832.	814.	682.	584.
540.	451.	340.	309.	310.	252.	286.	253.	248.	210.
211.	240.	251.	228.	219.	212.	223.	227.	234.	255.
225.	238.	195.	215.	201.	186.	202.	190.	186.	162.
191.	166.	136.	191.	173.	154.	182.	145.	158.	197.
169.	145.	178.	173.	193.	206.	206.	202.	226.	248.
226.	248.	272.	312.	290.	277.	280.	337.	353.	349.
397.	346.	398.	393.	361.	385.	444.	424.	381.	420.
405.	360.	301.	320.	319.	259.	324.	276.	229.	250.
240.	262.	224.	222.	198.	218.	203.	201.	206.	168.
194.	176.	166.	207.	177.	152.	190.	206.	169.	184.
210.	224.	222.	207.	257.	239.	243.	307.	301.	292.
320.	326.	376.	332.	400.	433.	457.	428.	460.	505.
518.	475.	508.	497.	533.	505.	495.	477.	466.	446.
463.	363.	364.	375.	381.	320.	304.	251.	226.	250.
179.	205.	156.	185.	137.	151.	146.	130.	147.	135.
127.	116.	134.	124.	113.	110.	90.	95.	122.	83.
83.	101.	94.	89.	107.	112.	109.	93.	71.	79.
103.	108.	88.	107.	115.	110.	82.	86.	82.	88.
84.	82.	96.	98.	86.	77.	91.	92.	87.	94.
84.	96.	98.	87.	82.	69.	91.	94.	108.	99.
82.	82.	105.	88.	123.	99.	102.	118.	130.	119.
92.	103.	117.	87.	109.	107.	99.	92.	115.	102.
109.	79.	92.	152.	120.	105.	105.	138.	134.	130.
146.	159.	174.	166.	182.	196.	227.	229.	262.	276.
250.	233.	291.	313.	286.	322.	326.	391.	352.	397.
336.	365.	358.	337.	281.	336.	313.	285.	262.	247.
256.	244.	224.	240.	242.	193.	206.	215.	159.	220.
219.	186.	179.	204.	247.	168.	240.	197.	226.	216.
208.	210.	238.	220.	263.	239.	249.	262.	286.	261.
233.	244.	247.	240.	223.	227.	224.	274.	205.	232.
242.	240.	212.	222.	239.	255.	262.	232.	214.	189.
229.	214.	195.	213.	242.	180.	211.	201.	182.	195.
189.	203.	242.	237.	207.	226.	240.	242.	259.	251.
263.	279.	262.	298.	334.	325.	387.	347.	369.	354.
356.	358.	381.	386.	433.	431.	465.	476.	486.	493.
528.	544.	519.	512.	599.	552.	514.	552.	545.	520.
545.	518.	496.	537.	488.	498.	456.	466.	388.	398.
417.	363.	341.	304.	305.	292.	246.	242.	237.	211.
182.	176.	177.	186.	163.	142.	146.	148.	128.	141.
143.	122.	146.	147.	137.	136.	147.	129.	133.	145.
123.	125.	132.	117.	108.	141.	126.	127.	124.	123.
121.	131.	135.	111.	145.	155.	158.	164.	179.	154.
144.	120.	142.	139.	126.	134.	141.	172.	149.	155.
135.	125.	128.	124.	137.	122.	140.	171.	121.	123.
132.	122.	154.	140.	115.	136.	109.	129.	124.	99.
127.	116.	117.	118.	154.	122.	132.	129.	100.	105.
109.	139.	119.	113.	141.	122.	129.	143.	108.	137.
106.	123.	123.	159.	165.	141.	154.	163.	158.	180.
178.	211.	214.	231.	228.	247.	240.	234.	258.	254.
252.	259.	294.	301.	361.	334.	342.	342.	347.	330.
318.	334.	285.	292.	270.	226.	249.	196.	166.	183.
165.	137.	139.	130.	146.	140.	139.	140.	159.	140.
119.	139.	159.	131.	148.	167.	174.	167.	160.	170.
192.	183.	222.	207.	175.	194.	211.	213.	201.	173.
229.	261.	184.	255.	207.	192.	243.	234.	208.	228.
210.	200.	205.	230.	218.	219.	196.	215.	189.	218.
196.	187.	217.	218.	217.	163.	190.	187.	177.	192.
186.	176.	171.	160.	130.	145.	156.	140.	151.	127.
146.	101.	116.	108.	100.	139.	101.	123.	100.	108.
104.	97.	68.	100.	93.	65.	92.	65.	88.	81.
87.	96.	73.	90.	93.	89.	63.	86.	76.	75.
79.	71.	77.	83.	78.	73.	65.	86.	78.	77.
62.	83.	68.	76.	69.	80.	95.	83.	81.	65.

92.	78.	83.	64.	84.	85.	89.	97.	78.	94.
108.	89.	88.	84.	90.	94.	102.	99.	90.	82.
88.	103.	100.	106.	84.	95.	99.	72.	106.	78.
89.	77.	90.	100.	110.	100.	104.	105.	108.	102.
121.	112.	102.	104.	98.	84.	116.	99.	103.	110.
107.	122.	115.	84.	97.	104.	98.	104.	101.	97.
96.	102.	95.	92.	86.	94.	92.	97.	79.	68.
91.	85.	97.	70.	88.	88.	72.	73.	94.	84.
89.	83.	91.	89.	88.	76.	88.	79.	80.	91.
90.	89.	83.	100.	83.	66.	74.	90.	78.	76.
75.	85.	69.	83.	80.	73.	79.	61.	80.	77.
93.	77.	74.	67.	104.	100.	80.	79.	89.	81.
64.	79.	83.	61.	83.	69.	63.	80.	64.	94.
75.	83.	86.	82.	86.	80.	72.	78.	67.	101.
74.	70.	88.	90.	88.	90.	82.	71.	92.	80.
90.	85.	99.	91.	84.	56.	71.	91.	83.	71.
88.	65.	77.	72.	89.	65.	56.	70.	67.	82.
83.	87.	74.	62.	80.	85.	90.	72.	84.	79.
62.	61.	92.	73.	74.	92.	76.	99.	92.	82.
68.	83.	95.	100.	94.	74.	96.	85.	96.	89.
92.	110.	123.	109.	87.	106.	87.	88.	115.	94.
91.	101.	87.	102.	105.	73.	97.	100.	90.	95.
95.	84.	105.	96.	111.	122.	130.	100.	108.	79.
106.	101.	92.	107.	115.	123.	100.	97.	85.	88.
117.	138.	122.	101.	138.	144.	106.	122.	143.	145.
137.	148.	115.	138.	113.	133.	139.	122.	155.	135.
149.	161.	140.	129.	120.	150.	124.	142.	115.	136.
148.	129.	136.	124.	158.	149.	133.	121.	173.	118.
138.	136.	130.	127.	132.	128.	129.	113.	131.	122.
112.	123.	104.	115.	116.	126.	124.	136.	105.	101.
124.	130.	124.	112.	123.	105.	126.	123.	120.	122.
134.	149.	130.	117.	116.	132.	145.	146.	173.	155.
167.	173.	157.	172.	193.	193.	160.	173.	179.	169.
165.	177.	222.	211.	196.	188.	175.	180.	174.	181.
180.	201.	169.	169.	173.	192.	135.	171.	132.	174.
188.	187.	183.	171.	185.	222.	212.	233.	188.	238.
215.	183.	200.	228.	212.	223.	221.	253.	241.	287.
248.	240.	252.	202.	235.	239.	238.	264.	254.	248.
264.	248.	271.	255.	292.	266.	269.	294.	280.	289.
352.	304.	325.	300.	336.	306.	310.	336.	314.	312.
332.	296.	327.	309.	327.	303.	328.	300.	331.	348.
327.	329.	301.	323.	288.	289.	272.	269.	281.	280.
296.	270.	242.	248.	255.	241.	261.	266.	224.	217.
281.	275.	248.	233.	216.	247.	243.	265.	238.	277.
253.	211.	276.	219.	285.	308.	256.	235.	238.	216.
240.	222.	199.	283.	228.	226.	203.	197.	208.	236.
193.	229.	230.	223.	198.	205.	237.	227.	196.	208.
206.	226.	198.	204.	164.	187.	186.	150.	195.	172.
179.	188.	183.	171.	159.	193.	145.	166.	182.	141.
207.	170.	140.	198.	151.	194.	165.	149.	163.	165.
151.	158.	168.	200.	198.	169.	175.	185.	151.	199.
161.	176.	169.	156.	175.	160.	147.	135.	159.	167.
168.	134.	140.	149.	147.	167.	150.	131.	133.	107.
137.	124.	135.	127.	119.	153.	141.	155.	133.	126.
115.	137.	128.	129.	120.	118.	108.	121.	128.	159.
125.	110.	100.	118.	100.	122.	113.	143.	127.	129.
137.	127.	104.	123.	125.	117.	117.	135.	129.	110.
114.	132.	128.	141.	122.	107.	123.	127.	130.	144.
131.	129.	144.	157.	131.	113.	111.	122.	135.	142.
137.	131.	125.	142.	140.	134.	140.	152.	148.	145.
133.	165.	165.	158.	150.	170.	143.	161.	164.	146.
138.	133.	133.	129.	175.	123.	140.	138.	147.	136.
146.	185.	167.	154.	146.	160.	177.	141.	128.	149.
170.	167.	191.	159.	184.	151.	186.	177.	180.	166.
173.	185.	178.	171.	168.	216.	198.	170.	204.	243.
224.	237.	212.	204.	229.	235.	213.	244.	210.	246.
257.	251.	244.	226.	249.	237.	201.	215.	207.	206.
223.	207.	257.	218.	216.	190.	186.	198.	201.	196.
195.	176.	182.	183.	203.	165.	182.	188.	157.	185.

166.	181.	175.	154.	183.	187.	184.	152.	207.	166.
186.	191.	230.	204.	225.	272.	264.	243.	301.	298.
318.	311.	341.	353.	351.	378.	391.	384.	392.	442.
460.	489.	464.	471.	522.	498.	499.	552.	509.	557.
591.	590.	571.	643.	560.	590.	650.	587.	604.	555.
561.	519.	507.	443.	403.	437.	366.	333.	323.	330.
288.	244.	242.	207.	205.	211.	213.	181.	216.	214.
153.	203.	185.	155.	188.	154.	155.	162.	185.	199.
187.	207.	211.	187.	154.	169.	167.	156.	194.	154.
169.	205.	154.	127.	182.	161.	138.	130.	113.	154.
125.	151.	129.	132.	126.	128.	110.	154.	132.	116.
131.	135.	128.	126.	129.	97.	97.	129.	100.	128.
114.	121.	105.	117.	103.	92.	118.	119.	116.	118.
84.	109.	81.	110.	102.	115.	109.	122.	99.	109.
101.	99.	99.	87.	107.	81.	112.	87.	113.	97.
87.	92.	109.	75.	86.	78.	109.	89.	70.	84.
90.	88.	95.	92.	94.	100.	84.	73.	93.	114.
77.	108.	105.	89.	89.	98.	115.	94.	87.	93.
83.	117.	104.	108.	113.	101.	89.	101.	96.	86.
124.	100.	79.	104.	100.	99.	115.	124.	95.	139.
110.	120.	108.	105.	100.	119.	93.	122.	111.	105.
111.	121.	121.	104.	92.	98.	87.	66.	79.	92.
105.	94.	94.	95.	83.	63.	97.	84.	93.	99.
90.	91.	86.	93.	82.	99.	103.	91.	112.	75.
94.	95.	111.	102.	79.	59.	86.	95.	67.	80.
90.	86.	66.	86.	78.	100.	85.	102.	79.	85.
96.	85.	88.	65.	94.	87.	82.	83.	92.	75.
99.	85.	83.	94.	96.	102.	98.	75.	99.	83.
72.	109.	74.	101.	106.	103.	92.	109.	104.	105.
123.	68.	118.	87.	90.	85.	105.	89.	99.	98.
78.	92.	90.	92.	102.	87.	107.	101.	84.	68.
100.	68.	82.	95.	82.	92.	96.	100.	93.	73.
102.	93.	79.	79.	91.	94.	96.	83.	96.	97.
77.	84.	73.	74.	85.	103.	97.	76.	74.	100.
99.	108.	91.	85.	114.	111.	96.	77.	111.	120.
112.	114.	96.	111.	81.	111.	116.	101.	95.	122.
96.	99.	107.	121.	94.	105.	105.	101.	115.	85.
106.	98.	108.	125.	109.	134.	120.	128.	149.	107.
107.	128.	132.	118.	135.	112.	132.	134.	113.	119.
127.	127.	131.	169.	139.	147.	150.	156.	147.	169.
173.	157.	186.	150.	173.	145.	156.	172.	175.	139.
200.	205.	188.	164.	176.	167.	150.	157.	199.	157.
180.	183.	169.	216.	169.	176.	174.	159.	169.	167.
191.	160.	192.	175.	185.	186.	168.	184.	186.	173.
148.	120.	169.	151.	167.	193.	179.	161.	125.	124.
142.	152.	162.	165.	172.	139.	141.	118.	144.	128.
126.	135.	108.	118.	101.	121.	106.	129.	98.	111.
135.	113.	116.	121.	93.	113.	98.	102.	102.	102.
114.	96.	91.	100.	115.	108.	104.	99.	103.	122.
108.	104.	88.	86.	86.	103.	89.	110.	77.	111.
105.	101.	106.	75.	103.	81.	79.	103.	113.	99.
109.	88.	98.	104.	105.	104.	103.	117.	104.	100.
114.	116.	96.	115.	96.	89.	116.	115.	118.	104.
110.	113.	103.	84.	123.	115.	112.	105.	90.	105.
79.	88.	101.	112.	111.	95.	89.	100.	82.	114.
82.	95.	110.	126.	103.	108.	121.	117.	105.	119.
126.	103.	87.	122.	115.	98.	112.	104.	99.	107.
112.	107.	116.	99.	145.	94.	101.	148.	110.	123.
116.	118.	153.	118.	145.	147.	166.	134.	146.	177.
155.	169.	203.	201.	196.	187.	206.	195.	197.	243.
214.	205.	211.	264.	232.	240.	241.	243.	280.	251.
263.	285.	277.	305.	282.	297.	295.	292.	275.	317.
286.	309.	276.	319.	285.	252.	302.	246.	273.	253.
288.	236.	238.	220.	246.	229.	199.	218.	201.	200.
183.	174.	190.	204.	199.	182.	185.	164.	179.	182.
172.	160.	146.	149.	146.	126.	138.	153.	133.	140.
114.	132.	112.	135.	162.	121.	123.	134.	167.	118.
145.	128.	122.	119.	117.	117.	165.	214.	122.	117.
138.	106.	149.	116.	154.	130.	145.	139.	132.	113.

124.	147.	133.	119.	147.	125.	161.	150.	134.	159.
140.	128.	162.	136.	137.	139.	133.	118.	137.	127.
160.	123.	161.	138.	155.	122.	176.	132.	137.	142.
124.	139.	124.	139.	117.	138.	105.	126.	121.	105.
118.	118.	130.	99.	116.	105.	118.	107.	107.	109.
117.	119.	141.	113.	123.	124.	115.	101.	83.	99.
121.	111.	90.	101.	101.	124.	118.	129.	113.	105.
111.	105.	126.	139.	97.	130.	101.	111.	121.	150.
139.	133.	132.	162.	128.	130.	129.	141.	159.	151.
133.	175.	143.	138.	137.	148.	143.	143.	143.	131.
165.	163.	168.	163.	181.	177.	157.	124.	147.	171.
161.	152.	181.	145.	164.	151.	164.	148.	170.	122.
142.	166.	129.	151.	129.	147.	140.	131.	135.	135.
117.	103.	97.	104.	118.	103.	124.	128.	97.	114.
110.	90.	108.	82.	103.	95.	100.	109.	107.	121.
102.	110.	80.	96.	81.	108.	99.	101.	90.	90.
106.	91.	98.	84.	119.	84.	103.	109.	135.	110.
115.	111.	120.	89.	122.	127.	117.	109.	97.	123.
98.	119.	114.	107.	101.	128.	128.	108.	90.	126.
123.	109.	105.	129.	97.	118.	110.	120.	98.	125.
123.	105.	105.	134.	113.	107.	134.	107.	108.	116.
110.	96.	106.	98.	117.	94.	107.	105.	109.	86.
115.	101.	91.	88.	113.	94.	115.	98.	88.	101.
97.	105.	113.	90.	94.	104.	92.	103.	91.	74.
91.	67.	84.	107.	75.	96.	90.	96.	71.	91.
120.	97.	84.	93.	85.	90.	93.	97.	111.	84.
84.	82.	85.	88.	80.	89.	73.	81.	96.	105.
84.	79.	126.	89.	91.	85.	103.	97.	81.	94.
88.	105.	99.	96.	92.	74.	95.	103.	100.	79.
93.	71.	83.	86.	89.	84.	94.	112.	85.	86.
89.	105.	101.	75.	81.	74.	81.	115.	94.	81.
83.	109.	95.	77.	80.	89.	97.	74.	86.	67.
91.	66.	87.	86.	108.	116.	94.	109.	93.	111.
83.	83.	107.	85.	98.	111.	84.	97.	91.	105.
81.	86.	93.	95.	103.	105.	99.	85.	94.	96.
100.	71.	90.	87.	103.	101.	86.	68.	87.	77.
92.	90.	92.	80.	95.	78.	86.	66.	83.	84.
77.	86.	69.	82.	85.	75.	90.	69.	51.	75.
75.	91.	64.	93.	73.	73.	80.	81.	91.	92.
75.	53.	82.	66.	72.	56.	72.	80.	63.	77.
71.	73.	76.	90.	73.	76.	68.	63.	51.	57.
75.	65.	77.	55.	74.	73.	65.	69.	59.	73.
66.	60.	69.	72.	75.	67.	95.	67.	79.	78.
59.	60.	80.	80.	68.	57.	78.	63.	69.	76.
65.	68.	53.	82.	71.	68.	58.	52.	70.	56.
49.	62.	65.	86.	69.	71.	72.	86.	64.	57.
77.	88.	70.	63.	71.	75.	70.	69.	70.	67.
64.	62.	76.	70.	66.	78.	52.	68.	79.	69.
65.	51.	79.	64.	90.	56.	76.	47.	51.	69.
76.	83.	84.	84.	60.	67.	73.	69.	62.	70.
65.	55.	67.	73.	62.	50.	48.	53.	59.	73.
50.	59.	54.	72.	65.	70.	72.	86.	64.	53.
68.	58.	44.	62.	77.	43.	64.	69.	49.	53.
76.	65.	80.	74.	55.	51.	49.	58.	71.	69.
52.	77.	75.	68.	74.	44.	69.	70.	66.	65.
73.	62.	78.	55.	73.	64.	75.	42.	49.	52.
92.	63.	76.	79.	56.	69.	73.	51.	64.	86.
66.	54.	65.	50.	73.	65.	53.	56.	68.	64.
40.	64.	64.	62.	62.	64.	87.	56.	74.	74.
79.	60.	62.	59.	60.	54.	71.	80.	83.	77.
68.	72.	66.	66.	73.	58.	74.	57.	56.	69.
80.	78.	64.	59.	84.	55.	80.	75.	59.	71.
67.	95.	74.	112.	102.	67.	76.	79.	72.	69.
77.	82.	83.	75.	96.	86.	71.	87.	78.	80.
106.	79.	89.	102.	91.	107.	109.	67.	95.	102.
82.	95.	113.	99.	101.	114.	101.	104.	92.	115.
86.	92.	87.	102.	89.	104.	122.	92.	92.	90.
110.	112.	89.	84.	82.	87.	87.	97.	80.	88.
105.	116.	111.	103.	80.	101.	102.	96.	96.	103.

83.	85.	81.	77.	85.	87.	86.	111.	107.	78.
91.	89.	95.	85.	87.	95.	72.	89.	98.	100.
103.	84.	73.	91.	90.	85.	66.	59.	87.	88.
86.	81.	93.	58.	64.	78.	53.	78.	67.	86.
87.	66.	84.	62.	75.	51.	66.	76.	80.	77.
77.	73.	79.	81.	79.	63.	71.	79.	60.	55.
76.	67.	67.	47.	48.	93.	68.	56.	54.	53.
48.	56.	70.	60.	54.	55.	59.	46.	59.	57.
57.	41.	70.	53.	48.	75.	47.	62.	50.	61.
49.	51.	53.	67.	77.	45.	61.	59.	57.	68.
60.	41.	47.	65.	55.	79.	56.	62.	65.	68.
65.	74.	72.	46.	55.	53.	53.	59.	52.	68.
53.	71.	90.	50.	56.	72.	59.	66.	56.	44.
50.	76.	70.	47.	92.	49.	64.	55.	46.	71.
68.	50.	63.	54.	64.	74.	47.	65.	66.	66.
80.	52.	54.	59.	54.	65.	58.	75.	61.	66.
72.	59.	62.	55.	68.	59.	75.	63.	64.	73.
52.	58.	70.	79.	68.	75.	56.	64.	70.	59.
91.	74.	63.	75.	69.	57.	70.	69.	76.	75.
80.	62.	74.	54.	100.	64.	76.	58.	75.	71.
70.	57.	66.	57.	64.	63.	68.	62.	66.	73.
62.	60.	68.	88.	54.	64.	69.	71.	71.	82.
62.	82.	72.	67.	70.	73.	80.	54.	70.	69.
71.	68.	78.	80.	71.	88.	51.	78.	75.	79.
94.	58.	71.	80.	76.	87.	77.	102.	86.	65.
76.	95.	71.	62.	83.	85.	66.	90.	74.	60.
70.	72.	73.	80.	66.	73.	58.	69.	77.	92.
87.	65.	59.	92.	79.	61.	80.	71.	82.	68.
64.	63.	71.	85.	73.	59.	74.	66.	66.	79.
54.	65.	70.	88.	80.	56.	62.	80.	74.	88.
75.	67.	64.	77.	73.	67.	49.	51.	72.	56.
57.	57.	53.	62.	50.	76.	52.	63.	65.	69.
57.	59.	54.	54.	56.	56.	72.	70.	55.	58.
76.	53.	58.	54.	61.	63.	55.	55.	56.	68.
58.	63.	68.	62.	67.	61.	51.	46.	60.	65.
45.	58.	73.	60.	64.	61.	61.	58.	74.	56.
60.	65.	59.	65.	62.	43.	62.	55.	57.	66.
51.	55.	75.	63.	64.	61.	63.	65.	57.	58.
49.	61.	52.	62.	67.	56.	55.	66.	69.	70.
68.	74.	62.	66.	61.	68.	58.	50.	38.	75.
66.	61.	66.	76.	66.	59.	64.	72.	55.	47.
64.	57.	55.	74.	70.	56.	60.	53.	79.	54.
72.	79.	60.	65.	93.	74.	76.	64.	62.	59.
66.	64.	80.	63.	44.	46.	59.	65.	56.	70.
57.	51.	71.	67.	59.	53.	59.	62.	75.	63.
54.	72.	47.	86.	62.	55.	85.	69.	68.	68.
48.	76.	68.	52.	57.	56.	61.	59.	57.	49.
57.	45.	51.	60.	63.	47.	63.	45.	65.	80.
55.	60.	64.	55.	54.	66.	61.	48.	48.	65.
57.	42.	52.	36.	55.	59.	55.	51.	60.	56.
66.	63.	53.	53.	66.	59.	57.	53.	46.	47.
51.	54.	56.	62.	52.	63.	47.	61.	45.	71.
56.	49.	55.	54.	59.	63.	55.	68.	46.	82.
51.	58.	52.	39.	74.	63.	62.	76.	65.	76.
64.	53.	55.	77.	79.	69.	78.	66.	59.	65.
65.	71.	67.	78.	59.	60.	82.	60.	69.	74.
70.	64.	70.	77.	60.	72.	82.	64.	83.	67.
69.	87.	80.	82.	73.	72.	83.	74.	69.	84.
87.	72.	87.	67.	93.	70.	61.	97.	78.	76.
92.	76.	77.	72.	80.	85.	92.	76.	79.	89.
71.	86.	101.	80.	96.	90.	73.	78.	74.	81.
73.	84.	82.	69.	111.	93.	86.	78.	72.	73.
81.	96.	72.	101.	86.	68.	69.	59.	89.	81.
85.	98.	88.	82.	100.	80.	98.	91.	89.	83.
83.	57.	76.	91.	64.	65.	68.	80.	74.	80.
61.	63.	79.	65.	68.	73.	62.	86.	67.	75.
83.	80.	82.	78.	76.	67.	93.	45.	83.	80.
85.	94.	73.	74.	83.	67.	69.	102.	80.	87.
92.	72.	77.	77.	69.	73.	74.	80.	70.	62.

82.	66.	57.	98.	74.	82.	64.	65.	72.	63.
79.	86.	77.	68.	76.	65.	63.	82.	59.	73.
61.	64.	57.	58.	62.	58.	71.	66.	75.	66.
58.	67.	69.	75.	76.	61.	95.	73.	79.	53.
77.	62.	74.	74.	81.	66.	57.	60.	67.	78.
72.	65.	83.	67.	60.	58.	69.	44.	55.	79.
59.	59.	76.	53.	83.	79.	55.	65.	58.	67.
67.	66.	63.	56.	79.	84.	71.	65.	65.	82.
63.	56.	67.	79.	60.	53.	61.	63.	78.	80.
92.	92.	70.	61.	77.	67.	82.	56.	57.	59.
73.	76.	78.	88.	74.	82.	86.	86.	63.	105.
78.	71.	86.	79.	92.	75.	79.	82.	80.	86.
87.	68.	86.	90.	91.	80.	80.	90.	88.	79.
96.	76.	86.	100.	78.	77.	96.	96.	84.	94.
86.	79.	84.	107.	72.	88.	89.	103.	90.	81.
82.	85.	93.	84.	88.	80.	100.	87.	103.	110.
89.	81.	74.	94.	97.	75.	74.	81.	70.	94.
79.	82.	64.	94.	87.	86.	89.	86.	85.	93.
81.	88.	88.	89.	83.	84.	84.	93.	86.	92.
91.	74.	104.	80.	99.	94.	63.	104.	89.	94.
96.	85.	70.	110.	79.	99.	91.	113.	124.	103.
128.	105.	99.	86.	99.	82.	83.	70.	95.	119.
97.	84.	106.	87.	115.	118.	126.	118.	122.	90.
95.	98.	119.	93.	125.	102.	108.	129.	95.	96.
124.	111.	132.	113.	93.	102.	121.	104.	102.	101.
101.	113.	99.	104.	111.	120.	105.	114.	95.	95.
123.	101.	85.	113.	95.	90.	82.	101.	85.	83.
123.	84.	92.	94.	87.	113.	81.	95.	91.	103.
99.	96.	84.	90.	84.	113.	95.	90.	77.	107.
101.	94.	91.	78.	84.	104.	111.	98.	93.	94.
81.	90.	82.	102.	101.	99.	87.	78.	102.	98.
68.	88.	92.	74.	81.	88.	64.	67.	93.	78.
59.	71.	72.	75.	74.	92.	75.	96.	64.	86.
94.	88.	73.	71.	97.	70.	72.	92.	74.	74.
75.	74.	52.	64.	75.	82.	94.	85.	61.	61.
65.	66.	72.	78.	64.	100.	59.	77.	94.	85.
69.	67.	62.	66.	84.	67.	73.	76.	67.	64.
86.	63.	67.	70.	67.	54.	77.	71.	69.	72.
58.	67.	48.	64.	83.	55.	68.	60.	51.	43.
72.	77.	66.	62.	56.	70.	55.	56.	75.	46.
71.	56.	70.	60.	51.	60.	67.	51.	64.	39.
65.	69.	75.	69.	62.	74.	64.	55.	74.	49.
63.	43.	66.	65.	55.	59.	65.	64.	75.	63.
69.	46.	53.	69.	60.	71.	70.	63.	65.	75.
56.	65.	50.	67.	48.	66.	72.	53.	46.	69.
52.	75.	67.	54.	58.	45.	54.	52.	45.	57.
60.	60.	59.	59.	54.	52.	50.	60.	64.	60.
59.	65.	69.	60.	51.	49.	53.	72.	72.	64.
75.	51.	76.	57.	59.	56.	73.	56.	78.	74.
54.	58.	63.	64.	61.	72.	51.	52.	60.	80.
70.	53.	66.	63.	77.	58.	56.	63.	70.	63.
67.	70.	68.	65.	78.	46.	63.	58.	56.	61.
76.	58.	53.	51.	55.	59.	53.	56.	56.	64.
67.	54.	62.	55.	74.	49.	53.	65.	70.	55.
62.	67.	60.	59.	51.	64.	56.	65.	55.	70.
63.	62.	60.	46.	71.	76.	72.	67.	66.	54.
65.	72.	51.	57.	54.	56.	68.	68.	65.	59.
59.	53.	63.	85.	50.	78.	57.	59.	48.	48.
54.	59.	65.	77.	57.	66.	65.	66.	67.	63.
65.	49.	46.	66.	62.	73.	54.	74.	56.	85.
66.	83.	67.	80.	53.	51.	79.	65.	68.	81.
56.	69.	60.	65.	68.	66.	61.	74.	52.	60.
63.	69.	65.	50.	58.	65.	59.	68.	58.	67.
49.	70.	63.	76.	45.	61.	45.	59.	52.	68.
78.	51.	68.	67.	64.	59.	59.	60.	55.	78.
70.	54.	54.	65.	64.	61.	60.	63.	66.	60.
72.	67.	59.	64.	52.	38.	43.	68.	65.	51.
45.	73.	74.	70.	54.	72.	64.	47.	53.	50.
66.	62.	66.	51.	90.	66.	48.	55.	52.	86.

43.	46.	53.	58.	42.	61.	58.	64.	63.	30.
66.	51.	64.	71.	82.	44.	50.	55.	50.	58.
66.	46.	61.	81.	54.	58.	44.	54.	61.	66.
68.	69.	59.	59.	61.	61.	56.	67.	48.	62.
63.	61.	59.	65.	56.	56.	60.	60.	64.	61.
62.	61.	58.	49.	51.	56.	43.	61.	58.	76.
54.	64.	52.	68.	58.	50.	66.	64.	60.	55.
58.	62.	56.	50.	69.	45.	62.	54.	66.	61.
60.	67.	53.	57.	59.	57.	79.	74.	60.	59.
59.	57.	63.	80.	54.	49.	73.	47.	58.	74.
73.	55.	73.	59.	68.	59.	68.	82.	65.	74.
71.	61.	42.	58.	49.	59.	74.	65.	51.	73.
53.	65.	72.	69.	78.	63.	67.	52.	70.	38.
65.	60.	66.	52.	57.	51.	60.	77.	62.	49.
72.	77.	57.	49.	72.	71.	82.	48.	83.	76.
72.	68.	66.	50.	74.	68.	61.	71.	55.	70.
39.	71.	74.	58.	64.	64.	58.	88.	83.	69.
62.	60.	78.	79.	65.	73.	61.	83.	85.	69.
66.	84.	67.	90.	75.	87.	49.	71.	73.	70.
84.	76.	69.	74.	56.	71.	74.	94.	63.	50.
74.	70.	71.	78.	66.	72.	71.	64.	91.	70.
71.	85.	80.	90.	76.	79.	76.	79.	80.	57.
96.									

Appendix S-1: Observed and calculated structure factors for olivine

h	k	l	10Fo	10Fc	10s
2	0	0	147	177	1
4	0	0	677	710	2
6	0	0	23	-13	1
1	1	0	49	-47	0
2	1	0	336	336	1
3	1	0	323	320	1
4	1	0	82	85	1
5	1	0	188	189	1
6	1	0	168	164	1
0	2	0	297	296	1
1	2	0	249	-249	1
2	2	0	57	57	1
3	2	0	271	-277	1
4	2	0	30	29	1
5	2	0	148	-153	1
6	2	0	45	-45	1
2	3	0	214	216	1
3	3	0	347	351	1
4	3	0	183	191	1
5	3	0	295	294	2
6	3	0	19	13	2
0	4	0	66	63	1
1	4	0	608	574	1
2	4	0	675	671	1
3	4	0	493	-505	1
4	4	0	306	308	2
5	4	0	80	78	1
6	4	0	374	367	2
1	5	0	339	334	1
2	5	0	72	-70	1
3	5	0	185	188	1
4	5	0	207	216	1
5	5	0	141	-141	1
6	5	0	82	-79	1
0	6	0	27	-30	1
1	6	0	169	166	1
2	6	0	87	-85	1
3	6	0	16	-7	1
4	6	0	171	176	1
5	6	0	47	41	1
6	6	0	191	189	1
1	7	0	662	660	1
2	7	0	172	-179	1
3	7	0	477	473	2
4	7	0	191	-192	1
5	7	0	164	162	1
0	8	0	135	126	1
1	8	0	113	-112	1
2	8	0	425	417	2
3	8	0	411	414	2
4	8	0	104	106	1
5	8	0	62	64	1
1	9	0	82	-77	1
2	9	0	154	-155	1
3	9	0	141	-139	1
4	9	0	118	-120	1
5	9	0	195	193	1
0	10	0	331	324	2
1	10	0	83	86	1
2	10	0	427	425	2
3	10	0	14	-9	2
4	10	0	64	62	1
1	11	0	178	178	1
2	11	0	22	12	1
3	11	0	215	214	1
4	11	0	90	86	1
0	12	0	320	318	2
1	12	0	35	-30	1
2	12	0	30	28	1
3	12	0	107	-106	1
1	13	0	14	-2	2
2	13	0	161	161	1
0	14	0	114	112	1
1	14	0	166	-161	1
1	0	1	289	-277	1
3	0	1	198	-206	1
5	0	1	91	-95	1
1	1	1	237	-213	1
2	1	1	350	347	1
3	1	1	234	-229	1
4	1	1	80	84	1
5	1	1	254	-256	1
6	1	1	128	125	1
0	2	1	459	-451	1
1	2	1	138	-136	1
2	2	1	64	51	1
3	2	1	143	-145	1
4	2	1	73	73	1
5	2	1	103	-104	1
6	2	1	218	215	1
2	6	7	89	-89	1
1	7	7	91	90	1
0	8	7	186	-180	1

h	k	l	10Fo	10Fc	10s
1	3	1	595	611	1
2	3	1	31	-29	1
3	3	1	373	380	1
4	3	1	26	-24	1
5	3	1	71	-73	1
6	3	1	18	14	2
0	4	1	367	-376	1
1	4	1	15	-2	1
2	4	1	413	-411	1
3	4	1	306	309	2
4	4	1	61	-60	1
5	4	1	101	103	1
6	4	1	34	31	1
1	5	1	208	-207	1
2	5	1	277	-285	1
3	5	1	65	-62	1
4	5	1	219	-222	1
5	5	1	190	-187	1
6	5	1	111	-109	1
0	6	1	590	597	1
1	6	1	31	-23	1
2	6	1	164	159	1
3	6	1	283	290	2
4	6	1	203	204	1
5	6	1	44	44	1
6	6	1	14	4	2
1	7	1	119	-117	1
2	7	1	104	-110	1
3	7	1	35	35	1
4	7	1	26	-23	1
5	7	1	139	140	1
0	8	1	127	134	1
1	8	1	88	95	1
2	8	1	165	-169	1
3	8	1	64	-59	1
4	8	1	135	-136	1
5	8	1	34	30	1
1	9	1	162	-165	1
2	9	1	48	45	1
3	9	1	44	-41	1
4	9	1	105	104	1
5	9	1	97	94	1
0	10	1	320	331	2
1	10	1	86	76	1
2	10	1	173	173	1
3	10	1	282	-281	2
4	10	1	142	144	1
1	11	1	18	-15	1
2	11	1	156	155	1
3	11	1	42	-39	1
4	11	1	172	170	1
0	12	1	342	-346	2
1	12	1	16	11	2
2	12	1	130	-128	1
3	12	1	162	-163	1
1	13	1	236	235	1
2	13	1	9	3	-4
0	14	1	166	-166	1
1	14	1	41	35	1
0	0	2	450	-445	1
2	0	2	159	-157	1
4	0	2	56	54	1
6	0	2	189	188	1
1	1	2	716	715	1
2	1	2	91	-95	1
3	1	2	397	401	1
4	1	2	267	-275	1
5	1	2	66	63	1
6	1	2	19	-9	2
0	2	2	153	152	1
1	2	2	508	-476	1
2	2	2	858	870	1
3	2	2	579	602	1
4	2	2	296	297	2
5	2	2	14	10	2
6	2	2	352	343	2
1	3	2	217	200	1
2	3	2	183	-188	1
3	3	2	17	-19	1
4	3	2	185	-194	1
5	3	2	242	241	1
6	3	2	12	-2	-3
0	4	2	211	212	1
1	4	2	49	51	1
2	4	2	284	281	1
3	4	2	177	178	1
4	4	2	16	-14	2
5	4	2	44	43	1
6	4	2	55	-55	1
1	5	2	273	267	1
0	0	8	486	504	2
2	0	8	237	243	2
1	1	8	15	-5	2

h	k	l	10Fo	10Fc	10s
2	5	2	95	-95	1
3	5	2	375	375	2
4	5	2	29	-29	1
5	5	2	362	363	2
6	5	2	72	-67	1
1	6	2	81	-84	1
2	6	2	211	208	1
3	6	2	51	-34	1
4	6	2	380	386	2
5	6	2	26	-21	1
1	7	2	139	-143	1
2	7	2	262	271	2
3	7	2	54	56	1
4	7	2	55	53	1
5	7	2	18	15	2
0	8	2	222	224	1
1	8	2	229	-239	1
2	8	2	139	139	1
3	8	2	165	-169	1
4	8	2	144	146	1
5	8	2	173	-170	1
1	9	2	522	541	2
2	9	2	162	164	1
3	9	2	332	333	2
4	9	2	89	88	1
5	9	2	184	180	1
0	10	2	123	-123	1
1	10	2	119	121	1
2	10	2	95	98	1
3	10	2	134	-133	1
4	10	2	98	94	1
1	11	2	142	143	1
2	11	2	88	-89	1
3	11	2	95	95	1
4	11	2	33	32	1
0	12	2	202	207	1
1	12	2	82	84	1
2	12	2	52	52	1
3	12	2	61	59	1
1	13	2	221	227	1
2	13	2	106	-107	1
0	14	2	77	78	1
1	0	3	89	-76	1
3	0	3	334	337	2
5	0	3	28	26	1
1	1	3	227	213	1
2	1	3	238	-234	1
3	1	3	127	121	1
4	1	3	120	-121	1
5	1	3	290	291	2
6	1	3	79	-77	1
0	2	3	62	67	1
1	2	3	227	222	1
2	2	3	156	155	1
3	2	3	67	64	1
4	2	3	143	-148	1
5	2	3	125	123	1
6	2	3	164	-160	1
1	3	3	513	-501	1
2	3	3	46	-41	1
3	3	3	316	-318	2
4	3	3	103	102	1
5	3	3	71	71	1
6	3	3	81	-75	1
0	4	3	536	524	1
1	4	3	112	104	1
2	4	3	207	201	1
3	4	3	329	-335	2
4	4	3	126	126	1
5	4	3	57	-57	1
1	5	3	143	140	1
2	5	3	270	274	2
3	5	3	128	122	1
4	5	3	173	171	1
5	5	3	111	109	1
0	6	3	463	-463	2
1	6	3	161	-164	1
2	6	3	153	-155	1
3	6	3	143	-144	1
4	6	3	167	-166	1
5	6	3	90	-90	1
1	7	3	134	135	1
2	7	3	125	126	1
3	7	3	69	-71	1
4	7	3	19	-13	1
5	7	3	75	-74	1
0	8	3	238	-242	1
1	8	3	26	-26	1
2	8	3	251	252	1
3	8	3	22	19	1
2	1	8	75	74	1
0	2	8	135	137	1

h	k	l	10Fo	10Fc	10s
4	8	3	60	61	1
5	8	3	16	-8	2
1	9	3	157	157	1
2	9	3	80	-79	1
3	9	3	38	35	1
4	9	3	43	-39	1
0	10	3	202	-199	1
1	10	3	14	5	2
2	10	3	216	-219	1
3	10	3	209	205	1
4	10	3	80	-80	1
1	11	3	15	3	2
2	11	3	129	-128	1
3	11	3	78	79	1
0	12	3	327	333	2
1	12	3	91	-93	1
2	12	3	105	104	1
1	13	3	199	-196	1
2	0	4	347	333	2
4	0	4	489	479	2
2	1	4	195	196	1
3	1	4	205	202	1
4	1	4	101	99	1
5	1	4	167	165	1
0	2	4	215	207	1
1	2	4	76	-81	1
2	2	4	26	22	1
3	2	4	259	-261	2
4	2	4	40	38	1
5	2	4	105	-102	1
1	3	4	470	470	1
2	3	4	162	167	1
3	3	4	300	290	2
4	3	4	159	155	1
5	3	4	211	205	1
0	4	4	149	137	1
1	4	4	224	223	2
2	4	4	414	407	2
3	4	4	326	-318	2
4	4	4	256	256	2
5	4	4	50	43	1
1	5	4	265	264	2
2	5	4	17	-16	1
3	5	4	130	129	1
4	5	4	145	143	1
5	5	4	107	-103	1
0	6	4	111	-111	1
1	6	4	103	103	1
2	6	4	18	-14	1
3	6	4	13	5	2
4	6	4	112	109	1
5	6	4	32	32	1
1	7	4	504	496	2
2	7	4	151	-156	1
3	7	4	349	349	2
4	7	4	139	-135	1
0	8	4	128	126	1
1	8	4	26	-22	1
2	8	4	294	294	2
3	8	4	295	295	2
4	8	4	94	94	1
1	9	4	73	-71	1
2	9	4	124	-125	1
3	9	4	93	-92	1
4	9	4	98	-95	1
0	10	4	279	282	2
1	10	4	37	35	1
2	10	4	317	314	2
3	10	4	22	16	1
1	11	4	139	139	1
2	11	4	24	20	1
0	12	4	223	225	2
1	12	4	32	-29	1
1	0	5	256	-263	2
3	0	5	68	-69	1
5	0	5	113	-110	1
1	1	5	94	-89	1
2	1	5	223	224	1
3	1	5	187	-184	1
4	1	5	45	44	1
5	1	5	139	-136	1
0	2	5	325	-335	2
1	2	5	18	-13	1
2	2	5	94	94	1
3	2	5	138	-137	1
4	2	5	9	0	-3
5	2	5	56	-53	1
1	3	5	386	385	2
2	3	5	57	-59	1
3	3	5	239	236	2
1	2	8	25	24	1
1	3	8	199	205	1

h	k	l	10Fo	10Fc	10s
4	3	5	37	34	1
5	3	5	53	-53	1
0	4	5	159	-155	1
1	4	5	89	90	1
2	4	5	326	-329	2
3	4	5	166	165	1
4	4	5	24	10	1
5	4	5	103	98	1
1	5	5	129	-129	1
2	5	5	176	-178	1
3	5	5	12	-2	2
4	5	5	183	-178	1
0	6	5	369	371	2
1	6	5	88	-89	1
2	6	5	112	110	1
3	6	5	278	272	2
4	6	5	155	150	1
1	7	5	76	-72	1
2	7	5	60	-58	1
3	7	5	6	-6	-6
4	7	5	44	-42	1
0	8	5	29	22	1
1	8	5	93	89	1
2	8	5	33	-31	1
3	8	5	65	-62	1
1	9	5	114	-112	1
2	9	5	25	11	1
3	9	5	36	-32	1
0	10	5	290	290	2
1	10	5	99	97	1
2	10	5	78	77	1
1	11	5	21	-16	1
0	0	6	315	-325	2
2	0	6	28	-20	1
4	0	6	17	-12	2
1	1	6	386	391	2
2	1	6	99	-97	1
3	1	6	210	209	1
4	1	6	139	-135	1
0	2	6	185	188	1
1	2	6	63	-60	1
2	2	6	387	386	2
3	2	6	289	282	2
4	2	6	208	204	1
1	3	6	76	75	1
2	3	6	121	-124	1
3	3	6	36	33	1
4	3	6	129	-125	1
0	4	6	194	195	1
1	4	6	29	-30	1
2	4	6	122	120	1
3	4	6	166	163	1
4	4	6	22	17	1
1	5	6	133	132	1
2	5	6	36	-32	1
3	5	6	205	204	1
4	5	6	53	-51	1
0	6	6	541	537	2
1	6	6	54	-52	1
2	6	6	207	209	1
3	6	6	23	-21	1
1	7	6	81	-79	1
2	7	6	152	148	1
3	7	6	23	19	1
0	8	6	160	159	1
1	8	6	86	-84	1
2	8	6	63	62	1
1	9	6	329	325	2
2	9	6	110	106	1
0	10	6	52	-48	1
1	0	7	55	-54	1
3	0	7	225	226	1
1	1	7	87	89	1
2	1	7	115	-115	1
3	1	7	45	43	1
0	2	7	27	25	1
1	2	7	118	117	1
2	2	7	124	122	1
3	2	7	29	25	1
1	3	7	258	-261	2
2	3	7	32	-29	1
3	3	7	169	-169	1
0	4	7	296	303	2
1	4	7	59	58	1
2	4	7	77	79	1
3	4	7	211	-207	1
1	5	7	61	61	1
2	5	7	161	160	1
0	6	7	231	-227	1
1	6	7	133	-131	1
0	4	8	94	98	1
1	4	8	36	32	1

Appendix S-2: Observed and calculated structure factors for diopside

h	k	l	10Fo	10Fc	10s
2	0	0	76	50	1
4	0	0	135	190	1
6	0	0	886	849	2
8	0	0	819	819	3
10	0	0	565	559	3
12	0	0	105	-96	1
1	1	0	30	-28	1
3	1	0	812	766	1
5	1	0	683	-661	2
7	1	0	419	412	2
9	1	0	51	-38	1
11	1	0	316	313	2
13	1	0	209	-205	2
0	2	0	240	230	1
2	2	0	661	-666	1
4	2	0	245	-231	2
6	2	0	222	-224	2
8	2	0	230	-219	2
10	2	0	33	-28	2
12	2	0	203	-198	2
1	3	0	162	170	1
3	3	0	676	670	2
5	3	0	444	441	2
7	3	0	65	-59	1
9	3	0	360	350	2
11	3	0	204	204	2
0	4	0	32	-57	1
2	4	0	155	173	1
4	4	0	669	-672	2
6	4	0	340	330	2
8	4	0	133	125	1
10	4	0	502	-486	3
12	4	0	215	209	2
1	5	0	1035	-999	2
3	5	0	649	-704	2
5	5	0	88	98	1
7	5	0	1228	-1187	3
9	5	0	131	-122	1
11	5	0	475	-459	3
0	6	0	1034	-1004	2
2	6	0	328	340	2
4	6	0	127	-130	1
6	6	0	90	94	1
8	6	0	172	-160	1
10	6	0	364	-352	2
1	7	0	30	-20	2
3	7	0	152	149	1
5	7	0	435	482	3
7	7	0	288	-286	2
9	7	0	245	227	2
0	8	0	69	-66	1
2	8	0	342	-347	2
4	8	0	433	-457	3
6	8	0	80	-84	1
8	8	0	120	-121	1
10	8	0	360	-350	2
1	9	0	63	-57	1
3	9	0	209	214	2
5	9	0	188	-199	1
7	9	0	147	155	1
9	9	0	95	-91	2
0	10	0	798	788	3
2	10	0	101	84	1
4	10	0	550	564	3
6	10	0	212	230	2
8	10	0	211	235	2
1	11	0	36	29	2
3	11	0	228	230	2
5	11	0	349	-348	2
0	12	0	417	407	3
2	12	0	287	-277	2
-13	1	1	30	-3	3
-11	1	1	316	-307	2
-9	1	1	62	-57	1
-7	1	1	399	-404	2
-5	1	1	140	134	1
-3	1	1	880	-895	2
-1	1	1	78	-92	1
1	1	1	190	-199	1
3	1	1	850	-822	2
5	1	1	37	18	1
7	1	1	310	-308	2
9	1	1	51	43	2
11	1	1	411	-419	3
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-10	2	1	24	16	3
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-6	2	1	503	494	2
-4	2	1	664	637	2
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-8	2	4	111	-117	1
-6	2	4	54	-44	1
-4	2	4	333	-348	2
-2	2	4	185	-192	1
0	2	4	140	144	4
2	2	4	611	-609	3
4	2	4	32	-17	2
6	2	4	26	-17	3
8	2	4	187	-189	2
-11	3	4	211	206	2
-9	3	4	259	268	2
-7	3	4	34	-25	2
-5	3	4	300	316	2
-3	3	4	292	314	2
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3	3	4	350	354	2
2	2	1	1162	1144	2
4	2	1	284	265	2
6	2	1	781	792	2
8	2	1	416	404	3
10	2	1	46	-38	2
12	2	1	496	496	3
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-11	3	1	269	256	2
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-7	3	1	485	-486	2
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-1	3	1	869	856	2
1	3	1	251	-205	2
3	3	1	392	368	2
7	3	1	215	-217	2
9	3	1	492	484	3
11	3	1	104	94	1
-12	4	1	278	270	2
-10	4	1	343	-331	3
-8	4	1	216	-213	2
-6	4	1	138	-136	1
-4	4	1	130	-139	1
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8	4	1	74	-75	1
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-3	5	1	140	-127	1
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3	5	1	177	-175	1
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7	5	1	86	87	1
9	5	1	84	80	1
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6	6	1	81	84	1
8	6	1	269	264	2
10	6	1	247	244	2
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-7	7	1	40	19	2
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1	7	1	620	-624	3
3	7	1	84	-77	1
5	7	1	505	-537	3
7	7	1	126	-127	1
9	7	1	567	-558	3
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-8	8	1	377	-371	2
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-2	8	1	1026	-988	3
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2	8	1	559	-569	3
4	8	1	162	-177	1
6	8	1	570	-597	3
8	8	1	167	-167	1
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-7	9	1	575	638	3
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3	9	1	192	199	1
5	9	1	268	-280	2
7	9	1	399	412	2
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-4	10	1	44	-39	2
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0	10	1	157	140	16
2	10	1	79	-76	1
4	10	1	104	-106	1
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-6	6	4	285	-302	2
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4	6	4	555	-565	3
6	6	4	348	350	2
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-7	7	4	164	-176	1
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1	7	4	38	32	2
3	7	4	72	66	1
5	7	4	162	155	1
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-3	11	1	118	-115	1
-1	11	1	132	-126	1
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3	11	1	188	-188	2
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-10	0	2	706	-699	3
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2	0	2	970	-900	2
4	0	2	1229	-1200	2
6	0	2	105	114	1
8	0	2	528	-535	3
10	0	2	797	-821	3
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-9	1	2	304	309	2
-7	1	2	966	-966	2
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-3	1	2	110	87	1
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7	1	2	522	-516	3
9	1	2	306	317	2
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-6	2	2	506	528	2
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-5	3	2	335	-369	2
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1	3	2	501	-497	2
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7	3	2	288	-293	2
9	3	2	175	-177	1
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6	4	2	38	-14	2
8	4	2	83	-79	1
10	4	2	94	93	2
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-7	5	2	915	952	3
-5	5	2	110	111	1
-3	5	2	1054	1081	2
-1	5	2	129	128	1
1	5	2	747	742	2
3	5	2	1120	1142	2
5	5	2	52	32	1
7	5	2	617	617	3
9	5	2	141	144	1
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-10	2	5	45	-41	2
-8	2	5	622	627	3
-6	2	5	148	145	1
-4	2	5	200	206	2
-2	2	5	479	477	3
0	2	5	164	163	3
2	2	5	789	788	3
4	2	5	174	-167	1
6	2	5	415	428	3
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-9	3	5	598	607	3
-7	3	5	118	117	1
-5	3	5	418	422	2
2	6	2	108	-109	1
4	6	2	191	188	1
6	6	2	224	-218	2
8	6	2	164	160	1
10	6	2	195	189	2
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-9	7	2	205	-194	2
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-3	7	2	116	110	1
-1	7	2	420	-412	3
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3	7	2	192	206	1
5	7	2	364	-369	2
7	7	2	51	-54	2
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4	8	2	294	306	2
6	8	2	278	286	2
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1	9	2	100	-94	1
3	9	2	61	-52	2
5	9	2	152	159	1
7	9	2	211	-210	2
-8	10	2	200	-177	2
-6	10	2	289	-267	2
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2	10	2	59	-61	2
4	10	2	705	-732	3
6	10	2	117	-118	1
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-3	11	2	175	-170	2
-1	11	2	167	151	2
1	11	2	151	-158	1
3	11	2	203	-208	2
-2	12	2	420	394	3
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5	1	3	217	210	2
7	1	3	303	303	2
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4	2	3	93	94	1
6	2	3	711	-721	3
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1	7	5	314	-310	2
3	7	5	313	-314	2
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-4	8	5	98	-96	1
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0	8	5	70	-71	4
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4	4	3	493	506	3
6	4	3	144	-143	1
8	4	3	137	132	1
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3	5	3	38	-30	2
5	5	3	109	105	1
7	5	3	63	-66	2
9	5	3	263	-269	2
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-8	6	3	139	-152	1
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-2	6	3	195	-199	1
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2	6	3	36	22	2
4	6	3	410	-429	3
6	6	3	141	-139	1
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-7	9	3	445	-446	3
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-3	9	3	195	-192	1
-1	9	3	365	354	2
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-2	10	3	169	164	2
0	10	3	44	6	6
2	10	3	243	245	2
4	10	3	132	-141	1
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1	11	3	206	204	2
-12	0	4	141	131	1
-10	0	4	423	418	3
-8	0	4	41	-16	2
-6	0	4	1054	1080	3
-4	0	4	726	729	2
-2	0	4	74	-74	1
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7	1	4	123	125	1
9	1	4	238	-243	2
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2	4	6	372	-363	3
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-5	5	6	67	63	2

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-6	4	4	60	10	1	2	8	4	127	-129	1	-10	4	5	288	-288	2	-4	0	6	694	-677	3	-2	6	6	38	-29	2
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6	4	4	133	132	1	1	9	4	28	17	3	2	4	5	230	232	2	-7	1	6	270	-257	2	-5	1	7	111	-103	1
8	4	4	69	65	2	3	9	4	107	105	1	4	4	5	522	-512	3	-5	1	6	254	247	2	-3	1	7	288	270	2
-11	5	4	217	-222	2	-4	10	4	322	309	2	6	4	5	39	-37	2	-3	1	6	369	-362	2	-1	1	7	106	105	1
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Appendix S-3: Observed and calculated structure factors for muscovite

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3	1	0	135	-124	14
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7	1	0	121	94	-25
0	2	0	396	357	5
2	2	0	545	497	6
4	2	0	547	520	8
6	2	0	116	121	-25
1	3	0	434	-388	5
3	3	0	364	-281	8
5	3	0	122	-122	21
7	3	0	102	-37	-36
0	4	0	358	-303	6
2	4	0	708	654	6
4	4	0	531	-529	8
6	4	0	107	69	-27
1	5	0	347	337	6
3	5	0	31	40	-31
5	5	0	154	-165	17
0	6	0	2558	-2481	18
2	6	0	1004	-985	9
4	6	0	678	-677	9
6	6	0	197	219	19
1	7	0	276	297	10
3	7	0	138	139	17
5	7	0	122	74	-25
0	8	0	357	-320	9
2	8	0	30	-45	-30
4	8	0	448	-430	11
1	9	0	542	529	9
3	9	0	412	407	10
5	9	0	222	209	16
0	10	0	258	-238	12
2	10	0	514	-552	9
4	10	0	148	121	21
1	11	0	148	-157	20
3	11	0	36	4	-36
0	12	0	732	721	10
2	12	0	197	191	17
-7	1	1	348	-362	13
-5	1	1	82	-85	-31
-3	1	1	53	-65	-53
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1	1	1	549	-536	5
3	1	1	316	-304	8
5	1	1	461	-464	9
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2	6	21	161	-160	18
-3	7	21	126	127	-25
-1	7	21	98	92	-29
1	7	21	355	333	12
-2	8	21	160	154	19
0	8	21	244	238	11
-4	0	22	345	333	12
-2	0	22	253	249	13
0	0	22	876	854	9
2	0	22	350	335	11
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-3	1	22	444	-423	10
-1	1	22	295	-309	12
1	1	22	357	-355	11
3	1	22	106	-135	-28
-4	2	22	155	174	21
-2	2	22	184	-188	14
0	2	22	61	95	-28
2	2	22	245	-282	15
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-1	5	22	344	339	11
1	5	22	298	302	13
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0	6	22	802	-757	10
2	6	22	114	-101	-26
-1	7	22	220	213	15
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-3	1	23	63	-71	-63

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-3	5	14	234	241	12
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2	6	14	412	405	9
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3	7	14	112	106	22
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-1	9	14	213	235	15
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3	9	14	36	-80	-36
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2	10	14	162	-160	18
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-3	5	16	83	-82	-31
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1	5	16	77	56	-29
3	5	16	31	-32	-31
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-2	6	16	32	-37	-32
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2	6	16	86	-94	-28
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-1	7	16	122	113	19
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3	1	17	338	321	10
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2	0	26	727	-662	11
-3	1	26	134	116	24

-2	0	18	1148	-1180	10
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3	3	18	169	157	16
-4	4	18	291	-305	13
-2	4	18	207	202	13
0	4	18	361	-354	18
2	4	18	216	219	12
4	4	18	144	-148	21
-5	5	18	214	-174	17
-3	5	18	62	-89	-62
-1	5	18	139	-143	17
1	5	18	82	90	-31
3	5	18	33	-20	-33
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3	7	18	34	-14	-34
-2	8	18	108	-80	-26
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-1	9	18	397	-382	12
1	9	18	347	-312	12
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-3	1	19	145	-154	17
-1	1	19	213	219	12
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3	1	19	217	213	13
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3	3	20	36	29	-36
-4	4	20	62	-53	-62
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0	4	20	76	-92	-27
2	4	20	181	-164	15
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-3	5	20	211	-198	14
-1	5	20	138	-161	19
1	5	20	419	-401	10
3	5	20	142	-162	22
-4	6	20	573	-578	11
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0	8	20	259	-246	11
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-2	4	26	35	-12	-35
0	4	26	181	-186	16
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1	1	27	36	-40	-36

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-1	3	23	350	-334	11
1	3	23	698	-666	10
3	3	23	336	319	13
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-2	4	23	198	194	16
0	4	23	352	332	8
2	4	23	160	167	22
-3	5	23	207	-201	17
-1	5	23	34	23	-34
1	5	23	125	-148	23
-2	6	23	79	106	-49
0	6	23	112	96	-23
-1	7	23	575	-531	11
-4	0	24	203	-197	17
-2	0	24	697	-656	10
0	0	24	609	568	7
2	0	24	289	250	13
-3	1	24	328	319	12
-1	1	24	77	117	-47
1	1	24	55	84	-55
3	1	24	36	-45	-36
-4	2	24	131	126	23
-2	2	24	51	38	-51
0	2	24	218	228	10
2	2	24	125	-143	-27
-3	3	24	53	-20	-53
-1	3	24	89	102	-36
1	3	24	104	-104	-57
-2	4	24	124	-129	24
0	4	24	411	-377	8
2	4	24	259	251	14
-3	5	24	236	-210	15
-1	5	24	192	-183	17
1	5	24	35	33	-35
-2	6	24	460	424	11
0	6	24	382	-343	9
-3	1	25	289	-300	14
-1	1	25	35	63	-35
1	1	25	36	33	-36
-2	2	25	194	-185	16
0	2	25	34	11	-24
2	2	25	35	33	-35
-2	2	27	37	-93	-37
0	2	27	36	-73	-25
-1	3	27	657	623	11
0	0	28	118	144	-24
-1	1	28	75	29	-75

Appendix S-4: Observed and calculated structure factors for phlogopite

h	k	l	10Fo	10Fc	10s
2	0	0	1066	1001	5
4	0	0	51	-30	6
6	0	0	107	100	5
1	1	0	366	-305	3
0	2	0	402	-355	3
2	2	0	462	436	3
4	2	0	278	288	3
6	2	0	172	171	4
1	3	0	612	576	4
3	3	0	541	-525	4
5	3	0	655	-668	5
0	4	0	498	490	4
2	4	0	54	-41	4
4	4	0	202	206	3
6	4	0	318	319	4
1	5	0	162	-158	3
3	5	0	106	-106	3
5	5	0	214	206	4
0	6	0	1477	1481	6
2	6	0	948	958	7
4	6	0	49	23	7
6	6	0	69	-57	6
1	7	0	265	-280	3
3	7	0	56	48	6
5	7	0	97	92	5
0	8	0	68	55	5
2	8	0	66	-62	5
4	8	0	141	127	4
1	9	0	335	345	3
3	9	0	373	-383	4
5	9	0	397	-389	4
0	10	0	100	-97	4
2	10	0	65	56	6
4	10	0	127	127	5
1	11	0	153	-151	4
3	11	0	74	53	6
0	12	0	752	754	5
2	12	0	371	366	4
-6	0	1	208	-208	4
-4	0	1	745	750	5
-2	0	1	634	578	5
0	0	1	424	-417	4
2	0	1	936	-910	5
4	0	1	610	-613	4
6	0	1	146	-148	4
-7	1	1	72	50	7
-5	1	1	90	-89	5
-3	1	1	242	-247	3
-1	1	1	187	-161	2
1	1	1	364	336	3
3	1	1	456	453	3
5	1	1	275	272	3
7	1	1	47	52	-11
-4	2	1	157	-156	3
-2	2	1	496	475	4
0	2	1	77	68	2
2	2	1	367	362	3
4	2	1	557	551	4
6	2	1	45	30	9
-7	3	1	63	-62	8
-5	3	1	476	464	4
-3	3	1	1508	1482	6
-1	3	1	1046	999	5
1	3	1	410	-399	3
3	3	1	121	100	3
5	3	1	248	244	3
7	3	1	126	126	5
-6	4	1	84	58	5
-4	4	1	74	72	4
-2	4	1	268	-272	2
0	4	1	402	397	2
2	4	1	504	493	4
4	4	1	207	193	3
6	4	1	168	160	4
-5	5	1	54	-51	7
-3	5	1	237	-252	3
-1	5	1	214	-211	2
1	5	1	299	300	3
3	5	1	304	304	3
5	5	1	207	203	4
-6	6	1	181	-178	4
-4	6	1	346	342	3
-2	6	1	744	749	5
0	6	1	531	-525	3
2	6	1	829	-817	6
4	6	1	280	-273	3
6	6	1	252	-245	4
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-3	7	1	133	-133	4
-1	7	1	42	-28	7
0	8	6	275	276	2
2	8	6	236	234	4
4	8	6	160	154	5
-3	9	6	157	162	4
-1	9	6	196	-195	4
1	9	6	611	-623	5
3	9	6	432	-435	4
-4	10	6	46	-27	-9
-2	10	6	67	71	7
0	10	6	148	131	3
2	10	6	286	279	4
-1	11	6	31	-6	-16
1	11	6	105	99	5
-6	0	7	305	305	4
-4	0	7	52	-46	6
-2	0	7	1077	-1137	7

h	k	l	10Fo	10Fc	10s
1	7	1	55	45	6
3	7	1	369	366	3
5	7	1	218	220	4
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-2	8	1	123	-124	4
0	8	1	158	159	2
2	8	1	303	300	3
4	8	1	192	189	4
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-3	9	1	764	779	5
-1	9	1	479	469	4
1	9	1	47	27	7
3	9	1	82	-68	5
5	9	1	113	119	5
-4	10	1	105	-98	5
-2	10	1	37	-25	-9
0	10	1	33	9	-14
2	10	1	175	169	4
4	10	1	197	206	4
-3	11	1	125	-119	5
-1	11	1	64	-56	6
1	11	1	13	-12	-13
3	11	1	211	206	4
-2	12	1	254	239	4
0	12	1	186	-181	11
2	12	1	389	-390	4
-6	0	2	773	778	5
-4	0	2	949	957	7
-2	0	2	413	-392	3
0	0	2	158	-113	1
-7	1	2	109	-107	5
-5	1	2	120	-120	4
-1	1	2	622	591	4
1	1	2	863	832	4
3	1	2	368	372	3
5	1	2	35	8	-10
7	1	2	63	-44	7
-6	2	2	42	-8	-9
-4	2	2	228	-225	3
-2	2	2	368	379	3
0	2	2	828	776	4
2	2	2	32	-4	-7
4	2	2	118	120	4
6	2	2	105	-112	5
-7	3	2	240	239	4
-5	3	2	347	341	3
-3	3	2	543	-520	4
-1	3	2	953	-908	5
1	3	2	303	-282	3
3	3	2	246	-246	3
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0	4	2	312	305	2
2	4	2	557	557	4
4	4	2	92	-92	4
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1	5	2	657	654	4
3	5	2	312	320	3
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0	6	2	117	105	2
2	6	2	135	122	3
4	6	2	253	246	3
6	6	2	247	242	4
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1	7	2	360	365	3
3	7	2	173	171	3
5	7	2	65	50	6
-4	8	2	21	5	-21
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0	8	2	227	226	2
2	8	2	276	282	3
4	8	2	71	-71	6
-5	9	2	257	241	4
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-1	9	2	671	-668	5
1	9	2	276	-277	3
3	9	2	150	-150	4
5	9	2	148	-153	5
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0	10	2	269	273	2
2	10	2	134	129	4
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2	8	7	110	118	5
-3	9	7	124	-119	5
-1	9	7	272	-269	4
1	9	7	216	220	4
3	9	7	306	305	4
-2	10	7	222	220	4
0	10	7	197	193	3
2	10	7	59	51	8
-1	11	7	178	173	4
-6	0	8	124	-116	5
-4	0	8	94	-104	4
-2	0	8	264	266	3
0	0	8	555	584	3
2	0	8	590	614	4
4	0	8	296	303	4

h	k	l	10Fo	10Fc	10s
4	10	2	60	42	7
-3	11	2	19	-11	-19
-1	11	2	274	274	4
1	11	2	240	231	4
3	11	2	123	117	5
-2	12	2	68	-54	7
0	12	2	65	-56	5
2	12	2	118	120	5
-6	0	3	385	-374	4
-4	0	3	814	-808	6
-2	0	3	298	-281	3
0	0	3	997	-1017	5
2	0	3	399	-409	3
4	0	3	162	174	3
6	0	3	158	162	4
-7	1	3	48	-32	9
-5	1	3	173	180	4
-1	1	3	799	758	4
1	1	3	361	365	3
3	1	3	50	42	5
5	1	3	53	-48	6
-4	2	3	183	190	3
-2	2	3	180	176	2
0	2	3	601	583	7
2	2	3	335	-334	3
4	2	3	188	-195	3
6	2	3	30	8	-15
-7	3	3	368	368	4
-5	3	3	57	30	6
-3	3	3	116	106	3
-1	3	3	956	947	5
1	3	3	634	630	5
3	3	3	588	599	4
5	3	3	805	803	6
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3	11	3	103	-106	5
-2	12	3	266	-263	4
0	12	3	251	-249	3
2	12	3	143	-151	5
-6	0	4	61	-65	7
-4	0	4	12	115	-12
-2	0	4	603	619	4
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4	0	4	817	855	6
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-4	0	9	32	-21	-10
-2	0	9	100	111	4
0	0	9	197	-187	3
2	0	9	136	127	4
4	0	9	122	-115	5
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-3	1	9	67	57	5
-1	1	9	69	-78	5

h	k	l	10Fo	10Fc	10s
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5	1	4	65	60	6
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4	2	4	114	-117	4
6	2	4	197	189	4
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3	3	4	413	437	4
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-5	7	4	305	303	4
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3	7	9	66	52	8
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-2	8	9	90	-80	5
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1	5	10	102	101	5
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-2	2	11	94	101	5
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-2	4	11	151	144	4
0	4	11	229	223	4

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-3	1	12	120	106	4
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1	1	12	50	33	9
-4	2	12	153	151	5
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2	2	12	60	56	8
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-1	3	12	484	-455	4
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-4	4	12	116	116	5
-2	4	12	-171	161	4
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0	2	13	120	-103	4
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1	3	13	362	339	4
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0	4	13	49	-40	7
-1	5	13	83	-67	6
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0	0	14	121	130	4
-1	1	14	94	-83	5
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Appendix S-5: Observed and calculated structure factors for chabazite

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-3	6	0	1420	1408	10
0	6	0	114	105	16
-2	7	0	982	-1031	29
-4	8	0	2633	2741	11
-1	8	0	172	56	7
-3	9	0	137	-51	9
0	9	0	2896	3009	32
-5	10	0	693	741	7
-2	10	0	656	-673	16
-4	11	0	543	-541	4
-1	11	0	548	-519	5
-6	12	0	184	-229	11
-3	12	0	428	450	5
0	12	0	683	703	13
-5	13	0	1086	1100	8
-2	13	0	406	-470	8
-7	14	0	516	-505	7
-4	14	0	432	388	6
-1	14	0	450	444	11
-6	15	0	167	-190	9
-3	15	0	196	-217	10
0	15	0	110	-111	17
-8	16	0	402	346	8
-5	16	0	373	-350	7
-2	16	0	419	-397	6
-7	17	0	247	-243	12
-4	17	0	889	857	6
-1	17	0	103	77	20
-9	18	0	998	925	9
-6	18	0	34	24	-24
-3	18	0	75	-100	-34
-8	19	0	274	-247	15
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0	2	1	1368	-1200	9
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-4	4	1	3937	3866	245
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-3	5	1	559	-533	7
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-11	12	1	359	-392	5
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-2	12	1	465	-501	5
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-10	13	1	47	13	-33
-7	13	1	163	-176	9
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-12	14	1	346	-295	8
-9	14	1	352	364	6
-6	14	1	31	-12	-22
-3	14	1	382	-371	6
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