ASPECTS OF THE CRYSTAL CHEMISTRY OF THE TOURMALINE-GROUP MINERALS

BY

CHRISTINE M. CLARK McCRACKEN

A Thesis

Submitted to the Faculty of Graduate Studies

In Partial Fulfillment of the Requirements

for the Degree of

DOCTOR OF PHILOSOPHY

Department of Geological Sciences

University of Manitoba

Winnipeg, Manitoba

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FACULTY OF GRADUATE STUDIES

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ABSTRACT

Tourmaline is a complex borosilicate with the general formula: $^{[9]}X\ ^{[6]}Y_3\ ^{[6]}Z_6\ ^{[4]}T_6\ O_{18}\ (^{[3]}BO_3)_3\ V_3\ W$; it is common as an accessory mineral throughout the rock cycle. Due to complexities in the chemical composition, including the presence of the light elements B, H and (often) Li, transition-metals in multiple valence states, and chemical heterogeneity, tourmaline is not as well understood as other common accessory minerals.

Tourmaline normalization procedures have been compared to determine which schemes provide the most accurate mineral formula when there is undetermined information. Normalization on 31 anions, assuming OH values if necessary, produces a more useful formula than schemes that ignore F or B. Iteration of Li may give a first approximation of Li content; Li_2O may be added to the calculations until $Y + Z + T = 15$ *apfu*.

A number of potential new tourmaline species have been described, including "fluordravite", ideally $Na\ Mg_3\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$; "fluorschorl", ideally $Na\ Fe^{2+}{}_3\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$; "fluorelbaite", ideally $Na\ (Li_{1.5}Al_{1.5})\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$; "hydroxyuvite", ideally $Ca\ Mg_3\ (Al_5Mg)\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ (OH)$; and "cralpoite", ideally $Na\ Cr^{3+}{}_3\ (Al_4Mg_2)\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ O$.

A suite of chromian tourmalines were investigated, with Cr_2O_3 values ranging up to ~35 wt%. Comparison of SREF and EMPA data show details of Cr site assignment. Included in this suite are "cralpoite" and chromdravite, whose approved formula may need to be revised to show Cr dominant at both the *Y*- and *Z*-sites. Problems remain with

some of the chromian tourmaline analyses, which may not be resolved until accurate H-values can be determined.

Comparison of SREF and EMPA data for povondraite show the best method for distributing species between the octahedral sites involves filling the *Z*-site in the order Al, Mg, Fe^{3+}; there is indication that minor amounts of Fe^{2+} also occur. Povondraite has the most K reported for any species of tourmaline, and in some analyses (Na + K) exceeds the structural maximum of 1 *apfu*. The nature of the excess alkalis has not yet been resolved, but cannot be real as no additional electron-density is seen in the refined crystal structures.

The triangular (BO_3) groups in tourmaline have thus far been assumed to be relatively constant in dimensions. SREF and EMPA data for a suite of 99 tourmalines indicate that the B-O2 and B-O8 bond lengths are not constant, but vary according to the chemical composition of the tourmaline. Statistical analysis of the bond-valence contributions for the *X*-O2, *Y*-O2, *Z*-O8 and *Z'*-O8 bonds as they relate to the B-O2/B-O8 bond-valence indicate that the geometry of the (BO_3) triangle is most influenced by the *Z'*-O8 bond.

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

Introduction

1.1 General information

The most common borosilicate mineral and the largest sink for B in rocks is tourmaline. Tourmaline occurs in igneous, metamorphic and sedimentary rocks (London *et al.* 1996). It is a sensitive petrologic indicator and has long been valued as a gemstone. Tourmaline is also a polar mineral, exhibiting both morphological and chemical asymmetry. This polarity leads to a number of industrial uses for the mineral (Henry and Dutrow 1996).

Although tourmaline is an important accessory mineral, it is not yet well understood. This has been commented on recently by a number of authors (*e.g.* Henry and Guidotti 1985, Hawthorne *et al.* 1993, Hawthorne 1996). There are several reasons for this lack of understanding. For a long time, tourmaline was thought to occur predominantly in rare-element pegmatites, and therefore not to be a common mineral. Also, tourmaline is difficult to dissolve for wet-chemical analysis. Additionally, it is commonly strongly zoned. Finally, a number of key components and features (*i.e.* H, Li, B, Fe^{3+}/Fe^{2+}, Mg/Al site-ordering) cannot be studied with the electron microprobe. The advent of new techniques of analysis coupled with better instrumentation are now allowing some of these issues to be addressed.

1.2 Tourmaline chemistry and nomenclature

1.2.1 General formula

Tourmaline has the general formula:

$$X\,Y_3\,Z_6\,T_6\,O_{18}\,(BO_3)_3\,V_3\,W$$

where

X = Na, Ca, □, K

Y = Mg, Al, Fe^{2+}, Fe^{3+}, Li, Cr^{3+}, Mn^{2+}, Ti^{4+}

Z = Al, Mg, Cr^{3+}, Fe^{3+}, V^{3+}, Fe^{2+}

T = Si, Al, (B)

V = O, (OH)

W = (OH), O, F

Silicon is by far the dominant cation at the *T*-site, with minor substitution of Al (≤ 1 *apfu*; atoms per formula unit). There have been proposals for substitution of B at this site (*e.g.* Barton 1969, Serdyuchenko 1982, Dyar *et al.* 1994), but until recently, there has been no direct evidence of tetrahedrally-coordinated B reported from either spectroscopic or crystal-structure refinement. Hughes *et al.* (2000) have recently reported a well-characterized tourmaline with strong evidence for $^{[4]}B$, however, this is most likely a rarity. Povondra (1981) and Grice and Ercit (1993) have suggested that Ti^{4+} substitutes at the *T*-site, but this is not supported by optical spectra (Rossman and Mattson 1986). The *Y*-site is occupied by a large variety of cations, including Li, Mg, Fe^{2+}, Mn^{2+}, Al, Fe^{3+}, Cr^{3+}, V^{3+} and Ti^{4+}. The *Z*-site is dominantly occupied by the trivalent cations Al, Fe^{3+}, Cr^{3+} and V^{3+}, but can contain significant quantities (up to ~1 *apfu*) of the divalent

cations Mg and Fe^{2+}. The *X*-site is occupied by Na, Ca, and □ (vacancy), and can also contain minor K (*e.g.* Grice *et al.* 1993).

There are eight crystallographically distinct anion sites in the tourmaline structure; these are labeled O1 through O8. The O2 and O4 to O8 sites are fully occupied by O. The O1 can contain either OH or O; the O3 site can contain OH, F and/or O.

1.2.2 Tourmaline nomenclature

The tourmaline structure can accommodate a wide variety of different elements. This is reflected in the increasing number of naturally-occurring and synthetic tourmaline species currently recognized (Table 1.1). It was only recently, however, that a systematic approach to the classification of tourmaline species was proposed (Hawthorne and Henry 1999). The classification scheme has been submitted to the Commission on New

TABLE 1.1: Current tourmaline end-member species

Species	*X*	Y_3	Z_6	T_6O_{18}	$(BO_3)_3$	V_3	*W*
Alkali Tourmalines							
Elbaite	Na	$Li_{1.5}Al_{1.5}$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
Dravite	Na	Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
Schorl	Na	$Fe^{2+}{}_3$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
Chromdravite	Na	Mg_3	Cr_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
Olenite	Na	Al_3	Al_6	Si_6O_{18}	$(BO_3)_3$	O_3	(OH)
Povondraite	Na	$Fe^{3+}{}_3$	$Fe^{3+}{}_4Mg_2$	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	O
Buergerite	Na	$Fe^{3+}{}_3$	Al_6	Si_6O_{18}	$(BO_3)_3$	O_3	F
Calcic Tourmalines							
Uvite	Ca	Mg_3	Al_5Mg	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F
Liddicoatite	Ca	Li_2Al	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	F
Hydroxyferuvite	Ca	Mg_3	Al_5Mg	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
X site-vacant tourmalines							
Foitite		Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
Rossmanite		$LiAl_2$	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)
Magnesiofoitite		Mg_3	Al_6	Si_6O_{18}	$(BO_3)_3$	$(OH)_3$	(OH)

(after Hawthorne and Henry 1999)

Minerals and New Mineral Names of the International Mineralogical Association (IMA); the results of this submission are pending.

Hawthorne and Henry's (1999) proposal draws strongly on the 50% rule as argued by Nickel (1992). In addition, they set forth strict guidelines as to the definition of an end-member composition, which was only briefly touched on in Nickel (1992). The two main defining points of an end-member are (1) an end-member composition must be fixed, and (2) an end-member may have more than one species at one site. Strict adherence to these two points requires some modification in original species formulae, as described by Hawthorne and Henry (1999).

Tourmaline species may be divided into three principal classes on the basis of their *X*-site occupancy (Figure 1.1). Tourmalines dominated by Na and K (*i.e.*, > 0.5 *apfu* Na + K) are referred to as *alkali* tourmalines. Likewise, Ca-dominant tourmalines fall into the *calcic* tourmaline group, and vacancy-dominant tourmalines may be referred to as X-*site-vacant* tourmalines. This follows the classification scheme of other complex mineral groups such as the amphiboles and pyroxenes (Hawthorne and Henry 1999).

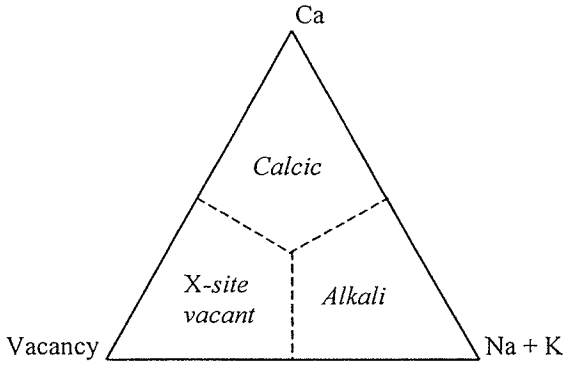

Figure1.1: Ternary plot of tourmaline principal classes

A key issue to come out of Hawthorne and Henry's (1999) classification is the differentiation of tourmaline species based on variations in occupancy of the *W*-site (Figure 1.2). Traditionally, the anion sites have been ignored in regards to tourmaline. However, an accurate and petrologically useful nomenclature should reflect the chemical composition at this site. Thus, the subdivisions within each of the three principal classes are defined on the occupancy of the *W*-site (Hawthorne and Henry 1999).

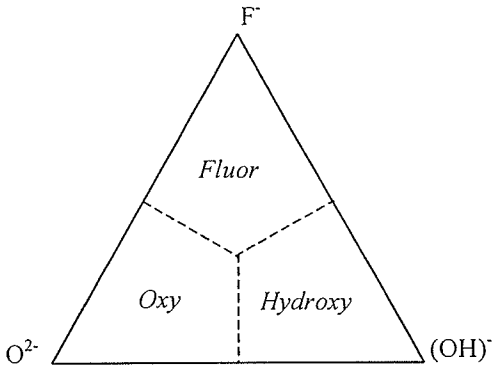

Figure1.2: Ternary plot of tourmaline subdivisions based on *W*-site occupancy

1.2.3 Tourmaline solid-solutions

Two continuous solid-solution series, schorl-dravite and schorl-elbaite, have traditionally been defined (*e.g.* Epprecht 1953) for tourmaline. These series are related by the substitution of Mg for Fe^{2+} and Li + Al for 2 Fe^{2+}, respectively (Table 1.2). Partial to complete solid-solution series have also been described for elbaite-liddicoatite, dravite-uvite, dravite-povondraite, feruvite-schorl, feruvite-uvite, and chromdravite-dravite (Dunn *et al.* 1977, Walenta and Dunn 1989, Dietrich 1985). Until recently, there was no evidence for solid solution between Li-rich tourmalines and Mg-rich tourmalines. A

TABLE 1.2: Important site-substitutions and corresponding exchange vectors

Site substitution	*Exchange vector*
$^{Y}Mg = {}^{Y}Fe^{2+}$	$FeMg_{-1}$
$^{Y}Mn = {}^{Y}Fe^{2+}$	$FeMn_{-1}$
$^{Z}Al = {}^{Z}Fe^{3+}$	$FeAl_{-1}$
$^{Z}Al = {}^{Z}Cr^{3+}$	$CrAl_{-1}$
$^{O1}OH = {}^{O1}F$	$F(OH)_{-1}$
$^{Y}Mg + {}^{Z}Al = {}^{Y}Al + {}^{Z}Mg$	$AlMgMg_{-1}Al_{-1}$
$2{}^{Y}Fe^{2+} = {}^{Y}Li + {}^{Y}Al$	$LiAlFe_{-2}$
$^{X}Na + {}^{Y}Mg = {}^{X}\square + {}^{Y}Al$	$\square AlNa_{-1}Mg_{-1}$
$^{X}Na + 2{}^{Y}Mg + {}^{O1}OH = {}^{X}\square + 2{}^{Y}Al + {}^{O1}O^{2-}$	$\square AlONa_{-1}Mg_{-2}(OH)_{-1}$
$^{Y}Mg + {}^{O3}OH = {}^{Y}Al + {}^{O3}O^{2-}$	$AlOMg_{-1}(OH)_{-1}$
$^{Y}Fe^{2+} + {}^{O3}OH = {}^{Y}Fe^{3+} + {}^{O3}O^{2-}$	$Fe^{3+}OFe^{2+}{}_{-1}(OH)_{-1}$
$^{Y}Mg + {}^{T}Si = {}^{Y}Al + {}^{T}Al$	$Al_2Mg_{-1}Si_{-1}$
$2{}^{Y}Al = {}^{Y}Mg + {}^{Y}Ti$	$TiMgAl_{-2}$
$^{X}Na + {}^{Y}Al = {}^{X}Ca + {}^{Y}Mg$	$CaMgNa_{-1}Al_{-1}$
$^{X}\square + {}^{Y}Al + {}^{O1}OH = {}^{X}Ca + {}^{Y}Mg + {}^{O1}O^{2-}$	$CaMgO\square_{-1}Al_{-1}(OH)_{-1}$
$2{}^{Y}Mg + {}^{Z}Al + {}^{O1}OH = 2{}^{Y}Al + {}^{Z}Mg + {}^{O1}O^{2-}$	$Al_2MgOMg_{-2}Al_{-1}(OH)_{-1}$

(after Henry and Dutrow 1996)

number of hypotheses for this apparent miscibility gap have been suggested. However, recent work on tourmalines from Bližná, Czech Republic, indicates solid solution between elbaite and dravite (Novák *et al.* 1999). The apparent miscibility gap is most likely due to the environments of formation of the Li-rich *vs.* Mg-rich tourmalines. Other significant substitutions can occur in the tourmaline group (Table 1.2) (Henry and Dutrow 1996).

1.2.4 Minor-element chemistry

A wide variety of minor and trace elements occur in tourmaline. The greatest diversity seems to occur in elbaite, due to its occurrence in complex, highly fractionated pegmatites in which minor- and trace-elements are concentrated (*e.g.* Dietrich 1985). Minor- and trace-element contents have been used for petrogenetic studies and as geochemical indicators of source rock (*e.g.* Conklin and Slack 1983, King *et al.* 1988).

1.3 The crystal structure of tourmaline

The tourmaline structure (Figure 1.3) consists of six-membered rings of tetrahedra (*T*-site), the apical oxygens of which are directed toward the -*c* pole of the crystal (Barton 1969). Parallel to the ring of tetrahedra are triangular (BO_3) groups that lie above the basal oxygens of the tetrahedra. Although B deficiency has been proposed (*e.g.* Dyar *et al.* 1994), crystal-structure refinement and spectroscopic data do not support this hypothesis (*e.g.* Tsang and Ghose 1973, Grice and Ercit 1993, Burns *et al.* 1994, Hawthorne 1996).

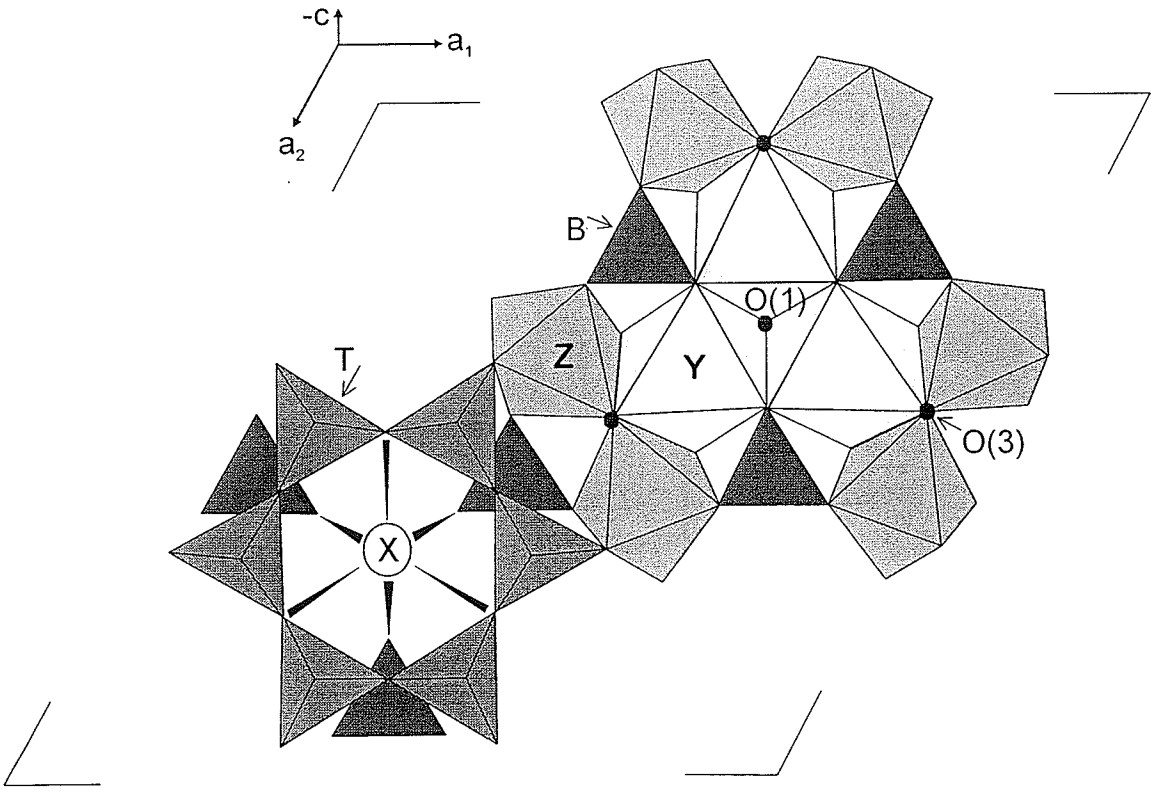

Figure 1.3: Portion of the tourmaline structure projected onto (0001), looking up the *c* axis (after Joliff *et al.* 1986).

The *Y*- and *Z*-sites are both octahedrally coordinated. Structure refinements indicate that there is no vacancy at either site. Substitution of a divalent cation at the *Z*-site usually can stabilize the structure when there is significant trivalent-cation occupancy of the *Y*-site and O^{2-} replacing OH at the *W*-site (Taylor *et al.* 1995, Hawthorne 1996). Each *Y* octahedron shares an edge with two adjacent *Y* octahedra, making a group of three octahedra with a common apical oxygen. Each *Y* octahedron also shares an edge with two *Z* octahedra. These *Z* octahedra link various structural fragments along the three-fold screw axis. The *X*-site is a [9]-coordinated trigonal antiprism sandwiched between the tetrahedral layer and the $(BO)_3$ groups along the three-fold axis.

There are eight distinct anion sites in the tourmaline structure; these are labeled O1 through O8. The O1 and O3 sites, which can have variable anion content, are referred to as follows: O1 = *W*, O3 = *V* (Hawthorne 1996, Hawthorne and Henry 1999). The O1 site is located on the three-fold axis and bonds to three *Y*-site cations. When OH occupies the O1 site, the H atom points toward the *X*-site; there is almost no hydrogen-bonding with the surrounding O atoms (Robert *et al.* 1993). Experimental and crystallographic studies show that F occurs in significant quantities solely at the O1 site; this assignment accounts for the apparent maximum of ~1.0 F *apfu* in extensive analytical data for tourmaline (*e.g.* Grew and Sandiford 1984, Grice and Ercit 1993, Robert *et al.* 1993, Dyar *et al.* 1994). Hawthorne (1996) proposed a substitution mechanism that links incorporation of O at the O1 site with disordering of Al and Mg at the *Y*- and *Z*-sites: $^{Y}Mg_2 + {}^{Z}Al + {}^{O1}OH = {}^{Y}Al_2 + {}^{Z}Mg + {}^{O1}O$. The O3 anion bonds to two *Z*-site cations and one *Y*-site cation. When OH occupies the O3 site, significant hydrogen bonding occurs with the adjacent O atoms (Robert *et al.* 1993).

1.4 Tourmaline properties

1.4.1 Physical properties

Tourmaline is a non-centrosymmetric rhombohedral borosilicate (space group $R3m$, Z = 3). It commonly forms vertically striated, prismatic crystals with a prominent trigonal prism and a subordinate hexagonal prism. The prism faces often round, forming a rounded triangular cross-section. Due to its polar character, crystals that are doubly-terminated usually exhibit different forms on opposite ends. Tourmaline may occur as single crystals or radiating to parallel columnar crystals. It may also be massive or compact (Klein and Hurlburt 1993).

Tourmaline occurs in a full rainbow of colors, as well as colorless and black varieties. Chemical composition does correlate with the color, but often quite dramatic color changes can be the result of slight variations in minor-element chemistry. Tourmaline has a vitreous to resinous luster, a hardness of 7-7.5, and conchoidal fracture (Klein and Hurlburt 1993).

1.4.2 Optical properties

Tourmaline is uniaxial-negative, with ω = 1.635-1.675, ε = 1.610-1.650. Crystals can be weakly to strongly pleochroic, $O > E$ (Klein and Hurlburt 1993).

1.4.3 Polar properties

Due to the non-centrosymmetric nature of tourmaline, it exhibits distinctive polar characteristics. Barton (1969) defined the absolute orientation of tourmaline with respect to the different poles, specifying the analogous pole as the $-c$ pole of the crystal. In most

tourmalines, this polar character results in pyroelectric and piezoelectric responses to changes in temperature or pressure (Henry and Dutrow 1996). Tourmaline can exhibit compositional polarity where different compositions of tourmaline develop simultaneously at each pole (Sperlich 1990, Henry and Dutrow 1992, Dutrow and Henry 1994).

1.5 Tourmaline occurrences

The most common B mineral by far is tourmaline (Anovitz and Grew 1996). Boron is required for tourmaline formation; as B is a trace element in the upper crust, it must be concentrated for the mineral to form. As B is mobile in most aqueous solutions, it is easy to concentrate or disperse in most geological processes. During formation, tourmaline is very reactive with its environment, including other minerals, fluids, H_2O activity, dissolved species, pressure and temperature. This often results in chemical zoning in the crystal, enhanced by the large number of elements that can be taken up into the tourmaline structure. However, once it forms, it does not easily change its composition; it remains unaltered in many geological environments. This early variability combined with post-formation stability makes tourmaline useful as a record of chemical history of formation (Henry and Dutrow 1996).

1.5.1 Igneous occurrences

Boron is a trace element in most magmas. When B is concentrated, it can play a major role in a melt by reducing the solidus and liquidus temperatures and decreasing the melt's viscosity. High levels of B generally occur in fractionated peraluminous magmas.

Tourmaline occurs in granites and granitic pegmatites, where it can occur in all zones, as well as in miarolitic cavities, veins, breccias and as disseminated grains. Each of these settings has different species most likely to be associated with it (though not necessarily restricted to it), depending on the other elements in the melt. Thus, schorl and dravite are common in border zones where Mg and Fe can be incorporated from the host rock. Elbaite and liddicoatite are more likely to be found in miarolitic cavities in a pegmatite, where the residual melt is enriched in Li (London *et al.* 1996).

1.5.2 Sedimentary occurrences

Tourmaline is one of the minerals most resistant to weathering; only nonmetamict zircon seems to be more stable (Thiel 1941). Henry and Dutrow (1996) note that tourmaline is used as a maturation-index mineral in clastic environments and is also useful as a provenance indicator. Additionally, tourmaline can form authigenically in sediments, precipitating during diagenesis and burial metamorphism (*e.g.* Awasthi 1961, Ricketts 1978). Extreme enrichment in B in pelitic and metavolcanic sequences can lead to the formation of tourmalinite (London *et al.* 1996).

1.5.3 Metamorphic occurrences

Tourmaline is the most likely borosilicate mineral to form under almost any metamorphic conditions (Grew 1996). It is stable in most bulk compositions and under most pressure-temperature regimes normally encountered in metamorphic terranes. In fact, other metamorphic borosilicates tend to be restricted to extreme environments, i.e. high values of B, pressure, temperature and a_{H_2O} (Grew 1996). Moreover, once formed,

tourmaline does not readily alter. London *et al.* (1996) note that tourmaline seems to be stable up to at least upper-amphibolite facies in regard to temperature, into eclogite facies with regard to pressure, and in strongly-to-weakly acidic conditions with regards to fluid composition.

1.5.4 Hydrothermal occurrences

Boron-bearing hydrothermal fluids can form tourmalines with a wide range of composition affected by the compositions of the host rock and the invading fluid (*e.g.* Caverretta and Puxeddu 1990). Boron metasomatism is commonly associated with precious-metal deposits, including Au, Ag, Zn, U and Mo (*e.g.* Fuchs and Maury 1995). The resultant tourmaline compositions may be dominated by the nature of the host rock, may be of mixed character, or dominated by the chemical composition of the fluid (Henry and Dutrow 1996).

1.6 Objectives

There are a number of crystal-chemical problems that are still not well understood with respect to tourmaline. This is in large part due to the complexity of the mineral and the chemical heterogeneity both within a sample and between crystals. I decided to examine a larger number of tourmalines from many localities with the following objectives in mind:

- Investigate various normalization schemes and assumptions in common use for tourmaline to determine the strengths and/or weaknesses of each and to clarify what assumptions about chemical content are valid and which are suspect.

- Investigate a broad suite of tourmalines using several analytical techniques to acquire precise and accurate chemical and crystallographic data over the range of compositions known to date. New species identified during this process will be fully characterized in preparation for submission to the Commission on New Minerals and Mineral Names.
- Develop a broad understanding of the nature of Cr in tourmaline including the range of site-occupancy and chemical variations.
- Develop a broad understanding of povondraite including site-occupancies and disorder between the sites and the range of chemical substitutions.
- Investigate the nature of the $^{[3]}B$-site in tourmaline, specifically how stereochemical variations at B are related to chemical variations at the cation sites.

CHAPTER 2

Experimental Methods

2.1 Analytical techniques

2.1.1 General Information

The analytical techniques used for this study, including specific information obtained from each technique, are listed below in Table 2.1.

TABLE 2.1: Techniques in this study

Technique	*Location*	*Analyst(s)*	*Information*
1. Electron-microprobe analysis (EMPA)	University of Manitoba; Louisiana State University, Baton Rouge, LA	Clark McCracken, C.M.; Chapman, R.; Henry, D.	Relative weight fractions of major and minor elements ($Z > 8$)
2. Single-crystal structure refinement	University of Manitoba	Clark McCracken, C.M.	Electron totals at crystallographic sites. Interatomic distances and angles
3. Gandolfi powder diffraction	University of Manitoba	Clark McCracken, C.M.; Ball, N.A.	X-ray powder pattern, limited sample
4. X-ray powder diffraction	University of Manitoba	Ball, N.A.; Dzikowski, T.J.	X-ray powder pattern, bulk sample
5. H-extraction line	Queens University, Kingston, ON	Kyser, K.	Weight fraction of the element H
6. Secondary-ion mass spectrometry (SIMS)	CNR-CSCC, Pavia, Italy	Ottolini, L.; Bottazzi, P.	Weight fraction of light elements (H, Li, B)

2.1.2 Sample preparation

Crystals for study were selected under a binocular microscope; preference was given to equidimensional crystal fragments that were typically 0.2-0.3 mm in size, free of cracks and inclusions, and with uniform color and high optical clarity. In some species choice was limited due to paucity of material, so smaller and/or less pristine crystals may have been chosen. Crystals for single-crystal structure refinement were prepared in two different ways, depending on the size of the crystal. For robust samples (>150 microns

approximate diameter), the crystals were ground to spheroids in order to minimize X-ray absorption anisotropy. For small samples, the crystals were mounted "as is". Each crystal was glued to the tip of a glass fiber fitted within a split brass pin. This pin assembly was then mounted onto a goniometer head that was subsequently mounted on a four-circle X-ray diffractometer. After diffraction-intensity data were collected, each crystal was removed from its glass fiber. The crystals were then set in a thermal-setting epoxy (PETROPOXY™) on one-inch plastic disks. The surface was polished and carbon-coated in preparation for EMPA. After EMPA analysis, these disks were then sent to Pavia, Italy, for SIMS analysis. In Italy, the carbon-coating was removed and replaced by a gold-coating approximately 50 nm in thickness.

Additional material was selected using a similar screening process from each sample if a powder-diffraction pattern or H-line extraction data were to be collected. For powder diffraction, a few crystals were isolated; for H-line extraction, approximately 30 mg of pure material were collected. In either case, the grain separates were ground using a clean mortar and pestle. Powder-diffraction granules were then mounted in epoxy on the tip of a glass fiber for data collection. H-extraction-line powder was sent to Queens University (Kingston, Ontario) for analysis.

2.2 Single-crystal structure refinement (SREF)

Intensity data were collected on a Siemens *P*3 single-crystal diffractometer using graphite-monochromated Mo*K*α X-radiation. The crystals were optically aligned within the X-ray beam. In ideal situations, crystals were centered on 13 reflections, either randomly collected or from a rotation photo. Once the crystal was centered, it was re-

centered on 13 standard *hkl*'s (Table 2.2). When crystals were exceptionally small, less than 13 reflections may have been used for centering. The cell parameters and orientation matrix were derived by least-squares refinement of the setting angles of the centered reflections. Crystal quality was assessed using the profiles of Bragg diffraction peaks and cell-parameter standard deviations; unsuitable candidates were rejected at this point. A single asymmetric unit of intensity data was collected ($4 \rightarrow 60^{\circ}$ 2θ; θ - 2θ scan mode, *hkl* from 0 0 -11 to 23 23 11). A standard reflection was collected every 50 measurements to monitor instrument stability. After the intensity data were collected, a second data-set was collected in order to acquire information for application of an empirical absorption correction. This second data-set consisted of between 8 and 15 strong reflections uniformly distributed with regard to 2θ and measured over 10° intervals of ψ (the azimuthal angle corresponding to rotation of the crystal about its diffraction vector) from $0 \rightarrow 360^{\circ}$ ψ.

Table 2.2: Standard *hkl* for tourmaline centering

Number	*h*	*k*	*l*
1	5	0	-1
2	0	5	1
3	0	0	3
4	0	0	-3
5	0	1	2
6	0	5	-5
7	1	5	2
8	2	7	1
9	4	3	-2
10	5	1	-2
11	6	0	-3
12	7	2	-1
13	10	0	1

The Siemens SHELXTL (PC Version) system of programs was used throughout this study. Data reduction included scaling on the standard reflections and applying

standard drift, Lorentz, polarization and background corrections. These data were then corrected for absorption using the ψ-scan data with the crystal modeled as an ellipsoid. The resulting data were reduced to structure factors and used for full-matrix least-squares structure refinement. The structure was refined on $|F|$ using neutral scattering factors and anomalous dispersion corrections from the *International Tables for Crystallography* (1992) for all cations.

The structures were refined in the space group $R3m$ using the positional coordinates of a dravite sample. The final cycles of refinement involved variable positional parameters, anisotropic-displacement parameters and site-scattering parameters for the *X*-, *Y*- and *Z*-sites. The residual Fourier peaks were scanned for H-atoms, particularly that bonded to O(3). When found, this site was constrained to be approximately 0.98 Å from the O(3) site. The final *R* indices generally fell between 1.3 and 3.0 %. Miscellaneous refinement information are provided in Appendix B, final atomic parameters are given in Appendix C, refined site-scattering values are provided in Appendix D and selected interatomic distances and angles are given in Appendix F.

2.3 Electron-microprobe analysis

Electron-microprobe analysis was done on a CAMECA SX-50 in wavelength-dispersive mode. The beam voltage for all elements was 15 kV and the spot diameter was 1 μm. Count times for peak and background determinations for all elements were 20 and 10 s, respectively. Data were collected with a beam current of 20 nA for Na, Fe, Ca, Al, Si, and Mg and 30 nA for F, Cr, V, Mn, Zn, K, Ti, and P. The standards and detection limits for wt% oxides are listed in Table 2.3.

The analytical data were reduced using the $\phi(\rho z)$ method of Pouchou and Pichoir (1984, 1985). Diopside, kyanite, fayalite, albite (jadeite), olivine, chromite and

Table 2.3: Tourmaline analysis by electron microprobe

Standard	*Element, line, crystal*	*Oxide*	*Beam current (nA)*	*Detection limit (wt%)*
VP_2O_7	P, K_α, PET	P_2O_5	30	0.07
Diopside	Si, K_α, PET	SiO_2	20	0.09
Titanite	Ti, K_α, PET	TiO_2	20	0.05
Kyanite	Al, K_α, TAP	Al_2O_3	20	0.04
VP_2O_7	V, K_α, LiF	V_2O_3	30	0.05
Chromite	Cr, K_α, LiF, PET*	Cr_2O_3	30	0.04
Olivine	Mg, K_α, TAP	MgO	20	0.01
Diopside	Ca, K_α, PET	CaO	20	0.04
Spessartine	Mn, K_α, LiF	MnO	20	0.08
Fayalite	Fe, K_α, LiF	FeO	20	0.10
Gahnite	Zn, K_α, LiF	ZnO	30	0.15
Albite	Na, K_α, TAP	Na_2O	20	0.04
Jadeite	Na, K_α, TAP	Na_2O	20	0.02
Orthoclase	K, K_α, PET	K_2O	30	0.03
Fluor-riebeckite	F, K_α, TAP	F	30	0.14

Detection limits are calculated using L.D. = $[3(\text{wt\% oxide})(R_b/t_b)^{1/2}] / (R_p-R_b)$ where R_b = background count rate (counts/s), t_b = background count time (s), R_p = peak count rate (counts/s)
* Samples with >15 wt% Cr_2O_3 were recollected using the PET crystal.

spessartine standards were each analyzed twice at the beginning of a run, followed by analysis of approximately 40 unknowns and two determinations of each standard. This sequence was repeated and the run ended with analysis of the standards. The K-values (intensity of unknown/intensity of standard) for the specific element for each of the standards (e.g. the K-values of Si in diopside) were averaged over the entire run. If the average K-value for each element was <0.99 or >1.01 (ideal K-value is 1.0), the data for the entire run were recalculated using the K-value ratio obtained for the standard.

2.4 Powder diffraction

Powder-diffraction data were collected for all new minerals. When sufficient material was available, the powder-diffraction data were collected on a Philips PW 1710 diffractometer with graphite-monochromated Cu$K\alpha$ radiation.

When new-mineral samples were limited in quantity, the powder-diffraction data were collected using a Gandolfi camera instead of a powder diffractometer. The sample was mounted in the Gandolfi camera, then exposed to graphite-monochromated Cu$K\alpha$ X-radiation. Run times were approximately 4 – 6 h, depending on the amount of sample. After the run, the film was developed and the position and intensity of the diffraction lines were measured. No correction was made for shrinkage and no internal standards were used.

Cell dimensions for both collection techniques were refined from the corrected *d*-values using the program CELREF (Appleman and Evans 1973).

2.5 Analysis of light elements

2.5.1 H-extraction line

Select tourmaline samples were analyzed at Queens University, Kingston, Ontario. Fragments and crystals of tourmaline were hand-selected to ensure that the material lacked visible zonation and inclusions, and ground to a powder. Samples were wrapped in molybdenum foil, placed in a platinum crucible, and suspended inside a quartz extraction vessel. The vessel and its contents were outgassed for 12 h in a vacuum at 150° C to remove surface-adsorbed water. The sample was then inductively heated at 1400° C for 20 minutes and the gases were collected in a trap that was held at -196° C.

The majority of the hydrogen released was in the form of water, though minor quantities of hydrocarbons or molecular hydrogen released or produced during this treatment were also collected in the trap. The accumulated water (representing the total amount of hydrogen in the samples) was separated from the other gases by differential-freezing techniques. This water was reacted with uranium at 750° C to produce H_2 which was collected on charcoal at -196° C. The volume of H_2 was measured manometrically. This method has a reproducibility of +/- 0.02 weight percent (Kyser and O'Neil 1984).

2.5.2 Secondary-ion mass spectrometry (SIMS)

Secondary-ion mass spectrometry (SIMS) analysis was attempted on a number of samples. Tourmaline samples were analyzed on a CAMECA IMS-4F ion-microprobe at CNR-CSCC, Pavia, Italy, for B, Li, and H. The $^{16}O^-$ primary beam was focused to a diameter of <10 μm on the sample surface at an accelerating voltage of 12.5 kV and a primary-current intensity of ~ 5 nA. Positive secondary ions were accelerated through 4.5 kV, and secondary ion at masses 1, 7, 11, 27, and 30 were collected under a 25 μm ion-image field. The selected-contrast diaphragm and field aperture were 400 and 1800 μm, respectively. Medium- to high-energy ions were used to reduce the influence of matrix composition; these were selected by offsetting the sample-accelerating voltage to –100 V. This was done while keeping the setting of the electrostatic-analyzer voltages constant and the width and the position of the energy slit to +/- 25 eV. Secondary ions were counted by an electron multiplier in the pulse-counting mode; Al^+ ions were counted in a Faraday cup. No corrections were made for dead time. Count times of 40 s for H and Li, 30 s for B and Si, and 20 s for Al over 10 cycles were used for a single

measurement. All measurements were done under steady-state sputtering conditions, which were achieved after approximately 9 minutes of bombardment (Ottolini *et al.* 1995; Ottolini and Hawthorne 1999).

CHAPTER 3

Structural-formula Calculation

3.1 Introduction

Mineral formulae are calculated by normalization of the [analyzed] chemical composition to a structurally defined number of anions or cations. The key issue is that the normalization scheme has to be correct. In an optimal situation, the complete quantitative chemical analysis of the elements in a mineral would be available, and the formula would be calculated by normalizing the cations to the total number of anions in the structure, as required by the electroneutrality principle. Normalization on anions is generally a more accurate method then normalization on a specific number of cations, as vacancies at anion sites are rare, whereas vacancies at cation sites are common, and additional complications are raised by the occurrence of specific cations at more than one site. However, mineral analyses are rarely complete, as light elements (H, Li, Be, B) and valence states of transition metals are frequently not analyzed. The goal in these situations is to develop a normalization scheme that is not affected by the information gaps.

Tourmaline formulae are calculated in a variety of ways. The difficulties in tourmaline formula calculation, and the reason why there are so many methods, lie in the number of undetermined species that commonly occur in chemical analyses of tourmalines. H, Li and B are all common components of tourmaline, but none of these components are easily measured. This is due to limitations in current methods of chemical analysis, where measurement of light elements usually relies on bulk sample.

Due to the prevalence of compositional variations in tourmaline, commonly seen in the frequency of zoned samples, bulk homogeneous material is uncommon. This leads to assumptions in normalization schemes (*e.g.* OH + F = 4 *apfu)* that may not be sound.

In addition to elements that are difficult to analyze, tourmalines also contain transition metals with variable valence states. Most notable of these is Fe, which can be either 2+ (ferrous) or 3+ (ferric). Additionally, Mn, Cr, V and Ti could potentially all have mixed valence states, though it is commonly assumed they do not in tourmaline.

3.2 Methods of structural-formula calculation

To get around the problems created by unknowns in our chemical compositions, various schemes have been developed and used (*e.g.* Grice and Ercit 1993, Hawthorne 1996, Taylor *et al.* 1995, King and Kerrich 1989, Michailidis *et al.* 1995, Dutrow and Henry 2000). If we had a complete composition, a simple normalization on 31 anions would give an accurate formula. In the absence of some of the data, the question becomes what are the possible normalization schemes? Methods in use include normalization on 31 anions (assuming OH + F = 4 *apfu*), on 27 anions (omitting O1 and O3), and on 24.5 anions (omitting O1, O3, and B_2O_3). Schemes that are normalized on cations include 19 total cations (*X, Y, Z, T* and *B*), 18 total cations (*Y, Z, T* and *B*), 15 total cations (*Y, Z* and *T*) and 9 total cations (*Y* and *Z*). When variables such as Li and Fe^{3+} / Fe^{2+} ratios are brought into bear, accurate normalizations can be exceedingly difficult.

In the absence of some of the chemical-compositional data for tourmaline, some assumptions are necessary in the normalization scheme. The method chosen should be based on what information is known about the material; not all schemes work equally

well and some are better for some compositions than others. For example, normalizing on total cations (19 cations) is generally not appropriate, as there is commonly a minor to significant vacancy at the *X*-site. Normalizing on 15 cations at *Y, Z* and *T* is not appropriate if Li is not determined or Fe^{3+} / Fe^{2+} is unknown. One method that can work well is normalizing on 6 *apfu* of Si at *T*; however, this is only true if *T* is fully occupied by Si. Although there are a variety of methods for formula calculation, there has not been a thorough review of the strengths and weaknesses of each method.

3.3 Structural-formula calculations

In order to evaluate the various formula-calculation schemes, I generated a suite of tourmaline formulae; six "ideal" end-members and six with small amounts of chemical variability (non-ideal). The weight % oxides were calculated from the theoretical atomic contents. Subsequently, I ran this suite through Ercit's "Formula" (1993) software several times, each time varying the number of unknowns, and therefore, the assumptions made in the calculation of the formulae. Table 3.1 lists the chemical compositions of the suite used. Formulae in Table 3.1 reflect an optimal situation; all chemical components are known and a straightforward normalization on 31 anions gives the true formulae. All subsequent calculated formulae should be compared back to Table 3.1 to see the extent of deviations from the correct formulae.

Table 3.1: Theoretical tourmaline compositions normalized to 31 anions

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*Iros*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	0.00	2.39	0.00	0.00	0.00	1.62	0.00	1.86	0.00	0.00	0.15	1.75
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	9.91	11.15	10.89	9.92	10.71	11.30	10.24	10.86	10.70	9.91	10.69	11.09
H_2O	3.42	3.85	3.76	0.00	2.77	3.90	3.36	3.37	3.69	0.09	2.58	3.63
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	100.01	99.99	100.00	100.00	100.00	100.00	100.01	99.99	99.99	99.99	100.00
Si^{4+}	6.00	6.00	6.00	6.00	6.00	6.00	6.00	5.90	6.00	6.00	5.80	6.00
Al^{3+}	6.00	7.50	6.00	6.00	5.00	8.00	6.20	7.30	6.20	6.00	6.00	7.60
Fe^{3+}	0.00	0.00	0.00	3.00	0.00	0.00	0.20	0.00	0.00	2.80	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	2.00	0.60	0.70	0.20	0.20	0.30
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.80	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.20	0.10	0.20	0.70	0.10
Li^{+}	0.00	1.50	0.00	0.00	0.00	1.00	0.00	1.20	0.00	0.00	0.10	1.10
Na^{+}	1.00	1.00	1.00	1.00	0.00	0.00	0.60	0.70	0.60	0.70	0.20	0.30
B^{3+}	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
H^{+}	4.00	4.00	4.00	0.00	3.00	4.00	3.80	3.60	4.00	0.11	2.80	3.80
F^{-}	0.00	0.00	0.00	1.00	1.00	0.00	0.20	0.40	0.00	1.00	1.00	0.20
O^{2-}	31.00	31.00	31.00	30.00	30.00	31.00	30.80	30.60	31.00	30.00	30.00	30.80
Cat Σ	19.00	19.00	19.00	19.00	19.00	18.00	18.60	18.90	18.70	18.90	18.90	18.41
An Σ	31	31	31	31	31	31	31	31	31	31	31	31

"Ideal" tourmalines: *ISch:* schorl, *IElb:* elbaite, *IDrv*: dravite, *IBur*: buergerite, *IUv*: uvite, *IRos*: rossmanite;
"Non-ideal" tourmalines: *Sch*: schorl, *Elb*: elbaite, *Drv*: dravite, *Bur*: buergerite, *Uv*: uvite, *Ros*: rossmanite

The second run assumed all chemical components except for B_2O_3 were known. As the vast majority of tourmalines to date have shown B fully occupying the *B*-site with no tetrahedral B (Hawthorne 1996, Burns *et al.* 1994, Hughes *et al.* 2000), when the amount of B_2O_3 is unknown, it is straightforward to assume a stoichiometric amount such that B = 3 *apfu*. Table 3.2 shows the chemical composition and formulae for a suite with unknown B_2O_3. B was calculated using stoichiometric arguments on the basis of 31 anions. As expected, the lack of quantitative B analysis does not affect the calculated formulae. Since the theoretical tourmalines were developed with 3 *apfu* of B,

Table 3.2: Formulae normalized to 31 anions with B calculated stoichiometrically

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*IRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	0.00	2.39	0.00	0.00	0.00	1.62	0.00	1.86	0.00	0.00	0.15	1.75
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	9.91	11.15	10.89	9.92	10.71	11.31	10.24	10.86	10.70	9.91	10.69	11.09
H_2O	3.42	3.85	3.76	0.00	2.77	3.90	3.36	3.37	3.69	0.09	2.58	3.63
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	100.01	99.99	100.00	100.00	100.01	100.00	100.00	99.99	99.99	99.99	100.00
Si^{4+}	6.00	6.00	6.00	6.00	6.00	6.00	6.00	5.90	6.00	6.00	5.80	6.00
Al^{3+}	6.00	7.50	6.00	6.00	5.00	8.00	6.20	7.30	6.20	6.00	6.00	7.60
Fe^{3+}	0.00	0.00	0.00	3.00	0.00	0.00	0.20	0.00	0.00	2.80	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	2.00	0.60	0.70	0.20	0.20	0.30
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.80	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.20	0.10	0.20	0.70	0.10
Li^{+}	0.00	1.50	0.00	0.00	0.00	1.00	0.00	1.20	0.00	0.00	0.10	1.10
Na^{+}	1.00	1.00	1.00	1.00	0.00	0.00	0.60	0.70	0.60	0.70	0.20	0.30
B^{3+}	3	3	3	3	3	3	3	3	3	3	3	3
H^{+}	4.00	4.00	4.00	0.00	3.00	4.00	3.80	3.60	4.00	0.11	2.80	3.80
F^{-}	0.00	0.00	0.00	1.00	1.00	0.00	0.20	0.40	0.00	1.00	1.00	0.20
O^{2-}	31.00	31.00	31.00	30.00	30.00	31.00	30.80	30.60	31.00	30.00	30.00	30.80
Cat Σ	19.00	19.00	19.00	19.00	19.00	18.00	18.60	18.90	18.70	18.90	18.90	18.41
An Σ	31	31	31	31	31	31	31	31	31	31	31	31

this is not surprising. Assuming stoichiometric amounts of B in tourmaline is a relatively benign assumption, only causing problems in the exceedingly rare cases where B ≠ 3 *apfu*.

Slightly more complicated, but very common, is a situation in which neither B_2O_3 or H_2O are measured. This is usually handled by assuming that OH + F = 4 *apfu*. Examination of Table 3.3 shows that this assumption generates formulae which are accurate except in those cases where O^{2-} is present at the O1 and/or O3 sites; this is the case for both end-member and non-ideal buergerite as well as uvite, which had O^{2-} assigned initially to O1 (see Table 3.1). Another way of dealing with unknown values of

Table 3.3: Formulae normalized to 31 anions with B and H calculated stoichiometrically

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*IRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	0.00	2.39	0.00	0.00	0.00	1.62	0.00	1.86	0.00	0.00	0.15	1.75
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
$B_2O_3^*$	9.91	11.15	10.89	10.53	10.71	11.31	10.24	10.86	10.70	10.50	10.73	11.09
H_2O^*	3.42	3.85	3.76	2.78	2.77	3.90	3.36	3.37	3.69	2.77	2.78	3.64
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	100.01	99.99	103.38	100.00	100.01	100.00	100.01	99.99	103.26	100.23	100.01
Si^{4+}	6.00	6.00	6.00	5.65	6.00	6.00	6.00	5.90	6.00	5.67	5.78	6.00
Al^{3+}	6.00	7.50	6.00	5.65	5.00	8.00	6.20	7.30	6.20	5.66	5.98	7.60
Fe^{3+}	0.00	0.00	0.00	2.83	0.00	0.00	0.20	0.00	0.00	2.64	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	2.00	0.60	0.70	0.19	0.20	0.30
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.79	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.20	0.10	0.19	0.70	0.10
Li^{+}	0.00	1.50	0.00	0.00	0.00	1.00	0.00	1.20	0.00	0.00	0.10	1.10
Na^{+}	1.00	1.00	1.00	0.94	0.00	0.00	0.60	0.70	0.60	0.66	0.20	0.30
B^{3+}	3	3	3	3	3	3	3	3	3	3	3	3
H^{+}	4.00	4.00	4.00	3.06	3.00	4.00	3.80	3.60	4.00	3.06	3.01	3.80
F^{-}	0.00	0.00	0.00	0.95	1.00	0.00	0.20	0.40	0.00	0.94	0.99	0.20
O^{2-}	31.00	31.00	31.00	30.06	30.00	31.00	30.80	30.60	31.00	30.06	30.01	30.80
Cat Σ	19.00	19.00	19.00	18.08	19.00	18.00	18.60	18.90	18.70	18.01	18.83	18.40
An Σ	31	31	31	31	31	31	31	31	31	31	31	31

B_2O_3 and H_2O is to solve the formulae on 24.5 anions, leaving both H and B out of the calculations (Table 3.4). This method, however, has a few problems. First, the fact that B_2O_3 and H_2O are left out of the wt% totals means that any systematic error will not be readily recognizable, as the sums are far off 100%. Additionally, the formulae generated in this manner are farther from the actual values than when B_2O_3 and H_2O are assumed by stoichiometric arguments (Table 3.3). For instance, buergerite, which has O^{2-} dominant at O3 and F at O1, will obviously have problems in a scheme where OH + F = 4 *apfu*. However, since it has F at O1, additional errors in the formula calculation are generated as normalizing on 24.5 anions leaves out the O1 site, essentially forcing the

Table 3.4: Formulae normalized to 24.5 anions

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*IRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	0.00	2.39	0.00	0.00	0.00	1.62	0.00	1.86	0.00	0.00	0.15	1.75
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	----	----	----	----	----	----	----	----	----	----	----	----
H_2O	----	----	----	----	----	----	----	----	----	----	----	----
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	86.66	85.01	85.34	90.08	86.52	84.80	86.40	85.78	85.60	89.99	86.72	85.28
Si^{4+}	6.00	6.00	6.00	5.55	5.88	6.00	5.98	5.85	6.00	5.56	5.66	5.98
Al^{3+}	6.00	7.50	6.00	5.55	4.90	8.00	6.17	7.24	6.20	5.56	5.86	7.57
Fe^{3+}	0.00	0.00	0.00	2.77	0.00	0.00	0.20	0.00	0.00	2.59	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	1.99	0.60	0.70	0.18	0.20	0.30
Mg^{2+}	0.00	0.00	3.00	0.00	3.92	0.00	0.60	0.00	2.10	0.00	2.73	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	0.98	0.00	0.00	0.20	0.10	0.18	0.68	0.10
Li^{+}	0.00	1.50	0.00	0.00	0.00	1.00	0.00	1.19	0.00	0.00	0.10	1.10
Na^{+}	1.00	1.00	1.00	0.92	0.00	0.00	0.60	0.70	0.60	0.65	0.19	0.30
B^{3+}	----	----	----	----	----	----	----	----	----	----	----	----
H^{+}	----	----	----	----	----	----	----	----	----	----	----	----
F^{-}	0.00	0.00	0.00	0.93	0.98	0.00	0.20	0.40	0.00	0.92	0.97	0.20
O^{2-}	24.50	24.50	24.50	23.57	23.52	24.50	24.30	24.10	24.50	23.58	23.53	24.30
Cat Σ	16.00	16.00	16.00	14.79	15.68	15.00	15.54	15.77	15.70	14.73	15.52	15.34
An Σ	24.50	24.50	24.50	24.50	24.50	24.50	24.50	24.50	24.50	24.50	24.50	24.50

normalization to accommodate the reported F in some other manner. This is also seen in the other theoretical tourmaline species with F, notably end-member uvite, as well as the non-ideal schorl, elbaite, uvite and rossmanite. Alternatively, F may be left out of the calculation, but this leads to inaccurate mineral nomenclature. Therefore, the use of a 24.5 anion normalization scheme is prone to errors and should not be used. Estimations assuming OH + F = 4 *apfu* and normalizing on 31 anions gives better results, as it accommodates F.

The next step was to make B_2O_3, H_2O and Li_2O all undetermined. In this situation, there are two ways of dealing with Li; either leave it out of the formula calculation or try to iterate for Li. Table 3.5 lists the resultant formulae when B and H

Table 3.5: Formulae normalized to 31 anions with B and H calculated stoichiometrically and Li unknown

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*IRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	----	----	----	----	----	----	----	----	----	----	----	----
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	9.91	10.81	10.89	10.53	10.71	11.07	10.24	10.59	10.70	10.50	10.71	10.84
H_2O	3.42	3.73	3.76	2.78	2.77	3.82	3.36	3.28	3.69	2.77	2.77	3.55
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	97.16	99.99	103.38	100.00	98.08	100.00	97.79	99.99	103.26	100.06	97.92
Si^{4+}	6.00	6.19	6.00	5.65	6.00	6.13	6.00	6.05	6.00	5.67	5.79	6.14
Al^{3+}	6.00	7.74	6.00	5.65	5.00	8.17	6.20	7.48	6.20	5.66	5.99	7.77
Fe^{3+}	0.00	0.00	0.00	2.83	0.00	0.00	0.20	0.00	0.00	2.64	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	2.00	0.62	0.70	0.19	0.20	0.31
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.80	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.21	0.10	0.19	0.70	0.10
Li^{+}	----	----	----	----	----	----	----	----	----	----	----	----
Na^{+}	1.00	1.03	1.00	0.94	0.00	0.00	0.60	0.72	0.60	0.66	0.20	0.31
B^{3+}	3	3	3	3	3	3	3	3	3	3	3	3
H^{+}	4.00	4.00	4.00	3.06	3.00	4.00	3.80	3.59	4.00	3.06	3.00	3.80
F^{-}	0.00	0.00	0.00	0.95	1.00	0.00	0.20	0.41	0.00	0.94	1.00	0.20
O^{2-}	31.00	31.00	31.00	30.06	30.00	31.00	30.80	30.59	31.00	30.06	30.00	30.80
Cat	19.00	17.96	19.00	18.08	19.00	17.29	18.60	18.07	18.70	18.01	18.77	17.63
An	31	31	31	31	31	31	31	31	31	31	31	31

are calculated stoichiometrically, but Li is left out. In minerals which should have Li included, the totals tend to run low and the cation *apfu* individually run high; this is most noticeable for Si. This trend may be hidden if the assumption OH + F = 4 *apfu* is not true and the amount of Li is not large. In the non-ideal uvite composition, for example, trace Li was included. The sum is close to the ideal 100 wt%, even though the 0.15 wt% Li_2O is not included. This is because the anion assumption to calculate H values is not correct for this sample.

Li can be calculated by iterating the formula calculations to achieve a set cation value. Table 3.6 contains the formulae as they would be if Li was iterated for by

Table 3.6: Formulae normalized to 31 anions, B and H determined by stoichiometry, Li by $Y + Z + T = 15$ *apfu*

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*IRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	0.00	2.39	0.00	1.88	0.00	1.62	0.00	1.87	0.00	1.81	0.29	1.75
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	9.91	11.15	10.89	10.80	10.71	11.31	10.24	10.86	10.70	10.76	10.75	11.09
H_2O	3.42	3.85	3.76	2.87	2.77	3.90	3.36	3.37	3.69	2.86	2.79	3.64
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	100.01	99.99	105.62	100.00	100.01	100.00	100.02	99.99	105.42	100.40	100.01
Si^{4+}	6.00	6.00	6.00	5.51	6.00	6.00	6.00	5.90	6.00	5.53	5.77	6.00
Al^{3+}	6.00	7.50	6.00	5.51	5.00	8.00	6.20	7.30	6.20	5.53	5.96	7.60
Fe^{3+}	0.00	0.00	0.00	2.76	0.00	0.00	0.20	0.00	0.00	2.58	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	2.00	0.60	0.70	0.18	0.20	0.30
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.78	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.20	0.10	0.18	0.70	0.10
Li^{+}	0.00	1.50	0.00	1.22	0.00	1.00	0.00	1.20	0.00	1.18	0.19	1.10
Na^{+}	1.00	1.00	1.00	0.92	0.00	0.00	0.60	0.70	0.60	0.65	0.20	0.30
B^{3+}	3	3	3	3	3	3	3	3	3	3	3	3
H^{+}	4.00	4.00	4.00	3.08	3.00	4.00	3.80	3.60	4.00	3.08	3.01	3.80
F^{-}	0.00	0.00	0.00	0.92	1.00	0.00	0.20	0.40	0.00	0.92	0.99	0.20
O^{2-}	31.00	31.00	31.00	30.08	30.00	31.00	30.80	30.60	31.00	30.08	30.01	30.80
Cat Σ	19.00	19.00	19.00	18.92	19.00	18.00	18.60	18.90	18.70	18.83	18.90	18.40
An Σ	31	31	31	31	31	31	31	31	31	31	31	31

assuming $Y + Z + T = 15$ *apfu*. This argument allows cation ordering at the sites to be unknown, including Al at *T*. Using this method and not checking the weight % sums can produce some odd results. Buergerite, since its cation *apfu* is low when OH + F = 4, could mistakenly be thought to contain Li. However, when Li is calculated such that $Y + Z + T = 15$ *apfu*, the weight % sum is much higher than it should be. Hence, care should be taken when iterating for Li, that the final results are reasonable in terms of weight % oxides as well as formula *apfu*.

Table 3.7 shows the results of formula calculation when B_2O_3, H_2O, Li_2O and Fe^{3+}/Fe^{2+} are all unknown. Unfortunately, this is the probably the most common

Table 3.7: Formulae normalized to 31 anions, B and H calculated stoichiometrically, Li and Fe^{3+} not measured

	lSch	*lElb*	*lDrv*	*lBur*	*lUv*	*lRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	----	----	----	----	----	----	----	----	----	----	----	----
FeO	20.46	0.00	0.00	20.49	0.00	0.00	15.50	4.48	5.15	20.46	2.21	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	----	----	----	----	----	----	----	----	----	----	----	----
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	9.91	10.81	10.89	9.92	10.71	11.07	10.20	10.59	10.70	9.93	10.69	10.84
H_2O	3.42	3.73	3.76	2.57	2.77	3.82	3.34	3.28	3.69	2.57	2.77	3.55
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	97.16	99.99	100.30	100.00	98.08	99.78	97.79	99.99	100.38	99.95	97.92
Si^{4+}	6.00	6.19	6.00	6.00	6.00	6.13	6.03	6.05	6.00	5.99	5.80	6.14
Al^{3+}	6.00	7.74	6.00	6.00	5.00	8.17	6.23	7.48	6.20	5.99	6.00	7.77
Fe^{3+}	----	----	----	----	----	----	----	----	----	----	----	----
Fe^{2+}	3.00	0.00	0.00	3.00	0.00	0.00	2.21	0.62	0.70	2.99	0.30	0.31
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.80	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.21	0.10	0.20	0.70	0.10
Li^{+}	----	----	----	----	----	----	----	----	----	----	----	----
Na^{+}	1.00	1.03	1.00	1.00	0.00	0.00	0.60	0.72	0.60	0.70	0.20	0.31
B^{3+}	3	3	3	3	3	3	3	3	3	3	3	3
H^{+}	4.00	4.00	4.00	3.00	3.00	4.00	3.80	3.59	4.00	3.00	3.00	3.80
F^{-}	0.00	0.00	0.00	1.00	1.00	0.00	0.20	0.41	0.00	1.00	1.00	0.20
O^{2-}	31.00	31.00	31.00	30.00	30.00	31.00	30.80	30.59	31.00	30.00	30.00	30.80
Cat Σ	19.00	17.96	19.00	19.00	19.00	17.29	18.66	18.07	18.70	18.87	18.80	17.63
An Σ	31	31	31	31	31	31	31	31	31	31	31	31

case of tourmaline analysis and formula calculations. Here, B and H are again calculated from stoichiometry and Li and Fe^{3+} are left out of the normalization. An interesting, but frightening result is that, with the assumption that all iron is 2+ and OH + F = 4 *apfu*, buergerite formulae end up appearing to be schorl. This leads to the speculation that buergerite as a species might not be as rare as assumed, as it could be mistaken for schorl with only EMPA data available. As Fe^{2+} and Fe^{3+} have different ionic radii, it may be possible to differentiate the two tourmalines using SREF data, though this is often complicated by the large number of chemical species that may populate the octahedral sites, and the details of the site-occupancies are not easy to clarify. Site-ordering curves

developed to date may contain data from buergerites that have been misidentified as schorls, potentially causing problems. Further work needs to be done on developing relations between bond-lengths and constituent-cation radii for tourmaline with known Fe^{3+}/Fe^{2+} ratios and H values. These types of relations are very useful for the pyroxenes and amphiboles (*e.g.* Cameron and Papike 1980, Hawthorne 1983), whose stereochemistry is better understood. Accurate classification of a tourmaline species directly affects our understanding of the geochemical environment in which the mineral formed, particularly the oxygen fugacity of the system.

Normalization schemes on cations are generally not appropriate, as the amounts of Li and Fe^{3+} are commonly not known. However, if the *T*-site is fully occupied by Si, normalization on 6 *apfu* of Si can give good results (Table 3.8), though problems can develop if Al is also present at the *T*-site (as is often the case). The formulae for the non-ideal elbaite and uvite do have some tetrahedral Al. The resultant cation sum for these two are greater than the possible 19 *apfu*, which should be sufficient indication that something is suspect with these normalizations. However, this might not be so readily apparent for elbaite if the Li_2O is not analytically determined. Normalization on 6 *apfu* of Si may be appropriate in those instances where total Al is low and Li is assumed not to occur. In my overall tourmaline sample suite, I ran normalizations on 6 *apfu* of Si for those tourmalines with unreasonably high Si *apfu* from a 31-anion formula calculation method (Appendix G.2). As Si > 6 *apfu* from the anion normalization, $^{[4]}Al$ was assumed not to occur in these samples and the cation normalization was deemed reasonable.

Table 3.8: Formulae normalized to 6 *apfu* Si^{4+}

	ISch	*IElb*	*IDrv*	*IBur*	*IUv*	*IRos*	*Sch*	*Elb*	*Drv*	*Bur*	*Uv*	*Ros*
SiO_2	34.22	38.49	37.60	34.26	36.97	39.03	35.35	36.86	36.93	34.22	35.66	38.28
Al_2O_3	29.04	40.82	31.90	29.07	26.14	44.15	30.99	38.69	32.38	29.03	31.30	41.14
Fe_2O_3	0.00	0.00	0.00	22.76	0.00	0.00	1.57	0.00	0.00	21.22	0.82	0.00
FeO	20.46	0.00	0.00	0.00	0.00	0.00	14.09	4.48	5.15	1.36	1.47	2.29
MgO	0.00	0.00	12.61	0.00	16.53	0.00	2.37	0.00	8.67	0.00	11.55	0.00
CaO	0.00	0.00	0.00	0.00	5.75	0.00	0.00	1.17	0.57	1.06	4.02	0.60
Li_2O	0.00	2.39	0.00	0.00	0.00	1.62	0.00	1.86	0.00	0.00	0.15	1.75
Na_2O	2.94	3.31	3.23	2.94	0.00	0.00	1.82	2.26	1.90	2.06	0.63	0.99
B_2O_3	9.91	11.15	10.89	9.92	10.71	11.30	10.24	10.86	10.70	9.91	10.69	11.09
H_2O	3.42	3.85	3.76	0.00	2.77	3.90	3.36	3.37	3.69	0.09	2.58	3.63
F	0.00	0.00	0.00	1.81	1.95	0.00	0.37	0.79	0.00	1.80	1.94	0.40
O=F	0.00	0.00	0.00	-0.76	-0.82	0.00	-0.16	-0.33	0.00	-0.76	-0.82	-0.17
Total	99.99	100.01	99.99	100.00	100.00	100.00	100.00	100.01	99.99	99.99	99.99	100.00
Si^{4+}	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00	6.00
Al^{3+}	6.00	7.50	6.00	6.00	5.00	8.00	6.20	7.42	6.20	6.00	6.21	7.60
Fe^{3+}	0.00	0.00	0.00	3.00	0.00	0.00	0.20	0.00	0.00	2.80	0.10	0.00
Fe^{2+}	3.00	0.00	0.00	0.00	0.00	0.00	2.00	0.61	0.70	0.20	0.21	0.30
Mg^{2+}	0.00	0.00	3.00	0.00	4.00	0.00	0.60	0.00	2.10	0.00	2.90	0.00
Ca^{2+}	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.20	0.10	0.20	0.73	0.10
Li^{+}	0.00	1.50	0.00	0.00	0.00	1.00	0.00	1.22	0.00	0.00	0.10	1.10
Na^{+}	1.00	1.00	1.00	1.00	0.00	0.00	0.60	0.71	0.60	0.70	0.21	0.30
B^{3+}	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.05	3.00	3.00	3.11	3.00
H^{+}	4.00	4.00	4.00	0.00	3.00	4.00	3.80	3.66	4.00	0.11	2.90	3.80
F^{-}	0.00	0.00	0.00	1.00	1.00	0.00	0.20	0.41	0.00	1.00	1.03	0.20
O^{2-}	31.00	31.00	31.00	30.00	30.00	31.00	30.80	31.12	31.00	30.00	31.04	30.80
Cat Σ	19.00	19.00	19.00	19.00	19.00	18.00	18.60	19.22	18.70	18.90	19.55	18.41
An Σ	31.00	31.00	31.00	31.00	31.00	31.00	31.00	31.52	31.00	31.00	32.07	31.00

3.4 Conclusions

Problems are routinely encountered when trying to calculate tourmaline formulae as the analysis data are commonly missing some information. The most logical approach to deriving an accurate formula is to start with as much accurate data as possible. When all constituents have been measured, a simple normalization on 31 anions produces an accurate formula. When there are unknowns, however, assumptions must be made, and the variations in available normalization schemes begin to show different results. Schemes which normalize on 27 or 24.5 anions, leaving out the O1 and O3 anions, also

leave out the site which contains F, making the formula for any F-bearing tourmaline incorrect. If F is simply omitted from the normalization, an accurate mineral name (including anion components) may be difficult to assign. As F is common as a trace to dominant constituent of the *W*-site (O1), these schemes are inappropriate in most instances. In almost all situations, the results are better if OH + F is assumed to equal 4 *apfu*. Adjusting this sum to lower values lowers the overall weight % sum and increases the total cation *apfu*.

Li may be iterated for by adding Li_2O to the calculation scheme until $Y + Z + T =$ 15 *apfu*. This gives a reasonable first approximation of Li content. Accurate Li values may be measured using SIMS, though the technique is still being improved.

Iron ratios can be quite difficult to determine in tourmaline, yet every effort should be made to attain these values. There is a significant difference in ionic radii for Fe^{2+} and Fe^{3+}, but the large number of constituents at the octahedral sites can make it difficult to get a good Fe^{3+}/Fe^{2+} ratio solely using structure data. As $Fe^{3+} + O^{2-}$ substitute for $Fe^{2+} + (OH)^-$, without an accurate measure of Fe^{3+}/Fe^{2+} or H, inaccurate categorization of tourmalines may be made, especially if there is no accompanying crystal-structure data.

Cation normalization schemes are less useful than anion-based approaches, as unknown amounts of vacancies may occur at cation sites. However, normalization on 6 *apfu* of Si at the *T*-site can be useful, especially if initial anion normalization led to >6 *apfu* Si. As Si has not been shown to occur at any site other than *T*, it cannot exceed 6 *apfu* in tourmaline. Therefore cation normalization on Si^{4+} can provide a more useful

formula in instances where normalization on 31 anions reports an unreasonably high Si *apfu*.

If information is known about certain samples prior to formula calculation, this information should be brought into the normalization scheme if appropriate. Examples include the likelihood of Li or Fe^{3+} in an environment, or restrictions based on crystal-structure data. Ultimately, the more data analytically determined, the more accurate the resultant formula.

CHAPTER 4

Potential New Species of Tourmaline

4.1 Criteria for new mineral species

The International Mineralogical Association's Commission on New Minerals and Mineral Names (CNMMN) is the body established for regulating mineral nomenclature. Nickel and Mandarino (1987), representing the CNMMN, defined two guidelines for defining a new mineral species. A mineral is a new species if, compositionally, at least one major structural site is occupied by a different chemical component than which occurs in the equivalent site in a recognized mineral. Crystallographically, a mineral is a new species if the structure of the mineral is topologically different from a recognized one. Nickel (1992), again representing the CNMMN, later clarified mineral nomenclature in cases of solid-solution. According to Nickel, a complete solid-solution series without structural order of the ions defining the end-members is arbitrarily divided at 50 mole %. In ternary systems, the 50% rule is applied between end-members, resulting in three bisectors of the ternary triangle, meeting at the center. Each end-member is named, and this name applies to the compositional range from the corner to the bisectors (Figure 4.1). Hawthorne and Henry (1999) proposed that tourmaline-group minerals should be differentiated on the basis of their anion component, as well as their cation components. Further discussion of this is given in Chapter 1.2.2.

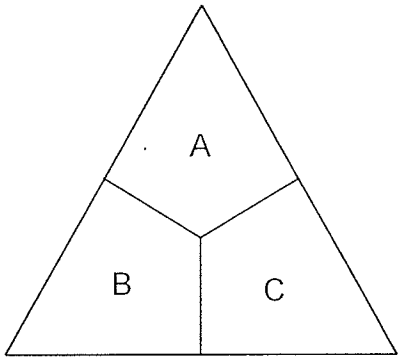

Figure 4.1: Nomenclature for a ternary solid-solution. A, B, and C represent three compositional fields which each deserve a mineral name (after Nickel, 1992).

Much of the work on potential new species of tourmaline is preliminary and further analyses need to be done on most samples, including analysis of light elements and measurement of the optical properties. For some samples, this will be done pending acceptance of the proposed tourmaline nomenclature scheme by the CNMMN. For the chrome tourmaline in particular, light-element analysis has been delayed until appropriate standards for SIMS analyses are developed.

4.2 "Fluordravite"

4.2.1 Occurrence

"Fluordravite" was discovered in material from the Crabtree Emerald Mine, North Carolina, USA. The Crabtree Pegmatite belongs to the Spruce Pine District pegmatites, which intrude mica schists and gneisses of Late Proterozoic age in the eastern Blue Ridge province. Unlike the mineralogically simple pegmatites that make up the majority of the Spruce Pine suite, the Crabtree pegmatite has a complex mineralogy, characterized by abundant tourmaline and emerald with plagioclase, K-feldspar, quartz. Accessory

minerals include muscovite, garnet, biotite and fluorite. This complex chemistry is a result of interactions between the pegmatitic fluids and the host, a highly altered plagioclase-chlorite-quartz-calcite metaconglomerate. The sample was obtained from the Smithsonian Institution where it is catalogued as sample 121341.

4.2.2 Physical and optical properties

"Fluordravite" is black and has a vitreous luster; it has a pale-brown streak and shows no fluorescence under long-wave or short-wave ultraviolet light. It occurs as striated prisms. "Fluordravite" has a Mohs hardness of ~7, no cleavage, and is brittle. The calculated density is 3.13 g/cm^3. Optical data has not been collected yet for this sample.

4.2.3 Chemical composition

"Fluordravite" was analyzed by electron microprobe by the method described in Chapter 2. The average composition is given in Table 4.2.1. The unit formula was

TABLE 4.2.1: Chemical composition (wt%) and formula unit (*apfu*) for "fluordravite"

SiO_2	36.02	Na	0.89	Si	5.92
TiO_2	0.25	Ca	0.04	Al	0.08
Al_2O_3	31.69	ΣX	0.93	ΣT	6.00
MgO	7.71				
FeO	6.41	Mg	1.89	Al	6.00
MnO	0.67	Fe^{2+}	0.88	Mg	0.00
CaO	0.25	Mn	0.09	ΣZ	6.00
Na_2O	2.80	Al	0.06		
F	1.45	Li	0.04	OH	3.25
Li_2O^*	0.05	Ti	0.03	F	0.75
$B_2O_3^*$	10.57	ΣY	2.99	$\Sigma V + W$	4.00
H_2O^*	2.96				
$O \equiv F$	-0.61				
Total	100.22				

* Calculated assuming 31 anions *pfu*; Li_2O, B_2O_3 and H_2O calculated from stoichiometry
Cr, V, Zn, K not detected

calculated on the basis of 31 anions assuming B = 3 *apfu* (atoms per formula unit), OH + F = 4 *apfu* and Li_2O calculated to ensure full occupancy at the *Y*, *Z* and *T*-sites. Further analysis will be done to collect quantitative B_2O_3, Li_2O and H_2O data.

4.2.4 Crystal structure

The powder-diffraction pattern was recorded on a Philips PW 1710 diffractometer as described in Chapter 2.4. Cell dimensions were refined using the program JADE 6.1. The systematic absences are compatible with the space group *R*3*m* that is observed for all other tourmaline species (Table 4.2.2).

TABLE 4.2.2: Indexed powder-diffraction pattern for "fluordravite"

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	*h,k,l*	I_{obs}	d_{obs} (Å)	d_{calc} (Å)	*h,k,l*
19.4	6.375	6.368	0,1,1	27.3	1.920	1.921	4,3,2
11.7	4.985	4.979	2,0,1	2.3	1.906	1.906	3,5,1
6.3	4.620	4.612	3,0,0	6.1	1.874	1.874	1,4,3
22.2	3.998	3.994	2,2,0	3.0	1.853	1.854	6,2,1
100.0	3.475	3.471	1,0,2	6.1	1.779	1.779	3,3,3
7.7	3.386	3.384	1,3,1	3.5	1.735	1.736	0,2,4
4.4	3.023	3.020	1,4,0	14.3	1.660	1.660	0,6,3
59.9	2.961	2.958	2,1,2	5.1	1.646	1.645	7,2,1
4.4	2.904	2.903	3,2,1	6.3	1.598	1.598	5,5,0
3.7	2.621	2.620	3,1,2	3.9	1.592	1.592	0,4,4
66.6	2.583	2.582	0,5,1	2.1	1.561	1.561	3,2,4
2.5	2.491	2.490	4,0,2	2.0	1.538	1.538	9,0,0
14.2	2.392	2.391	0,0,3	3.1	1.529	1.529	2,7,2
9.9	2.378	2.377	3,2,2	11.8	1.505	1.505	5,0,4
8.4	2.350	2.348	5,1,1	3.0	1.427	1.427	1,0,5
6.5	2.191	2.191	5,0,2	3.4	1.422	1.422	5,6,1
6.9	2.169	2.168	3,4,1	6.8	1.358	1.359	0,10,1
14.2	2.123	2.123	3,0,3	5.2	1.328	1.328	3,5,4
5.7	2.114	2.113	2,4,2	2.3	1.325	1.325	5,7,0
12.5	2.051	2.051	2,2,3	4.4	1.314	1.313	10,1,0
19.1	2.043	2.043	5,1,2	2.4	1.308	1.308	3,8,2
6.9	2.025	2.024	6,1,1	4.5	1.274	1.274	5,0,5

Cu*K*α (Ni-filtered) λ = 1.5406 Å; data for intensities > 2%; outlier rejected data (2σ) not listed; calculated powder pattern from single-crystal structure refinement used to aid indexing; no internal standard
a = 15.978(1), c = 7.172(1) Å, V = 1585.6 Å^3

A fragment of "fluordravite" was ground to an ellipsoid and mounted on a Nicolet *R*3*m* four-circle diffractometer. Cell dimensions and intensity data were collected

according to the experimental procedure described in Chapter 2. Refined unit-cell dimensions and selected data pertaining to crystal-structure refinement are given in Table 4.2.3.

TABLE 4.2.3: Unit-cell dimensions and data pertaining to crystal-structure refinement of "fluordravite" (Sample CT50)

a (Å)	15.955 (3)	radiation	Mo$K\alpha$
c	7.153 (2)	scan mode	θ-2θ
V (Å)^3	1576.9	θ range (°)	4-60
Space group	$R3m$	R(az) (%)	1.4 → 1.0
R (obs) (%)	1.61	Total $\|F\|$	1139
wR (%)	2.21	$\|F_{obs}\|$	1137
GOF	2.69		

Structure refinement was initiated with the atom coordinates of foitite (MacDonald *et al.* 1993) using the SHELTXL PC Plus system of programs. The final refinement for an anisotropic-displacement model converged to an R index of 1.61% for 1137 observed (5σ) reflections. Final atom parameters, refined site-scattering values, and selected interatomic distances and angles are given in Appendices C, D and F, respectively, as Sample CT50. Observed and calculated structure-factors will be deposited with the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada. The crystal used in the collection of the X-ray intensity data was subsequently analyzed using an electron microprobe.

4.2.5 Discussion

The composition of "fluordravite" (Table 4.2.1) may be generalized to the end-member composition Na Mg_3 Al_6 (Si_6O_{18}) $(BO_3)_3$ $(OH)_3$ F. An alkali tourmaline, it is distinct from dravite due to the presence of F, as opposed to (OH), at the O1 (= W)

crystallographic site. As Hawthorne and Henry (1999) discussed, this distinction between dominant anions in a crystallographic site is required in an end-member composition. This proposed new tourmaline species will be submitted to the CNMMN.

4.3 "Fluorelbaite"

4.3.1 Occurrence

"Fluorelbaite" was discovered in material from the Black Mountain granitic pegmatite, Rumford, in western Maine, USA. This pegmatite lies within the northern portion of the Oxford pegmatite field, which is near the Mooselookmeguntic, Rumford and Whitecap Mountain granitic plutons. The Black Mountain pegmatite intrudes sulfide-bearing mica schist, mica schist and impure quartzite. The pegmatite is strongly zoned and contains a wide array of rare-element minerals, including beryl, spodumene, cassiterite, columbite, amblygonite-montebrasite and lepidolite (Brown and Wise 2001). The sample was obtained from the Royal Ontario Museum where it is catalogued as sample M30977.

4.3.2 Physical and optical properties

"Fluorelbaite" is pale green and has a vitreous luster; it has a white streak and shows no fluorescence under long-wave or short-wave ultraviolet light. "Fluorelbaite" has a Mohs hardness of ~7, no cleavage, and is brittle. The calculated density is 3.02 g/cm^3. Optical data has not been collected yet for this sample.

4.3.3 Chemical composition

"Fluorelbaite" was analyzed by electron microprobe by the method described in Chapter 2. The average composition is given in Table 4.2.1. The initial unit formula was calculated on the basis of 6 apfu of Si assuming B = 3 *apfu* (atoms per formula unit), OH + F = 4 *apfu* and Li_2O calculated to ensure full occupancy at the *Y*, *Z* and *T*-sites. Further analyses will be done to collect quantitative B_2O_3, Li_2O and H_2O data.

TABLE 4.3.1: Chemical composition (wt%) and formula unit (*apfu*) for "fluorelbaite"

SiO_2	38.58	Na	0.61	Si	6.00
Al_2O_3	40.19	Ca	0.04	Al	0.00
MgO	0.04	ΣX	0.65	ΣT	6.00
FeO	1.65				
MnO	0.15	Al	1.37	Al	6.00
ZnO	0.13	Li	1.37	Mg	0.00
CaO	0.25	Fe^{2+}	0.22	ΣZ	6.00
Na_2O	2.01	Mn	0.02		
F	1.14	Zn	0.02	OH	3.44
Li_2O^*	2.19	Mg	0.01	F	0.56
$B_2O_3^*$	11.18	ΣY	3.01	$\Sigma V + W$	4.00
H_2O^*	3.32				
$O \equiv F$	-0.45				
Total	100.34				

* Calculated assuming Si = 6 *apfu*; Li_2O, B_2O_3 and H_2O calculated from stoichiometry
Cr, V, Ti, K not detected

4.3.4 Crystal structure

The powder-diffraction pattern was recorded on a Philips PW 1710 diffractometer as described in Chapter 2.4. Cell dimensions were refined using the program JADE 6.1. The systematic absences are compatible with the space group *R*3*m* that is observed for all other tourmaline species (Table 4.3.2).

TABLE 4.3.2: Indexed powder-diffraction pattern for "fluorelbaite"

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	h,k,l	I_{obs}	d_{obs} (Å)	d_{calc} (Å)	h,k,l
3.4	7.937	7.930	1,1,0	12.3	1.586	1.586	5,5,0
13.7	6.312	6.313	0,1,1	10.6	1.578	1.578	0,4,4
22.1	4.941	4.939	2,0,1	2.7	1.568	1.568	8,1,1
6.6	4.582	4.578	3,0,0	3.7	1.539	1.538	6,4,1
37.5	4.196	1.412	1,2,1	3.7	1.527	1.526	9,0,0
46.4	3.966	3.965	2,2,0	4.0	1.517	1.517	2,7,2
17.9	3.361	3.358	1,3,1	2.0	1.510	1.510	7,3,1
5.6	3.093	3.092	0,4,1	3.5	1.498	1.499	8,2,0
12.7	2.998	2.997	4,1,0	19.6	1.492	1.492	0,5,4
4.2	2.883	2.881	3,2,1	6.4	1.466	1.466	2,4,4
8.2	2.600	2.599	3,1,2	22.7	1.442	1.442	5,1,4
92.3	2.563	2.562	5,0,1	2.7	1.424	1.424	4,7,0
18.5	2.370	2.370	0,0,3	6.1	1.414	1.414	0,1,5
27.1	2.358	2.358	3,2,2	26.1	1.397	1.398	3,6,3
39.9	2.330	2.331	5,1,1	4.4	1.349	1.349	10,0,1
8.0	2.173	2.174	5,0,2	3.0	1.334	1.335	6,5,2
14.6	2.152	2.152	4,3,1	2.6	1.322	1.322	6,6,0
18.4	2.105	2.105	0,3,3	6.2	1.318	1.318	5,5,3
12.8	2.096	2.096	2,4,2	6.0	1.314	1.314	0,4,5
20.8	2.034	2.034	2,2,3	7.8	1.304	1.304	1,10,0
35.4	2.027	2.027	1,5,2	2.4	1.296	1.296	2,3,5
4.3	2.009	2.009	1,6,1	2.5	1.270	1.270	3,9,0
2.4	1.934	1.983	4,4,0	2.1	1.267	1.267	8,2,3
31.0	1.907	1.906	4,3,2	15.6	1.263	1.263	5,0,5
3.3	1.891	1.891	5,3,1	4.7	1.250	1.250	4,5,4
6.5	1.859	1.859	4,1,3	3.5	1.230	1.230	0,11,1
7.0	1.840	1.840	6,2,1	2.4	1.203	1.203	3,4,5
14.2	1.763	1.764	3,3,3	4.7	1.147	1.147	3,0,6
3.3	1.720	1.721	2,0,4	3.0	1.142	1.142	10,1,3
22.0	1.647	1.646	0,6,3	3.3	1.119	1.119	9,3,3
12.7	1.633	1.633	2,7,1				

Cu$K\alpha$ (Ni-filtered) $\lambda = 1.5406$ Å; data for intensities > 2%;outlier rejected data (2σ) not listed calculated powder pattern from single-crystal structure refinement used to aid indexing; no internal standard
$a = 15.860(1)$, $c = 7.109(1)$ Å, $V = 1548.5$ Å^3

A fragment of "fluorelbaite" was ground to an ellipsoid and mounted on a Nicolet *R*3*m* four-circle diffractometer. Cell dimensions and intensity data were collected according to the experimental procedure described in Chapter 2. Refined unit-cell dimensions and selected data pertaining to crystal-structure refinement are given in Table 4.3.3.

TABLE 4.3.3: Unit-cell dimensions and data pertaining to crystal-structure refinement of "fluorelbaite" (Sample CT27)

a (Å)	15.851 (2)	radiation	Mo$K\alpha$
c	7.103 (3)	scan mode	θ-2θ
V (Å)^3	1545.5	θ range (°)	4-60
Space group	$R3m$		
R (obs) (%)	1.96	Total $\|F\|$	1109
wR (%)	2.28	$\|F_{obs}\|$	1083
GOF	1.98		

The structure refinement was initiated with the atom coordinates of foitite (MacDonald *et al.* 1993) using the SHELTXL PC Plus system of programs. The final refinement for an anisotropic-displacement model converged to an R index of 1.96% for 1083 observed (5σ) reflections. Final atom parameters, refined site-scattering values, and the selected interatomic distances and angles are given in Appendices C, D and F, respectively, as Sample CT31. Observed and calculated structure-factors will be deposited with the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada. The crystal used in the collection of the X-ray intensity data was subsequently analyzed using an electron microprobe.

4.3.5 Discussion

The composition of "fluorelbaite" (Table 4.3.1) may be generalized to the end-member composition Na $(Li_{1.5}Al_{1.5})$ Al_6 (Si_6O_{18}) $(BO_3)_3$ $(OH)_3$ F. An alkali tourmaline, it is distinct from elbaite due to the presence of F, as opposed to (OH), at the O1 (= W) crystallographic site. This proposed new tourmaline species will be submitted to the CNMMN.

4.4 "Fluorschorl"

4.4.1 Occurrence

"Fluorschorl" was discovered in material from San Diego County, California, USA. The sample was obtained from a gem dealer, but the locality indicates that it is of pegmatite origin.

4.4.2 Physical and optical properties

"Fluorschorl" is black and has a vitreous luster; it has a pale-brown streak and shows no fluorescence under long-wave or short-wave ultraviolet light. It occurs as striated prisms. "Fluorschorl" has a Mohs hardness of ~7, no cleavage, and is brittle. The calculated density is 3.13 g/cm^3. Optical data has not been collected yet for this sample.

4.4.3 Chemical composition

"Fluorschorl" was analyzed by electron microprobe by the method described in Chapter 2. The average composition is given in Table 4.4.1. The unit formula was calculated on the basis of 31 anions assuming B = 3 *apfu* (atoms per formula unit), OH + F = 4 *apfu* and Li_2O calculated to ensure full occupancy at the *Y*, *Z* and *T*-sites. Further analysis will be done to collect quantitative B_2O_3, Li_2O and H_2O data.

TABLE 4.4.1: Chemical composition (wt%) and formula unit (*apfu*) for "fluorschorl"

SiO_2	35.89	Na	0.69	Si	5.86
TiO_2	0.77	Ca	0.17	Al	0.14
Al_2O_3	35.80	ΣX	0.86	ΣT	6.00
MgO	0.63				
FeO	7.71	Fe^{2+}	1.05	Al	6.00
MnO	0.65	Li	0.84	Mg	0.00
CaO	0.96	Al	0.76	ΣZ	6.00
Na_2O	2.17	Mg	0.15		
F	1.08	Ti	0.10	OH	3.44
Li_2O^*	1.28	Mn	0.09	F	0.56
$B_2O_3^*$	10.64	ΣY	2.99	$\Sigma V + W$	4.00
H_2O^*	3.16				
$O \equiv F$	-0.45				
Total	100.27				

* Calculated assuming 31 anions *pfu*; Li_2O, B_2O_3 and H_2O calculated from stoichiometry
Cr, V, Zn, K not detected

4.4.4 Crystal structure

The powder-diffraction pattern was recorded on a Philips PW 1710 diffractometer as described in Chapter 2.4. Cell dimensions were refined using the program JADE 6.1. The systematic absences are compatible with the space group *R*3*m* that is observed for all other tourmaline species (Table 4.4.2).

A fragment of "fluorschorl" was ground to an ellipsoid and mounted on a Nicolet *R*3*m* four-circle diffractometer. Cell dimensions and intensity data were collected according to the experimental procedure described in Chapter 2. Refined unit-cell dimensions and selected data pertaining to crystal-structure refinement are given in Table 4.4.3.

TABLE 4.4.2: Indexed powder-diffraction pattern for "fluorschorl"

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	h,k,l	I_{obs}	d_{obs} (Å)	d_{calc} (Å)	h,k,l
35.0	6.350	6.336	1,0,1	2.5	1.687	1.687	1,2,4
25.1	4.978	4.960	0,2,1	21.9	1.654	1.653	6,0,3
13.9	4.614	4.604	3,0,0	10.5	1.641	1.642	4,3,3
61.0	4.219	4.212	2,1,1	9.6	1.594	1.595	5,5,0
58.2	3.990	3.987	2,2,0	5.3	1.584	1.584	6,4,0
100.0	3.458	3.453	4,0,0	2.0	1.555	1.556	5,5,1
10.1	3.378	3.374	1,3,1	2.3	1.546	1.547	6,4,1
2.9	3.108	3.108	4,0,1	3.4	1.525	1.525	2,7,2
8.7	3.014	3.014	4,1,0	17.2	1.499	1.500	0,9,1
92.9	2.947	2.944	2,1,2	3.9	1.472	1.472	1,8,2
8.6	2.897	2.895	2,3,1	20.0	1.448	1.448	5,6,0
6.3	2.611	2.610	2,4,0	2.3	1.431	1.432	7,4,0
92.5	2.576	2.576	5,0,1	7.1	1.420	1.419	5,6,1
2.9	2.483	2.480	5,1,0	12.6	1.403	1.404	1,1,5
24.1	2.380	2.377	0,0,3	2.2	1.375	1.376	2,1,5
15.1	2.342	2.342	1,0,3	6.1	1.355	1.356	10,0,1
2.2	2.301	2.302	1,4,2	3.0	1.341	1.341	5,6,2
2.5	2.281	2.278	1,1,3	4.9	1.324	1.324	5,5,3
17.6	2.183	2.183	0,5,2	5.5	1.319	1.318	6,4,3
10.9	2.163	2.163	1,2,3	5.8	1.310	1.311	1,10,0
18.1	2.115	2.112	2,5,1	3.4	1.306	1.306	6,6,1
46.9	2.037	2.036	5,1,2	3.1	1.301	1.301	7,5,1
6.6	2.018	2.020	3,1,3	3.0	1.273	1.273	8,2,3
36.3	1.915	1.915	3,4,2	10.3	1.268	1.267	0,5,5
3.1	1.901	1.901	3,2,3	2.2	1.256	1.256	11,0,0
7.4	1.868	1.866	4,1,3	2.3	1.236	1.236	1,5,5
5.9	1.849	1.850	6,2,1	2.5	1.152	1.151	12,0,0
9.1	1.770	1.768	5,4,0	3.0	1.147	1.148	10,1,3
3.5	1.728	1.726	8,0,0	2.0	1.124	1.124	0,4,6

Cu$K\alpha$ (Ni-filtered) $\lambda = 1.5406$ Å; data for intensities > 2%;outlier rejected data (2σ) not listed calculated powder pattern from single-crystal structure refinement used to aid indexing; no internal standard
$a = 15.947(2)$, $c = 7.130(1)$ Å, $V = 1570.3$ Å^3

TABLE 4.4.3: Unit-cell dimensions and data pertaining to crystal-structure refinement of "fluorschorl" (Sample CT63)

a (Å)	15.932 (1)	radiation	Mo$K\alpha$
c	7.134 (1)	scan mode	θ-2θ
V (Å)^3	1568.1	θ range (°)	4-60
Space group	$R3m$	R(az) (%)	1.4 → 0.8
R (obs) (%)	2.08	Total $\|F\|$	1129
wR (%)	2.20	$\|F_{obs}\|$	1091
GOF	1.73		

The structure refinement was initiated with the atom coordinates of foitite (MacDonald *et al.* 1993) using the SHELTXL PC Plus system of programs. The final

refinement for an anisotropic-displacement model converged to an *R* index of 2.08% for 1091 observed (5σ) reflections. Final atom parameters, refined site-scattering values, and the selected interatomic distances and angles are given in Appendices C, D and F, respectively, as Sample CT63. Observed and calculated structure-factors will be deposited with the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada. The crystal used in the collection of the X-ray intensity data was subsequently analyzed using an electron microprobe.

4.4.5 Discussion

The composition of "fluorschorl" (Table 4.5.1) may be generalized to the end-member composition $Na\ Fe_3\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$. An alkali tourmaline, it is distinct from schorl due to the presence of F, as opposed to (OH), at the O1 (= *W*) crystallographic site. This proposed new tourmaline species will be submitted to the CNMMN.

4.5 "Hydroxyuvite"

4.5.1 Occurrence

"Hydroxyuvite" was discovered in material from the Brumado mine in Bahia, Brazil. Brumado is the largest town in southern Bahia and lies to the west-southwest of Salvador. The area consists primarily of Precambrian gneisses and schists with granitic intrusions and amphibolite [*sic*] dikes. These basement materials are overlain by a metamorphosed sequence of quartzite and dolomite which has been correlated with the Minas series in southern Minas Gerias. Four distinct stages of mineralization have been

described in the area, associated with periods of fracturing. Stages 1,2 and 4 were characterized by deposition of magnesite and/or alteration of pre-existing minerals to Mg-rich varieties, with stage 4 also having deposition of opal and calcite. Silica and aluminosilicates, as well as hematite, tourmaline and beryl, characterize the third stage of mineralization (Cassedanne and Cassedanne 1978). "Hydroxyuvite" occurs as euhedral orange crystals, both as single crystals and as aggregates. The sample was obtained from a mineral dealer.

4.5.2 Physical and optical properties

"Hydroxyuvite" is orange and has a vitreous luster; it has a pale-orange streak and shows no fluorescence under long-wave or short-wave ultraviolet light. It occurs as aggregates and singles of terminated crystals up to 1cm in size, and shortened on the *c*-axis. "Hydroxyuvite" has a Mohs hardness of ~7, no cleavage, and is brittle. The density, measured by flotation, is 3.10(4) g/cm^3, close to the calculated density of 3.07 g/cm^3.

In transmitted light, "hydroxyuvite" is dichroic, O = orange, E = pale yellow. It is uniaxial negative with indices of refraction ω = 1.646(2), ϵ = 1.624(2), measured with gel-filtered Na light (λ = 589.9 nm).

4.5.3 Chemical composition

"Hydroxyuvite" was analyzed by electron microprobe by the method described in Chapter 2. The H_2O content was analyzed by hydrogen-line extraction as described in

Chapter 2.5.2. The average composition is given in Table 4.5.1. The unit formula was calculated on the basis of 31 anions assuming B = 3 *apfu* (atoms per formula unit).

TABLE 4.5.1: Chemical composition (wt%) and formula unit (*apfu*) for "hydroxyuvite"

SiO_2	35.77	Ca	0.58	Si	5.90
TiO_2	0.40	Na	0.36	Al	0.10
Al_2O_3	28.55	ΣX	0.94	ΣT	6.00
MgO	11.52				
FeO	3.67	Mg	2.27	Al	5.44
CaO	3.30	Fe^{2+}	0.51	Mg	0.56
Na_2O	1.12	Ti	0.05	ΣZ	6.00
H_2O	3.77	ΣY	2.83		
F	0.43			OH	4.14
B_2O_3*	10.47			F	0.22
$O \equiv F$	-0.18			$\Sigma V + W$	4.36
Total	100.27				

* Calculated assuming 31 anions *pfu*; B_2O_3 calculated from stoichiometry
Cr, V, Mn, Zn, Li, K not detected

4.5.4 Crystal structure

The powder-diffraction pattern was recorded on a Gandolfi camera with Cu$K\alpha$ X-radiation. Cell dimensions were refined using the program CELREF (Appleman and Evans 1973). The systematic absences are compatible with the space group *R*3*m* that is observed for all other tourmaline species (Table 4.5.2). There was no correction for shrinkage and no internal standards were used.

A fragment of "hydroxyuvite" was ground to an ellipsoid and mounted on a Nicolet *R*3*m* four-circle diffractometer. Cell dimensions and intensity data were collected according to the experimental procedure described in Chapter 2. Refined unit-cell dimensions and selected data pertaining to crystal-structure refinement are given in Table 4.5.3.

TABLE 4.5.2: Indexed powder-diffraction pattern for "hydroxyuvite"

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	h,k,l	I_{obs}	d_{obs} (Å)	d_{calc} (Å)	h,k,l
50	6.385	6.402	-1,1,1	5	1.882	1.882	-1,5,3
50	4.981	4.996	0,2,1	5	1.857	1.855	-6,8,1
50	4.596	4.613	0,3,0	5	1.786	1.786	-3,6,3
90	4.234	4.236	-2,3,1	5	1.695	1.695	-2,8,2
100	3.978	3.995	-2,4,0	20	1.665	1.665	-6,6,3
70	3.491	3.494	0,1,2	20	1.665	1.665	0,6,3
15	3.394	3.389	-1,4,1	20	1.647	1.646	-2,9,1
5	3.021	3.020	-1,5,0	30	1.598	1.598	-5,10,0
80	2.969	2.972	-1,3,2	5	1.549	1.551	-4,10,1
5	2.913	2.907	-3,5,1	5	1.533	1.531	-7,9,2
5	2.624	2.630	-3,4,2	20	1.512	1.513	0,5,4
90	2.582	2.585	0,5,1	5	1.485	1.486	-2,6,4
10	2.408	2.407	0,0,3	30	1.460	1.461	-5,6,4
10	2.384	2.384	-2,5,2	10	1.437	1.437	0,1,5
15	2.353	2.350	-5,6,1	15	1.414	1.434	-4,7,4
5	2.303	2.307	0,6,0	5	1.359	1.359	-10,10,1
5	2.197	2.197	-5,5,2	5	1.346	1.346	-5,11,2
10	2.169	2.170	-4,7,1	15	1.333	1.333	-3,8,4
10	2.137	2.134	0,3,3	15	1.333	1.333	0,4,5
10	2.137	2.134	-3,3,3	15	1.333	1.332	-6,12,0
40	2.048	2.048	-1,6,2	15	1.333	1.331	-5,10,3
5	2.027	2.026	-1,7,1	15	1.314	1.314	-1,11,0
5	1.998	1.998	-4,8,0	15	1.281	1.280	-5,5,5
30	1.925	1.925	-3,7,2				

114.6 Debye-Scherrer camera with Gandolfi attachment; Cu$K\alpha$ (Ni-filtered) $\lambda = 1.5418$ Å; observed intensities visually estimated; calculated powder pattern from single-crystal structure refinement used to aid indexing; no correction for shrinkage; no internal standard;
$a = 15.981(3)$, $c = 7.222(2)$ Å, $V = 1597.3(5)$ Å^3

TABLE 4.5.3: Unit-cell dimensions and data pertaining to crystal-structure refinement of "hydroxyuvite" (Sample CT79)

a (Å)	15.954 (1)	radiation	Mo$K\alpha$
c	7.214 (1)	scan mode	θ - 2θ
V (Å)^3	1590.0	θ range (°)	4 - 60
Space group	$R3m$	R(az) (%)	1.0 → 0.8
R (obs) (%)	1.77	Total $\|F\|$	1147
wR (%)	2.13	$\|F_{obs}\|$	1127
GOF	1.97		

The structure refinement was initiated with the atom coordinates of foitite (MacDonald *et al.* 1993) using the SHELTXL PC Plus system of programs. The final refinement for an anisotropic-displacement model converged to an R index of 1.8% for

1127 observed (5σ) reflections. Final atom parameters, refined site-scattering values, and the selected interatomic distances and angles are given in Appendices C, D and F, respectively, as Sample CT79. Observed and calculated structure-factors will be deposited with the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada. The crystal used in the collection of the X-ray intensity data was subsequently analyzed using an electron microprobe.

4.5.5 Discussion

The composition of "hydroxyuvite" (Table 4.5.1) may be generalized to the end-member composition $Ca\ Mg_3\ Al_6'\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ (OH)$. A calcic tourmaline, it is distinct from uvite due to the presence of (OH), as opposed F, at the O1 (= *W*) crystallographic site. This proposed new tourmaline species has been submitted to the CNMMN.

4.6 "Cralpoite"

4.6.1 Occurrence

"Cralpoite" was discovered in material from the chromite deposits of Nausahi, Keonjhar District, India. It occurs as thin anastomosing veins replacing chromite along fractures and as encrustations on the surface of chromite. Larger crystals occur in vugs within the host (Mukherjee 1966). The sample was obtained from the Smithsonian Institution where it is catalogued as sample 120534.

4.6.2 Physical and optical properties

"Cralpoite" is dark green and has a vitreous luster; it has a pale-green streak and shows no fluorescence under long-wave or short-wave ultraviolet light. It occurs as acicular striated single crystals up to 0.4 cm in the *c*-axis direction and granular masses of crystals. "Cralpoite" has a Mohs hardness of ~7, no cleavage, and is brittle. The calculated density is 3.14 g/cm^3.

In transmitted light, "cralpoite" is dichroic, O = dark emerald green with a distinct blue tint, E = medium intensity yellow-green. It is uniaxial negative with indices of refraction ω = 1.746(2), ϵ = 1.702(2), measured with gel-filtered Na light (λ = 590.0 nm).

4.6.3 Chemical composition

"Cralpoite" was analyzed by electron microprobe by the method described in Chapter 2. The average composition is given in Table 4.6.1. The unit formula was

TABLE 4.6.1: Chemical composition (wt%) and formula unit (*apfu*) for "cralpoite"

SiO_2	33.25	Na	0.92	Si	5.89
TiO_2	0.15	Ca	0.04	Al	0.11
Al_2O_3	11.72	K	0.01	ΣT	6.00
Cr_2O_3	29.68	ΣX	0.97		
MgO	7.57			Al	2.34
FeO	0.07	Cr	2.50	Mg	2.00
CaO	0.23	Li	0.46	Cr	1.66
Na_2O	2.67	Ti	0.02	ΣZ	6.00
K_2O	0.05	Fe^{2+}	0.01		
F	0.69	ΣY	2.99	OH	3.61
Li_2O^*	0.64			F	0.39
$B_2O_3^*$	9.81			$\Sigma V + W$	4.00
H_2O^*	3.06				
$O \equiv F$	-0.29				
Total	100.34				

* Calculated assuming 31 anions *pfu*; Li_2O, B_2O_3 and H_2O calculated from stoichiometry
V, Zn, Mn not detected

calculated on the basis of 31 anions assuming B = 3 *apfu* (atoms per formula unit), OH + F = 4 *apfu* and Li_2O calculated to ensure full occupancy at the *Y*, *Z* and *T*-sites. Further analysis will be done to collect quantitative B_2O_3, Li_2O and H_2O data.

4.6.4 Crystal structure

The powder-diffraction pattern was recorded on a Gandolfi camera with Cu*K*α X-radiation. Cell dimensions were refined using the program CELREF (Appleman and Evans 1973). The systematic absences are compatible with the space group *R*3*m* that is observed for all other tourmaline species (Table 4.6.2). There was no correction for shrinkage and no internal standards were used.

TABLE 4.6.2: Indexed powder-diffraction pattern for "cralpoite"

I_{obs}	d_{obs} (Å)	d_{calc} (Å)	*h,k,l*	I_{obs}	d_{obs} (Å)	d_{calc} (Å)	*h,k,l*
60	6.487	6.489	1,0,1	5	2.214	2.212	5,0,2
20	5.033	5.039	0,2,1	5	2.166	2.163	3,0,3
20	4.642	4.618	3,0,0	20	2.059	2.060	1,5,2
30	4.262	4.264	2,1,1	10	1.938	1.936	3,4,2
50	4.010	3.999	2,2,0	5	1.679	1.680	6,0,3
30	3.545	3.550	0,1,2	5	1.599	1.600	5,5,0
35	3.013	3.023	4,1,0	5	1.540	1.539	9,0,0
35	3.013	3.007	1,2,2	5	1.529	1.531	0,5,4
100	2.598	2.592	0,5,1	5	1.478	1.477	5,1,4
5	2.392	2.403	2,3,2	5	1.432	1.435	3,7,2
5	2.354	2.357	5,1,1	5	1.432	1.430	4,3,4

114.6 Debye-Scherrer camera with Gandolfi attachment; Cu*K*α (Ni-filtered) λ = 1.5418 Å; observed intensities visually estimated; calculated powder pattern from single-crystal structure refinement used to aid indexing; no correction for shrinkage; no internal standard;
a = 15.997(9), c = 7.345(6) Å, V = 1627.8(17) Å^3

A fragment of "cralpoite" was ground to an ellipsoid and mounted on a Nicolet *R*3*m* four-circle diffractometer. Cell dimensions and intensity data were collected according to the experimental procedure described in Chapter 2. Refined unit-cell dimensions and selected data pertaining to crystal-structure refinement are given in Table 4.6.3.

TABLE 4.6.3: Unit-cell dimensions and data pertaining to crystal-structure refinement of "cralpoite" (Sample CT92)

a (Å)	16.035 (1)	radiation	Mo$K\alpha$
c	7.313 (1)	scan mode	θ-2θ
V (Å)^3	1628.4	θ range (°)	4-60
Space group	$R3m$	R(az) (%)	1.4 → 0.9
R (obs) (%)	3.27	Total $\|F\|$	1177
wR (%)	2.22	$\|F_{obs}\|$	851
GOF	1.03		

The structure refinement was initiated with the atom coordinates of foitite (MacDonald *et al.* 1993) using the SHELTXL PC Plus system of programs. The final refinement for an anisotropic-displacement model converged to an R index of 3.3% for 851 observed (5σ) reflections. Final atom parameters, refined site-scattering values, and the selected interatomic distances and angles are given in Appendices C, D and F, respectively, as Sample CT92. Observed and calculated structure-factors will be deposited with the Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada. The crystal used in the collection of the X-ray intensity data was subsequently analyzed using an electron microprobe.

4.6.5 Discussion

The composition of "cralpoite" (Table 4.6.1) may be generalized to the end-member composition Na Cr^{3+}_3 (Al_4Mg_2) (Si_6O_{18}) (BO_3)$_3$ (OH)$_3$ O, essentially the Cr^{3+}/Al analogue of povondraite. An alkali tourmaline, it is distinct from chromdravite by virtue of the presence of Cr^{3+} at the Y-site and Al (+ Mg) at the Z-site. This proposed new tourmaline species will be submitted to the CNMMN pending collection of hydrogen data.

4.7 Discussion

Correct mineral nomenclature is an invaluable tool to mineralogists, petrologists and geologists in general. An accurate mineral name should be precise enough to succinctly convey important information regarding chemical make-up and crystal structure. A verification of the importance anion content has to an accurate interpretation of petrologic environment can be seen in Selway's (1999) work on tourmalines from pegmatites (Figure 4.2). It is apparent from these graphs that the relation of Na to F

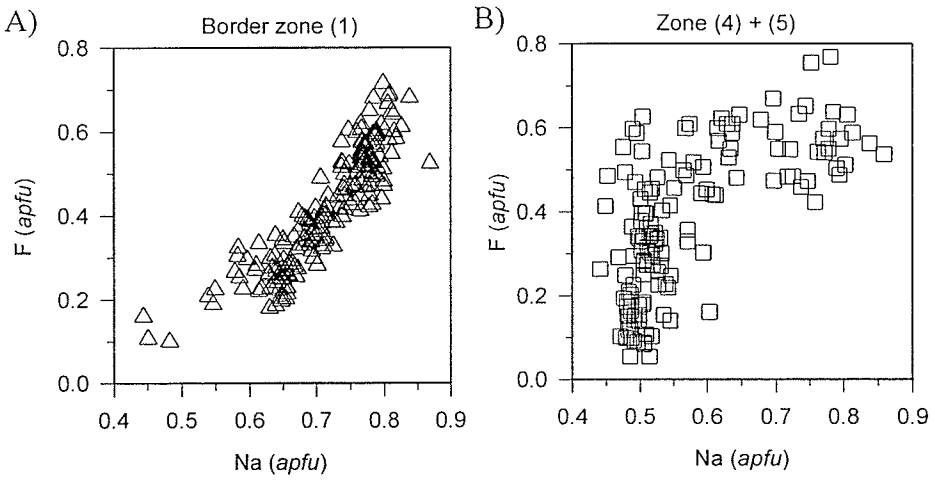

Figure 4.2: Na *vs.* F plots for tourmaline from the Tanco pegmatite, Manitoba. Graph a) is for tourmalines from the border zone; graph b) is for tourmalines from the intermediate zones (from Selway 1999).

is different for different zones in the pegmatite. It is key to a complete understanding of the petrologic environment of formation that anion content of tourmaline (and all minerals) is completely analyzed for and variations in content be reported in mineral names. Differences in F, (OH) and O^{2-} content, in addition to cation variations, must be considered if we are to understand the behavior of tourmaline in geologic environments.

Additional new species of tourmaline are likely to be discovered and described, based on variations in both the cation and anion content. As instrumentation becomes

more advanced and more available, tourmaline species will be better analyzed. The result will be not only new species of tourmaline, but also a better understanding of the petrologic environments these minerals formed in.

CHAPTER 5

Crystal Chemistry of Chromian Tourmaline Minerals

5.1 Introduction

Chromium in tourmaline can occur in amounts ranging from 0 - >35 wt% Cr_2O_3, though in the majority of tourmaline minerals, it contributes less than 1 wt%. Chromium can occur at the *Y*- and *Z*-sites, apparently dependent both on the amount of Cr^{3+} as well as the amounts of other cations (*e.g.* Al, Mg, Fe) present. As Cr levels can vary quite significantly, in this thesis the terms "Cr-bearing tourmaline", "Cr-rich tourmaline", "Cr-tourmaline" and "chromian tourmaline" are used to signify tourmalines with varying amounts of Cr. This nomenclature is explained in Table 5.1, based on the nomenclature of Selway and Novák (1997) and, although somewhat arbitrary, is based on relative proportion of Cr to other components. "Chromian tourmaline" will be used to

Table 5.1: Nomenclature of chromian tourmaline minerals

	Lower limit	Upper limit
Cr-bearing tourmaline	0.2 *apfu* (or ~7 % of *Y*-site)	0.6 *apfu*
Cr-rich tourmaline	0.6 *apfu*	1.0 *apfu*
Cr-tourmaline	1.0 *apfu*	------
Chromian tourmaline	0.2 *apfu*	------

refer to any tourmaline with a Cr-content greater than 0.2 *apfu*; "Cr-tourmaline" will be used to designate any tourmaline with significant Cr content (> 1 *apfu* or roughly 5 – 6 wt%).

5.1.1 Previous work

Elevated levels of Cr (>1.00 wt% Cr_2O_3) in tourmaline have been reported from only a few localities. Most chromian tourmaline minerals are dravites. The only

approved species of tourmaline with Cr as a dominant component is chromdravite, ideally Na Mg_3 $Cr^{3+}{}_6$ Si_6O_{18} $(BO_3)_3$ $(OH)_3$ (OH), found associated with chromian phengite in metasomatized sediments in central Karelia (Rumyantseva 1983). Table 5.2 lists the published information on chromian tourmaline minerals.

Table 5.2: Compilation of published chromian tourmaline data

Location	Cr_2O_3 wt%	Site Occupancy	References
Timmins-Porcupine, ON	0.42 – 1.52	*Y*	King and Kerrich, 1989
Krivoi Rog, Russia	1.60	*Y*	Shenderova, 1955
Zimbabwe	2.26 – 4.93	*Y*	Schreyer *et al.*, 1981
Line Pit, PA-MD	2.60 – 5.40	*Y* + *Z*	Foord *et al.*, 1981
Vavdos, Greece	3.81 – 13.90	*Y* + *Z*	Michailidis *et al.*, 1995
Etchison, MD	4.32	*Y*	Gill, 1889
Swat, Pakistan	8.50	*Y* + *Z*	Jan *et al.*, 1972
Kaavi, Finland	8.87	*Y* + *Z*	Peltola *et al.*, 1968
Outokumpu, Finland	9.60	*Y* + *Z*	Peltola *et al.*, 1968
Urals, Russia	10.86 (5.96)	*Y*	Cossa and Arzruni, 1883; Dunn, 1977
Orissa, India	17.84 – 22.85	*Y* + *Z*	Mukherjee, 1968
Karelia, Russia	31.6	*Y* + *Z*	Rumyantseva, 1983

5.1.2 Petrogenetic environments of chromian tourmaline

Chromian tourmalines incorporate an element usually associated with ultramafic environments (Cr) with elements generally concentrated by fractionation of granitic rocks (B, Li, Na). Tourmalines with significant Cr must form in some sort of contact zone between ultramafic and peraluminous rocks, melts or fluids.

The Cr-tourmalines from Orissa, India, occur in chromite deposits associated with layered ultramafic rocks which intruded the host meta-sedimentary sequence. These rocks were later intruded by a granite with a number of associated pegmatites in the area (Mukherjee 1966, Pattnaik *et al.* 1984). As the tourmaline post-dates the chromite, in this locality the B-bearing fluids from the pegmatitic bodies likely invaded the ultramafic suite, and the Cr-tourmalines formed as an alteration of primary chromite.

Rumyantseva (1983) reports metasomatic chromdravite occurring with Cr-micas in faults within a sequence of carbonates and clays. Although the origin of the Cr is not clear in this instance, it can be assumed that it was brought into the environment by metasomatic fluids which mobilized B from the pelitic sequence to form chromdravite.

5.2 Chromian tourmaline sample suite

5.2.1 General information

There are fifteen tourmalines in my sample suite with Cr_2O_3 content larger than 1.00 wt%. It is this subset to which I will be referring throughout the rest of this chapter. Table 5.3 is an excerpt from Appendix A, listing the sample information for this subset.

Table 5.3: Sample list of chromian tourmaline samples

Sample	Species	Locale
CT34	*"Cralpoite"*	Kokka, Finland
CT40	Dravite	Kaavi, Finland
CT41	Dravite	Etchison, Maryland
CT42	Dravite	Etchison, Maryland
CT43	Dravite	Etchison, Maryland
CT80	*"Hydroxyuvite"*	unknown
CT90	*"Cralpoite"*	Nausahi, Keonjhar District, India
CT91	*"Cralpoite"*	Nausahi, Keonjhar District, India
CT92	*"Cralpoite"*	Nausahi, Keonjhar District, India
CT93	*"Cralpoite"*	Nausahi, Keonjhar District, India
CT94	*"Cralpoite"*	Nausahi, Keonjhar District, India
CT95	*"Cralpoite"*	Nausahi, Keonjhar District, India
CT96	Chromdravite	Urals, Russia
CT97	Chromdravite	Urals, Russia
CT98	Chromdravite	Urals, Russia

As with the rest of my larger sample suite, these tourmalines were analyzed by SREF and EMPA.

5.2.2 Chemical analysis

Chemical data were collected by EMPA using the method described in Chapter 2. Preliminary formulae calculations were done according to the methods described in Chapters 2 and 3 (Table 5.4). According to this method, the *Z*-site was filled first with Al, followed by Mg. Cr was only assigned to *Z* if Al + Mg < 6 *apfu*. All Fe was initially assumed to be divalent, and OH + F = 4 *apfu* was assumed.

In several samples the total wt% sums differ significantly from 100 %. Sums that vary by ± 1.00 % are not generally commented on as these discrepancies can usually be explained by random error. However, samples CT80, CT96, CT97 and CT98 are +2.46, -3.16, -2.43, and -4.20 wt% from 100 %, respectively. A discrepancy of ± 2 wt% can be potentially explained by error in the assumed amount of OH in the sample, but discrepancies of > 3 wt% must be significant. These samples were re-collected a number of times (*e.g.* sample CT98 in Table 5.5), initially by the same method, but additional runs were done using a different Cr-standard as well as at a different facility to rule out local lab error. The only significant variation between the results collected at the U of M and those from the outside facility (Louisiana State University) is in the amount of F. This is due to the researcher at LSU reporting the wavelength of the F peak occurring on the flanks of another peak, which he assumed was probably a high-order Cr peak. Thus he narrowed the wavelength range for F significantly and reported a much lower F value (D. Henry, *personal comm.*). Though the potential overlap bears further investigation, it does not resolve the greater issue of low totals.

Table 5.4: Chemical analyses of chromian tourmaline samples

	CT34	CT40	CT41	CT42	CT43	CT80	CT90	CT91	CT92	CT93
SiO2	34.86	35.98	36.32	36.41	37.2	35.54	35.20	35.5	33.25	36.05
TiO2	0.01	0.07	0.11	0.02	0.0	0.68	0.08	0.1	0.15	0.12
Al2O3	27.04	29.49	31.27	32.68	32.9	29.08	20.21	21.9	11.72	21.68
V2O3	0.00	0.29	0.13	0.06	0.0	5.25	0.04	0.0	0.04	0.07
Cr2O3	10.80	8.21	5.35	4.74	4.0	1.80	15.80	13.3	29.68	13.27
MgO	8.41	9.41	9.22	8.78	9.6	9.88	10.13	10.2	7.57	10.37
CaO	0.98	1.18	0.71	0.31	0.1	2.60	0.21	0.2	0.23	0.19
MnO	0.01	0.01	0.00	0.00	0.0	0.03	0.05	0.0	0.01	0.01
FeO	0.05	0.06	0.65	0.42	0.4	1.25	0.18	0.1	0.07	0.26
ZnO	0.00	0.02	0.00	0.00	0.0	0.02	0.04	0.0	0.03	0.03
CuO	0.00	---	---	---	---	---	---	---	---	---
Na2O	2.05	2.08	2.33	2.45	2.1	1.20	2.67	2.6	2.67	2.73
K2O	0.08	0.07	0.02	0.02	0.0	0.09	0.02	0.0	0.05	0.03
F	0.33	0.28	0.09	0.18	0.0	0.59	0.39	0.2	0.69	0.25
Li2O*	0.55	0.46	0.40	0.42	0.2	0.42	0.27	0.2	0.64	0.42
B2O3*	10.45	10.83	10.83	10.88	11.0	10.83	10.20	10.2	9.81	10.35
H2O*	3.45	3.60	3.70	3.67	3.7	3.46	3.33	3.4	3.06	3.45
O=F	-0.14	-0.12	-0.04	-0.08	-0.0	-0.25	-0.16	-0.1	-0.29	-0.11
Total	99.06	101.92	101.09	100.96	101.7	102.46	98.65	98.5	99.37	99.17
Na	0.661	0.647	0.725	0.759	0.652	0.373	0.882	0.879	0.918	0.889
K	0.017	0.014	0.004	0.004	0.00	0.018	0.004	0.00	0.011	0.006
Ca	0.175	0.203	0.122	0.053	0.03	0.447	0.038	0.03	0.044	0.034
Vacancy	0.147	0.136	0.149	0.184	0.31	0.162	0.076	0.07	0.027	0.071
X Total	1.000	1.000	1.000	1.000	1.00	1.000	1.000	1.00	1.000	1.000
Li	0.372	0.296	0.259	0.270	0.14	0.269	0.184	0.20	0.457	0.283
Mg	1.182	1.606	1.945	2.065	2.26	1.571	0.634	0.96	0.000	0.889
Ti4+	0.018	0.008	0.013	0.002	0.00	0.082	0.010	0.01	0.020	0.015
V3+	0.000	0.037	0.017	0.008	0.01	0.676	0.005	0.00	0.006	0.009
Cr3+	1.420	1.042	0.679	0.599	0.50	0.228	2.129	1.77	2.501	1.762
Mn2+	0.001	0.001	0.000	0.000	0.00	0.004	0.007	0.00	0.002	0.001
Fe2+	0.007	0.008	0.087	0.056	0.05	0.168	0.026	0.02	0.010	0.037
Cu	0.000	---	---	---	---	---	---	---	---	---
Zn	0.000	0.002	0.000	0.000	0.00	0.002	0.005	0.00	0.004	0.004
Al	0.000	0.000	0.000	0.000	0.01	0.000	0.000	0.00	0.000	0.000
Y Total	3.000	3.000	3.000	3.000	3.00	3.000	3.000	3.00	3.000	3.000
Cr	0.000	0.000	0.000	0.000	0.00	0.000	0.000	0.00	1.658	0.000
Mg	0.903	0.646	0.260	0.027	0.00	0.793	1.940	1.61	2.000	1.708
Al	5.097	5.354	5.740	5.973	6.00	5.207	4.060	4.38	2.342	4.292
Z Total	6.000	6.000	6.000	6.000	6.00	6.000	6.000	6.00	6.000	6.000
Al	0.203	0.225	0.173	0.182	0.11	0.295	0.000	0.00	0.106	0.000
Si	5.797	5.775	5.827	5.818	5.88	5.705	6.000	6.01	5.894	6.056
T Total	6.000	6.000	6.000	6.000	6.00	6.000	6.000	6.01	6.000	6.056
OH	3.826	3.858	3.954	3.909	3.97	3.700	3.790	3.84	3.613	3.867
F	0.174	0.142	0.046	0.091	0.025	0.300	0.210	0.155	0.387	0.133

Table 5.4 *(continued)*

	CT94	CT95	CT96	CT97	CT98
SiO2	33.68	33.01	31.10	32.40	32.2
TiO2	0.19	0.11	0.09	0.08	0.0
Al2O3	12.25	11.00	1.25	0.65	2.3
V2O3	0.06	0.05	0.02	0.02	0.0
Cr2O3	27.25	30.36	33.54	34.77	29.2
MgO	8.64	7.19	9.98	9.89	9.4
CaO	0.38	0.21	0.00	0.01	0.0
MnO	0.03	0.03	0.51	0.45	0.3
FeO	0.17	0.05	5.09	3.84	6.8
ZnO	0.01	0.02	0.07	0.05	0.0
CuO	---	---	---	---	---
Na2O	2.56	2.60	2.72	2.56	2.6
K2O	0.05	0.06	0.30	0.34	0.2
F	0.52	0.59	0.71	0.86	0.6
Li2O*	0.50	0.69	0.00	0.14	0.1
B2O3*	9.84	9.70	9.00	9.13	8.9
H2O*	3.15	3.07	2.77	2.74	2.7
O=F	-0.22	-0.25	-0.30	-0.36	-0.2
Total	99.06	98.48	96.84	97.57	95.8
Na	0.877	0.904	1.019	0.945	0.98
K	0.011	0.014	0.074	0.083	0.06
Ca	0.072	0.040	0.000	0.002	0.00
Vacancy	0.040	0.042	0.000	0.000	0.00
X Total	1.000	1.000	1.093	1.030	1.05
Li	0.354	0.497	0.000	0.108	0.07
Mg	0.000	0.000	0.000	0.000	0.00
Ti4+	0.025	0.015	0.013	0.011	0.01
V3+	0.008	0.007	0.003	0.003	0.00
Cr3+	2.583	2.466	2.284	2.187	1.74
Mn2+	0.004	0.005	0.083	0.073	0.05
Fe2+	0.025	0.007	0.823	0.611	1.11
Cu	---	---	---	---	---
Zn	0.001	0.003	0.010	0.007	0.00
Al	0.000	0.000	0.000	0.000	0.00
Y Total	3.000	3.000	3.216	3.000	3.00
Cr	1.223	1.837	2.840	3.047	2.73
Mg	2.276	1.921	2.875	2.807	2.73
Al	2.501	2.242	0.285	0.146	0.53
Z Total	6.000	6.000	6.000	6.000	6.00
Al	0.050	0.082	0.000	0.000	0.00
Si	5.950	5.918	6.009	6.168	6.24
T Total	6.000	6.000	6.009	6.168	6.24
OH	3.709	3.665	3.566	3.482	3.60
F	0.291	0.335	0.434	0.518	0.39

TABLE 5.5: EMPA results for CT98

	Run 1	Run 2	Run 3	Run 4	Run 5
SiO_2	32.28	32.02	32.34	32.30	31.94
TiO_2	0.08	0.07	0.08	0.09	0.11
Al_2O_3	2.33	3.72	3.18	3.05	2.80
V_2O_3	0.00	0.00	0.02	0.05	0.01
Cr_2O_3	29.24	26.07	27.09	26.35	27.31
MgO	9.49	9.22	9.53	10.48	10.62
CaO	0.00	0.00	0.00	0.00	0.01
MnO	0.32	0.14	0.17	0.17	0.06
FeO	6.88	9.91	8.34	8.96	8.32
ZnO	0.03	0.00	0.03	0.04	0.07
Na_2O	2.62	2.90	2.63	2.63	2.63
K2O	0.28	0.27	0.31	0.32	0.34
F	0.65	0.57	0.61	0.60	0.04
B_2O_3*	8.97	9.00	8.99	9.04	9.26
H_2O*	2.79	2.83	2.81	2.84	3.18
O=F	-0.27	-0.24	-0.26	-0.25	-0.02
Total	95.68	96.50	95.87	96.68	96.68

Runs 1, 2, 5 collected with chromite standard, runs 3, 4 collected with Cr metal standard, runs 1-4 collected at UM, run 5 collected by D. Henry at LSU.

There are several possibilities as to why these sums are low. As runs were collected using different standards and at a different facility, the basic data-collection scheme does not appear faulty. A physical problem that may contribute to the low sum is the small size of the grains. These grains, which are significantly harder than the epoxy in which they were mounted, were often rounded during the polishing process. If a grain's edges are rounded, any data collected from a rounded area is suspect, as the angle of the ejected electrons is not optimal. Other reasons for the low sums are based on problems with normalization assumptions, which will be discussed further in section 5.2.3.

Light-element analysis was not done on the Cr-tourmalines. These tourmalines occur as very small crystals (150 μm *c*-axis) and are compositionally heterogeneous between individual crystals, making analysis by a bulk technique (such as H-extraction-

line) fruitless. For this same reason, Fe^{3+}/Fe^{2+} ratios were not collected. Though samples were sent for SIMS analysis, data were not collected as the large amount of transition metals are likely to cause matrix effects which cannot be adjusted for at this time.

5.2.3 Formula normalization

The unit formulae for these tourmalines were calculated initially assuming 31 anions *pfu*, OH + F = 4 *apfu* and all Fe^{2+}. For several samples, these initial assumptions are questionable; most obviously seen in Si > 6 *apfu* (samples CT91, CT93, CT96, CT97 and CT98). These tourmalines were recalculated to bring Si = 6 *apfu*. Table 5.6 lists several normalization results for Sample CT98. Although the simplest way to do this is to renormalize on 6 *apfu* of Si, this method requires a significant amount of (assumed) Li to be introduced in order to bring the $Y + Z + T$ cation sum to 15 *apfu*. It is unclear as to whether Li in large quantities is a reasonable assumption for Cr tourmalines, and attempts to collect Li values by SIMS analysis have so far been unsuccessful.

Another method to improve the normalization results is to change the valence state of one or more of the transition metals, which tends to raise overall weight percent sums and lower cation *apfu*. As these ratios were not determined due to difficulties in analysis and size of samples, the relative proportions of ions like Fe^{3+}/Fe^{2+} is unknown.

Table 5.6 is a summary of the results of several normalization schemes for sample CT98. Formulae were calculated on the basis of 31 anions, on 6 *apfu* Si, with and without Li assumed, and with different valence states of the transition metals Fe, Mn, and Cr. Fe^{3+} and Mn^{3+}, though not commonly initially assumed in tourmaline, have been reported in previous studies. Cr^{6+} has not been reported in any silicate mineral to date.

Table 5.6: Various normalization results for CT98

	31 anions, Fe^{2+}, Mn^{2+}, Li	Si = 6 *apfu*, Fe^{2+}, Mn^{2+}, Li	31 anions, Fe^{3+}, Mn^{2+}	31 anions, Fe^{3+}, Mn^{3+}	31 anions, Fe^{3+}, Mn^{3+}, some Cr^{6+}	31 anions, Fe^{3+}, Mn^{2+}, from D.H.
CrO_3	-----	-----	-----	-----	1.32	-----
SiO_2	32.28	32.28	32.28	32.28	32.28	31.94
TiO_2	0.08	0.08	0.08	0.08	0.08	0.11
Al_2O_3	2.33	2.33	2.33	2.33	2.33	2.80
Cr_2O_3	29.24	29.24	29.24	29.24	28.24	27.31
Fe_2O_3	-----	-----	7.64	7.64	7.64	9.25
Mn_2O_3	-----	-----	-----	0.36	0.36	-----
MgO	9.49	9.49	9.49	9.49	9.49	10.62
MnO	0.32	0.32	0.32	-----	-----	0.06
FeO	6.88	6.88	-----	-----	-----	-----
Na_2O	2.62	2.62	2.62	2.62	2.62	2.63
K_2O	0.28	0.28	0.28	0.28	0.28	0.34
F	0.65	0.65	0.65	0.65	0.65	0.04
Li_2O*	0.10	0.57	-----	-----	-----	-----
B_2O_3*	8.98	9.35	9.17	9.18	9.26	9.26
H_2O*	2.79	2.92	2.86	2.86	2.89	3.18
O=F	-0.27	-0.27	-0.27	-0.27	-0.27	-0.02
Total	95.80	96.76	96.71	96.76	97.20	97.63
Na	0.983	0.944	0.963	0.962	0.953	0.957
K	0.069	0.066	0.068	0.068	0.067	0.081
Vacancy	-----	-----	-----	-----	-----	-----
ΣX	1.052	1.010	1.031	1.030	1.020	1.040
Cr^{6+}	-----	-----	-----	-----	0.149	-----
Si	6.247	6.000	6.118	6.112	6.056	5.993
Ti^{4+}	0.012	0.011	0.011	0.011	0.011	0.016
Al	0.531	0.510	0.520	0.520	0.515	0.619
Cr^{3+}	4.474	4.297	4.382	4.377	4.189	4.052
Fe^{3+}	-----	-----	1.090	1.089	1.079	1.306
Mn^{3+}	-----	-----	-----	0.052	0.051	-----
Mg	2.738	2.630	2.682	2.679	2.654	2.971
Fe^{2+}	1.114	1.069	-----	-----	-----	-----
Mn^{2+}	0.052	0.050	0.051	-----	-----	0.010
Li	0.075	0.429	-----	-----	-----	-----
$\Sigma Y+Z+T$	15.247	14.996	14.858	14.844	14.704	14.979
OH	3.602	3.618	3.610	3.611	3.614	3.976
F	0.398	0.382	0.390	0.389	0.386	0.024

*All normalizations done with the assumption OH + F = 4 *apfu* as lowering this sum serves to bring down wt% and bring up cation *apfu*, opposite of the results needed.

The difficulty with Cr^{6+} lies in the fact that it would be very difficult to determine its presence. Cr^{6+} would occur in tetrahedral coordination in tourmaline, and one might hope to be able to look at bond-lengths or site-scattering intensities to support this theory. However, as all other cation sites in tourmaline have variable content, one cation site must have a fixed scattering intensity to serve as the standard for all of the other sites. Although the B-site is the most likely site to be stable in content, the intensity from the site is too low to serve as a suitable standard for the other sites. The *T*-site, therefore, must have its scattering fixed, and Cr cannot be found from scattering intensities. Bond-lengths cannot be used, as Cr^{6+} in tetrahedral coordination has an ionic radius of 0.26 Å (Shannon 1976), the same radius of Si in tetrahedral coordination; therefore, Cr^{6+} at the *T*-site would not alter the <*T*-O> length. Table 5.6 shows that no method tried so far has resulted in a satisfactory formula.

5.3 Crystal Chemistry

5.3.1 Introduction

Cr^{3+} has an ionic radius of 0.615 Å in octahedral coordination (Shannon 1976) and therefore substitutes readily at both the *Y*- and *Z*-sites in tourmaline. Table 5.2 includes a column that lists the site to which the researchers assigned Cr. When structure data are lacking, there has been some confusion as to which site Cr is located. Cr has been assigned based on assumed substitution for either Mg (*e.g.* King and Kerrich 1989) or Al (*e.g.* Rumyantseva 1983), usually based on circumstantial evidence; Rumyantseva (1983) assigned Cr to *Z* based on the size of the unit cell.

Crystal-structure refinement can give a clear indication of the location of Cr, using both the bond-lengths and the X-ray scattering intensity at a site. Using SREF data, the chromian tourmalines of my sample suite have Cr occurring at both *Y* and *Z*. I will now discuss the site-assignments of the Cr-tourmalines in detail.

5.3.2 Sample CT34:

Sample CT34 is from Kokka, Finland, and has 10.80 wt% Cr_2O_3. Table 5.7 is a comparison of site-scattering information. The *epfu* reported from EMPA is slightly low

Table 5.7: Site-scattering values (*epfu*) for CT34

	SREF	EMPA
X	11.5(1)	11.1
Y	52.1(2)	50.0
Z	79.1(2)	77.1
T	84	83.80

for all of the sites, but there seems to be no major discrepancy in the manner of site assignment. This suggests that, for CT34, Cr is preferentially located at *Y*, substituting in for Mg. The average bond-length for *Y* is 1.993 Å, shorter than the average for dravite (2.011 Å, Appendix F). The <*Z*-O> is 1.935 Å, equal to the <*Z*-O> for dravite (1.931 Å). This supports the argument that Cr^{3+} (0.615 Å) is substituting for Mg (0.72 Å) at *Y*, resulting in a shorter <*Y*-O>. The resulting formula for CT34 is $^{[X]}(Na_{0.66}\ Ca_{0.17}\ \square_{0.15}\ K_{0.02})\ ^{[Y]}(Cr_{1.42}\ Mg_{1.18}\ Li_{0.37}\ Ti_{0.02}\ Fe^{2+}_{0.01})\ ^{[Z]}(Al_{5.10}\ Mg_{0.90})\ ^{[T]}(Si_{5.80}\ Al_{0.20})\ O_{18}\ (BO_3)_3\ ^{[V]}(OH)_3\ ^{[W]}((OH)_{0.83}\ F_{0.17})$. This formula does not belong to a currently approved tourmaline species but has been grouped with dravite in my suite. However, if the species "cralpoite" is accepted by the IMA, it will be classified as such (see Chapter 4.6).

5.3.3 Sample CT40

Sample CT40 is from Kaavi, Finland, and has 8.21 wt% Cr_2O_3. Table 5.8 is a comparison of site-scattering information. Examination of the bond-lengths at the *Y*-

Table 5.8: Site-scattering values (*epfu*) for CT40

	SREF	EMPA
X	11.0(1)	11.4
Y	46.1(2)	46.5
Z	78	77.4
T	84	83.8

(2.002 Å) and *Z*- (1.936 Å) sites shows that <*Y*-O> is shorter than the average for dravite and <*Z*-O> is statistically equal. The bond-lengths information combined with the *epfu* data suggest that Cr is primarily located at the *Y*-site in CT40. The resulting formula for CT40 is $^{[X]}(Na_{0.65}\ Ca_{0.20}\ \square_{0.15})\ ^{[y]}(Mg_{1.61}\ Cr_{1.04}\ Li_{0.30}\ V_{0.04}\ Fe^{2+}_{0.01})\ ^{[Z]}(Al_{5.35}\ Mg_{0.65})\ ^{[T]}(Si_{5.78}\ Al_{0.22})\ O_{18}\ (BO_3)_3\ ^{[v]}(OH)_3\ ^{[w]}((OH)_{0.86}\ F_{0.14})$. As Mg is still the dominant cation at *Y*, this mineral can be termed "chromian dravite".

5.3.4. Samples CT90-95: "Cralpoite"

Samples CT90-95 are from Orissa, India, and have been fully described in Chapter 4.6. Table 5.9 is a comparison of the site-scattering information. The *epfu*

Table 5.9: Site-scattering values (*epfu*) for CT90-95

	CT90		CT91		CT92		CT93		CT94		CT95	
	SREF	EMP	SREF	EMP	SREF	EMP	SREF	EMP	SREF	EMP	SREF	EMP
X	11.9(2)	10.5	11.5(1)	10.5	11.8(2)	11.2	12.1(1)	10.5	12.7(1)	11.3	12.5(1)	11.0
Y	56.6(5)	60.6	49.6(3)	55.9	64.4(7)	62.4	53.5(3)	54.5	58.2(3)	64.6	64.4(4)	61.6
Z	92.2(5)	76.1	83.6(3)	76.4	94.7(7)	94.3	85.4(3)	76.3	95.6(4)	89.2	95.4(4)	96.3
T	84	84.0	84	84	84	83.9	84	84	84	84.0	84	83.9

EMP = EMPA; EMPA *epfu* for CT91 and CT93 calculated from Si = 6 *apfu* normalization

reported from EMPA was calculated by filling *T* in the order Si then Al; *Z* in the order Al, Mg, Cr; and *Y* was filled with the remaining cations. Li was added to bring the $Y + Z$

+ *T* sum to 15 *apfu*. Examination of the *epfu* data shows that the majority of the samples have too many electrons assigned by EMPA to *Y* and not enough assigned to *Z*. This suggests that there is significant Cr at both the *Y*- and *Z*-sites in these samples. <*Y*-O> bond-lengths for these samples are shorter and <*Z*-O> are longer than for dravite. This is due to the overall low amount of Al occurring in these samples, resulting in significant Mg and Cr at *Z*. Based on SREF scattering information, these tourmalines are best represented by the ideal formula $^{[X]}Na\ ^{[Y]}Cr_3\ ^{[Z]}(Mg_2Al_4)\ ^{[T]}Si_6\ O_{18}\ (BO_3)_3\ ^{[V]}(OH)_3\ ^{[W]}(O)$, making it a Cr-Al analogue of povondraite.

5.3.5. Sample CT96-98: Chromdravite

Samples CT96-98 are from Karelia, Russia, from the type locality of chromdravite. Table 5.10 is a comparison of site-scattering information. The *epfu*

Table 5.10: Site-scattering values (*epfu*) for CT96-98

	CT96		CT97		CT98	
	SREF	EMPA	SREF	EMPA	SREF	EMPA
X	11.1(2)	12.4	11.9(3)	11.7	11.3(3)	11.6
Y	65.2(6)	73.7	61.0(8)	65.9	64.2(11)	65.2
Z	114.3(7)	107.8	112.2(10)	109.7	115.0(14)	106.8
T	84	83.9	84	84	84	84

EMPA *epfu* for CT96 calculated with $Fe^{3+} + Fe^{2+}$; CT97-98 calculated from Si = 6 *apfu* normalization

reported from EMPA was calculated by filling *T* in the order Si then Al; *Z* in the order Al, Mg, Cr; *Y* was filled with the remaining cations. Li was added to bring the $Y + Z + T$ sum to 15 *apfu*. The formula normalization for CT96 required some Fe to be trivalent in order to bring $Y + Z + T = 15$ *apfu* and Si ≤ 6 *apfu*. Examination of the *epfu* data shows that all three samples have too many electrons assigned to *Y* and not enough electrons assigned to *Z* by EMPA. Examination of average bond-lengths for *Y* and *Z* shows <*Y*-

O> for the three samples to be 2.018 Å, slightly longer than the average for dravite (2.011 Å). The <Z-O> length for these samples is 2.006 Å, significantly longer than the <Z-O> for dravite (1.931 Å). The *epfu* results and the average bond-lengths suggest that the above scheme for the assignment of cations between the *Y*- and *Z*-sites is incorrect; more Cr should be assigned to *Z* with disorder of Mg between the *Y*- and *Z*-sites. This would result in an ideal formula for chromdravite of $^{[X]}Na\ ^{[Y]}(Cr_2\ Mg_1)\ ^{[Z]}(Cr_4Mg_2)\ ^{[T]}Si_6\ O_{18}\ (BO_3)_3\ ^{[V]}(OH)_3\ ^{[W]}(OH)$. This formula, with Cr dominant at both *Y* and *Z* and Cr and Mg disordered over the two sites is different than the IMA-approved formula for chromdravite, which has Mg solely at *Y* and Cr solely at *Z*. As there have been difficulties with the collection of data for these high Cr tourmalines, this conclusion is still preliminary.

5.4 Discussion

Though Cr generally does not occur in large amounts in tourmaline, it can be a major constituent. Cr in tourmaline can substitute at the *Y*-site, the *Z*-site, or both sites. The proposed new tourmaline species, "cralpoite", has Cr dominant at *Y*, which has not been shown for any Cr-tourmaline before. Chromdravite, whose approved formula specifies Mg dominant at *Y* and Cr dominant at *Z*, may need to be revised to show Cr dominant at both sites.

Cr-tourmalines tend to present a number of difficulties in analysis. Samples with high Cr_2O_3 wt% tend to be small crystals that are chemically heterogeneous from crystal to crystal. Zoning within the crystals also occurs. This makes analysis of light elements or ion ratios difficult by any bulk technique. SIMS, the microbeam technique most

suitable to measurement of light elements, does not yet have standards for tourmalines with high transition metal content.

Additional problems with Cr-tourmaline data include low wt% totals, which have not yet been fully explained. These totals are low regardless of standards or correction procedures used, and were low when collected at another facility. This is still being investigated to determine the cause. Ultimately, better chemical analyses must be done to determine the correct anion content so that the rest of the formula may be determined by stoichiometric arguments. This includes the presence or absence of Li, Fe^{3+}, Mn^{3+} and $^{[4]}Cr^{6+}$.

CHAPTER 6

Crystal Chemistry of Povondraite

6.1 General Information

6.1.1 Introduction

Walenta and Dunn (1979) described a new species of tourmaline of ideal composition Na Mg_3 Fe^{3+}_6 Si_6 O_{18} B_3 $(O, OH)_{30}$ (OH,F) that they named "ferridravite", as they assigned all Mg to the *Y*-group and all Fe^{3+} to the *Z*-group. However, Grice *et al.* (1993) refined the crystal structure of this mineral, and showed that the site assignment suggested by Walenta and Dunn (1979) is incorrect. Their refinement shows that both the *Y* and the *Z* sites are occupied predominantly by Fe^{3+}, giving the ideal formula Na Fe^{3+}_3 Fe^{3+}_6 (BO_3) $(Si_6$ $O_{18})$ $(O, OH)_4$. As this formula is not "the ferric analog of dravite" (Walenta and Dunn 1979), they recommended renaming the mineral povondraite, after the Czech researcher who has done extensive work on tourmaline-group minerals (Grice *et al.*, 1993). However, as noted by Hawthorne and Henry (1999), the "ideal end-member" formula given by Grice *et al.* (1993) is not of fixed composition, and hence cannot be an end-member. In fact, the above formula requires a $V + W$ anion composition of O_3 (OH) *apfu* (atoms per formula unit) for the formula to be electroneutral. However, Walenta and Dunn (1979) report an H_2O content (loss on ignition) of 3.5 wt%, corresponding to approximately 3.5 (OH) *pfu*; this value is nothing like that assigned to the end-member formula. If the formula of the povondraite crystal refined by Grice *et al.* (1993) is written with $Fe^{3+} = Fe^{3+} + Al$ and $Mg = Mg + Al$ (Hawthorne and Henry 1999), we obtain the following:

$$Na\ (Fe^{3+}_{2.28}\ Mg_{0.80})\ (Fe^{3+}_{4.61}\ Mg_{1.36})\ (Si_6\ O_{18})\ (BO_3)\ (OH)_{3.12}\ O_{0.88}$$

As indicated by Hawthorne and Henry (1999), the ideal end-member corresponding to this composition is as follows:

$$Na\ Fe^{3+}_3\ (Fe^{3+}_4\ Mg_2)\ (Si_6\ O_{18})\ (BO_3)\ (OH)_3\ O$$

In addition to Walenta and Dunn (1979) and Grice *et al.* (1993), a team of Czech researchers characterized a suite of tourmalines corresponding to povondraite – "oxydravite" – dravite solid-solution from the type locality of povondraite (Žáček *et al.* 2000). They looked extensively at the exchange vectors that describe the substitutions in this series. The present work is intended to investigate Fe^{3+}/Fe^{2+} ratios in order to develop a good chemical formula based on a combination of SREF and EMPA data.

6.1.2 Occurrence

Povondraite occurs as the rim of black euhedral crystals coating the country rock at the San Francisco mine, Alto Chapare, Cochamba Department, Bolivia. The host schist is composed of quartz, potassium feldspar, alkali amphibole and muscovite, with accessory schorl. This schist is a component of a sequence of metasedimentary rocks, probably of Cambrian age (Walenta and Dunn 1979, Grice *et al.* 1993).

6.2 Chemical Composition

6.2.1 General information

Several crystals identified as povondraite were chemically analyzed by EMPA, using the procedure described in Chapter 2.3. The majority of samples discussed in this chapter are not included in my larger data-set because of a lack of SREF data. Sample

CT99 is a povondraite from my general set and is included in the povondraite subset discussed here. Sample points were chosen from four distinct regions of the crystals: the core, central, edge and rim zones (Figure 6.1).

Representative chemical compositions are summarized in Table 6.1. Structural formulae were calculated on the basis of 31 anions, assuming stoichiometric amounts of H_2O (as $(OH)^-$, *i.e.* OH + F = 4 *apfu*) and B_2O_3 (B = 3 *apfu*). In the initial calculation, Fe was assumed to be trivalent, as previous authors had reported all ferric iron. However, this assumption should be investigated for validity.

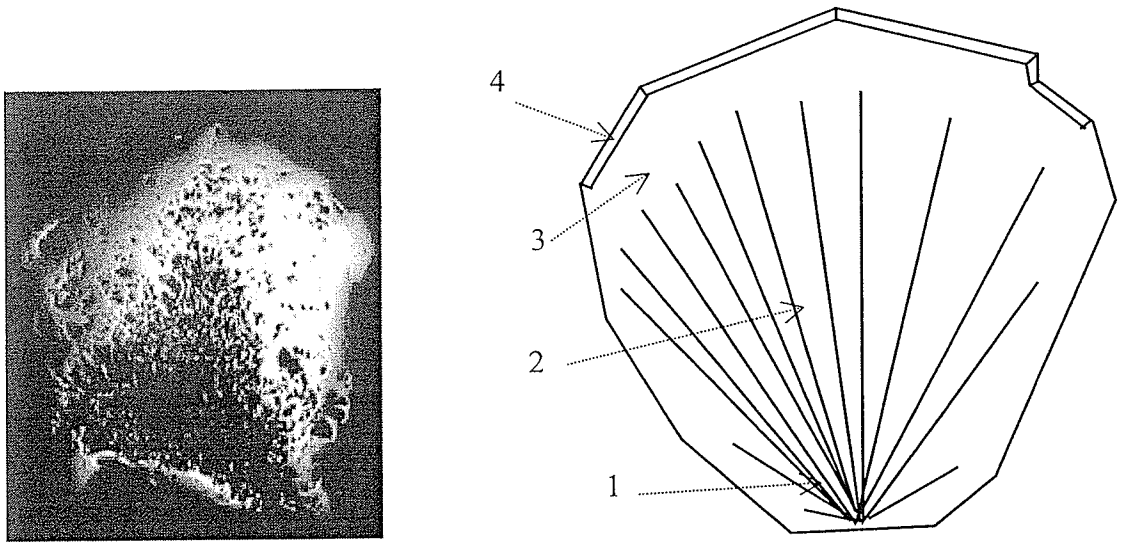

Figure 6.1: Reflected light image and schematic drawing of a povondraite-containing crystal with representative regions labeled as follows: (1) core, (2) central, (3) edge and (4) rim. Long axis of crystal ~500 μm.

Table 6.1:Chemical compositions (wt%) and unit formulae (*apfu*) of povondraite

Zone	Core	Core	Central	Central	Central	Rim	Rim	Rim	Edge
Point	20-21	20-23	20-26	20-29	20-34	19a16	20-5	20-15	CT99
SiO_2	34.88	34.74	35.41	33.87	32.65	33.20	31.38	33.94	32.04
TiO_2	0.29	0.09	0.59	0.90	1.77	1.68	2.43	1.32	2.49
Al_2O_3	27.39	26.46	24.55	20.37	15.30	13.62	13.11	10.69	6.36
V_2O_3	0.26	0.26	0.25	0.29	0.25	0.00	0.06	0.07	0.09
Fe_2O_3	12.15	14.48	15.85	22.81	28.21	29.53	30.10	33.45	36.81
MgO	8.92	8.02	8.25	7.32	6.64	6.72	7.80	6.72	7.21
Na_2O	3.09	3.04	3.03	2.70	2.40	2.47	2.46	2.05	1.96
K_2O	0.11	0.15	0.19	0.40	0.79	0.75	0.96	1.09	1.39
B_2O_3 *	10.36	10.29	10.33	10.08	9.72	9.68	9.61	9.68	9.53
H_2O **	2.68	2.66	2.67	2.61	2.52	2.50	2.49	2.51	3.28
TOTAL	100.13	100.2	101.13	101.35	100.25	100.15	100.4	101.52	101.23
Na	1.005	0.995	0.988	0.903	0.832	0.860	0.862	0.713	0.708
K	0.024	0.032	0.041	0.088	0.180	0.172	0.221	0.250	0.330
ΣX	1.029	1.027	1.029	0.991	1.012	1.032	1.083	0.963	1.038
Mg	2.231	2.019	2.068	1.882	1.769	1.799	2.103	1.798	2.001
Fe^{3+}	0.802	0.972	0.827	0.940	0.852	0.833	0.563	0.778	0.520
Ti	0.037	0.011	0.075	0.117	0.238	0.227	0.330	0.178	0.349
V^{3+}	0.035	0.035	0.034	0.040	0.036	0.000	0.009	0.010	0.013
ΣY	3.105	3.037	3.004	2.979	2.895	2.859	3.005	2.764	2.883
Al	5.268	5.132	4.821	3.980	3.058	2.843	2.468	2.261	1.362
Fe^{3+}	0.732	0.868	1.179	2.020	2.942	3.157	3.532	3.739	4.638
ΣZ	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Si	5.852	5.866	5.955	5.840	5.835	5.961	5.674	6.091	5.966
Al	0.148	0.134	0.045	0.160	0.165	0.039	0.326	0.000	0.034
ΣT	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.091	6.000
B	3	3	3	3	3	3	3	3	3
H	3	3	3	3	3	3	3	3	3

Number of cations based on 31 anions; * B_2O_3 from B = 3 *apfu*; ** H_2O based on OH = 3 *apfu*; Mn, Cr, Zn, P, Ca, F not detected

Examination of the data in Table 6.1 shows that a number of points analyzed are not actually povondraite in composition. Figure 6.2 is a ternary plot of the data that shows there is a trend in composition, from dravite at the core of the tourmaline crystals to povondraite at the edge.

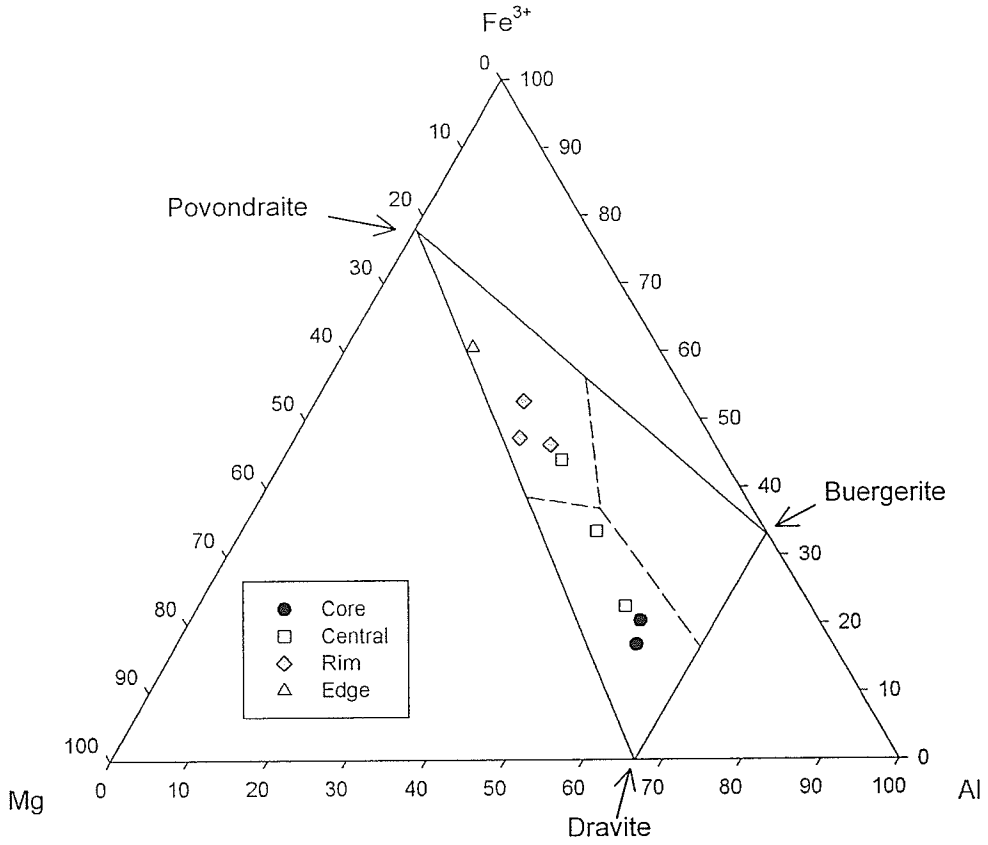

Figure 6.2: Ternary plot of $(Y + Z)$ cations, normalized for 100% Fe^{3+}, Mg and Al. Inner triangle represents actual tourmaline species compositions, with the apices labeled according to appropriate species. All Fe was assumed to be 3+, although in dravitic compositions, there is likely to be a strong ferrous component in the overall iron.

Although analytical data for H_2O would be extremely useful for determination of relative percentages of Fe^{3+}/Fe^{2+} and the correct occupancies at the *V*- and *W*-sites, I was not able to make such measurements for povondraite. Several attempts were made to collect such data, but the lack of bulk homogeneous povondraite made H-extraction-line analysis impossible. Moreover, H could not be analyzed by SIMS, as povondraite has far more transition metals than most other tourmalines, and there are currently no appropriate standards for SIMS analysis.

6.2.2 X-site occupancy

Povondraite has the highest reported values of K for any tourmaline (*e.g.* Table 6.1, Žáček *et al.* 2000, Grice *et al.* 1993), with several researchers reporting analyses in which K > Na, representing a new tourmaline species with the ideal formula: K Fe^{3+}_3 ($Mg_2Fe^{3+}_4$) (Si_6O_{18}) (BO_3)$_3$ (OH)$_3$ O. Unfortunately, full characterization of this new mineral species is difficult due to the nature of the material; Žáček *et al.* (2000) reported parts of povondraite crystals that were K-dominant being no larger than several tens of microns in size. Likewise, Grice *et al.* report their K-dominant povondraite as a thin (10 μm) outer rim.

The *X*-site in povondraite is unlike many other tourmalines in that there seems to be very little vacancy. A scan through Appendix G shows that most tourmalines in my suite have some vacancy at *X*, with uvite having the least vacancy in (or the most fully occupied) *X* of the tourmaline species. However, both my sample of povondraite as well as some of Žáček's *et al.* (2000) reported samples have *X*-site sums greater than 1 *apfu*. Structurally, this is impossible. When the data was normalized so that Na + K = 1 *apfu*, the resultant $Y + Z + T$ sum was significantly less than the optimal 15 *apfu*. Altering the normalization by varying the amount of OH or Fe^{3+} / Fe^{2+} does not ameliorate the situation, as any change which decreases the *X*-site sum also serves to decrease the $Y + Z + T$ sum, which is already low. Interestingly, the wt% total for my sample (Žáček *et al.* (2000) did not include B_2O_3 or H_2O in their sums) is well-behaved. This indicates if any element was missed in the analysis, there cannot be a large quantity of it.

The most obvious explanation is that there is an analysis error. As both Žáček *et al.* (2000) and my analysis show this result, the error would most likely be due to some

unforeseen difficulty in this particular material, potentially because of overlap of peaks during EMPA, the high Fe content causing some sort of interference, or because some rare element is in the tourmaline but was not analyzed for. A likely suspect is Zr, which commonly substitutes for Ti in minerals. As these tourmalines have higher than average Ti content, the presence of Zr is conceivable. As the calculated *epfu* from EMPA is lower than the *epfu* calculated from SREF, adding a heavier element does increase the total *epfu* from EMPA, bringing it closer to the value from SREF. Other possible explanations include some interstitial K, though interstitial cations are generally not reported for tourmaline and there is no void space which could easily accommodate this large cation. Another possibility is that the alkali values are incorrect due to mobilization by the microbeam. A third possibility is a substitution of Na into an octahedral site. This would serve to lower the *X*-site sum and raise the $Y + Z + T$ sum, however this hypothesis is not supported by the bond-lengths of either the *Y*- or *Z*-site.

Several samples of povondraite were re-analyzed by EMPA to try to solve this problem. Initially, the Na and K values were re-collected to verify their agreement with original values. The beam was allowed to collect on the sample for several minutes, with data collected at five-second intervals in order to test the theory of alkali mobilization. The values remained consistent throughout the entire 130-second run. Secondly, the K peak was closely examined to determine if there was any distortion of the peak due to possible overlaps with higher order peaks from other components; the peak was found undistorted. Finally, additional elements were tested for by checking for anomalous peaks as well as analyzing for specific elements (As, Cu, Zr, Sr, Co, Sn, Y, Sc, Nb, Ba,

Pb and S). Neither method revealed any unknown constituent of significant quantity; the largest reported wt% from this study was 0.10 wt% CuO.

The impossibly high values of alkalis reported by Žáček *et al.* (2000) as well as myself cannot be easily explained by errors in chemical analysis or missed constituents. The structural data does not support interstitial K or Na substituting at an octahedral site. Further work needs to be done explain why the Na + K > 1 *apfu* for these samples.

6.2.3 Substitution mechanisms

Substitution of Fe^{3+} into the tourmaline structure seems to be at the expense of Al (Figure 6.3). Additionally, there is a positive correlation between Fe^{3+} and K in several of these tourmalines, though Žáček's *et al.* (2000) "B" group, which they report is the

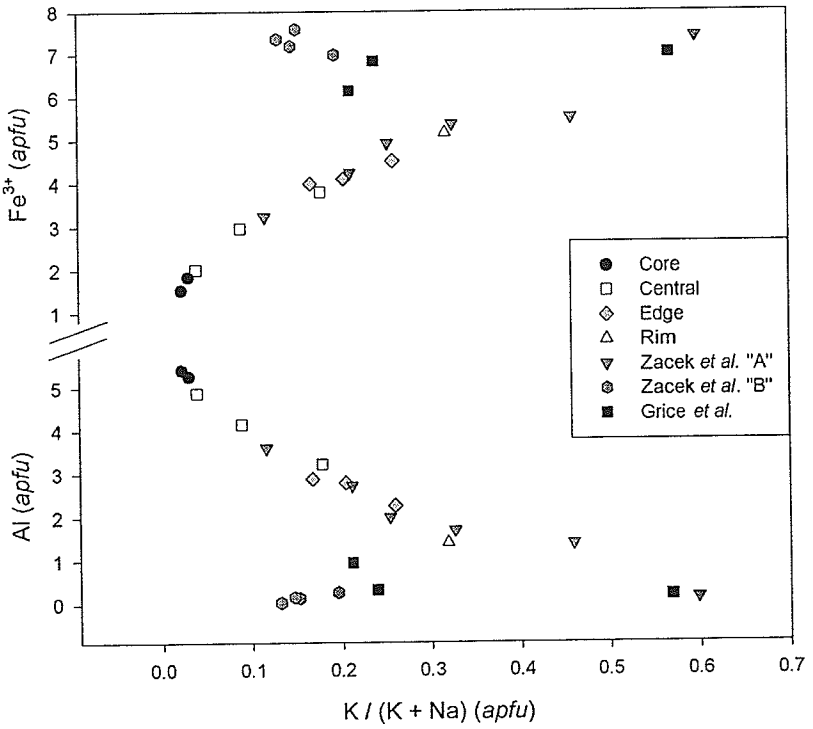

Figure 6.3: Chemical zoning of Fe^{3+} and Al in povondraite in relation to location in the crystal and increasing K content. Data from Žáček *et al.* (2000) and Grice *et al.* (1993) are included for comparison.

closest to ideal povondraite, and two of the three compositions Grice *et al.* (1993) do not follow this trend. As there seems to be no crystal-chemical reason why K has not substituted into these tourmalines to a greater degree, the lower K values must be geochemically controlled.

Grice *et al.* (1993) and Žáček *et al.* (2000) report various trends for Ti, V and Mg as a function of the K/(K+Na) ratio. Data from these two researchers were combined with my data. As Grice *et al.* (1993) calculated Fe^{3+}/Fe^{2+} ratios from stoichiometry based on H_2O values from bond-valence arguments, their data was renormalized with all Fe^{3+} so it could be directly compared to the other data sets. Žáček *et al.* (2000) do not report V. Figure 6.4 shows Mg as a function of K/(K + Na) where a weak negative correlation can be seen. Plots of Ti and V *vs.* K/(K + Na) show no conclusive trend.

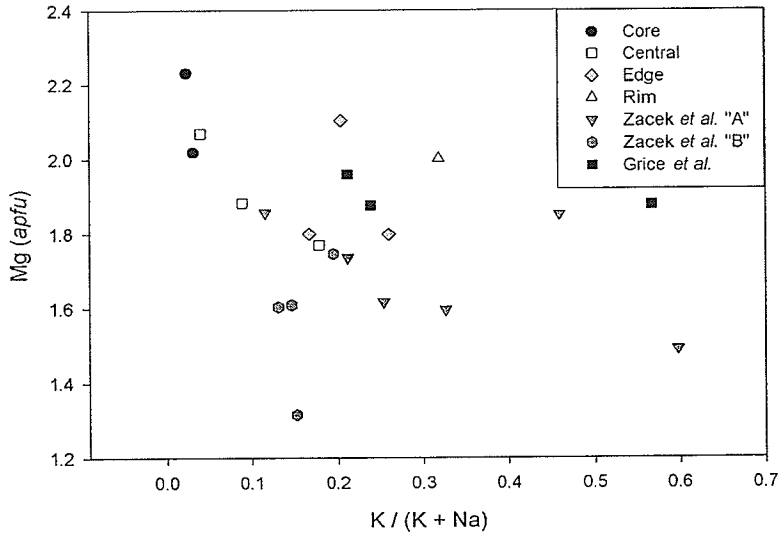

Figure 6.4: Chemical variation of Mg in povondraite with increasing K content. Data from Žáček *et al.* (2000) and Grice *et al.* (1993) are included for comparison

6.3 Crystal structure

A single crystal of povondraite was obtained for structure refinement by grinding away material until only the outer, iron-rich rim remained. This wafer of material was analyzed by SREF using the method described in Chapter 2.2, then subsequently chemically analyzed by electron-microprobe (sample CT99). Table 6.2 lists the refinement data for this sample, which was refined to an *R*-value of 2.09%. The size of the unit cell of povondraite is significantly larger than those of other tourmaline, in agreement with the observations of Grice *et al.* (1993). Table 6.3 presents the site-scattering (SREF and EMPA) data.

Table 6.2: Unit-cell parameters and SREF collection data for CT99

a (Å)	16.243(2)	N	6349
c (Å)	7.493(1)	#I $\|F_o\| > 5\sigma\Phi$	1208
		R (%)	2.09
V (Å^3)	1712.1	wR(%)	2.39
		GOF	1.415

Table 6.3: Site-scattering data (*epfu*) for CT99

	SREF data	**Probe data, Fe^{2+}	*Probe data, Fe^{3+}	**Probe data, Fe^{3+}
X	14.16	15.40	14.06	14.06
Y	70.97	95.88	45.52	73.52
Z	128.06	105.63	138.29	110.28
T	84.00	84[§]	83.97	83.97

Fe^{2+} formula calculated with OH = 4 *apfu*, Fe^{3+} formula calculated with OH = 3 *apfu*
* *Z* filled with Al + Fe^{3+}; ** *Z* filled with Al + Mg + Fe. [§] Si *apfu* calculated with all Fe^{2+} greatly exceeds the possible 6 *apfu*, thus the calculated *epfu* is above the allowable 84 *epfu* by 7.22 *epfu*.

6.4 Discussion

Site-scattering data from SREF should be relatively consistent no matter what element is assigned at a site (within reason) and provides a good check on methods for site assignment from chemical data. Sample CT99 was refined with the scattering

species Na + K at *X*, Fe + Al at *Y*, and Fe + Mg at *Z*. This assignment for the *Y*- and *Z*-sites, though not standard, was done based on the ideal end-member having considerable Mg at *Z*. As Mg and Al have very similar scattering powers, there should be no significant difference in the refinement if there is disorder between Mg and Al.

Comparing the site-scattering data from SREF with that assigned from the unit formula, it is apparent that one assignment has a better fit to the SREF data than the other assignments. Column 2 is the chemical data with all iron assumed to be ferrous. There are a number of problems here, but the most obvious is that the calculated *epfu* at the *T*-site exceeds the crystallographically possible 84 *epfu* for sites fully occupied by Si, indicative of an impossible Si > 6 *apfu*. This result supports the premise that the majority of the iron is trivalent.

Column 3 shows the site-scattering when all iron is assumed to be ferric. Site populations were assigned by first assigning Al to the *T*-site such that Si + $^{[4]}$Al = 6 *apfu*. Remaining Al was assigned to the *Z*-site, followed by Fe^{3+}. The *Y*-site was filled with the remaining Fe^{3+}, and by Mg, V and Ti. Total *apfu* for the *Y*-site is less than 3. Comparing the site-scattering values from this method of site-assignment to the SREF data, there is reasonable agreement for the *X*- and *T*-sites. However, there is a significant difference in the data for the *Y*- and *Z*-sites, most apparent for the *Y*-site. Because the *epfu* assigned to this site from the unit formula is significantly less than the *epfu* calculated from the SREF data, this suggests that a larger amount of "heavy" elements need to be assigned to this site. Likewise, the *Z*-site apparently has too much heavy element assigned here. This suggests that the above site-assignment scheme is not optimal.

In column 4, the method of assigning elements to sites was altered. Here, the *T*-site was filled the same way as in column 3, but now the *Z*-site was filled in the order Al, Mg, and Fe^{3+}. This method leaves only Fe^{3+}, V, and Ti to be assigned to *Y*. Although there still is some discrepancy between the site-scattering calculated from this method and that from the SREF data, the agreement is much closer than from the other two methods.

Based on these observations, the best method for distributing species between the *Y*- and *Z*-sites in povondraite involves filling the *Z*-site in the order Al, Mg, Fe^{3+}. The discrepancies between this method and the *epfu* calculated from the refinement data are most likely due to the presence of some Fe^{2+} and minor disorder of Mg and Al over the *Y*- and *Z*-sites.

In addition to site-scattering data, bond-lengths may also be used to determine chemical constituents at a site. Bond-lengths are most useful when the number of potential components is small, as minor elements can shift overall bond-lengths and it is easier to determine what is controlling an average length if the number of contributors is small. The <Z-O> length for sample CT99 is 2.018 Å. We can calculate the ideal average bond-length from the proposed methods of assigning components by using the ideal ionic radii of Shannon (1976). The three sets of probe data shown in Table 6.3 were used to calculate what the <Z-O> bond-lengths would be for the three site-assignment and Fe^{2+} *vs.* Fe^{3+} combinations listed; with all Fe^{2+} and $Z = Al + Mg + Fe^{2+}$, <Z-O> = 2.056 Å, with all Fe^{3+} and $Z = Al + Fe^{3+}$, <Z-O> = 1.984 Å, and with all Fe^{3+} and $Z = Al + Mg + Fe^{3+}$, <Z-O> = 2.007 Å. As the calculated bond-length which most closely resemble the observed length is 2.007 Å, this argument supports the premise that the *Z*-

site is filled with Al + Mg + Fe^{3+}. As the calculated value is slightly shorter than the observed, and this cannot be increased by adding more Mg (all Mg is already assigned to *Z*), there is further evidence that a small percentage of Fe may be 2+ (Fe^{2+} ionic radius = 0.78 Å) (Shannon 1976).

Povondraite has the most K reported for any tourmaline, with some individual analytical points reporting as K dominant at the *X*-site (Grice *et al.* 1993, Žáček *et al.* 2000). An idea is that this is due to the large amount of Fe in the structure. Fe^{3+}, with an ionic radius significantly larger than Al, could effectively expand the structure, allowing K to substitute for the smaller Na in greater quantity than is normally the case in the tourmaline structure. This feature is well-characterized in the amphiboles (*e.g.* K + Cl → Na + (OH) in calcic amphiboles (Oberti *et al.* 1993)). More work needs to be done on povondraite (as well as other tourmalines with enlarged cells) in order to determine whether this is a crystallographically-controlled phenomenon.

The alkali contents of both CT99 and samples from Žáček *et al.* (2000) exceed the structurally allowed 1 *apfu*. This may be due to an element missed in data collection, errors in data collection due to peak interference or mobilization of the alkalis, or mis-assignment in the structure. Further work needs to be done characterizing the exact nature of this problem and testing the various hypotheses.

CHAPTER 7

Stereochemistry of the $^{[3]}B$-site

7.1 Introduction

Boron is an essential component of all tourmalines, and SREF and bond-valence calculations indicate that B = 3 *apfu* in all tourmalines structurally analyzed to date, indicating the *B*-site is fully occupied by B. In almost all tourmalines analyzed to date, boron occurs only in triangular coordination (Hawthorne 1996). The only exception to this is the Austrian olenite of Hughes *et al.* (2000) which shows direct evidence of B > 3 *apfu*.

There is one triangularly coordinated site (the *B*-site) in tourmaline (Figure 7.1). The central cation is bonded to one O2 and two O8 anions. The *B*-site is thought

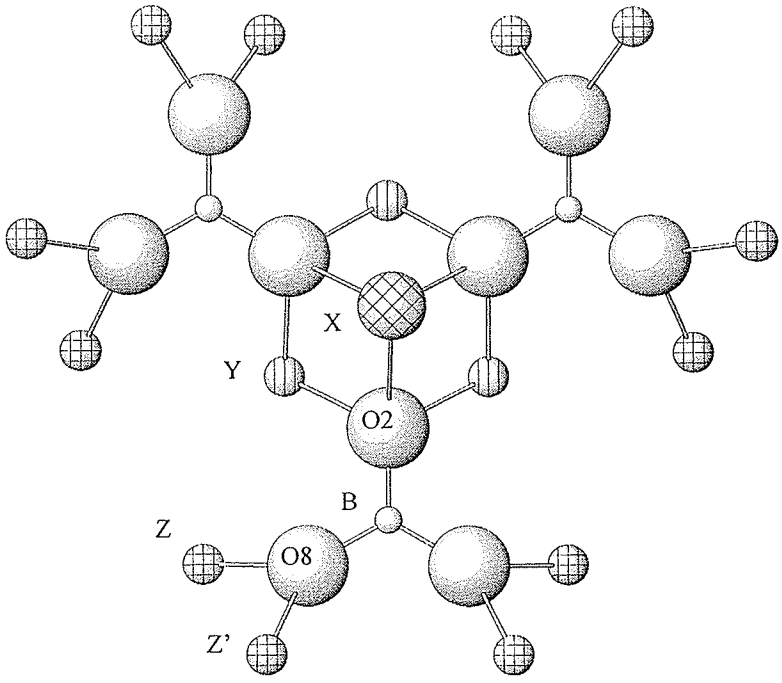

Figure 7.1: A fragment of the tourmaline structure looking down the *c*-axis, showing the local environment around the BO_3 triangle.

to be relatively rigid in the tourmaline structure.

7.2 Description of problem

While investigating the tourmalines in my sample suite, some systematics in the stereochemistry about the *B*-site became apparent. Table 7.1 lists the average <B-O> distances for my sample suite. Due to SREF *R*-values >3.0%, I excluded eight tourmaline samples from this particular study (samples CT41, CT58, CT73, CT90, CT92, CT96, CT97, and CT98). The <B-O> bond length is 1.374, with <B-O2> = 1.360 and <B-O8> = 1.381 Å. These distances are in agreement with values reported for a variety

TABLE 7.1: Average B–O bond lengths for tourmaline

Species	#	<B-O2> Å	<B-O8> Å	<B-O> Å
Elbaite	14	1.358	1.381	1.373
Oxy-elbaite	1	1.356	1.382	1.373
Fluorelbaite	17	1.354	1.384	1.374
Dravite	11	1.368	1.376	1.373
Fluordravite	7	1.356	1.386	1.376
Schorl	6	1.354	1.384	1.374
Fluorschorl	5	1.354	1.384	1.374
Uvite	9	1.369	1.379	1.376
Hydroxyuvite	7	1.370	1.377	1.374
Liddicoatite	4	1.355	1.384	1.374
Foitite	3	1.345	1.385	1.372
Oxy-foitite	1	1.346	1.385	1.372
Buergerite	1	1.380	1.374	1.376
Cralpoite	4	1.378	1.368	1.371
Povondraite	1	1.388	1.367	1.374
TOTAL	91	1.360	1.381	1.374

of tourmaline species in the literature (*e.g.* Burns *et al.* 1994, Grice and Ercit 1993, Selway *et al.* 1998, MacDonald and Hawthorne 1995). In all of the tourmaline species investigated, the <B-O> bond length is fairly constant. However, there is significant variation in the B-O2 and B-O8 lengths for different tourmaline species. For example, in elbaite, B-O2 < B-O8, in hydroxyuvite B-O2 ≈ B-O8, and in povondraite B-O2 > B-O8, but the <B-O> distances for these tourmalines are about the same.

Figure 7.2 shows the variation in <B-O2> as a function of <B-O8>; for brevity, tourmaline minerals with variations only at *W* have been grouped together under one species name. There is a relatively well-developed inverse correlation. The dotted line is a regression line, and most points fall within 2 standard deviations of this line. Points on this graph are not randomly distributed, but occur in chemical groupings. This suggests that the dominant cations at the *X*-, *Y*-, and *Z*-sites control this behavior.

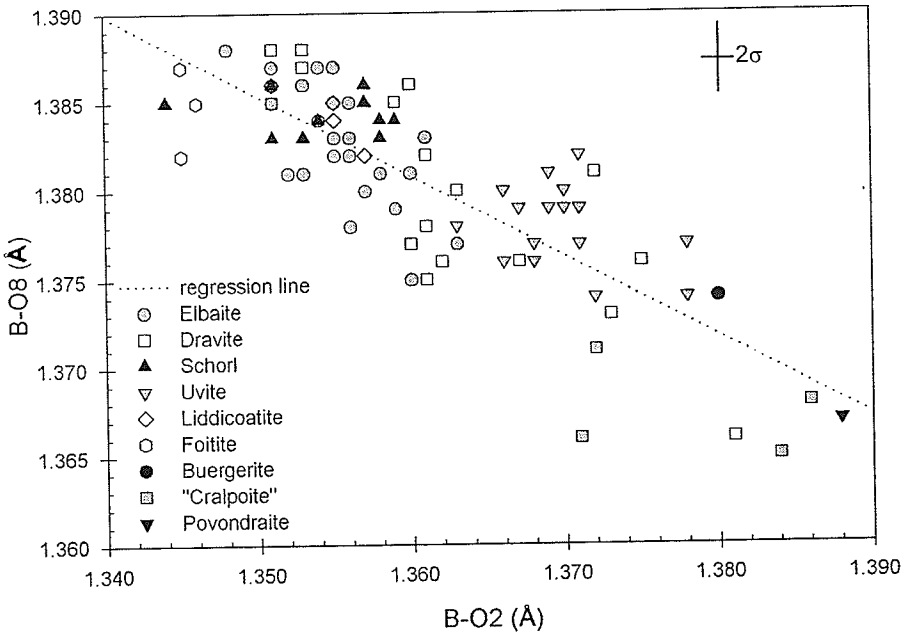

Figure 7.2: Observed B – O2 *vs.* B – O8 distances in tourmaline

Re-examination of Figure 7.1 shows why the B-O2 and B-O8 distances vary between different chemical groups of tourmaline. With different *X*- and *Y*-site populations, the strength of the interactions between *X*, *Y* and O2 vary, and the B-O2 distance varies as a result. Similarly, variations in the *Z*-site population cause a variation in the strength of the *Z*-O8 interaction, and the B-O8 distance varies as a result. In addition, B-O2 and B-O8 distances must vary inversely in order for the bond-valence

requirements of the central B cation to be satisfied. In order to put this argument onto a more quantitative basis, I will examine this situation using bond-valence theory.

7.3 Bond-valence theory

Bond-valence theory is essentially a development of Pauling's second rule, which relates the strength of a bond to the coordination of the central cation (or anion) Pauling's second rule also went on to say that the sum of bond strengths incident at an atom are approximately equal to the formal valence of that atom (Pauling 1929). With bond-valence theory, the strength of a bond is related to its length as well as the types of cations involved (Brown 1981). There are several different formulae for calculating bond-valences (*e.g.* Donnay and Allmann 1970, Brown 1981, Brown and Altermatt 1985, Brese and O'Keeffe 1990), each with different pros and cons. A major advantage to the universal curves of Brown (1981) is that it has one set of constants for Na, Mg, Al and Si. This is beneficial for tourmaline as details of site-ordering between Mg and Al are not required. Therefore, bond-valences were calculated using Brown (1981):

$$s = \exp[(R_0 - R) / B]$$

where R is the bond length, and R_0 and B are fitted constants. The advantage to using bond-valence curves is that they combine chemical and crystallographic data, taking into account variations both in site populations and bond lengths. Figure 7.3 shows the bond-valence interactions that can affect the geometry of the (BO_3) triangle. Multiple regression was used determine which interactions are more significant.

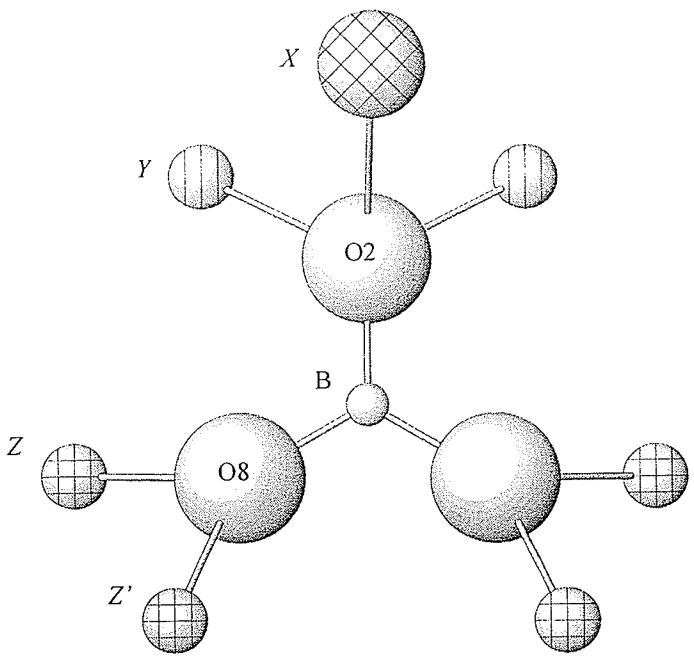

Figure 7.3: Geometry of the (BO_3) triangle, showing the bonds that can affect the stereochemistry of the site.

7.4 Statistical methods

The variation in stereochemistry of the (BO_3) triangle is constrained by the fact that the mean <B-O> distance is constant. Therefore, I used the ratio of the B-O2 and B-O8 bond-valences as dependent variable. Possible independent variables which may effect this ratio are *X*-O2, 2 * (*Y*-O2), *Z*-O8, and *Z'*-O8. Forward stepwise linear regression gave the formula:

$$\text{B-O2/B-O8} = -0.58(10) + 0.10(3) * [2 * (Y\text{-O2})] + 3.02(18) * Z'\text{-O8}$$

with an R^2 value of 0.772. This equation shows that the principal independent variable controlling the shape of the (BO_3) triangle is the *Z'*-O8 bond-valence, with minor contributions from the *Y*-site cations.

7.5 Discussion

The primary control on the geometry of the (BO_3) triangle is the *Z*'-O8 bond. Figure 7.4 is a plot of calculated *vs.* observed B-O2/B-O8 ratios and Figure 7.5 shows the original data.

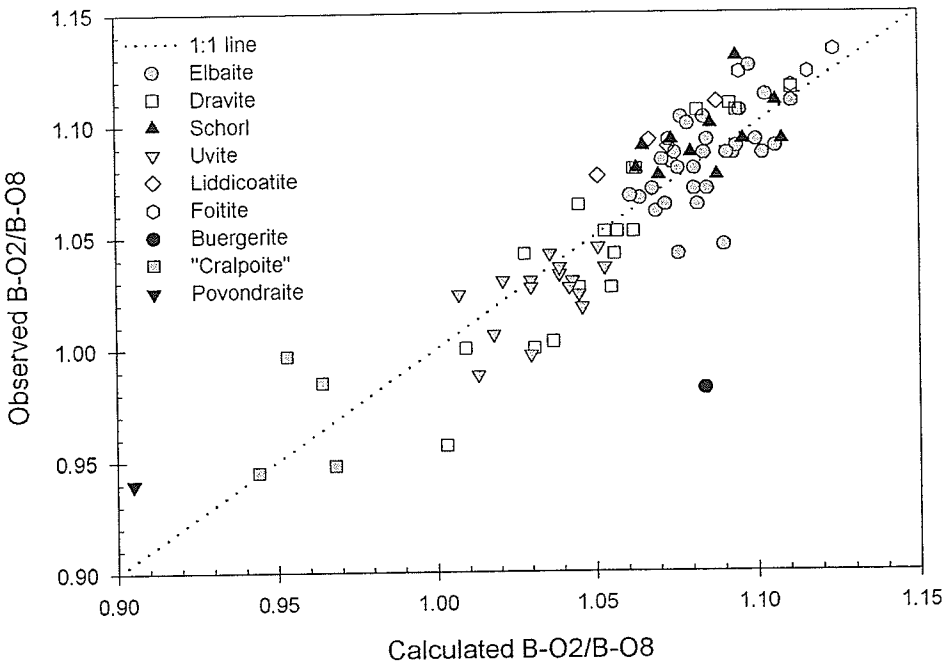

Figure 7.4: Calculated B-O2/B-O8 *vs.* observed B-O2/B-O8. Calculated values from the formula given in the text.

An examination of this plot, along with Figure 7.5, shows that the chemical groupings originally observed are actually groupings based on variations in the *Z*-site population. In Figure 7.5, boundaries have been drawn around species with similar *Z*-site chemistry. Elbaite, schorl, liddicoatite, and foitite all have six Al assigned to *Z*, and they all plot together. Likewise, uvite and dravite both have significant Mg at *Z* and are similarly grouped. The tourmaline samples that plot on the far right of the graph all have significant variation in their *Z*-site chemistry, with considerable-to-dominant amounts of

Cr or Fe^{3+}. It seems that the mean ionic radius of the *Z* cations increases toward the lower right of Figure 7.5.

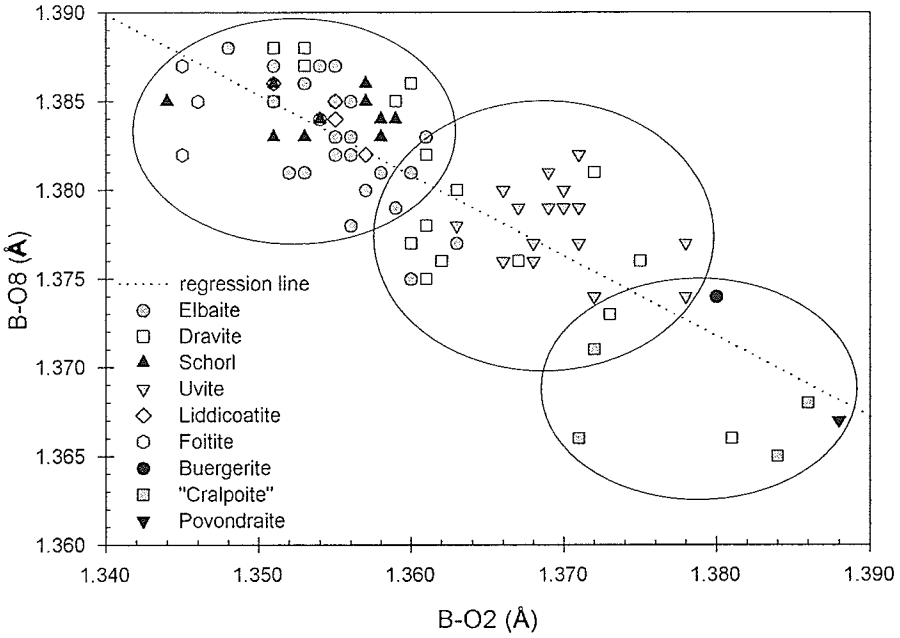

Figure 7.5: Observed B-O2 *vs.* B-O8 distances, with approximate chemical groupings shown. Some points of a given composition may not fall in the same field as others; this is assumed to be due to variation in chemistry away from end-member compositions.

In conclusion, the *B*-site in tourmaline is a relatively rigid structural element. However, inversely coupled variation does occur between the B-O2 and B-O8 bonds. As the *Z*-site increases in size, B-O8 decreases and B-O2 increases. Regardless of the individual bond-lengths, the <B-O> distance remains relatively constant in all tourmaline minerals.

CHAPTER 8

Discussion and Summary

8.1 Structural-formula calculation

Chemical analyses of tourmaline are usually incomplete due to difficulties in the analysis of light elements, valence states of transition metals, and problems with the heterogeneity of crystals. When there are undetermined components, assumptions must be made in order to develop a structural formula. Normalization on 31 anions with assumed OH + F = 4 *apfu* usually provides the most accurate formula, though care should be taken to ensure total wt% sums are near 100 % and cation *apfu* are reasonable (*e.g.* Si $\leq$ 6 *apfu*).

Li, if not measured, may be iterated for by adding Li_2O to the calculation scheme until $Y + Z + T = 15$ *apfu*.

Fe is often assumed to be 2+ in tourmaline, unless there is strong evidence that ferric iron may occur. This assumption may have lead to the misidentification of some buergerite, as the calculated formula of buergerite, when Fe^{2+} and OH + F = 4 *apfu* are assumed, is equivalent to the formula for schorl. Every effort must be made in tourmaline chemical analysis to determine the correct valence state of Fe. As most methods for valence determinations currently available require bulk sample, direct measurement of the Fe^{3+}/Fe^{2+} ratio might not be possible. However, this can be accurately determined if it is the only undetermined value in a chemical data set. If the valence state cannot be measured, stoichiometric arguments can be accurately used, provided all other constituents have been measured.

Normalization on 6 *apfu* of Si at *T* can be useful if the initial anion normalization led to >6 *apfu* Si.

Whenever possible, additional information should be incorporated when calculating structural formula. This includes data from structure analysis or the petrologic environment. Accurate normalization schemes are imperative in order to accurately classify the tourmaline by species and to use the chemical information that the mineral provides.

8.2 Potential new species of tourmaline

Pending approval of Hawthorne and Henry's (1999) proposed nomenclature scheme for tourmaline, there are several potential new species of tourmaline based on variation of anions at the *W*-site included in my suite. In addition, there is one new Cr-tourmaline that will be submitted after further chemical analysis is made.

"Fluordravite" is the F-dominant analogue of dravite, with an ideal end-member formula: $Na\ Mg_3\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$.

"Fluorelbaite" is the F-dominant analogue of elbaite, with an ideal end-member formula: $Na\ (Li_{1.5}Al_{1.5})\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$.

"Fluorschorl" is the F-dominant analogue of schorl, with an ideal end-member formula: $Na\ Fe^{2+}_3\ Al_6\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ F$.

"Hydroxyuvite" is the OH-dominant analogue of uvite, with an ideal end-member formula: $Ca\ Mg_3\ (Al_5Mg)\ (Si_6O_{18})\ (BO_3)_3\ (OH)_3\ (OH)$.

"Cralpoite" is the Cr-Al analogue of povondraite, with an ideal end-member formula: Na Cr^{3+}_3 (Al_4Mg_2) (Si_6O_{18}) $(BO_3)_3$ $(OH)_3$ O. It is distinct from chromdravite by virtue of the presence of Cr^{3+} at the *Y*-site and Al (+ Mg) at the *Z*-site.

8.3 Crystal chemistry of chromian tourmaline minerals

Tourmaline with significant amounts of Cr (> 1 wt% Cr_2O_3), though rare, do occur at a few localities. Cr can occur at the *Y*-site, the *Z*-site, or both. "Cralpoite" is a proposed new species of tourmaline with the ideal formula: Na Cr^{3+}_3 (Al_4Mg_2) (Si_6O_{18}) $(BO_3)_3$ $(OH)_3$ O; as such, it is the first tourmaline to have Cr dominant at *Y*. Chromdravite, currently Na Mg_3 Cr^{3+}_6 (Si_6O_{18}) $(BO_3)_3$ $(OH)_3$ (OH), may need to be revised to show Cr dominant at both the *Y*- and *Z*-sites.

There are a number of problems with the analysis of Cr tourmaline. The tourmalines tend to occur as small, internally zoned crystals that are chemically heterogeneous from crystal to crystal; therefore bulk analytical techniques are not appropriate for light-element analysis. SIMS standards have not yet been developed for tourmaline with high transition-metal content.

In addition to difficulties in collecting data due to crystal size and character, EMPA data that have been collected report low wt% sums. This has not been fully explained and is still being investigated.

8.4 Crystal chemistry of povondraite

Povondraite, a ferric tourmaline, has the most K reported for any species of tourmaline. This may be due to the large amount of Fe^{3+} present, which could effectively

expand the structure, allowing K to substitute for Na in greater quantity than is usually found.

The best method for distribution of species at the *Y*- and *Z*-sites for povondraite involves filling the *Z*-site in the order Al, Mg, Fe^{3+}. This argument is based on examination of bond-lengths and comparison of *epfu* calculated from SREF and EMPA, for each site.

The reported alkali contents for some povondraite samples exceed the structurally allowed 1 *apfu*. It is still unclear as to what is causing this anomaly.

8.5 Stereochemistry of the $^{[3]}B$-site

The (BO_3) triangle in tourmaline, though relatively rigid, shows inversely coupled variations between B-O2 and B-O8. Regression analysis shows that the primary control on this relation is the *Z'*-O8 bond. As the constituent *Z* cation increases in size, B-O8 decreases and B-O2 increases. Regardless of individual variations, the <B-O> distance remains relatively constant in all tourmaline.

8.6 Unresolved issues

A number of unanswered questions regarding tourmaline would be significantly aided by accurate analysis of light-element contents (Li_2O, B_2O_3 and H_2O). Due to the ubiquitous zoning in tourmaline and chemical inhomogeneity between crystals, accurate analysis by bulk techniques is usually impossible. Analysis by SIMS is possible provided appropriate standards are available. Currently, this is not the case for tourmaline with high transition-metal content (Cr tourmaline and povondraite). However, I am currently

investigating the development of an appropriate synthetic tourmaline for use as a standard. Accurate analysis of H_2O, B_2O_3 and H_2O would allow complete characterization of the proposed new species "fluordravite", "fluorschorl", "fluorelbaite" and "cralpoite", as well as potentially recognizing oxy-tourmaline species. In addition to characterization of new species, these data would allow stoichiometric arguments to be used in unresolved issues concerning low weight-percent totals in Cr tourmaline and excess alkalis in povondraite. Ultimately, with standardization of SIMS techniques for light-element analysis, all tourmaline investigations will improve, as normalization schemes will no longer need to be based on assumed OH content.

Another area where there is room for considerable work is the development of site-ordering curves based on a combination of SREF, EMPA and SIMS data. This would allow a better understanding of the substitution mechanisms in tourmaline and the petrologic environment of formation, increasing the usefulness of tourmaline to petrologists.

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APPENDIX A

Tourmaline Samples

Abbreviations used in Appendix A:

Museum or collection of:

a: California Institute of Technology; **b**: National Museum of Natural Sciences; **c**: Dalhousie University; **d**: Royal Ontario Museum; **e**: University of Manitoba; **f**: American Museum of Natural History; **g**: University of Maine; **h**: Smithsonian Institute; **i**: Nova Scotia Department of Mines and Energy; **j**: purchased from dealer; **k**: Moravian Museum, Brno;

Provided by:

l: Frank C. Hawthorne; **m**: Mark A. Cooper; **n**: Dan J. MacDonald; **o**: Bradley S. Wilson; **p**: Christine M. Clark McCracken; **q**: dealer

Analyses run on each sample:

S: single-crystal structure refinement; **P**: electron-microprobe analyses; **X**: X-ray powder diffraction; **H**: H-extraction line

* denotes holotype of potential new tourmaline species

Sample	Species	Locale	Other Number	Source	Data
CT1	Elbaite	Sverdlouskoblast, Ural Mts, Russia	T-15, 43216	b	S,P
CT2	Elbaite	Brazil	T-31	e	S,P
CT3	Elbaite	Lilly Pads, ON	T-33	e,m	S,P
CT4	Elbaite	Tanco Mine, Bernic Lake, MB	T-34	e,n	S,P
CT5	Elbaite	Baja, CA	T-37	e	S,P
CT6	Elbaite	Northern Africa	T-39		S,P
CT7	Elbaite	Minas Gerais, Brazil	T-45, M20916	d	S,P
CT8	Elbaite	Elba, Italy	T-47, E1454	d	S,P
CT9	Elbaite	Pesrig, Saxony, Germany	T-48, M6101	d	S,P
CT10	Elbaite	Minas Gerais, Brazil	T-50, M31184	d	S,P
CT11	Elbaite	Paraiba, Brazil	T-54	b	S,P
CT12	Elbaite	Paraiba, Brazil	T-55	b	S,P
CT13	Elbaite	Brazil	T-82	l	S,P
CT14	Elbaite		MT10A		S,P
CT15	Elbaite	Tanco Mine, Bernic Lake, MB	TCR-1	e,p	S,P
CT16	"Fluorelbaite"	Santa Rosa, Minas Gerais, Brazil	T-12, 43276	b	S,P
CT17	"Fluorelbaite"	South Africa	T-13, 43215	b	S,P
CT18	"Fluorelbaite"	San Diego Co., CA	T-16	c	S,P
CT19	"Fluorelbaite"	San Diego Co., CA	T-18	c	S,P
CT20	"Fluorelbaite"	San Diego Co., CA	T-19	c	S,P
CT21	"Fluorelbaite"	San Diego Co., CA	T-25	c	S,P
CT22	"Fluorelbaite"	San Diego Co., CA	T-26	c	S,P
CT23	"Fluorelbaite"	San Diego Co., CA	T-29	c	S,P
CT24	"Fluorelbaite"	San Diego Co., CA	T-30	c	S,P
CT25	"Fluorelbaite"	Baja, CA	T-36	e	S,P
CT26	"Fluorelbaite"	Minas Gerais, Brazil	T-49, M41979	d	S,P
CT27*	"Fluorelbaite"	Black Mt., Rumford, ME	T-51, M30977	d	S,P,X
CT28	"Fluorelbaite"	Havey Mine, Poland, ME	T-52, M19027	d	S,P
CT29	"Fluorelbaite"	Brazil	T-83	l	S,P
CT30	"Fluorelbaite"	Tanco Mine, Bernic Lake, MB	TCGT-1	e,p	S,P
CT31	"Fluorelbaite"	Brazil	T-96m	e,l	S,P
CT32	"Fluorelbaite"	Lastovicky	MT13A, LA3-2	k	S,P
CT33	Dravite	Osarara, Kenya	T-9, TDRV	a	S,P
CT34	"Cralpoite"	Kokka, Finland	T-38, MOC3532	b	S,P
CT35	Dravite	Modoc, ON	T-41, M31665	d	S,P
CT36	Dravite	Karsten, Germany	T-42, M19631	d	S,P
CT37	Dravite	Monmouth Twp., ON	T-56, M42863	d	S,P
CT38	Dravite	Minas Gerais, Brazil	T-64, M39701	d	S,P
CT39	Dravite	Tanzania	T-85, 143901	h	S,P
CT40	Dravite	Kaavi, Finland	119820X	h	S,P
CT41	Dravite	Etchison, Maryland	CrE-1, 78452	h	S,P
CT42	Dravite	Etchison, Maryland	CrE-2, 78452	h	S,P
CT43	Dravite	Etchison, Maryland	CrE-4, 78452	h	S,P
CT44	Dravite	unknown	T-92m, M1141	e	S,P
CT45	"Fluordravite"	Pierrepont, NY	T-66, E2666	d	S,P
CT46	"Fluordravite"	Langanbach quarry, Binntal Wallis, Switzerland	T-67		S,P
CT47	"Fluordravite"	Burma	133839C		S,P
CT48	"Fluordravite"	Burma	133839M		S,P

Sample	Species	Locale	Other Number	Source	Data
CT49	"Fluordravite"	Crabtree Emerald Mine, NC	123688A		S,P
CT50*	"Fluordravite"	Crabtree Emerald Mine, NC	MT14A, 121341	h	S,P,X
CT51	"Fluordravite"	Nedevice	TNE5B	k	S,P
CT52	Schorl	Villeneuve Mine, Papineau Co, PQ	T-10, 43261	b	S,P
CT53	Schorl	Lydoch Tp, ON	T-11, 43251	b	S,P
CT54	Schorl	Buckingham, Papineau Co, PQ	T-14, 43262	b	S,P
CT55	Schorl	San Diego Co., CA	T-20b	c	S,P
CT56	Schorl	Hatchet Lake, South Mt. Batholith, NS	T-87, D12-0033-3	i	S,P
CT57	Schorl	Nephton (Blue Mtn.), Methuer Twp, ON	108747	e,q	S,P
CT58	Schorl	Bayer's Lake blast pit, NS	T-99m	e,n	S,P
CT59	"Fluorschorl"	San Diego Co., CA	T-20a	c	S,P
CT60	"Fluorschorl"	San Diego Co., CA	T-21	c	S,P
CT61	"Fluorschorl"	Geco Mine	T-53, M25206	d	S,P
CT62	"Fluorschorl"	San Diego Co., CA	T-90m	c	S,P
CT63*	"Fluorschorl"	San Diego Co., CA	T-94m	c	S,P,X
CT64	Uvite	Laxton Twp., ON	T-23, M20414	d	S,P
CT65	Uvite	Sri Lanka	T-44, M34554	d	S,P
CT66	Uvite	Brazil	T-57, CB20	e	S,P
CT67	Uvite	Franklin, NJ	T-59m, C80699	f	S,P
CT68	Uvite	Hamburg, NJ	T-62m, 39870	f	S,P
CT69	Uvite	Galway Twp., ON	T-63, M18478	d	S,P
CT70	Uvite	Richville, NY	T-70, M31658	d	S,P
CT71	Uvite		MT12		S,P
CT72	Uvite	Mt. Isa, Queensland, Australia	T95m, M1179	e	S,P
CT73	Uvite	Burma	133839E		S,P
CT74	Uvite	Hamburg, NJ	T-65m, 607	d	S,P
CT75	"Hydroxyuvite"	Bahia, Brazil	T-46, M44381	d	S,P
CT76	"Hydroxyuvite"	Pierrepont, NY	T-58, 41080	b	S,P
CT77	"Hydroxyuvite"	unknown	T-61m	e	S,P
CT78	"Hydroxyuvite"	Umba, Tansania	CrU-1	h	S,P
CT79*	"Hydroxyuvite"	Brumado, Bahia, Brazil	MT6A	l	S,P, X,H
CT80	"Hydroxyuvite"		V012998	h	S,P
CT81	Liddicoatite	Franklin, NJ	T-40, M37600	d	S,P
CT82	Liddicoatite	Antsirabe, Malagasy Rep.	T-43, M34669	d	S,P
CT83	Liddicoatite	Madagascar	T-81	l	S,P
CT84	Liddicoatite	Madagascar	T-98m, 165836	h	S,P
CT85	Foitite	San Diego Co., CA	T-27	c	S,P
CT86	Foitite	San Diego Co., CA	T-28m	c	S,P
CT87	Foitite	San Diego Co., CA	T-28mb	c	S,P
CT88	Foitite	Erongo, Namibia	MT15A, C35B	l	S,P
CT89	Buergerite	Mexquito, San Luis, Potosi, Mexico	MT5A		S,P
CT90	"Cralpoite"	Nausahi, Keonjhar District, India	MT1A, 120534	h	S,P
CT91	"Cralpoite"	Nausahi, Keonjhar District, India	MT1B_2, 120534	h	S,P
CT92*	"Cralpoite"	Nausahi, Keonjhar District, India	MT1D, 120534	h	S,P,X

Sample	Species	Locale	Other Number	Source	Data
CT93	"Cralpoite"	Nausahi, Keonjhar District, India	MT1E, 120534	h	S,P
CT94	"Cralpoite"	Nausahi, Keonjhar District, India	MT1F, 120534	h	S,P
CT95	"Cralpoite"	Nausahi, Keonjhar District, India	MT1G, 120534	h	S,P
CT96	Chromdravite		MT4A, 123711	h	S,P
CT97	Chromdravite		MT4C, 123711	h	S,P
CT98	Chromdravite		MT4D, 123711	h	S,P
CT99	Povondraite		MT3B, Ktour		S,P

APPENDIX B

SREF Miscellaneous Information

This appendix lists miscellaneous data concerning each sample including cell dimensions (Å), SREF crystal size (μm), color, and statistical parameters regarding crystal structure refinements. An explanation of terms and abbreviations used in this appendix are as follows:

N = number of total observed reflections
#I $|F_0| > 5\sigma$ = subset of reflections of total observed reflections with absolute values of structure factors > 5 standard errors
R (%) = *R* index, not weighted
w*R* (%) = *R* index, weighted
GOF = goodness of fit parameter

		CT1	CT2	CT3	CT4	CT5
Cell Parameters	*a* (Å)	15.838(3)	15.841(2)	15.822(3)	15.823(3)	15.811(3)
	c	7.095(1)	7.100(1)	7.095(2)	7.091(1)	7.094(2)
	V (Å^3)	1541.3	1542.9	1538.1	1537.4	1535.7
Crystal Dimensions	'X'(μ)	280	450	260	320	350
	'Y'	350	430	280	340	350
	'Z'	310	430	300	360	350
Color		pink	light green	pink	pink	pink
N		1109	1106	1108	1108	1103
#I $\|F_0\| > 5\sigma$		1101	1106	1098	1104	1100
***R* (%)**		1.80	1.67	1.95	1.82	1.70
w*R* (%)		2.32	2.40	2.53	2.60	2.45
GOF		2.718	3.861	3.080	3.503	4.144

		CT6	CT7	CT8	CT9	CT10
Cell Parameters	*a* (Å)	15.830(2)	15.828(4)	15.792(3)	15.800(4)	15.828(2)
	c	7.086(1)	7.092(3)	7.091(3)	7.093(2)	7.097(1)
	V (Å^3)	1537.8	1538.8	1531.5	1533.4	1539.8
Crystal Dimensions	'X'(μ)	380	330	370	400	200
	'Y'	390	320	360	420	220
	'Z'	400	320	380	440	240
Color		light blue	pink	colorless	pink	light green
N		1106	1107	1101	1102	1107
#I $\|F_0\| > 5\sigma$		1103	1100	1096	1098	1100
***R* (%)**		1.68	1.73	1.62	1.80	2.03
w*R* (%)		2.24	2.38	2.24	2.77	2.60
GOF		3.338	3.192	3.329	4.406	3.479

		CT11	CT12	CT13	CT14	CT15
Cell Parameters	*a* (Å)	15.818(2)	15.805(2)	15.851(2)	15.824(2)	15.811(1)
	c	7.088(1)	7.084(1)	7.104(1)	7.089(1)	7.093(1)
	V (Å^3)	1535.8	1532.6	1545.7	1537.3	1535.6
Crystal Dimensions	'X'(μ)	480	440	480	200	200
	'Y'	440	450	520	200	200
	'Z'	420	440	500	200	200
Color		blue	light blue	green	colorless	dark pink
N		1098	1086	1107	1109	1109
#I $\|F_0\| > 5\sigma$		1095	1085	1107	1105	1102
***R* (%)**		1.99	1.85	2.12	2.46	1.68
w*R* (%)		2.74	2.56	2.88	3.00	2.25
GOF		4.424	4.283	5.177	3.599	2.467

		CT16	CT17	CT18	CT19	CT20
Cell Parameters	*a* (Å)	15.908(2)	15.909(3)	15.906(3)	15.883(2)	15.887(2)
	c	7.135(2)	7.128(2)	7.127(1)	7.113(1)	7.116(1)
	V (Å^3)	1563.6	1562.2	1561.5	1554.1	1555.4
Crystal Dimensions	'X'(μ)	330	310	400	400	420
	'Y'	330	350	350	400	400
	'Z'	360	370	350	370	380
Color		green	light blue	green	light green	light blue
N		1127	1121	1121	1115	1116
#I $\|F_0\| > 5\sigma$		1122	1112	1117	1111	1114
***R* (%)**		2.03	1.89	1.95	2.41	2.06
w*R* (%)		2.52	2.44	2.41	2.92	2.91
GOF		3.184	3.202	3.127	4.434	4.812

		CT21	CT22	CT23	CT24	CT25
Cell Parameters	*a* (Å)	15.880(2)	15.907(2)	15.909(2)	15.874(2)	15.852(2)
	c	7.113(3)	7.120(1)	7.118(2)	7.111(1)	7.106(1)
	V (Å^3)	1553.4	1560.2	1560.0	1551.9	1546.4
Crystal Dimensions	'X'(μ)	440	400	280	600	400
	'Y'	460	390	300	540	380
	'Z'	500	400	320	420	380
Color		aqua-blue	blue-grey	light blue	sky blue	green
N		1110	1120	1121	1108	1109
#I $\|F_0\| > 5\sigma$		1109	1116	1118	1107	1104
***R* (%)**		2.08	2.26	2.26	1.93	1.76
w*R* (%)		2.82	3.24	2.95	2.63	2.49
GOF		4.687	5.181	4.298	4.329	3.923

		CT26	CT27	CT28	CT29	CT30
Cell Parameters	*a* (Å)	15.842(3)	15.851(2)	15.808(3)	15.842(2)	15.889(1)
	c	7.096(3)	7.103(3)	7.096(3)	7.100(2)	7.117(1)
	V (Å^3)	1542.3	1545.5	1535.6	1543.0	1556.2
Crystal Dimensions	'X'(μ)	400	200	380	340	200
	'Y'	420	200	400	360	200
	'Z'	380	120	300	350	200
Color		green	light green	light green	pink	green
N		1099	1109	1106	1107	1118
#I $\|F_0\| > 5\sigma$		1096	1083	1103	1103	1110
***R* (%)**		1.83	1.96	2.20	2.28	1.88
w*R* (%)		2.51	2.28	2.82	2.88	2.40
GOF		4.062	1.976	4.020	4.158	2.812

		CT31	CT32	CT33	CT34	CT35
Cell Parameters	*a* (Å)	15.843(1)	15.915(1)	15.947(2)	15.920(3)	15.921(4)
	c	7.104(1)	7.128(1)	7.214(1)	7.204(2)	7.219(2)
	V (Å^3)	1544.1	1563.6	1588.9	1581.3	1584.5
Crystal Dimensions	'X'(μ)	130	230	380	480	400
	'Y'	130	230	380	500	380
	'Z'	130	230	380	500	400
Color		pink	pink	brown	green	golden brown
N		1111	1121	1136	1119	1139
#I $\|F_0\| > 5\sigma$		1079	1117	1134	1118	1132
***R* (%)**		2.04	2.08	1.66	1.60	2.00
w*R* (%)		2.30	2.71	2.45	2.14	2.63
GOF		1.772	3.389	4.129	3.807	3.847

		CT36	CT37	CT38	CT39	CT40
Cell Parameters	*a* (Å)	15.914(3)	15.945(2)	15.896(2)	15.906(3)	15.936(1)
	c	7.185(3)	7.203(1)	7.168(2)	7.182(2)	7.207(1)
	V (Å^3)	1575.7	1585.9	1568.4	1573.7	1585.1
Crystal Dimensions	'X'(μ)	320	380		400	130
	'Y'	300	360		380	130
	'Z'	280	360		400	130
Color		golden brown	brown	golden brown	green	green
N		1135	1143	1129	1134	1141
#I $\|F_0\| > 5\sigma$		1128	1133	1125	1133	1118
***R* (%)**		1.70	1.70	1.93	2.03	1.74
w*R* (%)		2.41	2.37	2.68	2.84	1.98
GOF		3.087	3.076	3.478	6.263	1.873

		CT41	CT42	CT43	CT44	CT45
Cell Parameters	*a* (Å)	15.934(3)	15.916(3)	15.914(1)	15.966(1)	15.939(1)
	c	7.203(2)	7.204(2)	7.193(1)	7.199(1)	7.185(1)
	V (Å^3)	1583.9	1580.3	1577.6	1589.1	1580.7
Crystal Dimensions	'X'(μ)	240	260	180	200	450
	'Y'	240	260	200	200	460
	'Z'	280	260	220	230	480
Color		green	green	green	brown	golden brown
N		1171	1141	1137	1145	1131
#I $\|F_0\| > 5\sigma$		1120	1127	1133	1136	1129
***R* (%)**		3.47	2.31	1.59	1.52	1.91
w*R* (%)		4.18	2.70	1.97	1.97	2.63
GOF		3.555	2.344	2.119	2.404	4.314

		CT46	CT47	CT48	CT49	CT50
Cell Parameters	*a* (Å)	15.922	15.949(1)	15.961(1)	15.978(2)	15.955(3)
	c	7.165	7.158(1)	7.162(1)	7.166(1)	7.153(2)
	V (Å^3)	1573.0	1576.8	1580.1	1584.4	1576.9
Crystal Dimensions	'X'(μ)	360	200	200	200	230
	'Y'	380	200	200	200	230
	'Z'	390	200	200	200	230
Color		colorless	green	green		brown
N		1132	1139	1141	1141	1139
#I $\|F_0\| > 5\sigma$		1124	1132	1129	1136	1137
***R* (%)**		2.17	1.74	2.37	1.52	1.61
w*R* (%)		2.66	2.22	2.83	1.91	2.21
GOF		3.595	2.538	3.104	2.142	2.694

		CT51	CT52	CT53	CT54	CT55
Cell Parameters	*a* (Å)	15.972(2)	15.998(3)	16.002(3)	16.015(2)	15.916(2)
	c	7.164(1)	7.173(3)	7.184(2)	7.180(1)	7.127(2)
	V (Å^3)	1582.7	1589.8	1593.1	1594.8	1563.6
Crystal Dimensions	'X'(μ)	180	160	370	240	400
	'Y'	180	140	340	330	370
	'Z'	200	140	320	270	350
Color		black	brown	brown	blue	dark brown
N		1141	1143	1143	1148	1121
#I $\|F_0\| > 5\sigma$		1127	1130	1139	1141	1119
***R* (%)**		1.65	1.70	1.66	2.20	1.85
w*R* (%)		1.98	1.98	2.05	2.92	2.34
GOF		1.915	2.021	2.692	3.611	3.172

		CT56	CT57	CT58	CT59	CT60
Cell Parameters	*a* (Å)	15.972(1)	15.979(4)	15.982(1)	15.907(3)	15.907(3)
	c	7.156(1)	7.160(2)	7.147(1)	7.133(1)	7.119(2)
	V (Å^3)	1580.9	1583.2	1580.8	1563.1	1559.9
Crystal Dimensions	'X'(μ)	350	200	180	360	400
	'Y'	340	200	180	280	440
	'Z'	300	200	200	310	460
Color		black		black	dark green	blue-green
N		1137	1139	1139	1125	1120
#I $\|F_0\| > 5\sigma$		1135	1135	1129	1119	1118
***R* (%)**		2.03	1.56	3.60	2.17	2.00
w*R* (%)		2.54	2.04	4.44	2.65	2.60
GOF		3.546	2.343	4.428	3.430	4.187

		CT61	CT62	CT63	CT64	CT65
Cell	*a* (Å)	15.901(1)	15.932(2)	15.932(1)	15.941(3)	15.959(3)
Parameters	*c*	7.118(2)	7.132(1)	7.134(1)	7.189(3)	7.198(3)
	V (Å^3)	1558.6	1567.9	1568.1	1582.1	1587.6
Crystal	'X'(μ)	400	240	130	355	320
Dimensions	'Y'	380	160	130	370	320
	'Z'	380	100	130	380	290
Color		blue-purple	black	black	bronze	brown-bronze
N		1121	1129	1129	1139	1147
#I $\|F_0\| > 5\sigma$		1119	1116	1091	1130	1134
***R* (%)**		1.89	2.00	2.08	1.77	1.59
w*R* (%)		2.46	2.44	2.20	2.28	2.05
GOF		3.716	2.355	1.736	3.323	2.650

		CT66	CT67	CT68	CT69	CT70
Cell	*a* (Å)	15.927(4)	15.960(1)	15.960(1)	15.939(2)	15.946(1)
Parameters	*c*	7.202(1)	7.205(1)	7.201(1)	7.196(2)	7.197(1)
	V (Å^3)	1582.3	1589.4	1588.5	1583.0	1584.8
Crystal	'X'(μ)	360	100	180	360	320
Dimensions	'Y'	380	100	200	350	320
	'Z'	380	220	200	370	340
Color		dark brown	green	orange	brown	pale brown
N		1140	1147	1147	1136	1139
#I $\|F_0\| > 5\sigma$		1130	1121	1131	1124	1126
***R* (%)**		1.83	1.60	1.55	1.93	1.83
w*R* (%)		2.46	1.89	1.94	2.55	2.40
GOF		3.568	1.765	2.084	3.694	3.156

		CT71	CT72	CT73	CT74	CT75
Cell Parameters	*a* (Å)	15.940(1)	15.943(1)	15.980(2)	15.958(2)	15.943(3)
	c	7.197(1)	7.192(1)	7.177(1)	7.200(1)	7.195(2)
	V (Å^3)	1583.6	1583.0	1587.2	1587.9	1583.8
Crystal Dimensions	'X'(μ)	180	180	200	120	340
	'Y'	180	180	200	120	320
	'Z'	180	180	200	120	300
Color		green	dark brown	green	colorless	green
N		1141	1141	1141	1147	1139
#I $\|F_0\| > 5\sigma$		1120	1131	1118	1086	1126
***R* (%)**		1.70	1.60	3.29	2.00	1.69
w*R* (%)		2.05	1.99	4.11	2.26	2.20
GOF		1.849	1.997	4.231	1.764	2.929

		CT76	CT77	CT78	CT79	CT80
Cell Parameters	*a* (Å)	15.958(1)	15.985(1)	15.937(1)	15.954(1)	15.969(2)
	c	7.210(1)	7.223(1)	7.208(1)	7.214(1)	7.205(1)
	V (Å^3)	1590.0	1598.4	1585.6	1590.0	1591.18
Crystal Dimensions	'X'(μ)	360	180	320	100	200
	'Y'	360	180	320	200	200
	'Z'	370	200	340	200	200
Color		black-green	dark brown	green	orange	
N		1146	1151	1141	1147	1579
#I $\|F_0\| > 5\sigma$		1139	1140	1136	1127	1127
***R* (%)**		1.77	1.80	1.70	1.77	1.92
w*R* (%)		2.29	2.50	2.35	2.13	2.01
GOF		3.341	2.481	2.649	1.969	2.406

		CT81	CT82	CT83	CT84	CT85
Cell Parameters	*a* (Å)	15.841(3)	15.821(4)	15.854(2)	15.835(1)	15.967(2)
	c	7.091(3)	7.105(2)	7.109(1)	7.106(1)	7.126(2)
	V (Å^3)	1541.1	1540.2	1547.5	1543.1	1573.4
Crystal Dimensions	'X'(μ)	320	320	360	130	400
	'Y'	320	300	370	130	380
	'Z'	330	280	380	130	380
Color		olive green	green-bronze	light pink	colorless	purple-pink
N		1109	1112	1109	1111	1128
#I $\|F_0\| > 5\sigma$		1102	1102	1105	1072	1124
***R* (%)**		1.78	1.94	1.94	2.29	1.75
w*R* (%)		2.26	2.40	2.40	2.50	2.36
GOF		3.057	3.155	3.155	1.918	3.489

		CT86	CT87	CT88	CT89	CT90
Cell Parameters	*a* (Å)	15.965(3)	15.967(4)	15.882(2)	15.862(1)	16.033(1)
	c	7.128(2)	7.133(2)	7.114(1)	7.188(1)	7.312(1)
	V (Å^3)	1573.4	1574.9	1554.1	1566.3	1627.8
Crystal Dimensions	'X'(μ)	160	210	60	200	40
	'Y'	190	210	80	200	40
	'Z'	210	210	180	200	100
Color		blue-black	blue-black	blue-black	black	dark green
N		1133	1135	1117	1131	1177
#I $\|F_0\| > 5\sigma$		1121	1124	1088	1122	978
***R* (%)**		2.66	2.81	2.00	1.77	3.31
w*R* (%)		3.23	3.56	2.25	2.19	2.28
GOF		3.224	3.565	1.857	2.250	1.456

		CT91	CT92	CT93	CT94	CT95
Cell Parameters	*a* (Å)	15.973(1)	16.035(1)	15.991(1)	16.036(1)	16.040(2)
	c	7.267(1)	7.313(1)	7.276(1)	7.319(1)	7.316(1)
	V (Å^3)	1605.7	1628.4	1611.3	1630.0	1630.09
Crystal Dimensions	'X'(μ)	80	25	50	70	60
	'Y'	80	35	60	70	65
	'Z'	180	70	150	80	110
Color		dark green	dark green	dark green	dark green	dark green
N		1159	1177	1158	1177	5115
#I $\|F_0\| > 5\sigma$		1126	851	1097	1101	1091
***R* (%)**		2.24	3.27	2.35	2.31	1.97
w*R* (%)		2.25	2.22	2.17	1.72	1.79
GOF		1.680	1.030	1.429	1.615	1.552

		CT96	CT97	CT98	CT99
Cell Parameters	*a* (Å)	16.129(2)	16.151(4)	16.149(1)	16.243(2)
	c	7.411(3)	7.413(2)	7.420(1)	7.493(1)
	V (Å^3)	1669.64	1674.5	1675.8	1712.1
Crystal Dimensions	'X'(μ)	60	70	60	
	'Y'	70	70	60	
	'Z'	120	75	120	
Color		dark green	dark green	dark green	black
N		1201	1202	1203	6349
#I $\|F_0\| > 5\sigma$		1096	1101	1140	1208
***R* (%)**		3.18	4.18	5.06	2.09
w*R* (%)		2.35	3.45	4.26	2.39
GOF		1.539	2.718	2.859	1.415

APPENDIX C

Atomic Parameters

This appendix lists the refined positional and equivalent displacement factors (Ueq) for each sample. Standard deviations are also listed. Note that the symmetry operators defined at the beginning of Appendix E apply here.

The first part of this appendix (Section C.1) lists the atomic parameters for the *X, Y, Z, B, T,* and O(1) – O(8) sites. The second section of this appendix (Section C.2) lists the atomic parameters for those samples where H was located in coordination with O(3) and assigned. Section C.3 lists the atomic parameters for the on sample where the H coordinating O(1) was located and assigned.

H positions were refined isotropically with a fixed distance from their coordinating O. Generally, the Ueq value was allowed to refine for H, though for some samples this value was fixed.

Section C.1

		CT1		CT2		CT3		CT4		CT5	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0196	(10)	0.0225	(8)	0.0224	(13)	0.0175	(10)	0.0224	(9)
Y	x	0.06106	(4)	0.06161	(4)	0.06119	(5)	0.06149	(5)	0.06159	(5)
	y	0.93894	(4)	0.93839	(4)	0.93881	(5)	0.93851	(5)	0.93841	(5)
	z	0.43684	(50)	0.44380	(42)	0.43916	(63)	0.43920	(54)	0.44185	(48)
	Ueq	0.0072	(4)	0.0085	(3)	0.0075	(4)	0.0067	(4)	0.0071	(4)
Z	x	0.25984	(4)	0.26032	(4)	0.25995	(5)	0.26000	(4)	0.25991	(4)
	y	0.29653	(4)	0.29708	(4)	0.29667	(4)	0.29667	(4)	0.29668	(4)
	z	0.46462	(46)	0.46498	(39)	0.46425	(59)	0.46484	(49)	0.46685	(42)
	Ueq	0.0064	(2)	0.0065	(2)	0.0066	(2)	0.0063	(2)	0.0062	(2)
T	x	0.18970	(4)	0.18990	(3)	0.18978	(4)	0.18983	(4)	0.18987	(3)
	y	0.19171	(3)	0.19192	(3)	0.19183	(4)	0.19191	(4)	0.19190	(3)
	z	0.07283	(46)	0.07523	(39)	0.07318	(60)	0.07400	(49)	0.07657	(42)
	Ueq	0.0057	(2)	0.0055	(2)	0.0056	(2)	0.0054	(2)	0.0053	(2)
B	x	0.89095	(11)	0.89071	(11)	0.89090	(12)	0.89104	(12)	0.89098	(11)
	y	0.10905	(11)	0.10929	(11)	0.10910	(12)	0.10896	(12)	0.10902	(11)
	z	0.61998	(59)	0.62094	(53)	0.61989	(73)	0.62057	(64)	0.62237	(58)
	Ueq	0.0063	(8)	0.0067	(8)	0.0074	(9)	0.0069	(9)	0.0070	(8)
O1	x	0		0	(0)	0		0		0	
	y	0		0	(0)	0		0		0	
	z	0.29609	(64)	0.29402	(64)	0.29558	(77)	0.29511	(71)	0.29528	(66)
	Ueq	0.0285	(12)	0.0418	(15)	0.0322	(14)	0.0337	(14)	0.0386	(14)
O2	x	0.93967	(7)	0.93931	(7)	0.93950	(8)	0.93971	(8)	0.93979	(7)
	y	0.06033	(7)	0.06069	(7)	0.06050	(8)	0.06029	(8)	0.06021	(7)
	z	0.58368	(55)	0.58851	(48)	0.58474	(69)	0.58580	(60)	0.58845	(52)
	Ueq	0.0133	(7)	0.0161	(8)	0.0148	(8)	0.0150	(8)	0.0149	(73)
O3	x	0.13142	(9)	0.13323	(8)	0.13181	(9)	0.13218	(9)	0.13271	(9)
	y	0.86858	(9)	0.86677	(8)	0.86819	(9)	0.86782	(9)	0.86729	(9)
	z	0.56541	(52)	0.56694	(47)	0.56619	(65)	0.56751	(56)	0.56849	(49)
	Ueq	0.0127	(6)	0.0118	(6)	0.0130	(7)	0.0126	(6)	0.0123	(6)
O4	x	0.90595	(8)	0.90656	(7)	0.90610	(8)	0.90631	(8)	0.90638	(7)
	y	0.09405	(8)	0.09344	(7)	0.09390	(8)	0.09369	(8)	0.09362	(7)
	z	-0.00055	(52)	0.00324	(45)	-0.00006	(65)	0.00112	(55)	0.00349	(47)
	Ueq	0.0095	(6)	0.0094	(6)	0.0091	(6)	0.0096	(6)	0.0091	(6)
O5	x	0.09362	(8)	0.09353	(7)	0.09378	(8)	0.09360	(8)	0.09358	(8)
	y	0.90638	(8)	0.90647	(7)	0.90622	(8)	0.90640	(8)	0.90642	(8)
	z	-0.02268	(530	-0.01985	(46)	-0.02201	(66)	-0.02143	(56)	-0.01879	(50)
	Ueq	0.0101	(6)	0.0092	(5)	0.0097	(6)	0.0097	(6)	0.0092	(6)
O6	x	0.18411	(9)	0.18567	(9)	0.18468	(10)	0.18455	(10)	0.18492	(9)
	y	0.19458	(9)	0.19604	(9)	0.19517	(10)	0.19512	(10)	0.19528	(9)
	z	0.29924	(49)	0.30057	(44)	0.29926	(63)	0.30014	(54)	0.30212	(48)
	Ueq	0.0079	(5)	0.0081	(5)	0.0080	(5)	0.0078	(5)	0.0082	(5)
O7	x	0.28606	(8)	0.28606	(9)	0.28623	(9)	0.28624	(9)	0.28608	(9)
	y	0.28660	(9)	0.28610	(9)	0.28658	(10)	0.28658	(10)	0.28625	(9)
	z	-0.00389	(49)	-0.00358	(42)	-0.00451	(62)	-0.00373	(52)	-0.00198	(45)
	Ueq	0.0070	(5)	0.0073	(5)	0.00708	(5)	0.0072	(5)	0.0068	(5)
O8	x	0.27011	(10)	0.27038	(10)	0.27029	(11)	0.27003	(11)	0.27003	(10)
	y	0.20956	(10)	0.20964	(10)	0.20968	(11)	0.20954	(11)	0.20958	(10)
	z	0.63528	(49)	0.63570	(43)	0.63497	(63)	0.63569	(5)	0.63718	(46)
	Ueq	0.0077	(5)	0.0085	(5)	0.0082	(5)	0.0080	(5)	0.0082	(5)

		CT6		CT7		CT8		CT9		CT10	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0203	(8)	0.0178	(10)	0.0228	(11)	0.0241	(15)	0.0197	(11)
Y	x	0.06150	(4)	0.06148	(5)	0.06069	(4)	0.06090	(5)	0.06174	(5)
	y	0.93850	(4)	0.93852	(5)	0.93931	(4)	0.93910	(5)	0.93826	(5)
	z	0.44135	(43)	0.43925	(50)	0.43511	(55)	0.43731	(70)	0.44133	(55)
	Ueq	0.0076	(3)	0.0070	(4)	0.0077	(3)	0.0085	(4)	0.0064	(5)
Z	x	0.26016	(4)	0.25992	(4)	0.25968	(4)	0.25974	(5)	0.25989	(5)
	y	0.29681	(4)	0.29671	(4)	0.29652	(4)	0.29648	(4)	0.29677	(4)
	z	0.46498	(39)	0.46384	(45)	0.46300	(51)	0.46444	(65)	0.46422	(49)
	Ueq	0.0064	(2)	0.0062	(2)	0.0066	(2)	0.0064	(2)	0.0058	(2)
T	x	0.18983	(3)	0.18989	(4)	0.18969	(3)	0.18974	(4)	0.18991	(4)
	y	0.19191	(3)	0.19191	(3)	0.19165	(3)	0.19176	(4)	0.19196	(4)
	z	0.07432	(39)	0.07368	(45)	0.07103	(52)	0.07296	(66)	0.07462	(49)
	Ueq	0.0055	(2)	0.0051	(2)	0.0056	(2)	0.0055	(2)	0.0047	(2)
B	x	0.89089	(10)	0.89102	(11)	0.89090	(10)	0.89094	(12)	0.89098	(12)
	y	0.10911	(10)	0.10898	(11)	0.10910	(10)	0.10906	(12)	0.10902	(12)
	z	0.62092	(53)	0.61981	(59)	0.61775	(62)	0.61890	(77)	0.61998	(7)
	Ueq	0.0069	(8)	0.0068	(8)	0.0068	(8)	0.0066	(9)	0.0063	(9)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29574	(61)	0.29156	(66)	0.29531	(68)	0.29574	(84)	0.29118	(75)
	Ueq	0.0369	(13)	0.0388	(14)	0.0272	(11)	0.0278	(14)	0.0399	(17)
O2	x	0.93962	(7)	0.93971	(7)	0.93958	(7)	0.93968	(8)	0.93967	(8)
	y	0.06038	(7)	0.06029	(7)	0.06042	(7)	0.06032	(8)	0.06033	(8)
	z	0.58695	(48)	0.58652	(55)	0.58114	(58)	0.58185	(73)	0.58695	(60)
	Ueq	0.0156	(7)	0.0156	(7)	0.0134	(6)	0.0138	(8)	0.0153	(8)
O3	x	0.13246	(8)	0.13286	(9)	0.13126	(8)	0.13161	(10)	0.13312	(9)
	y	0.86754	(8)	0.86714	(9)	0.86874	(8)	0.86839	(10)	0.86688	(9)
	z	0.56735	(46)	0.56624	(51)	0.56335	(57)	0.56539	(71)	0.56640	(56)
	Ueq	0.0129	(5)	0.0126	(6)	0.0125	(6)	0.0126	(7)	0.0117	(7)
O4	x	0.90631	(7)	0.90647	(7)	0.90577	(7)	0.90585	(8)	0.90665	(8)
	y	0.09369	(7)	0.09353	(7)	0.09423	(7)	0.09415	(8)	0.09335	(8)
	z	0.00203	(44)	0.00139	(50)	-0.00214	(56)	-0.00002	(70)	0.00218	(55)
	Ueq	0.0094	(5)	0.0088	(6)	0.0093	(5)	0.0091	(6)	0.0085	(6)
O5	x	0.09367	(7)	0.09359	(7)	0.09369	(7)	0.09382	(8)	0.09366	(8)
	y	0.90633	(7)	0.90641	(7)	0.90631	(7)	0.90618	(8)	0.90634	(8)
	z	-0.02098	(47)	-0.02106	(52)	-0.02381	(57)	-0.02240	(71)	-0.02022	(57)
	Ueq	0.0102	(5)	0.0090	(6)	0.0097	(5)	0.0094	(6)	0.0085	(6)
O6	x	0.18490	(9)	0.18519	(9)	0.18417	(9)	0.18424	(11)	0.18539	(10)
	y	0.19549	(9)	0.19553	(9)	0.19447	(9)	0.19497	(11)	0.19564	(10)
	z	0.30044	(44)	0.29929	(50)	0.29700	(55)	0.29870	(70)	0.29983	(54)
	Ueq	0.0082	(4)	0.0082	(5)	0.0081	(4)	0.0084	(5)	0.0075	(5)
O7	x	0.28631	(8)	0.28598	(9)	0.28607	(8)	0.28625	(10)	0.28611	(9)
	y	0.28649	(9)	0.28625	(9)	0.28649	(9)	0.28644	(10)	0.28622	(10)
	z	-0.00346	(42)	-0.00468	(48)	-0.00554	(54)	-0.00416	(68)	-0.00424	(52)
	Ueq	0.0073	(4)	0.0070	(5)	0.0071	(4)	0.0072	(5)	0.0063	(5)
O8	x	0.27014	(9)	0.27003	(10)	0.27026	(9)	0.27014	(11)	0.27001	(11)
	y	0.20946	(9)	0.20952	(10)	0.20962	(9)	0.20948	(11)	0.20951	(11)
	z	0.63576	(43)	0.63482	(49)	0.63345	(54)	0.63468	(69)	0.63505	(53)
	Ueq	0.0082	(4)	0.0081	(5)	0.0081	(4)	0.0080	(5)	0.0077	(5)

		CT11		CT12		CT13		CT14		CT15	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0255	(11)	0.0256	(12)	0.0196	(8)	0.0239	(14)	0.0248	(13)
Y	x	0.06154	(4)	0.06101	(4)	0.06177	(5)	0.06155	(5)	0.06075	(4)
	y	0.93846	(4)	0.93899	(4)	0.93823	(5)	0.93845	(5)	0.93925	(4)
	z	0.43952	(54)	0.43867	(55)	0.44520	(45)	0.44103	(68)	0.43621	(60)
	Ueq	0.0093	(4)	0.0084	(3)	0.0085	(4)	0.0083	(5)	0.0089	(3)
Z	x	0.26005	(5)	0.25995	(4)	0.26022	(5)	0.26003	(5)	0.25960	(4)
	y	0.29683	(4)	0.29669	(4)	0.29710	(5)	0.29670	(5)	0.29644	(4)
	z	0.46437	(50)	0.46462	(52)	0.46491	(40)	0.46499	(62)	0.46433	(57)
	Ueq	0.0077	(2)	0.0068	(2)	0.0061	(2)	0.0074	(2)	0.0074	(2)
T	x	0.18983	(4)	0.18973	(3)	0.18995	(4)	0.18981	(4)	0.18973	(3)
	y	0.19191	(4)	0.19176	(3)	0.19193	(4)	0.19190	(4)	0.19173	(3)
	z	0.07355	(50)	0.07320	(52)	0.07579	(39)	0.07455	(63)	0.07181	(58)
	Ueq	0.0069	(2)	0.0057	(2)	0.0050	(2)	0.0065	(2)	0.0063	(2)
B	x	0.89072	(12)	0.89071	(11)	0.89061	(13)	0.89096	(13)	0.89098	(10)
	y	0.10928	(12)	0.10929	(11)	0.10939	(13)	0.10904	(13)	0.10902	(10)
	z	0.61915	(65)	0.61969	(63)	0.62141	(60)	0.62066	(78)	0.61903	(67)
	Ueq	0.0087	(9)	0.0075	(8)	0.0074	(9)	0.0083	(10)	0.0074	(7)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29445	(75)	0.29661	(710	0.29300	(75)	0.29486	(83)	0.29847	(69)
	Ueq	0.0378	(16)	0.0308	(13)	0.0455	(19)	0.0359	(16)	0.0206	(9)
O2	x	0.93961	(8)	0.93944	(7)	0.93949	(9)	0.93962	(9)	0.93949	(7)
	y	0.06039	(8)	0.06056	(7)	0.06051	(9)	0.06038	(9)	0.06051	(7)
	z	0.58391	(60)	0.58260	(59)	0.59083	(54)	0.58589	(74)	0.58090	(64)
	Ueq	0.0159	(8)	0.0138	(7)	0.0170	(9)	0.0162	(9)	0.0136	(6)
O3	x	0.13228	(10)	0.13175	(9)	0.13356	(10)	0.13246	(10)	0.13055	(8)
	y	0.86772	(10)	0.86825	(9)	0.86644	(10)	0.86754	(10)	0.86945	(8)
	z	0.56640	(57)	0.56605	(58)	0.56715	(50)	0.56755	(69)	0.56476	(62)
	Ueq	0.0140	(7)	0.0125	(6)	0.0113	(7)	0.0137	(7)	0.0133	(5)
O4	x	0.90616	(8)	0.90587	(7)	0.90665	(9)	0.90627	(9)	0.90555	(7)
	y	0.09384	(8)	0.09413	(7)	0.09335	(9)	0.09373	(9)	0.09445	(7)
	z	0.00082	(56)	0.00068	(56)	0.00355	(47)	0.00175	(68)	-0.00195	(62)
	Ueq	0.0110	(6)	0.0093	(6)	0.0090	(6)	0.0099	((7)	0.0101	(5)
O5	x	0.09365	(8)	0.09377	(7)	0.09328	(9)	0.09384	(9)	0.09387	(7)
	y	0.90635	(8)	0.90623	(7)	0.90672	(9)	0.90616	(9)	0.90613	(7)
	z	-0.02239	(58)	-0.02285	(58)	-0.01904	(50)	-0.02069	(69)	-0.02367	(61)
	Ueq	0.0115	(6)	0.0099	(6)	0.0087	(6)	0.0106	(7)	0.0106	(5)
O6	x	0.18460	(10)	0.18444	(9)	0.18607	(11)	0.18485	(11)	0.18372	(8)
	y	0.19546	(10)	0.19517	(9)	0.19621	(11)	0.19537	(11)	0.19430	(8)
	z	0.29937	(55)	0.29943	(56)	0.30064	(46)	0.30036	(67)	0.29856	(60)
	Ueq	0.0097	(5)	0.0085	(5)	0.0082	(6)	0.0092	(5)	0.0088	(4)
O7	x	0.28625	(10)	0.28644	(9)	0.28576	(10)	0.28619	(10)	0.28637	(8)
	y	0.28641	(10)	0.28650	(9)	0.28583	(11)	0.28641	(11)	0.28692	(8)
	z	-0.00412	(53)	-0.00381	(55)	-0.00391	(44)	-0.00371	(66)	-0.00439	(60)
	Ueq	0.0085	(5)	0.0079	(5)	0.0068	(5)	0.0081	(5)	0.0081	(4)
O8	x	0.26995	(11)	0.27028	(10)	0.27039	(12)	0.26998	(12)	0.27029	(9)
	y	0.20945	(11)	0.20944	(10)	0.20972	(12)	0.20954	(12)	0.20957	(9)
	z	0.63492	(54)	0.63518	(55)	0.63532	(45)	0.63581	(66)	0.63500	(60)
	Ueq	0.0095	(5)	0.0082	(5)	0.0082	(6)	0.0094	(6)	0.0089	(4)

		CT16		CT17		CT18		CT19		CT20	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0227	(8)	0.0239	(8)	0.0219	(8)	0.0241	(9)	0.0233	(10)
Y	x	0.06193	(3)	0.06185	(3)	0.06191	(3)	0.06195	(4)	0.06206	(3)
	y	0.93807	(3)	0.93815	(3)	0.93809	(3)	0.93805	(4)	0.93794	(3)
	z	0.44891	(39)	0.44690	(41)	0.44870	(38)	0.44885	(44)	0.44975	(48)
	Ueq	0.0086	(3)	0.0087	(3)	0.0084	(3)	0.0092	(3)	0.0090	(3)
Z	x	0.26071	(5)	0.26070	(4)	0.26066	(4)	0.26069	(5)	0.26079	(5)
	y	0.29756	(4)	0.29742	(4)	0.29747	(4)	0.29753	(5)	0.29767	(5)
	z	0.46563	(37)	0.46508	(38)	0.46592	(35)	0.46561	(42)	0.46617	(46)
	Ueq	0.0068	(2)	0.0072	(2)	0.0066	(2)	0.0080	(2)	0.0069	(2)
T	x	0.19000	(4)	0.18995	(4)	0.18998	(4)	0.19000	(4)	0.18997	(4)
	y	0.19198	(4)	0.19194	(3)	0.19193	(3)	0.19196	(4)	0.19194	(4)
	z	0.07743	(36)	0.07606	(38)	0.07728	(35)	0.07730	(41)	0.07775	(45)
	Ueq	0.0055	(2)	0.0060	(2)	0.0052	(2)	0.0067	(2)	0.0056	(2)
B	x	0.89048	(12)	0.89064	(11)	0.89055	(11)	0.89051	(14)	0.89053	(14)
	y	0.10952	(12)	0.10936	(11)	0.10945	(11)	0.10949	(14)	0.10947	(14)
	z	0.62243	(54)	0.62201	(54)	0.62265	(52)	0.62239	(64)	0.62258	(66)
	Ueq	0.0069	(9)	0.0077	(8)	0.0068	(8)	0.0094	(10)	0.0077	(10)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29271	(7)	0.29367	(64)	0.29321	(65)	0.29271	(79)	0.29411	(82)
	Ueq	0.0599	(22)	0.0512	(18)	0.0543	(20)	0.0582	(25)	0.0634	(26)
O2	x	0.93900	(8)	0.93913	(8)	0.93915	(8)	0.93907	(10)	0.93904	(10)
	y	0.06100	(8)	0.06087	(8)	0.06085	(8)	0.06093	(10)	0.06096	(10)
	z	0.59338	(48)	0.56135	(48)	0.59332	(46)	0.59356	(55)	0.59291	(58)
	Ueq	0.0175	(9)	0.0177	(8)	0.0178	(8)	0.0193	(10)	0.0180	(10)
O3	x	0.13460	(8)	0.13388	(8)	0.13422	(8)	0.13444	(10)	0.13435	(10)
	y	0.86540	(8)	0.86612	(8)	0.86578	(8)	0.86556	(10)	0.86565	(10)
	z	0.56786	(45)	0.56747	(46)	0.56799	(44)	0.56764	(52)	0.56781	(56)
	Ueq	0.0106	(6)	0.0119	(6)	0.0109	(6)	0.0111	(7)	0.0100	(7)
O4	x	0.90696	(8)	0.90668	(8)	0.90693	(7)	0.90688	(9)	0.90681	(9)
	y	0.09304	(8)	0.09332	(8)	0.09307	(7)	0.09312	(9)	0.09319	(9)
	z	0.00663	(45)	0.00462	(46)	0.00607	(43)	0.00598	(51)	0.00662	(54)
	Ueq	0.0087	(6)	0.0099	(6)	0.0086	(6)	0.0101	(7)	0.0091	(7)
O5	x	0.09327	(8)	0.09338	(8)	0.09327	(8)	0.09321	(9)	0.09343	(9)
	y	0.90673	(8)	0.90662	(8)	0.90673	(8)	0.90679	(9)	0.90657	(9)
	z	-0.01576	(45)	-0.01791	(46)	-0.01632	(43)	-0.01649	(52)	-0.01515	(54)
	Ueq	0.0091	(6)	0.0100	(6)	0.0090	(6)	0.0104	(7)	0.0094	(7)
O6	x	0.18713	(10)	0.18652	(10)	0.18683	(10)	0.18707	(12)	0.18699	(12)
	y	0.19719	(10)	0.19683	(10)	0.19699	(10)	0.19722	(12)	0.19719	(12)
	z	0.30230	(42)	0.30120	(43)	0.30194	(40)	0.30155	(48)	0.30245	(52)
	Ueq	0.0087	(5)	0.0091	(5)	0.0085	(5)	0.0093	(6)	0.0088	(6)
O7	x	0.28572	(9)	0.28600	(9)	0.28583	(9)	0.28585	(11)	0.28584	(11)
	y	0.28552	(10)	0.28594	(9)	0.28574	(9)	0.28565	(12)	0.28552	(12)
	z	-0.00274	(41)	-0.00337	(42)	-0.00267	(39)	-0.00324	(46)	-0.00253	(50)
	Ueq	0.0076	(5)	0.0078	(5)	0.0072	(5)	0.0085	(6)	0.0073	(6)
O8	x	0.27057	(11)	0.27037	(10)	0.27048	(10)	0.27059	(13)	0.27068	(13)
	y	0.20988	(11)	0.20980	(10)	0.20987	(10)	0.20993	(12)	0.21000	(12)
	z	0.63620	(41)	0.63578	(43)	0.63642	(40)	0.63575	(47)	0.63642	(50)
	Ueq	0.0086	(5)	0.0093	(5)	0.0084	(5)	0.0010	(6)	0.0084	(6)

		CT21		CT22		CT23		CT24		CT25	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0241	(9)	0.0261	(12)	0.0232	(9)	0.0227	(9)	0.0259	(10)
Y	x	0.06203	(4)	0.06222	(4)	0.06220	(3)	0.06181	(3)	0.06166	(4)
	y	0.93797	(4)	0.93778	(4)	0.93780	(3)	0.93819	(3)	0.93834	(4)
	z	0.44980	(42)	0.44915	(55)	0.44928	(40)	0.44634	(45)	0.44494	(49)
	Ueq	0.0085	(3)	0.0085	(3)	0.0074	(3)	0.0085	(31)	0.0087	(4)
Z	x	0.26067	(5)	0.26092	(6)	0.26096	(5)	0.26062	(5)	0.26029	(4)
	y	0.29758	(5)	0.29784	(6)	0.29771	(5)	0.29745	(5)	0.29704	(4)
	z	0.46607	(40)	0.46516	(53)	0.46539	(38)	0.46471	(42)	0.46495	(45)
	Ueq	0.0072	(2)	0.0070	(3)	0.0064	(2)	0.0067	(2)	0.0065	(2)
T	x	0.19001	(4)	0.19002	(5)	0.18997	(4)	0.19004	(4)	0.18991	(4)
	y	0.19195	(4)	0.19199	(5)	0.19195	(4)	0.19198	(4)	0.19194	(4)
	z	0.07783	(39)	0.07665	(53)	0.07691	(37)	0.07586	(42)	0.07541	(45)
	Ueq	0.0059	2)	0.0058	(2)	0.0051	(2)	0.0055	(2)	0.0054	(2)
B	x	0.89033	(13)	0.89024	(16)	0.89053	(14)	0.89049	(12)	0.89084	(12)
	y	0.10967	(13)	0.10976	(16)	0.10947	(14)	0.10951	(12)	0.10916	(12)
	z	0.62247	(60)	0.62100	(77)	0.62235	(56)	0.62136	(59)	0.62149	(59)
	Ueq	0.0075	(10)	0.0078	(12)	0.0070	(10)	0.0072	(9)	0.0070	(8)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29287	(78)	0.29243	(98)	0.29250	(66)	0.29187	(72)	0.29400	(70)
	Ueq	0.0601	(25)	0.0595	(29)	0.0566	(24)	0.0514	(21)	0.0460	(17)
O2	x	0.93903	(9)	0.93868	(10)	0.93883	(9)	0.93910	(8)	0.93947	(8)
	y	0.06097	(9)	0.06132	(10)	0.06117	(9)	0.06090	(8)	0.06053	(8)
	z	0.59372	(53)	0.59179	(67)	0.59224	(51)	0.59097	(53)	0.58958	(56)
	Ueq	0.0192	(10)	0.0171	(11)	0.0183	(10)	0.0173	(9)	0.0172	(8)
O3	x	0.13441	(9)	0.13442	(11)	0.13439	(9)	0.13393	(9)	0.13337	(9)
	y	0.86559	(9)	0.86558	(11)	0.86561	(9)	0.86607	(9)	0.86663	(9)
	z	0.56829	(50)	0.56650	(64)	0.56757	(48)	0.56710	(51)	0.56722	(53)
	Ueq	0.0100	(7)	0.0100	(8)	0.0094	(7)	0.0111	(6)	0.0126	(6)
O4	x	0.90689	(9)	0.90687	(10)	0.90690	(9)	0.90667	(8)	0.90652	(8)
	y	0.09311	(9)	0.09313	(10)	0.09310	(9)	0.09333	(8)	0.09348	(8)
	z	0.00662	(48)	0.00579	(63)	0.00563	(46)	0.00431	(49)	0.00375	(50)
	Ueq	0.0091	(7)	0.0093	(8)	0.0083	(7)	0.0094	(6)	0.0088	(6)
O5	x	0.09327	(9)	0.09340	(10)	0.09329	(9)	0.09331	(8)	0.09365	(8)
	y	0.90673	(9)	0.90660	(10)	0.90671	(9)	0.90669	(8)	0.90635	(8)
	z	-0.01571	(49)	-0.01705	(63)	-0.01714	(45)	-0.01802	(50)	-0.01900	(53)
	Ueq	0.0095	(6)	0.0094	(8)	0.0087	(7)	0.0093	(6)	0.0096	(6)
O6	x	0.18715	(11)	0.18732	(13)	0.18730	(11)	0.18663	(10)	0.18588	(10)
	y	0.19726	(11)	0.19756	(13)	0.19745	(11)	0.19687	(10)	0.19620	(10)
	z	0.30234	(46)	0.30114	(60)	0.30152	(43)	0.30073	(47)	0.30098	(5)
	Ueq	0.0089	(6)	0.0089	(7)	0.0072	(5)	0.0083	(5)	0.0087	(5)
O7	x	0.28576	(10)	0.28588	(12)	0.28589	(11)	0.28589	(10)	0.28595	(9)
	y	0.28544	(11)	0.28554	(13)	0.28551	(12)	0.28576	(10)	0.28593	(10)
	z	-0.00260	(44)	-0.00373	(59)	-0.00367	(42)	-0.00422	(46)	-0.00343	(48)
	Ueq	0.0076	(5)	0.0076	(6)	0.0068	(5)	0.0073	(5)	0.0071	(5)
O8	x	0.27062	(12)	0.27076	(14)	0.27064	(12)	0.27062	(11)	0.27035	(11)
	y	0.21000	(12)	0.21007	(14)	0.20998	(11)	0.20990	(11)	0.20966	(10)
	z	0.63637	(44)	0.63550	(59)	0.63574	(43)	0.63512	(46)	0.63560	(49)
	Ueq	0.0090	(6)	0.0089	(7)	0.0082	(6)	0.0087	(5)	0.085	(5)

		CT26		CT27		CT28		CT29		CT30	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0216	(8)	0.0211	(10)	0.0225	(11)	0.0221	(10)	0.0255	(9)
Y	x	0.06188	(4)	0.06167	(4)	0.06158	(5)	0.06165	(5)	0.06184	(3)
	y	0.93812	(4)	0.93833	(4)	0.93842	(5)	0.93835	(5)	0.93816	(3)
	z	0.44683	(40)	0.44284	(51)	0.44410	(55)	0.44159	(55)	0.44732	(41)
	Ueq	0.0082	(3)	0.0079	(4)	0.0086	(4)	0.0073	(5)	0.0093	(3)
Z	x	0.26035	(4)	0.26018	(4)	0.26015	(5)	0.26013	(5)	0.26068	(4)
	y	0.29719	(4)	0.29693	(4)	0.29691	(5)	0.29688	(5)	0.29746	(4)
	z	0.46597	(36)	0.46476	(47)	0.46596	(50)	0.46400	(49)	0.46453	(39)
	Ueq	0.0068	(2)	0.0066	(2)	0.0068	(2)	0.0058	(2)	0.0074	(2)
T	x	0.18996	(4)	0.18986	(4)	0.18985	(4)	0.18991	(4)	0.18993	(3)
	y	0.19196	(3)	0.19191	(4)	0.19187	(4)	0.19193	(4)	0.19191	(3)
	z	0.07690	(36)	0.07482	(47)	0.07609	(50)	0.07408	(49)	0.07553	(39)
	Ueq	0.0057	(2)	0.0056	(2)	0.0058	(2)	0.0048	(2)	0.0062	(2)
B	x	0.89068	(11)	0.89074	(12)	0.89092	(13)	0.89096	(13)	0.89049	(10)
	y	0.10932	(11)	0.10926	(12)	0.10908	(13)	0.10904	(13)	0.10951	(10)
	z	0.62188	(54)	0.62111	(63)	0.62169	(66)	0.62020	(66)	0.62120	(53)
	Ueq	0.0074	(8)	0.0078	(9)	0.0075	(9)	0.0068	(9)	0.0073	(8)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29345	(67)	0.29381	(68)	0.29490	(75)	0.29174	(77)	0.29265	(62)
	Ueq	0.0488	(18)	0.0384	(16)	0.0408	(17)	0.0413	(18)	0.0522	(18)
O2	x	0.93936	(8)	0.93953	(8)	0.93957	(9)	0.93961	(9)	0.93910	(7)
	y	0.06064	(8)	0.06047	(8)	0.06043	(9)	0.06039	(9)	0.06090	(7)
	z	0.59116	(48)	0.58769	(58)	0.58928	(61)	0.58748	(62)	0.59092	(49)
	Ueq	0.0168	(8)	0.0159	(8)	0.0163	(9)	0.0159	(9)	0.0181	(8)
O3	x	0.13369	(9)	0.13290	(9)	0.13309	(10)	0.13305	(10)	0.13387	(8)
	y	0.86631	(9)	0.86710	(9)	0.86691	(10)	0.86695	(10)	0.86613	(8)
	z	0.56785	(45)	0.56714	(54)	0.56844	(58)	0.56647	(57)	0.56673	(46)
	Ueq	0.0117	(6)	0.0123	(7)	0.0128	(7)	0.0121	(7)	0.0118	(6)
O4	x	0.90671	(8)	0.90651	(8)	0.90656	(9)	0.90650	(9)	0.90665	(7)
	y	0.09329	(8)	0.09349	(8)	0.09344	(9)	0.09350	(9)	0.09335	(7)
	z	0.00458	(43)	0.00248	(54)	0.00423	(56)	0.00240	(56)	0.00423	(45)
	Ueq	0.0094	(6)	0.0093	(6)	0.0093	(6)	0.0089	(6)	0.0097	(52)
O5	x	0.09347	(8)	0.09364	(8)	0.09362	(9)	0.09362	(9)	0.09348	(7)
	y	0.90563	(8)	0.90636	(8)	0.90638	(9)	0.90638	(9)	0.90652	(7)
	z	-0.01777	(45)	-0.02028	(54)	-0.01849	(59)	-0.02065	(58)	-0.01820	(45)
	Ueq	0.0093	(6)	0.0091	(6)	0.0096	(6)	0.0093	(6)	0.0100	(5)
O6	x	0.18618	(10)	0.18544	(10)	0.18546	(11)	0.18547	(11)	0.18670	(9)
	y	0.19632	(10)	0.19587	(10)	0.19581	(11)	0.19572	(11)	0.19696	(9)
	z	0.30168	(42)	0.30034	(51)	0.30171	(55)	0.29960	(55)	0.30057	(43)
	Ueq	0.0083	(5)	0.0083	(5)	0.0085	(5)	0.0077	(5)	0.0092	(5)
O7	x	0.28592	(9)	0.28598	(9)	0.28596	(10)	0.28607	(10)	0.28603	(8)
	y	0.28583	(9)	0.28628	(10)	0.28594	(11)	0.28623	(11)	0.28593	(9)
	z	-0.00279	(40)	-0.00383	(51)	-0.00248	(54)	-0.00459	(53)	-0.00410	(42)
	Ueq	0.0073	(5)	0.0073	(5)	0.0074	(5)	0.0054	(5)	0.0083	(4)
O8	x	0.27038	(10)	0.27014	(11)	0.27028	(12)	0.27016	(12)	0.27042	(10)
	y	0.20972	(10)	0.20957	(10)	0.20962	(12)	0.20970	(12)	0.20976	(10)
	z	0.63620	(41)	0.63546	(51)	0.63671	(54)	0.63439	(54)	0.63514	(43)
	Ueq	0.0085	(5)	0.0084	(5)	0.0088	(6)	0.0080	(5)	0.0092	(5)

		CT31		CT32		CT33		CT34		CT35	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0183	(9)	0.0267	(8)	0.0243	(8)	0.0172	(5)	0.0216	(7)
Y	x	0.06190	(5)	0.06223	(3)	0.06131	(2)	0.06166	(2)	0.06278	(4)
	y	0.93810	(5)	0.93777	(3)	0.93869	(2)	0.93834	(2)	0.93722	(4)
	z	0.44266	(47)	0.44999	(38)	0.43582	(34)	0.42884	(27)	0.44720	(37)
	Ueq	0.0088	(5)	0.0107	(3)	0.0070	(2)	0.0055	(2)	0.0093	(3)
Z	x	0.25986	(4)	0.26108	(4)	0.26149	(4)	0.26176	(4)	0.26185	(5)
	y	0.29686	(4)	0.29788	(4)	0.29776	(4)	0.29775	(4)	0.29828	(5)
	z	0.46458	(41)	0.46293	(36)	0.46170	(33)	0.45521	(27)	0.46660	(34)
	Ueq	0.0071	(2)	0.0081	(2)	0.0070	(2)	0.0060	(2)	0.0071	(2)
T	x	0.19004	(4)	0.19004	(4)	0.18973	(3)	0.18934	(3)	0.19010	(4)
	y	0.19210	(4)	0.19197	(3)	0.19157	(3)	0.19118	(3)	0.19194	(4)
	z	0.07546	(41)	0.07540	(36)	0.07214	(33)	0.06469	(26)	0.07966	(33)
	Ueq	0.0059	(2)	0.0068	(2)	0.0063	(2)	0.0061	(2)	0.0060	(2)
B	x	0.89080	(12)	0.89015	(11)	0.89004	(11)	0.89010	(10)	0.89008	(13)
	y	0.10920	(12)	0.10985	(11)	0.10996	(11)	0.10990	(10)	0.10992	(13)
	z	0.62120	(59)	0.62065	(53)	0.61771	(48)	0.61233	(44)	0.62398	(54)
	Ueq	0.0073	(9)	0.0083	(8)	0.0090	(8)	0.0087	(8)	0.0080	(9)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29129	(66)	0.29096	(67)	0.30217	(48)	0.29844	(46)	0.30692	(59)
	Ueq	0.0428	(17)	0.0715	(25)	0.0119	(7)	0.0151	(8)	0.0128	(9)
O2	x	0.93953	(8)	0.93885	(8)	0.93904	(7)	0.93934	(6)	0.93884	(8)
	y	0.06047	(8)	0.06115	(8)	0.06096	(7)	0.06066	(6)	0.06116	(8)
	z	0.58903	(54)	0.59378	(48)	0.58430	(39)	0.57767	(35)	0.59537	(44)
	Ueq	0.0167	(8)	0.0218	(9)	0.0116	(6)	0.0097	(5)	0.0115	(7)
O3	x	0.13348	(9)	0.13476	(8)	0.13051	(8)	0.12947	(7)	0.13273	(9)
	y	0.86652	(9)	0.86524	(8)	0.86949	(8)	0.87053	(7)	0.86727	(9)
	z	0.56694	(49)	0.56534	(44)	0.56185	(40)	0.55454	(34)	0.56764	(44)
	Ueq	0.0123	(7)	0.0116	(6)	0.0139	(6)	0.0121	(5)	0.0119	(7)
O4	x	0.90690	(8)	0.90686	(8)	0.90618	(7)	0.90699	(7)	0.90717	(9)
	y	0.09310	(8)	0.09314	(8)	0.09382	(7)	0.09301	(7)	0.09283	(9)
	z	0.00290	(48)	0.00435	(44)	0.00120	(41)	-0.00772	(36)	0.01001	(44)
	Ueq	0.0098	(6)	0.0103	(6)	0.0119	(5)	0.0124	(5)	0.0108	(7)
O5	x	0.09349	(8)	0.09315	(8)	0.09242	(7)	0.09196	(7)	0.09168	(9)
	y	0.90651	(8)	0.90685	(8)	0.90758	(7)	0.90804	(7)	0.90832	(9)
	z	-0.01952	(50)	-0.01740	(44)	-0.02030	(39)	-0.02854	(34)	-0.01063	(44)
	Ueq	0.0094	(6)	0.0102	(6)	0.0112	(5)	0.0117	(5)	0.0104	(6)
O6	x	0.18591	(10)	0.18765	(10)	0.18437	(10)	0.18351	(9)	0.18630	(11)
	y	0.19600	(10)	0.19740	(10)	0.19448	(9)	0.19338	(9)	0.19622	(11)
	z	0.30034	(45)	0.29933	(41)	0.29498	(37)	0.28752	(32)	0.30194	(39)
	Ueq	0.0088	(5)	0.0099	(5)	0.0101	(5)	0.0094	(4)	0.0094	(6)
O7	x	0.28584	(9)	0.28560	(9)	0.28483	(8)	0.28466	(8)	0.28473	(10)
	y	0.28605	(10)	0.28535	(10)	0.28497	(9)	0.28490	(9)	0.28465	(11)
	z	-0.00371	(45)	-0.00560	(40)	-0.00543	(36)	-0.01099	(30)	-0.00003	(38)
	Ueq	0.0075	(5)	0.0087	(5)	0.0099	(4)	0.0107	(4)	0.0094	(6)
O8	x	0.26994	(11)	0.27083	(11)	0.27008	(9)	0.26953	(9)	0.27017	(12)
	y	0.20936	(11)	0.21012	(10)	0.20926	(9)	0.20871	(9)	0.20954	(11)
	z	0.63513	(45)	0.63332	(41)	0.63283	(37)	0.62646	(31)	0.63775	(39)
	Ueq	0.0087	(5)	0.0102	(5)	0.0107	(4)	0.0115	(5)	0.0103	(6)

		CT36		CT37		CT38		CT39		CT40	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0222	(7)	0.0163	(4)	0.0198	(8)	0.0185	(10)	0.0154	(6)
Y	x	0.06249	(3)	0.06266	(3)	0.06190	(4)	0.06182	(5)	0.06175	(2)
	y	0.93751	(3)	0.93734	(3)	0.93810	(4)	0.93818	(5)	0.93825	(2)
	z	0.44530	(37)	0.43742	(24)	0.43647	(43)	0.43458	(55)	0.43097	(29)
	Ueq	0.0073	(3)	0.0091	(3)	0.0072	(3)	0.0068	(5)	0.0053	(2)
Z	x	0.26152	(4)	0.26178	(4)	0.26139	(5)	0.26135	(7)	0.26164	(4)
	y	0.29789	(4)	0.29815	(4)	0.29762	(5)	0.29759	(6)	0.29768	(4)
	z	0.46612	(35)	0.45608	(22)	0.45938	(40)	0.45807	(51)	0.45619	(29)
	Ueq	0.0067	(2)	0.0059	(2)	0.0065	(2)	0.0061	(3)	0.0062	(2)
T	x	0.18989	(4)	0.19006	(4)	0.18982	(4)	0.18986	(5)	0.18955	(3)
	y	0.19182	(3)	0.19184	(3)	0.19175	(4)	0.19173	(5)	0.19142	(3)
	z	0.07798	(34)	0.06902	(21)	0.07004	(40)	0.06904	(50)	0.06630	(29)
	Ueq	0.0055	(2)	0.0053	(2)	0.0054	(2)	0.0051	(3)	0.0063	(2)
B	x	0.89036	(11)	0.89025	(12)	0.89037	(12)	0.89035	(17)	0.89036	(11)
	y	0.10964	(11)	0.10975	(12)	0.10963	(12)	0.10965	(17)	0.10964	(11)
	z	0.62286	(51)	0.61572	(45)	0.61630	(58)	0.61572	(77)	0.61337	(47)
	Ueq	0.0071	(8)	0.0075	(8)	0.0075	(9)	0.0066	(12)	0.0080	(8)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.30668	(54)	0.29365	(48)	0.29906	(60)	0.29880	(8)	0.29827	(49)
	Ueq	0.0107	(8)	0.0152	(9)	0.0143	(11)	0.0105	(12)	0.0096	(8)
O2	x	0.93906	(7)	0.93913	(7)	0.93908	(8)	0.93923	(11)	0.93933	(7)
	y	0.06094	(7)	0.06087	(7)	0.06092	(8)	0.06077	(11)	0.06067	(7)
	z	0.59141	(44)	0.59129	(33)	0.58288	(5)	0.58311	(66)	0.58015	(38)
	Ueq	0.0115	(6)	0.0100	(6)	0.0118	(7)	0.0118	(10)	0.0112	(6)
O3	x	0.13160	(8)	0.13359	(8)	0.13096	(9)	0.13102	(13)	0.13015	(8)
	y	0.86840	(8)	0.86641	(8)	0.86904	(9)	0.86898	(13)	0.86985	(8)
	z	0.56666	(43)	0.55703	(33)	0.56013	(49)	0.55934	(65)	0.55614	(37)
	Ueq	0.0131	(6)	0.0114	(6)	0.0137	(7)	0.0138	(10)	0.0135	(6)
O4	x	0.90678	(8)	0.90769	(8)	0.90639	(8)	0.90649	(12)	0.90678	(7)
	y	0.09322	(8)	0.09231	(8)	0.09361	(8)	0.09351	(12)	0.09322	(7)
	z	0.00750	(43)	-0.00232	(34)	-0.00132	(49)	-0.00228	(64)	-0.00533	(38)
	Ueq	0.0106	(6)	0.0102	(6)	0.0106	(6)	0.0107	(9)	0.0121	(6)
O5	x	0.09215	(8)	0.09108	(8)	0.09232	(8)	0.09203	(12)	0.09199	(7)
	y	0.90785	(8)	0.90892	(8)	0.90768	(8)	0.90797	(12)	0.90801	(7)
	z	-0.01427	(43)	-0.02199	(34)	-0.02302	(49)	-0.02348	(64)	-0.02672	(37)
	Ueq	0.0105	(6)	0.0097	(6)	0.0106	(6)	0.0100	(9)	0.0115	(6)
O6	x	0.18521	(10)	0.18672	(10)	0.18455	(11)	0.18455	(15)	0.18415	(9)
	y	0.19553	(10)	0.19585	(10)	0.19499	(10)	0.19482	(15)	0.19413	(9)
	z	0.30060	(39)	0.29054	(29)	0.29352	(45)	0.29265	(59)	0.28946	(34)
	Ueq	0.0093	(5)	0.0088	(5)	0.0090	(5)	0.0090	(8)	0.0095	(5)
O7	x	0.28487	(9)	0.28433	(9)	0.28517	(10)	0.28498	(14)	0.28474	(8)
	y	0.28508	(9)	0.28474	(10)	0.28540	(11)	0.28520	(15)	0.28505	(9)
	z	-0.00099	(39)	-0.01141	(27)	-0.00805	(44)	-0.00889	(57)	-0.01044	(33)
	Ueq	0.0087	(5)	0.0092	(5)	0.0086	(5)	0.0086	(7)	0.0104	(5)
O8	x	0.26995	(10)	0.27022	(11)	0.27003	(11)	0.27007	(16)	0.26946	(10)
	y	0.20933	(10)	0.20964	(10)	0.20934	(11)	0.20931	(15)	0.20888	(9)
	z	0.63732	(39)	0.62679	(29)	0.63048	(46)	0.62962	(59)	0.62728	(34)
	Ueq	0.0099	(5)	0.0099	(5)	0.0098	(5)	0.0097	(8)	0.0112	(5)

		CT41		CT42		CT43		CT44		CT45	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0206	(15)	0.0207	(10)	0.0246	(8)	0.0155	(3)	0.0144	(5)
Y	x	0.06173	(6)	0.06158	(3)	0.06195	(2)	0.06298	(2)	0.06291	(3)
	y	0.93827	(6)	0.93842	(3)	0.93805	(2)	0.93702	(2)	0.93709	(3)
	z	0.43532	(71)	0.43388	(49)	0.43911	(37)	0.43628	(16)	0.43972	(27)
	Ueq	0.0074	(5)	0.0053	(3)	0.0072	(2)	0.0092	(2)	0.0076	(3)
Z	x	0.26138	(9)	0.26142	(5)	0.26142	(3)	0.26180	(3)	0.26159	(5)
	y	0.29768	(9)	0.29756	(5)	0.29766	(3)	0.29821	(3)	0.29796	(40
	z	0.46024	(68)	0.45990	(48)	0.46274	(36)	0.45349	(14)	0.45641	(23)
	Ueq	0.0081	(4)	0.0070	(2)	0.0071	(2)	0.0071	(2)	0.0063	(2)
T	x	0.18972	(8)	0.18955	(4)	0.18964	(3)	0.19020	(3)	0.19014	(4)
	y	0.19160	(7)	0.19136	(4)	0.19156	(3)	0.19191	(3)	0.19185	(4)
	z	0.07057	(68)	0.06961	(48)	0.07295	(36)	0.06674	(14)	0.06957	(22)
	Ueq	0.0073	(4)	0.0072	(2)	0.0072	(1)	0.0066	(1)	0.0052	(2)
B	x	0.89029	(24)	0.89032	(15)	0.89044	(9)	0.89012	(9)	0.89012	(12)
	y	0.10971	(24)	0.10968	(15)	0.10956	(9)	0.10988	(9)	0.10988	(12)
	z	0.61750	(103)	0.61648	(68)	0.61911	(48)	0.61452	(34)	0.61596	(47)
	Ueq	0.0093	(18)	0.0092	(11)	0.0094	(7)	0.0088	(6)	0.0064	(9)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.30185	(108)	0.30185	(72)	0.30313	(49)	0.28834	(36)	0.29537	(47)
	Ueq	0.0132	(18)	0.0128	(11)	0.0143	(7)	0.0162	(7)	0.0104	(9)
O2	x	0.93896	(14)	0.93920	99)	0.93896	(6)	0.93940	(6)	0.93911	(7)
	y	0.06104	(14)	0.06080	(9)	0.06104	(6)	0.06060	(6)	0.06089	(7)
	z	0.48318	(86)	0.58004	(58)	0.58365	(42)	0.59207	(24)	0.59189	(35)
	Ueq	0.0120	(13)	0.0120	(8)	0.0131	(5)	0.0109	(5)	0.0095	(7)
O3	x	0.13007	(18)	0.12948	(10)	0.13023	(7)	0.13420	(6)	0.13369	(8)
	y	0.86993	(18)	0.87052	(10)	0.86977	(7)	0.86580	(6)	0.86631	(8)
	z	0.56015	(85)	0.56001	(57)	0.56300	(42)	0.55504	(24)	0.55822	(34)
	Ueq	0.0154	(14)	0.0143	(8)	0.0150	(5)	0.0118	(5)	0.0100	(6)
O4	x	0.90662	(16)	0.90651	(10)	0.90643	(6)	0.90803	(6)	0.90740	(8)
	y	0.09338	(16)	0.09349	(10)	0.09357	(6)	0.09197	(6)	0.09260	(8)
	z	0.00064	(86)	-0.00228	(58)	0.00249	(43)	-0.00495	(24)	-0.00185	(35)
	Ueq	0.0134	(13)	0.0131	(8)	0.0130	(5)	0.0113	(5)	0.0102	(6)
O5	x	0.09222	(15)	0.09233	(9)	0.09259	(6)	0.09092	(6)	0.09141	(8)
	y	0.90778	(15)	0.90767	(9)	0.90741	(6)	0.90908	(6)	0.90859	(8)
	z	-0.02128	(85)	-0.02297	(56)	-0.01938	(41)	-0.02473	(25)	-0.02177	(35)
	Ueq	0.0119	(12)	0.0120	(7)	0.0126	(5)	0.0110	(4)	0.0095	(6)
O6	x	0.18422	(19)	0.18379	(12)	0.18433	(8)	0.18720	(8)	0.18685	(10)
	y	0.19447	(20)	0.19379	(12)	0.19472	(8)	0.19618	(8)	0.19602	(10)
	z	0.29386	(78)	0.29273	(53)	0.29627	(39)	0.28866	(20)	0.29174	(30)
	Ueq	0.0112	(11)	0.0102	(6)	0.0109	(4)	0.0099	(4)	0.0083	(5)
O7	x	0.28463	(18)	0.28497	(11)	0.28514	(7)	0.28430	(7)	0.28438	(10)
	y	0.28523	(19)	0.28527	(12)	0.28517	(8)	0.28483	(8)	0.28465	(10
	z	-0.00570	(77)	-0.00640	(53)	-0.00398	(39)	-0.01445	(19)	-0.01127	(28)
	Ueq	0.0109	(11)	0.0110	(6)	0.0110	(4)	0.0103	(4)	0.0083	(5)
O8	x	0.26950	(21)	0.26982	(13)	0.26964	(8)	0.27014	(8)	0.27061	(11)
	y	0.20889	(20)	0.20894	(12)	0.20901	(8)	0.20959	(8)	0.20971	(10)
	z	0.63114	(77)	0.63135	(53)	0.63379	(40)	0.62436	(20)	0.62731	(29)
	Ueq	0.0113	(11)	0.0127	(6)	0.0125	(4)	0.0112	(4)	0.0090	(5)

		CT46		CT47		CT48		CT49		CT50	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0190	(7)	0.0176	(5)	0.0181	(6)	0.0209	(6)	0.0209	(6)
Y	x	0.06293	(4)	0.06291	(3)	0.06298	(4)	0.06316	(2)	0.06312	(2)
	y	0.93707	(4)	0.93709	(3)	0.93702	(4)	0.93684	(2)	0.93688	(2)
	z	0.44321	(36)	0.43677	(25)	0.43768	(32)	0.44589	(28)	0.44473	(31)
	Ueq	0.0074	(3)	0.0080	(3)	0.0083	(4)	0.0074	(2)	0.0088	(2)
Z	x	0.26150	(5)	0.26149	(3)	0.26148	(5)	0.26182	(3)	0.26174	(4)
	y	0.29784	(5)	0.29779	(3)	0.29778	(5)	0.29836	(3)	0.29827	(4)
	z	0.45854	(33)	0.46335	(22)	0.45357	(28)	0.45845	(28)	0.45757	(30)
	Ueq	0.0064	(2)	0.0066	(2)	0.0068	(2)	0.0057	(2)	0.0071	(2)
T	x	0.19009	(4)	0.19024	(3)	0.19027	(4)	0.19005	(3)	0.19009	(3)
	y	0.19191	(4)	0.19215	(3)	0.19211	(4)	0.19189	(3)	0.19191	(3)
	z	0.07128	(33)	0.06526	(21)	0.06576	(28)	0.07137	(28)	0.07041	(30)
	Ueq	0.0055	(2)	0.0062	(2)	0.0064	(2)	0.0053	(1)	0.0067	(2)
B	x	0.89036	(13)	0.89039	(10)	0.89035	(13)	0.88985	(9)	0.88998	(10)
	y	0.10964	(13)	0.10961	(10)	0.10965	(13)	0.11015	(9)	0.11002	(10)
	z	0.61746	(54)	0.61300	(40)	0.61350	(52)	0.61683	(43)	0.61615	(46)
	Ueq	0.0074	(9)	0.0074	(7)	0.0079	(9)	0.0075	(7)	0.0082	(7)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29791	(53)	0.29229	(39)	0.29225	(51)	0.19158	(44)	0.29119	(48)
	Ueq	0.0113	(9)	0.0131	(8)	0.0126	(10)	0.0181	(8)	0.0197	(8)
O2	x	0.93884	(8)	0.93912	(6)	0.93910	(8)	0.93829	(6)	0.93841	(6)
	y	0.06116	(8)	0.06088	(6)	0.06090	(8)	0.06171	(6)	0.06159	(6)
	z	0.59077	(43)	0.58653	(32)	0.58784	(41)	0.59107	(35)	0.59029	(38)
	Ueq	0.0104	(7)	0.0114	(6)	0.0112	(7)	0.0103	(5)	0.0122	(6)
O3	x	0.13354	(9)	0.13367	(7)	0.13378	(9)	0.13498	(6)	0.13491	(7)
	y	0.86646	(9)	0.86633	(7)	0.86622	(9)	0.86502	(6)	0.86509	(7)
	z	0.56074	(42)	0.55580	(30)	0.55587	(39)	0.56000	(35)	0.55913	(38)
	Ueq	0.0107	(7)	0.0106	(5)	0.0106	(7)	0.0101	(5)	0.0114	(5)
O4	x	0.90698	(9)	0.90712	(7)	0.90714	(9)	0.90705	(6)	0.90702	(7)
	y	0.09302	(9)	0.09288	(7)	0.09286	(9)	0.09295	(6)	0.09298	(7)
	z	0.00093	(43)	-0.00613	(31)	-0.00532	(40)	0.00171	(34)	0.00075	(37)
	Ueq	0.0101	(6)	0.0115	(5)	0.0114	(7)	0.0092	(5)	0.0109	(5)
O5	x	0.09233	(9)	0.09202	(7)	0.09207	(9)	0.09281	(6)	0.09271	(7)
	y	0.90767	(9)	0.90798	(7)	0.90793	(9)	0.90719	(6)	0.90729	(7)
	z	-0.02006	(44)	-0.02851	(32)	-0.02686	(41)	-0.01904	(34)	-0.02049	(37)
	Ueq	0.0100	(6)	0.0119	(5)	0.0117	(7)	0.0091	(4)	0.0108	(5)
O6	x	0.18675	(11)	0.18657	(8)	0.18667	(11)	0.18833	(8)	0.18803	(9)
	y	0.19629	(11)	0.19647	(8)	0.19637	(11)	0.19772	(8)	0.19746	(8)
	z	0.29482	(39)	0.28978	(27)	0.29037	(34)	0.29461	(32)	0.29369	(35)
	Ueq	0.0085	(5)	0.0088	(4)	0.0091	(6)	0.0083	(4)	0.0094	(4)
O7	x	0.28500	(10)	0.28560	(8)	0.28546	(10)	0.28532	(7)	0.28527	(8)
	y	0.28500	(11)	0.28590	(9)	0.28584	(11)	0.28495	(8)	0.28493	(9)
	z	-0.00904	(38)	-0.01491	(26)	-0.01471	(33)	-0.00990	(31)	-0.01074	(33)
	Ueq	0.0079	(5)	0.0086	(4)	0.0088	(5)	0.0079	(4)	0.0092	(4)
O8	x	0.27075	(11)	0.28035	(9)	0.27049	(11)	0.27108	(8)	0.27133	(9)
	y	0.20991	(11)	0.20968	(9)	0.20975	(11)	0.21027	(8)	0.21031	(9)
	z	0.62958	(39)	0.62457	(27)	0.62478	(34)	0.62854	(32)	0.62784	(34)
	Ueq	0.0088	(5)	0.0091	(4)	0.0093	(6)	0.0085	(4)	0.0100	(4)

		CT51		CT52		CT53		CT54		CT55	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0220	(7)	0.0243	(9)	0.0221	(8)	0.0238	(12)	0.0174	(6)
Y	x	0.06322	(2)	0.06142	(2)	0.06237	(2)	0.06241	(3)	0.06179	(3)
	y	0.93678	(2)	0.93858	(2)	0.93763	(2)	0.93759	(3)	0.93821	(3)
	z	0.44393	(31)	0.43325	(41)	0.43840	(38)	0.44080	(56)	0.44290	(31)
	Ueq	0.0081	(2)	0.0087	(2)	0.0089	(2)	0.0109	(2)	0.0085	(2)
Z	x	0.26180	(4)	0.26150	(4)	0.26181	(4)	0.26187	(5)	0.26093	(4)
	y	0.29845	(4)	0.29817	(4)	0.29855	(4)	0.29860	(5)	0.29780	(4)
	z	0.45697	(31)	0.45320	(41)	0.45461	(38)	0.45821	(56)	0.46062	(30)
	Ueq	0.0066	(2)	0.0051	(2)	0.0046	(2)	0.0062	(3)	0.0064	(2)
T	x	0.19001	(3)	0.18997	(4)	0.18998	(4)	0.18998	(5)	0.19015	(4)
	y	0.19189	(3)	0.19187	(3)	0.19184	(3)	0.19186	(5)	0.19201	(3)
	z	0.06968	(31)	0.06368	(41)	0.06632	(38)	0.07015	(57)	0.07226	(29)
	Ueq	0.0062	(2)	0.0057	(2)	0.0058	(2)	0.0086	(2)	0.0055	(2)
B	x	0.88984	(11)	0.88992	(12)	0.88969	(11)	0.88979	(16)	0.89027	(11)
	y	0.11016	(11)	0.11008	(12)	0.11031	(11)	0.11021	(16)	0.10973	(11)
	z	0.61486	(48)	0.61036	(57)	0.61195	(54)	0.61480	(79)	0.61810	(5)
	Ueq	0.0085	(8)	0.0085	(9)	0.0082	(8)	0.0108	(12)	0.0072	(8)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.28905	(50)	0.28193	(69)	0.28138	(64)	0.28830	(91)	0.28517	(66)
	Ueq	0.0210	(10)	0.0374	(14)	0.0352	(12)	0.0334	(17)	0.0529	(19)
O2	x	0.93823	(6)	0.93833	(7)	0.93814	(7)	0.93818	(10)	0.93852	(8)
	y	0.06177	(6)	0.06167	(7)	0.06186	(7)	0.06182	(10)	0.06148	(8)
	z	0.58795	(40)	0.58144	(50)	0.58460	(47)	0.58609	(70)	0.59097	(41)
	Ueq	0.0122	(6)	0.0138	(7)	0.0138	(7)	0.0159	(10)	0.0169	(8)
O3	x	0.13492	(7)	0.13421	(8)	0.13496	(8)	0.13451	(11)	0.13474	(8)
	y	0.86508	(7)	0.86579	(8)	0.86504	(8)	0.86549	(11)	0.86526	(8)
	z	0.55827	(38)	0.55382	(48)	0.55545	(45)	0.55869	(66)	0.56231	(39)
	Ueq	0.0112	(5)	0.0121	(6)	0.0122	(6)	0.0145	(8)	0.0102	(6)
O4	x	0.90706	(7)	0.90684	(7)	0.90710	(7)	0.90722	(10)	0.90710	(7)
	y	0.09294	(7)	0.09316	(7)	0.09290	(7)	0.09278	(10)	0.09290	(7)
	z	0.00038	(38)	-0.00546	(48)	-0.00284	(454)	0.00170	(65)	0.00103	(38)
	Ueq	0.0102	(5)	0.0103	(6)	0.0104	(6)	0.0124	(8)	0.0089	(6)
O5	x	0.09289	(7)	0.09330	(8)	0.09315	(7)	0.09299	(11)	0.09309	(8)
	y	0.90711	(7)	0.90670	(8)	0.90685	(7)	0.90701	(11)	0.90691	(8)
	z	-0.02087	(38)	-0.02736	(47)	-0.02440	(45)	-0.02008	(65)	-0.02090	(38)
	Ueq	0.0102	(5)	0.0103	(6)	0.0101	(5)	0.0120	(8)	0.0095	(6)
O6	x	0.18826	(9)	0.18753	(10)	0.18805	(10)	0.18790	(14)	0.18774	(10)
	y	0.19772	(9)	0.19741	(10)	0.19783	(9)	0.19769	(14)	0.09746	(9)
	z	0.29290	(36)	0.28810	(46)	0.28988	(44)	0.29355	(64)	0.29661	(36)
	Ueq	0.0095	(5)	0.0088	(5)	0.0095	(5)	0.0114	(7)	0.0085	(5)
O7	x	0.28514	(8)	0.28567	(9)	0.28538	(10)	0.28532	(13)	0.28575	(9)
	y	0.28470	(9)	0.28531	(10)	0.28490	(9)	0.28492	(13)	0.28561	(10)
	z	-0.01131	(34)	-0.01541	(45)	-0.01378	(42)	-0.01000	(62)	-0.00846	(34)
	Ueq	0.0090	(4)	0.0085	(5)	0.0090	(5)	0.0108	(7)	0.0075	(5)
O8	x	0.27094	(9)	0.27065	(10)	0.27083	(10)	0.27044	(14)	0.27065	(10)
	y	0.21023	(9)	0.20989	(10)	0.21003	99)	0.20980	(14)	0.20996	(10)
	z	0.62692	(35)	0.62315	(45)	0.62440	(42)	0.62797	(61)	0.63080	(35)
	Ueq	0.0096	(5)	0.0098	(5)	0.0105	(5)	0.0124	(7)	0.0087	(5)

		CT56		CT57		CT58		CT59		CT60	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0244	(15)	0.0276	(7)	0.0284	(27)	0.0212	(9)	0.0257	(8)
Y	x	0.06228	(2)	0.06130	(2)	0.06274	(4)	0.06203	(3)	0.06228	(3)
	y	0.93771	(2)	0.93870	(2)	0.93726	(4)	0.93797	(3)	0.93772	(3)
	z	0.43920	(67)	0.43138	(32)	0.43937	(11)	0.44812	(45)	0.44961	(41)
	Ueq	0.0089	(2)	0.0094	(1)	0.0083	(4)	0.0082	(3)	0.0092	(3)
Z	x	0.26153	(5)	0.26163	(4)	0.26168	(8)	0.26093	(5)	0.26096	(5)
	y	0.29839	(5)	0.29831	(4)	0.29868	(8)	0.29774	(5)	0.29782	(5)
	z	0.45630	(68)	0.45386	(32)	0.45454	(11)	0.46412	(44)	0.46485	(40)
	Ueq	0.0043	(2)	0.0056	(2)	0.0062	(4)	0.0059	(2)	0.0081	(2)
T	x	0.18986	(4)	0.19023	(3)	0.18994	(8)	0.19003	(4)	0.18997	(4)
	y	0.19186	(4)	0.19216	(3)	0.19198	(7)	0.19198	(4)	0.19196	(4)
	z	0.06688	(68)	0.06389	(33)	0.06520	(11)	0.07581	(43)	0.07656	(39)
	Ueq	0.0059	(2)	0.0059	(2)	0.0069	(4)	0.0049	(2)	0.0068	(2)
B	x	0.89000	(14)	0.89009	(10)	0.88994	(24)	0.89021	(13)	0.89035	(12)
	y	0.11000	(14)	0.10991	(10)	0.11006	(24)	0.10979	(13)	0.10965	(12)
	z	0.61190	(82)	0.61178	(48)	0.60963	(14)	0.62095	(62)	0.62104	(58)
	Ueq	0.0090	(10)	0.0080	(8)	0.0097	(18)	0.0064	(10)	0.0090	(9)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.28821	(93)	0.28226	(62)	0.28430	(16)	0.29104	(78)	0.29210	(74)
	Ueq	0.0461	(18)	0.0279	(11)	0.0494	(36)	0.0559	(23)	0.0612	(23)
O2	x	0.93812	(9)	0.93862	(7)	0.93818	(15)	0.93877	(9)	0.93881	(8)
	y	0.06188	(9)	0.06138	(7)	0.06182	(15)	0.06123	(9)	0.06119	(8)
	z	0.57949	(76)	0.58337	(42)	0.57813	(132)	0.59240	(55)	0.59209	(51)
	Ueq	0.0163	(9)	0.0136	(63)	0.0172	(16)	0.0169	(10)	0.0191	(9)
O3	x	0.13385	(10)	0.13417	(7)	0.13440	(17)	0.13474	(9)	0.13456	(9)
	y	0.86615	(10)	0.86583	(7)	0.86560	(17)	0.86526	(9)	0.86544	(9)
	z	0.55754	(73)	0.55475	(40)	0.55616	(124)	0.56622	(52)	0.56703	(48)
	Ueq	0.0137	(7)	0.0109	(5)	0.0137	(13)	0.0097	(7)	0.0109	(6)
O4	x	0.90686	(9)	0.90693	(7)	0.90686	(15)	0.90694	(9)	0.90695	(8)
	y	0.09314	(9)	0.09307	(7)	0.09314	(15)	0.09306	(9)	0.09305	(8)
	z	-0.00173	(73)	-0.00585	(40)	-0.00287	(122)	0.00589	(52)	0.00610	(47)
	Ueq	0.0114	(7)	0.0113	(5)	0.0115	(12)	0.0085	(7)	0.0102	(6)
O5	x	0.09371	(9)	0.09329	(7)	0.09378	(16)	0.09323	(9)	0.09328	(8)
	y	0.90629	(9)	0.90671	(7)	0.90622	(16)	0.90677	(9)	0.90672	(8)
	z	-0.02452	(73)	-0.02782	(39)	-0.02633	(122)	-0.01668	(52)	-0.01635	(47)
	Ueq	0.0105	(7)	0.0108	(5)	0.0121	(12)	0.0089	(7)	0.0105	(6)
O6	x	0.18717	(12)	0.18758	(9)	0.18766	(20)	0.18749	(11)	0.18727	(10)
	y	0.19767	(12)	0.19782	(9)	0.19813	(20)	0.19757	(11)	0.19765	(10)
	z	0.29146	(73)	0.28982	(37)	0.29009	(122)	0.30049	(49)	0.30125	(45)
	Ueq	0.0098	(6)	0.0088	(4)	0.0097	(10)	0.0079	(6)	0.0095	(5)
O7	x	0.28591	(11)	0.28633	(8)	0.28581	(19)	0.28571	(10)	0.28584	(10)
	y	0.28523	(11)	0.28582	(8)	0.28509	(20)	0.28543	(11)	0.28555	(10)
	z	-0.01195	(71)	-0.01497	(36)	-0.01422	(118)	-0.00450	(48)	-0.00363	(44)
	Ueq	0.0093	(6)	0.0080	(4)	0.0094	(10)	0.0068	(5)	0.0087	(5)
O8	x	0.27048	(12)	0.27027	(9)	0.27048	(21)	0.27071	(12)	0.27069	(11)
	y	0.20974	(12)	0.20963	(9)	0.20979	(20)	0.20991	(12)	0.21001	(11)
	z	0.62605	(71)	0.62403	(36)	0.62431	(118)	0.63454	(48)	0.63525	(44)
	Ueq	0.0107	(6)	0.0095	(5)	0.0110	(11)	0.0081	(6)	0.0102	(5)

		CT61		CT62		CT63		CT64		CT65	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0238	(8)	0.0170	(7)	0.0188	(8)	0.0142	(4)	0.0108	(2)
Y	x	0.06206	(3)	0.06196	(3)	0.06188	(3)	0.06274	(3)	0.06336	(3)
	y	0.93794	(3)	0.93804	(3)	0.93812	(3)	0.93726	(3)	0.93664	(3)
	z	0.44920	(39)	0.44448	(34)	0.44489	(37)	0.43732	(22)	0.43878	(17)
	Ueq	0.0077	(2)	0.0074	(3)	0.0079	(3)	0.0082	(3)	0.0070	(3)
Z	x	0.26094	(4)	0.26092	(4)	0.26082	(5)	0.26169	(94)	0.26176	(4)
	y	0.29781	(4)	0.29785	(4)	0.29779	(5)	0.29799	(4)	0.29807	(4)
	z	0.46522	(38)	0.46151	932)	0.46194	(35)	0.45584	(19)	0.45553	(14)
	Ueq	0.0064	(2)	0.0070	(2)	0.0065	(2)	0.0072	(2)	0.0059	(2)
T	x	0.19001	(4)	0.19014	(4)	0.19017	(4)	0.19014	(3)	0.19021	(3)
	y	0.19194	(3)	0.19205	(4)	0.19204	(4)	0.19189	(3)	0.19189	(3)
	z	0.07692	(38)	0.07331	(32)	0.07352	(35)	0.06886	(18)	0.06919	(13)
	Ueq	0.0053	(2)	0.0061	(2)	0.0057	(2)	0.0061	(2)	0.0048	(2)
B	x	0.89016	(12)	0.89011	(12)	0.89034	(13)	0.89009	(10)	0.89025	(10)
	y	0.10984	(12)	0.10989	(12)	0.10966	(13)	0.10991	(10)	0.10975	(10)
	z	0.62161	(55)	0.61841	(53)	0.61959	(58)	0.61598	(41)	0.61757	(36)
	Ueq	0.0072	(8)	0.0080	(9)	0.0084	(10)	0.0079	(8)	0.0064	(7)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29224	(70)	0.28627	(70)	0.28837	(8)	0.29488	(43)	0.29425	(37)
	Ueq	0.0560	(22)	0.0501	(20)	0.0523	(20)	0.0122	(8)	0.0112	(7)
O2	x	0.93874	(8)	0.93885	(8)	0.93883	(8)	0.93935	(7)	0.93980	(6)
	y	0.06126	(8)	0.06115	(8)	0.06117	(8)	0.06065	(7)	0.06020	(6)
	z	0.59224	(49)	0.59135	(46)	0.59158	(48)	0.59174	(31)	0.59697	(25)
	Ueq	0.0170	(8)	0.0172	(8)	0.0157	(9)	0.0110	(6)	0.0076	(5)
O3	x	0.13452	(8)	0.13473	(8)	0.13477	(9)	0.13339	(7)	0.13395	(7)
	y	0.86548	(8)	0.86527	(8)	0.86523	(9)	0.86661	(7)	0.86605	(7)
	z	0.56736	(45)	0.56320	(42)	0.56350	(44)	0.55737	(30)	0.55746	(26)
	Ueq	0.0094	(6)	0.0109	(6)	0.0108	(7)	0.0119	(6)	0.0100	(5)
O4	x	0.90686	(8)	0.90710	(8)	0.90721	(8)	0.90764	(7)	0.90845	(7)
	y	0.09314	(8)	0.09290	(8)	0.09279	(8)	0.09236	(7)	0.09155	(7)
	z	0.00578	(45)	0.00247	(42)	0.00292	(44)	-0.00296	(30)	-0.00342	(26)
	Ueq	0.0084	(6)	0.0099	(6)	0.0096	(7)	0.0114	(5)	0.0099	(5)
O5	x	0.09325	(8)	0.09303	(8)	0.09314	(8)	0.09106	(7)	0.08998	(7)
	y	0.90678	(8)	0.90697	(8)	0.90686	(8)	0.90894	(7)	0.91002	(7)
	z	-0.01594	(45)	-0.01978	(42)	-0.01888	(45)	-0.02278	(31)	-0.02269	(27)
	Ueq	0.0088	(6)	0.0097	(6)	0.0089	(6)	0.0109	(5)	0.0092	(5)
O6	x	0.18728	(10)	0.18767	(10)	0.18765	(10)	0.18649	(9)	0.18664	(8)
	y	0.19740	(10)	0.19748	(10)	0.19757	(11)	0.19567	(9)	0.19552	(9)
	z	0.30168	(43)	0.29776	(38)	0.29799	(41)	0.29100	(26)	0.29063	(21)
	Ueq	0.0081	(5)	0.0089	(5)	0.0083	(5)	0.0096	(5)	0.0083	(4)
O7	x	0.28594	(9)	0.28574	(9)	0.28569	(10)	0.28445	(9)	0.28380	(8)
	y	0.28569	(10)	0.28563	(10)	0.28541	(11)	0.28499	(9)	0.28473	(9)
	z	-0.00348	(42)	-0.00764	(37)	-0.00670	(40)	-0.01193	(24)	-0.01228	(20)
	Ueq	0.0071	(5)	0.0081	(5)	0.0080	(5)	0.0098	(5)	0.0088	(4)
O8	x	0.27065	(11)	0.27049	(11)	0.27035	(11)	0.27008	(10)	0.26983	(9)
	y	0.21010	(10)	0.20992	(10)	0.20965	(11)	0.20945	(9)	0.20927	(9)
	z	0.63551	(42)	0.63188	(37)	0.63201	(40)	0.62704	(25)	0.62692	(21)
	Ueq	0.0085	(5)	0.0093	(5)	0.0086	(6)	0.0103	(5)	0.0095	(4)

		CT66		CT67		CT68		CT69		CT70	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0104	(4)	0.0130	(3)	0.0137	(2)	0.0127	(3)	0.0128	(4)
Y	x	0.06296	(4)	0.06312	(3)	0.06352	(3)	0.06319	(4)	0.06299	(3)
	y	0.93704	(4)	0.93688	(3)	0.93648	(3)	0.93681	(4)	0.93701	(3)
	z	0.43834	(23)	0.43701	(18)	0.43981	(16)	0.43858	(22)	0.43898	(24)
	Ueq	0.0074	(3)	0.0075	(3)	0.0086	(2)	0.0086	(3)	0.0072	(3)
Z	x	0.26175	(4)	0.26162	(3)	0.26174	(3)	0.26162	(5)	0.26162	(4)
	y	0.29803	(4)	0.29796	(3)	0.29811	(3)	0.29796	(4)	0.29800	(4)
	z	0.45676	(19)	0.45379	(15)	0.45468	(13)	0.45531	(18)	0.45596	(20)
	Ueq	0.0066	(2)	0.0069	(2)	0.0072	(2)	0.0065	(2)	0.0064	(2)
T	x	0.19020	(4)	0.19016	(3)	0.19024	(3)	0.19013	(4)	0.19018	(4)
	y	0.19188	(4)	0.19190	(3)	0.19192	(3)	0.19182	(4)	0.19188	(3)
	z	0.06991	(18)	0.06722	(14)	0.06854	(13)	0.06889	(17)	0.06922	(19)
	Ueq	0.0054	(2)	0.0060	(2)	0.0062	(1)	0.0053	(2)	00053	(2)
B	x	0.89025	(12)	0.89029	(10)	0.89034	(9)	0.89030	(12)	0.89012	(11)
	y	0.10975	(12)	0.10971	(10)	0.10966	(9)	0.10970	(12)	0.10988	(11)
	z	0.61759	(44)	0.61477	(35)	0.61656	(33)	0.61680	(45)	0.61622	(44)
	Ueq	0:0072	(9)	0.0075	(7)	0.0078	(7)	0.0072	(9)	0.0068	(8)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29516	(45)	0.29328	(35)	0.29253	(33)	0.29422	(46)	0.29537	(45)
	Ueq	0.0105	(9)	0.0110	(7)	0.0133	(7)	0.0151	(9)	0.0113	(9)
O2	x	0.93941	(7)	0.93947	(6)	0.93962	(6)	0.93963	(8)	0.93931	(7)
	y	0.06059	(7)	0.06053	(6)	0.06038	(6)	0.06037	(8)	0.06069	(7)
	z	0.59475	(32)	0.59183	(26)	0.59526	(24)	0.59516	(32)	0.59317	(32)
	Ueq	0.0101	(6)	0.0101	(5)	0.0095	(5)	0.0097	(7)	0.0101	(6)
O3	x	0.13332	(8)	0.13344	(7)	0.13425	(6)	0.13386	(8)	0.13364	(8)
	y	0.86668	(8)	0.86656	(7)	0.86575	(6)	0.86614	(8)	0.86636	(8)
	z	0.55838	(32)	0.55569	(25)	0.55641	(24)	0.55663	(32)	0.55757	(31)
	Ueq	0.0114	(6)	0.0114	(5)	0.0109	(5)	0.0109	(7)	0.0104	(6)
O4	x	0.90785	(8)	0.90784	(6)	0.90817	(6)	0.90809	(8)	0.90766	(8)
	y	0.09215	(8)	0.09216	(6)	0.09183	(6)	0.09191	(8)	0.09234	(8)
	z	-0.00189	(32)	-0.00495	(26)	-0.00377	(24)	-0.00374	(32)	-0.00234	(32)
	Ueq	0.0106	(6)	0.0110	(5)	0.0111	(5)	0.0106	(6)	0.0102	(6)
O5	x	0.09066	(8)	0.09086	(7)	0.09042	(6)	0.09032	(8)	0.09107	(8)
	y	0.90934	(8)	0.90914	(7)	0.90958	(6)	0.90968	(8)	0.90893	(8)
	z	-0.02143	(33)	-0.02460	(26)	-0.02321	(25)	-0.02272	(33)	-0.02210	(33)
	Ueq	0.0101	(6)	0.0112	(5)	0.0106	(5)	0.0099	(6)	0.0101	(6)
O6	x	0.18654	(10)	0.18651	(8)	0.18701	(8)	0.18649	(10)	0.18668	(10)
	y	0.19566	(10)	0.19554	(8)	0.19579	(8)	0.19540	(11)	0.19577	(10)
	z	0.29161	(27)	0.28927	(21)	0.29010	(19)	0.29051	(26)	0.29123	(27)
	Ueq	0.0090	(5)	0.0092	(4)	0.0093	(4)	0.0091	(5)	0.0088	(5)
O7	x	0.28412	(10)	0.28438	(8)	0.28407	(7)	0.28388	(10)	0.28431	(9)
	y	0.28468	(10)	0.28501	(8)	0.28482	(8)	0.28475	(11)	0.28487	(10)
	z	-0.01091	(25)	-0.01383	(20)	-0.01323	(18)	-0.01235	(24)	-0.01174	(25)
	Ueq	0.0090	(5)	0.0097	(4)	0.0099	(4)	0.0093	(5)	0.0087	(5)
O8	x	0.26991	(11)	0.26992	(9)	0.26997	(8)	0.27002	(11)	0.27031	(10)
	y	0.20938	(10)	0.20942	(8)	0.20951	(8)	0.20945	(10)	0.20971	(10)
	z	0.62821	(26)	0.62486	(21)	0.62584	(19)	0.62671	(26)	0.62707	(27)
	Ueq	0.0100	(5)	0.0108	(4)	0.0108	(4)	0.0100	(5)	0.0094	(5)

		CT71		CT72		CT73		CT74		CT75	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0132	(3)	0.0187	(6)	0.0135	(6)	0.0109	(4)	0.0101	(4)
Y	x	0.06298	(3)	0.06187	(2)	0.06345	(6)	0.06350	(4)	0.06296	(3)
	y	0.93702	(3)	0.93813	(2)	0.93655	(6)	0.93650	(4)	0.93704	(3)
	z	0.43730	(20)	0.43621	(26)	0.43727	(38)	0.43878	(23)	0.43790	(21)
	Ueq	0.0085	(3)	0.0089	(2)	0.0093	(6)	0.0080	(4)	0.0070	(3)
Z	x	0.26156	(4)	0.26161	(3)	0.26158	(7)	0.26175	(5)	0.26166	(4)
	y	0.29795	(4)	0.29801	(3)	0.29793	(7)	0.29799	(5)	0.29800	(4)
	z	0.45453	(16)	0.45870	(25)	0.45321	(31)	0.45420	(18)	0.45624	(18)
	Ueq	0.0071	(2)	0.0071	(2)	0.0074	(4)	0.0066	(2)	0.0063	(2)
T	x	0.19014	(3)	0.19000	(3)	0.19046	(6)	0.19032	(4)	0.19019	(3)
	y	0.19187	(3)	0.19181	(3)	0.19219	(6)	0.19206	(4)	0.19191	(3)
	z	0.06783	(16)	0.07026	(25)	0.06554	(30)	0.06803	(18)	0.06930	(17)
	Ueq	0.0062	(2)	0.0066	(2)	0.0072	(3)	0.0057	(2)	0.0050	(2)
B	x	0.89035	(10)	0.89016	(10)	0.89023	(20)	0.89049	(14)	0.89026	(10)
	y	0.10965	(10)	0.10984	(10)	0.10977	(20)	0.10951	(14)	0.10974	(10)
	z	0.61515	(38)	0.61668	(41)	0.61558	(74)	0.61655	(48)	0.61714	(40)
	Ueq	0.0076	(7)	0.0084	(7)	0.0083	(15)	0.0069	(10)	0.0067	(8)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29463	(38)	0.29590	(46)	0.29195	(73)	0.29310	(48)	0.29485	(41)
	Ueq	0.0111	(7)	0.0173	(9)	0.0128	(15)	0.0013	(8)	0.0107	(8)
O2	x	0.93944	(6)	0.93892	(6)	0.93957	(12)	0.93970	(8)	0.93942	(7)
	y	0.06056	(6)	0.06108	(6)	0.06043	(12)	0.06030	(8)	0.06058	(7)
	z	0.59163	(28)	0.58735	(34)	0.59225	(53)	0.59522	(34)	0.59334	(29)
	Ueq	0.0106	(6)	0.0129	(6)	0.0096	(11)	0.0083	(7)	0.0101	(6)
O3	x	0.13342	(7)	0.13235	(7)	0.13425	(14)	0.13416	(9)	0.13331	(7)
	y	0.86658	(7)	0.86765	(7)	0.86575	(14)	0.86584	(9)	0.86669	(7)
	z	0.55571	(27)	0.55889	(33)	0.55555	(52)	0.55624	(32)	0.55794	(29)
	Ueq	0.0122	(6)	0.0142	(5)	0.0109	(11)	0.0093	(7)	0.0111	(6)
O4	x	0.90782	(7)	0.90712	(6)	0.90787	(14)	0.90817	(9)	0.90777	(7)
	y	0.09218	(7)	0.09288	(6)	0.09213	(14)	0.09183	(9)	0.09223	(7)
	z	-0.00440	(27)	-0.00040	(34)	-0.00622	(54)	-0.00444	(33)	-0.00237	(29)
	Ueq	0.0107	(5)	0.0120	(5)	0.0132	(11)	0.0109	(7)	0.0101	(5)
O5	x	0.09080	(7)	0.09189	(7)	0.09088	(14)	0.09040	(9)	0.09080	(7)
	y	0.90920	(7)	0.90811	(7)	0.90912	(14)	0.90960	(9)	0.90920	(7)
	z	-0.02406	(28)	-0.02123	(33)	-0.02714	(56)	-0.02379	(35)	-0.02210	(30)
	Ueq	0.0109	(5)	0.0120	(5)	0.0124	(10)	0.0106	(7)	0.0102	(5)
O6	x	0.18639	(8)	0.18597	(8)	0.18687	(16)	0.18726	(11)	0.18633	(9)
	y	0.19558	(9)	0.19586	(8)	0.19629	(17)	0.19617	(11)	0.19557	(9)
	z	0.28952	(22)	0.29326	(30)	0.28955	(44)	0.29018	(26)	0.29152	(24)
	Ueq	0.0095	(5)	0.0099	(4)	0.0099	(9)	0.0086	(6)	0.0085	(5)
O7	x	0.28424	(8)	0.28490	(7)	0.28489	(16)	0.28436	(10)	0.28423	(9)
	y	0.28497	(9)	0.28512	(8)	0.28582	(17)	0.28509	(11)	0.28493	(9)
	z	-0.01315	(22)	-0.00882	(29)	-0.01506	(42)	-0.01390	(26)	-0.01130	(23)
	Ueq	0.0096	(4)	0.0101	(4)	0.0101	(9)	0.0090	(6)	0.0086	(5)
O8	x	0.26999	(9)	0.27003	(9)	0.26994	(18)	0.26971	(11)	0.27003	(10)
	y	0.20944	(9)	0.20942	(8)	0.20939	(17)	0.20919	(11)	0.20932	(9)
	z	0.62544	(22)	0.62970	(29)	0.62466	(43)	0.62527	(27)	0.62758	(24)
	Ueq	0.0104	(5)	0.0111	(4)	0.0101	(9)	0.0100	(6)	0.0094	(5)

		CT76		CT77		CT78		CT79		CT80	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0148	(4)	0.0151	(5)	0.0141	(4)	0.0156	(4)	0.0155	(6)
Y	x	0.06189	(3)	0.06224	(3)	0.06175	(3)	0.06193	(3)	0.06192	(30
	y	0.93811	(3)	0.93776	(3)	0.93825	(3)	0.93807	(3)	0.93808	(3)
	z	0.43206	(23)	0.43444	(23)	0.42738	(22)	0.43149	(22)	0.42883	(26)
	Ueq	0.0087	(2)	0.0090	(3)	0.0079	(3)	0.0090	(3)	0.0073	(3)
Z	x	0.26178	(40	0.26180	(4)	0.26138	(4)	0.26159	(4)	0.26146	(4)
	y	0.29806	(4)	0.29824	(4)	0.29768	(4)	0.29797	(4)	0.29773	(4)
	z	0.45425	(22)	0.45498	(22)	0.45301	(19)	0.45531	(20)	0.45143	(25)
	Ueq	0.0056	(2)	0.0061	(2)	0.0061	(2)	0.0071	(2)	0.0059	(2)
T	x	0.18999	(4)	0.18997	(4)	0.18992	(3)	0.19007	(3)	0.18990	(4)
	y	0.19171	(3)	0.19168	(4)	0.19172	(3)	0.19181	(3)	0.19167	(4)
	z	0.06668	(21)	0.06785	(22)	0.06439	(19)	0.06744	(20)	0.06250	(25)
	Ueq	0.0056	(2)	0.0072	(2)	0.0051	(2)	0.0069	(2)	0.0067	(2)
B	x	0.89013	(12)	0.89007	(12)	0.89044	(11)	0.89023	(11)	0.89020	(13)
	y	0.10987	(12)	0.10993	(12)	0.10956	(11)	0.10977	(11)	0.10980	(13)
	z	0.61454	(45)	0.61513	(48)	0.61179	(40)	0.61483	(41)	0.61069	(50)
	Ueq	0.0077	(9)	0.0092	(9)	0.0068	(8)	0.0083	(8)	0.0093	(10)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29075	(49)	0.29076	(52)	0.29291	(45)	0.29467	(44)	0.29145	(52)
	Ueq	0.0155	(10)	0.0167	(10)	0.0165	(9)	0.0093	(7)	0.0106	(9)
O2	x	0.93917	(7)	0.93916	(8)	0.93979	(7)	0.93942	(7)	0.93913	(8)
	y	0.06083	(7)	0.06084	(8)	0.06021	(7)	0.06058	(7)	0.06087	(8)
	z	0.59001	(33)	0.59152	(4)	0.58326	(32)	0.58839	(32)	0.58285	(37)
	Ueq	0.0109	(7)	0.0117	(7)	0.0113	(6)	0.0124	(6)	0.0126	(7)
O3	x	0.13326	(8)	0.13342	(9)	0.13125	(8)	0.13218	(8)	0.13191	(9)
	y	0.86674	(8)	0.86658	(9)	0.86875	(8)	0.86782	(8)	0.86809	(9)
	z	0.55478	(34)	0.55544	(35)	0.55280	(31)	0.55597	(31)	0.55215	(37)
	Ueq	0.0120	(6)	0.0129	(7)	0.0143	(6)	0.0141	(6)	0.0132	(7)
O4	x	0.90775	(8)	0.90785	(8)	0.90749	(8)	0.90758	(7)	0.90730	(9)
	y	0.09225	(8)	0.09215	(8)	0.09251	(8)	0.09242	(7)	0.09270	(9)
	z	-0.00453	(34)	-0.00349	(35)	-0.00843	(31)	-0.00406	(31)	-0.00899	(37)
	Ueq	0.0109	(6)	0.0121	(6)	0.0109	(6)	0.0118	(6)	0.0122	(7)
O5	x	0.09110	(8)	0.09100	(8)	0.09076	(8)	0.09102	(7)	0.09174	(9)
	y	0.90890	(8)	0.90900	(8)	0.90924	(8)	0.90898	(7)	0.90826	(9)
	z	-0.02426	(34)	-0.02283	(35)	-0.02875	(32)	-0.02465	(31)	-0.02949	(37)
	Ueq	0.0103	(6)	0.0118	(6)	0.0105	(6)	0.0117	(5)	0.0118	(7)
O6	x	0.18656	(10)	0.18683	(10)	0.18451	(9)	0.18582	(9)	0.18560	(11)
	y	0.19573	(10)	0.19578	(10)	0.19432	(9)	0.19538	(9)	0.19524	(11)
	z	0.28831	(29)	0.28929	(30)	0.28680	(26)	0.28934	(26)	0.28538	(30)
	Ueq	0.0092	(5)	0.0107	(5)	0.0090	(5)	0.0101	(5)	0.0104	(6)
O7	x	0.28405	(10)	0.28410	(10)	0.28439	(9)	0.28443	(8)	0.28466	(10)
	y	0.28452	(10)	0.28464	(10)	0.28514	(10)	0.28500	(9)	0.28509	(11)
	z	-0.01317	(27)	-0.01252	(28)	-0.01402	(24)	-0.01225	(25)	-0.01644	(31)
	Ueq	0.0098	(5)	0.0111	(5)	0.0095	(5)	0.0107	(5)	0.0102	(6)
O8	x	0.27015	(11)	0.27011	(11)	0.26953	(10)	0.26968	(10)	0.26965	(11)
	y	0.20946	(10)	0.20939	(11)	0.20891	(10)	0.20901	(9)	0.20911	(11)
	z	0.62523	(29)	0.62569	(30)	0.62450	(26)	0.62640	(26)	0.62222	(32)
	Ueq	0.0107	(5)	0.0128	(6)	0.0100	(5)	0.0116	(5)	0.0109	(6)

		CT81		CT82		CT83		CT84		CT85	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0130	(3)	0.0128	(4)	0.0140	(4)	0.0136	(5)	0.0338	(32)
Y	x	0.06185	(5)	0.06193	(6)	0.06209	(5)	0.06211	(7)	0.06219	(2)
	y	0.93815	(5)	0.93807	(6)	0.93791	(5)	0.93789	(7)	0.93781	(2)
	z	0.44486	(27)	0.44424	(28)	0.45101	(29)	0.44476	(35)	0.45023	(142)
	Ueq	0.0078	(5)	0.0077	(5)	0.0083	(5)	0.0084	(7)	0.0086	(18)
Z	x	0.25972	(4)	0.25965	(4)	0.26020	(5)	0.25953	(5)	0.26152	(4)
	y	0.29682	(4)	0.29681	(4)	0.29725	(5)	0.29671	(5)	0.29824	(4)
	z	0.46762	(18)	0.46720	(18)	0.46864	(22)	0.46787	(22)	0.46390	(142)
	Ueq	0.0063	(2)	0.0068	(2)	0.0065	(2)	0.0070	(3)	0.0058	(2)
T	x	0.19012	(3)	0.19018	(4)	0.19017	(4)	0.19015	(4)	0.18994	(4)
	y	0.19203	(3)	0.19207	(4)	0.19209	(4)	0.19212	(4)	0.19196	(4)
	z	0.07944	(18)	0.07919	(17)	0.08100	(21)	0.07985	(22)	0.07461	(142)
	Ueq	0.0051	(2)	0.0056	(2)	0.0051	(2)	0.0059	(2)	0.0054	(2)
B	x	0.89113	(10)	0.89106	(11)	0.89076	(13)	0.89105	(14)	0.88975	(12)
	y	0.10887	(10)	0.10894	(11)	0.10924	(13)	0.10895	(14)	0.11025	(12)
	z	0.62527	(40)	0.62502	(43)	0.62650	(51)	0.62569	(51)	0.61901	(148)
	Ueq	0.0069	(8)	0.0075	(9)	0.0070	(10)	0.0077	(11)	0.0087	(9)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29146	(57)	0.29051	(59)	0.29252	(73)	0.29147	(66)	0.29434	(149)
	Ueq	0.0478	(16)	0.0463	(17)	0.0578	(24)	0.0475	(20)	0.0331	(14)
O2	x	0.94006	(7)	0.94008	(8)	0.93956	(9)	0.94008	(9)	0.93765	(8)
	y	0.05994	(7)	0.05992	(8)	0.06044	(9)	0.05992	(9)	0.06235	(8)
	z	0.59944	(33)	0.60049	(34)	0.60215	(41)	0.60034	(43)	0.58598	(147)
	Ueq	0.0170	(8)	0.0173	(8)	0.0189	(10)	0.0177	(10)	0.0191	(9)
O3	x	0.13465	(8)	0.13483	(8)	0.13492	(9)	0.13482	(10)	0.13418	(9)
	y	0.86535	(8)	0.86517	(8)	0.86508	(9)	0.86518	(10)	0.86582	(9)
	z	0.56973	(29)	0.56960	(30)	0.57101	(36)	0.56993	(36)	0.56586	(144)
	Ueq	0.0106	(5)	0.0106	(6)	0.0100	(7)	0.0116	(8)	0.0113	(6)
O4	x	0.90772	(7)	0.90796	(8)	0.90757	(9)	0.90798	(9)	0.90639	(8)
	y	0.09228	(7)	0.09204	(8)	0.09243	(9)	0.09202	(9)	0.09361	(8)
	z	0.00548	(29)	0.00484	(30)	0.00790	(35)	0.00551	(36)	0.00791	(142)
	Ueq	0.0087	(5)	0.0088	(6)	0.0083	(7)	0.0090	(7)	0.0093	(6)
O5	x	0.09211	(7)	0.09194	(8)	0.09234	(9)	0.09211	(9)	0.09445	(8)
	y	0.90789	(7)	0.90806	(8)	0.90766	(9)	0.90789	(9)	0.90555	(8)
	z	-0.01615	(30)	-0.01681	(32)	-0.01327	(38)	-0.01644	(37)	-0.01592	(142)
	Ueq	0.0089	(5)	0.0093	(6)	0.0088	(6)	0.0093	(7)	0.0094	(6)
O6	x	0.18621	(9)	0.18625	(10)	0.18696	(11)	0.18629	(11)	0.18778	(10)
	y	0.19595	(9)	0.19598	(10)	0.19650	(11)	0.19598	(11)	0.19834	(10)
	z	0.30369	(25)	0.30365	(25)	0.30515	(30)	0.30403	(30)	0.29988	(144)
	Ueq	0.0079	(5)	0.0080	(5)	0.0079	(6)	0.0083	(6)	0.0083	(5)
O7	x	0.28539	(8)	0.28531	(9)	0.28542	(11)	0.28523	(10)	0.28602	(10)
	y	0.28587	(9)	0.28589	(10)	0.28561	(11)	0.28608	(11)	0.28499	(10)
	z	-0.00169	(23)	-0.00248	(24)	-0.00040	(28)	-0.00138	(29)	-0.00455	(144)
	Ueq	0.0069	(4)	0.0072	(5)	0.0070	(5)	0.0074	(6)	0.0076	(5)
O8	x	0.27016	(9)	0.27023	(10)	0.27050	(12)	0.27005	(12)	0.27124	(11)
	y	0.20956	(9)	0.20973	(10)	0.20993	(12)	0.20946	(12)	0.21023	(11)
	z	0.63808	(24)	0.63772	(24)	0.63899	(29)	0.63808	(29)	0.63384	(142)
	Ueq	0.0080	(5)	0.0084	(5)	0.0082	(6)	0.0084	(6)	0.0093	(5)

		CT86		CT87		CT88		CT89		CT90	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0346	(43)	0.0313	(41)	0.0342	(44)	0.0255	(8)	0.0210	(17)
Y	x	0.06221	(3)	0.06218	(3)	0.06152	(3)	0.06644	(2)	0.06227	(5)
	y	0.93779	(3)	0.93782	(3)	0.93848	(3)	0.93356	(2)	0.93773	(5)
	z	0.44819	(198)	0.44672	(185)	0.43598	(183)	0.43435	(35)	0.43597	(68)
	Ueq	0.0095	(3)	0.0096	(3)	0.0073	(3)	0.0128	(2)	0.0067	(5)
Z	x	0.26145	(6)	0.26147	(7)	0.26047	(5)	0.25905	(4)	0.26193	(9)
	y	0.29822	(6)	0.29823	(7)	0.29711	(5)	0.29889	(4)	0.29788	(8)
	z	0.46247	(197)	0.46126	(185)	0.45664	(183)	0.45101	(36)	0.46266	(67)
	Ueq	0.0067	(3)	0.0068	(3)	0.0068	(3)	0.0080	(2)	0.0072	(5)
T	x	0.18996	(6)	0.18999	(6)	0.18964	(4)	0.19052	(4)	0.18900	(10)
	y	0.19196	(5)	0.19195	(5)	0.19161	(4)	0.19162	(3)	0.19073	(9)
	z	0.07301	(197)	0.07196	(185)	0.06394	(183)	0.05588	(35)	0.07308	(67)
	Ueq	0.0060	(3)	0.0065	(3)	0.0058	(2)	0.0070	(2)	0.0079	(5)
B	x	0.88971	(17)	0.88958	(18)	0.89044	(13)	0.89025	(12)	0.89059	(32)
	y	0.11029	(17)	0.11042	(18)	0.10956	(13)	0.10975	(12)	0.10941	(32)
	z	0.61793	(207)	0.61667	(197)	0.61160	(187)	0.60308	(55)	0.61894	(112)
	Ueq	0.0087	(13)	0.0095	(14)	0.0082	(10)	0.0090	(8)	0.0104	(25)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.29294	(208)	0.29233	(201)	0.29583	(185)	0.28573	(56)	0.30540	(119)
	Ueq	0.0361	(21)	0.0411	(26)	0.0201	(11)	0.0120	(8)	0.0098	(23)
O2	x	0.93763	(11)	0.93746	(12)	0.93830	(8)	0.93971	(7)	0.93937	(16)
	y	0.06237	(11)	0.06254	(12)	0.06170	(8)	0.06029	(7)	0.06063	(16)
	z	0.58468	(206)	0.58326	(195)	0.57271	(187)	0.56952	(46)	0.58500	(85)
	Ueq	0.0184	(12)	0.0185	(13)	0.0123	(8)	0.0113	(6)	0.0110	(16)
O3	x	0.13396	(12)	0.13386	(13)	0.13055	(9)	0.13215	(8)	0.12917	(20)
	y	0.86604	(12)	0.86614	(13)	0.86945	(9)	0.86785	(8)	0.87083	(20)
	z	0.56386	(202)	0.56258	(190)	0.55578	(184)	0.53551	(43)	0.56196	(86)
	Ueq	0.0124	(9)	0.0133	(10)	0.0141	(7)	0.0103	(6)	0.0138	(17)
O4	x	0.90629	(11)	0.90627	(11)	0.90532	(8)	0.90561	(7)	0.90822	(18)
	y	0.09371	(11)	0.09373	(11)	0.09468	(8)	0.09439	(7)	0.09178	(18)
	z	0.00599	(200)	0.00493	(188)	-0.00658	(185)	-0.02027	(43)	0.00397	(83)
	Ueq	0.0103	(9)	0.0107	(10)	0.0099	(7)	0.0107	(6)	0.0126	(16)
O5	x	0.09422	(11)	0.09423	(12)	0.09440	(8)	0.09097	(8)	0.09159	(18)
	y	0.90578	(11)	0.90577	(12)	0.90560	(8)	0.90903	(8)	0.90841	(18)
	z	-0.01719	(198)	-0.01862	(187)	-0.02880	(184)	-0.02908	(44)	-0.01709	(85)
	Ueq	0.0095	(8)	0.0104	(9)	0.0100	(7)	0.0119	(6)	0.0117	(15)
O6	x	0.18792	(15)	0.18792	(16)	0.18500	(10)	0.18657	(10)	0.18345	(24)
	y	0.19824	(15)	0.19814	(16)	0.19554	(11)	0.19306	(9)	0.19286	(26)
	z	0.29792	(202)	0.29679	(190)	0.29047	(185)	0.28106	(40)	0.29435	(77)
	Ueq	0.0091	(7)	0.0099	(8)	0.0088	(6)	0.0099	(5)	0.0103	(14)
O7	x	0.28592	(13)	0.28590	(15)	0.28631	(9)	0.28621	(9)	0.28284	(21)
	y	0.28503	(14)	0.28498	(16)	0.28597	(10)	0.28682	(10)	0.28268	(22)
	z	-0.00649	(199)	-0.00722	(187)	-0.01178	(184)	-0.01972	(39)	-0.00160	(76)
	Ueq	0.0083	(7)	0.0091	(8)	0.0080	(5)	0.0090	(5)	0.0105	(13)
O8	x	0.27103	(15)	0.27100	(16)	0.27075	(11)	0.26983	(10)	0.26864	(23)
	y	0.21022	(15)	0.21011	(16)	0.20991	(11)	0.20951	(10)	0.20764	(22)
	z	0.63221	(199)	0.63110	(187)	0.62657	(184)	0.61675	(40)	0.63279	(76)
	Ueq	0.0096	(7)	0.0104	(8)	0.0088	(6)	0.0092	(5)	0.0128	(14)

		CT91		CT92		CT93		CT94		CT95	
X	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0237	(9)	0.0155	(18)	0.0229	(10)	0.0197	(9)	0.0225	(8)
Y	x	0.06249	(3)	0.06178	(6)	0.06214	(3)	0.06215	(3)	0.06168	(2)
	y	0.93751	(3)	0.93822	(6)	0.93786	(3)	0.93785	(3)	0.93832	(2)
	z	0.44069	(40)	0.43027	(76)	0.43584	(42)	0.43447	(41)	0.42756	(32)
	Ueq	0.0055	(3)	0.0050	(5)	0.0057	(3)	0.0059	(3)	0.0060	(2)
Z	x	0.26194	(5)	0.26169	(10)	0.26193	(5)	0.26190	(5)	0.26186	(4)
	y	0.29818	(5)	0.29756	(10)	0.29795	(5)	0.29781	(5)	0.29775	(4)
	z	0.46513	(39)	0.45889	(76)	0.46180	(42)	0.46144	(40)	0.45633	(32)
	Ueq	0.0068	(2)	0.0058	(6)	0.0064	(3)	0.0068	(3)	0.0069	(2)
T	x	0.18947	(4)	0.18853	(11)	0.18918	(5)	0.18885	(6)	0.18845	(4)
	y	0.19130	(4)	0.19020	(11)	0.19099	(5)	0.19063	(5)	0.19025	(4)
	z	0.07657	(39)	0.06759	(76)	0.07253	(42)	0.07158	(41)	0.06523	(32)
	Ueq	0.0065	(2)	0.0077	(7)	0.0066	(3)	0.0070	(3)	0.0080	(3)
B	x	0.89034	(14)	0.89026	(39)	0.89013	(17)	0.89065	(19)	0.89066	(15)
	y	0.10966	(14)	0.10974	(39)	0.10987	(17)	0.10935	(19)	0.10934	(15)
	z	0.62236	(60)	0.61404	(133)	0.61765	(67)	0.61676	(71)	0.61141	(59)
	Ueq	0.0077	(10)	0.0084	(26)	0.0081	(13)	0.0091	(14)	0.0104	(12)
O1	x	0		0		0		0		0	
	y	0		0		0		0		0	
	z	0.30842	(62)	0.30385	(145)	0.30543	(68)	0.30429	(71)	0.30130	(58)
	Ueq	0.0100	(10)	0.0094	(29)	0.0093	(12)	0.0091	(14)	0.0096	(10)
O2	x	0.93911	(8)	0.93986	(20)	0.93930	(9)	0.93925	(10)	0.93965	(8)
	y	0.06089	(8)	0.06014	(20)	0.06070	(9)	0.06075	(10)	0.06035	(8)
	z	0.58876	(50)	0.57856	(94)	0.58377	(54)	0.58342	(52)	0.57557	(43)
	Ueq	0.0103	(7)	0.0080	(19)	0.0097	(9)	0.0091	(10)	0.0095	(8)
O3	x	0.13018	(9)	0.12906	(22)	0.12985	(11)	0.12932	(12)	0.12828	(9)
	y	0.86982	(9)	0.87094	(22)	0.87015	(11)	0.87068	(12)	0.87172	(9)
	z	0.56518	(48)	0.55692	(92)	0.56093	(52)	0.56014	(51)	0.55554	(43)
	Ueq	0.0125	(8)	0.0087	(20)	0.0125	(9)	0.0114	(10)	0.0128	(8)
O4	x	0.90736	(9)	0.90763	(21)	0.90733	(10)	0.90781	(11)	0.90757	(8)
	y	0.09264	(9)	0.09237	(21)	0.09267	(10)	0.09219	(11)	0.09243	(8)
	z	0.00636	(50)	-0.00483	(95)	0.00187	(52)	0.00143	(53)	-0.00633	(43)
	Ueq	0.0120	(7)	0.0115	(18)	0.0123	(8)	0.0119	(10)	0.0137	(8)
O5	x	0.09190	(9)	0.09163	(20)	0.09168	(10)	0.09131	(11)	0.09148	(8)
	y	0.90810	(9)	0.90837	(20)	0.90832	(10)	0.90869	(11)	0.90852	(8)
	z	-0.01419	(47)	-0.02447	(970	-0.01908	(51)	-0.01888	(52)	-0.02548	(41)
	Ueq	0.0109	(7)	0.0092	(18)	0.0106	(8)	0.0110	(9)	0.0118	(8)
O6	x	0.18460	(11)	0.18207	(28)	0.18395	(13)	0.18313	(14)	0.18226	(11)
	y	0.19439	(12)	0.19154	(31)	0.19375	(13)	0.19290	(16)	0.19184	(12)
	z	0.29748	(45)	0.28760	(86)	0.29316	(49)	0.29134	(47)	0.28502	(39)
	Ueq	0.0095	(6)	0.0092	(16)	0.0089	(7)	0.0088	(8)	0.0098	(7)
O7	x	0.28411	(10)	0.28283	(25)	0.28382	(12)	0.28314	(13)	0.28296	(10)
	y	0.28429	(11)	0.28299	(26)	0.28388	(13)	0.28326	(14)	0.28308	(11)
	z	-0.00037	(44)	-0.00569	(86)	-0.00351	(47)	-0.00320	(46)	-0.00819	(38)
	Ueq	0.0106	(6)	0.0110	(16)	0.0105	(7)	0.0107	(8)	0.0124	(7)
O8	x	0.26873	(12)	0.26853	(27)	0.26888	(13)	0.26842	(14)	0.26799	(12)
	y	0.20818	(12)	0.20774	(25)	0.20811	(13)	0.20771	(14)	0.20749	(11)
	z	0.63609	(45)	0.62964	(88)	0.63241	(48)	0.63186	(47)	0.62694	(40)
	Ueq	0.0129	(6)	0.0116	(16)	0.0124	(8)	0.0120	(8)	0.0136	(7)

		CT96		CT97		CT98		CT99	
X	x	0		0		0		0	
	y	0		0		0		0	
	z	0.84080		0.84080		0.84080		0.84080	
	Ueq	0.0262	(18)	0.0312	(27)	0.0262	(35)	0.0223	(7)
Y	x	0.06205	(4)	0.06202	(6)	0.06190	(8)	0.06126	(2)
	y	0.93795	(4)	0.93798	(6)	0.93810	(8)	0.93874	(2)
	z	0.42870	(74)	0.42670	(110)	0.42917	(137)	0.42042	(26)
	Ueq	0.0066	(4)	0.0051	(6)	0.0065	(8)	0.0107	(2)
Z	x	0.26203	(6)	0.26198	(9)	0.26184	(11)	0.26282	(3)
	y	0.29805	(6)	0.29796	(9)	0.29788	(12)	0.29896	(3)
	z	0.45944	(74)	0.45805	(109)	0.46055	(136)	0.45174	(25)
	Ueq	0.0054	(33)	0.0067	(5)	0.0065	(7)	0.0094	(2)
T	x	0.18778	(8)	0.18758	(12)	0.18805	(16)	0.18763	(4)
	y	0.18964	(8)	0.18935	(12)	0.18961	(16)	0.18915	(4)
	z	0.06985	(74)	0.06812	(110)	0.07073	(137)	0.06466	(26)
	Ueq	0.0063	(4)	0.0086	(7)	0.0084	(9)	0.0094	(2)
B	x	0.89182	(28)	0.89303	(42)	0.89147	(55)	0.89029	(12)
	y	0.10818	(28)	0.10697	(42)	0.10853	(55)	0.10971	(12)
	z	0.61435	(111)	0.61308	(181)	0.61541	(217)	0.60698	(51)
	Ueq	0.0086	(21)	0.0138	(34)	0.0090	(39)	0.0107	(10)
O1	x	0		0		0		0	
	y	0		0		0		0	
	z	0.30343	(120)	0.29866	(176)	0.30306	(226)	0.29339	(56)
	Ueq	0.0093	(20)	0.0153	(35)	0.0094	(40)	0.0143	(9)
O2	x	0.93912	(15)	0.93861	(23)	0.93940	(29)	0.93867	(8)
	y	0.06088	(15)	0.06139	(23)	0.06060	(29)	0.06133	(8)
	z	0.57721	(88)	0.57573	(129)	0.57807	(166)	0.57063	(41)
	Ueq	0.0081	(13)	0.0101	(21)	0.0098	(28)	0.0124	(7)
O3	x	0.12776	(17)	0.12696	(24)	0.12768	(32)	0.12856	(9)
	y	0.87224	(17)	0.87304	(24)	0.87232	(32)	0.87144	(9)
	z	0.55858	(87)	0.55702	(130)	0.56202	(158)	0.55169	(38)
	Ueq	0.0120	(15)	0.0120	(22)	0.0088	(28)	0.0134	(7)
O4	x	0.90845	(16)	0.90872	(24)	0.90815	(32)	0.90796	(9)
	y	0.09155	(16)	0.09128	(24)	0.09185	(32)	0.09204	(9)
	z	0.00083	(89)	-0.00515	(138)	-0.00196	(172)	-0.00413	(40)
	Ueq	0.0120	(14)	0.0174	(23)	0.0147	(28)	0.0142	(7)
O5	x	0.09162	(15)	0.09143	(24)	0.09155	(31)	0.09138	(9)
	y	0.90838	(15)	0.90857	(24)	0.90845	(31)	0.90862	(9)
	z	-0.01883	(87)	-0.02196	(131)	-0.01929	(164)	-0.02209	(37)
	Ueq	0.0103	(14)	0.0137	(22)	0.0112	(27)	0.0134	(6)
O6	x	0.18204	(21)	0.18196	(32)	0.18190	(40)	0.18319	(12)
	y	0.19132	(23)	0.19104	(34)	0.19113	(44)	0.19207	(12)
	z	0.28656	(82)	0.28160	(124)	0.28557	(153)	0.28004	(35)
	Ueq	0.0087	(12)	0.0115	(18)	0.0088	(23)	0.0124	(6)
O7	x	0.28229	(19)	0.28306	(30)	0.28241	(38)	0.28127	(11)
	y	0.28146	(20)	0.28233	(29)	0.28215	(40)	0.28047	(11)
	z	-0.00373	(79)	-0.00596	(117)	-0.00334	(148)	-0.01138	(31)
	Ueq	0.0096	(11)	0.0123	(18)	0.0113	(24)	0.0129	(6)
O8	x	0.26459	(21)	0.26571	(31)	0.26621	(40)	0.26736	(12)
	y	0.20497	(19)	0.20593	(30)	0.20576	(38)	0.20654	(12)
	z	0.63128	(82)	0.63067	(125)	0.63243	(155)	0.62243	(33)
	Ueq	0.0108	(12)	0.0156	(19)	0.0144	(24)	0.0141	(6)

Section C.2

		CT1		CT2		CT3		CT4		CT5	
H3	x	0.1264	(15)	0.1308	(15)	0.1257	(14)	0.1267	(18)	0.1327	(19)
	y	0.8736	(15)	0.8692	(15)	0.8743	(14)	0.8734	(18)	0.8673	(19)
	z	0.7021	(10)	0.7047	(6)	0.7022	(12)	0.7040	(12)	0.7066	(5)
	Ueq	0.0263	(108)	0.0308	(114)	0.0145	(99)	0.0385	(140)	0.0542	(156)

		CT6		CT7		CT8		CT9		CT10	
H3	x	0.1309	(14)	0.1286	(15)	0.1305	(16)	0.1308	(23)	0.1316	(18)
	y	0.8691	(14)	0.8714	(15)	0.8696	(16)	0.8692	(23)	0.8684	(18)
	z	0.7055	(5)	0.7034	(9)	0.7015	(6)	0.7035	(8)	0.7043	(7)
	Ueq	0.0284	(103)	0.0285	(114)	0.0432	(125)	0.0633	(190)	0.0380	(144)

		CT11		CT12		CT13		CT14		CT15	
H3	x	0.1383	(18)	0.1369	(17)	0.1426	(19)	0.1268	(19)	0.1272	(15)
	y	0.8617	(18)	0.8632	(17)	0.8575	(19)	0.8732	(19)	0.8728	(15)
	z	0.7027	(13)	0.7030	(11)	0.7007	(20)	0.7040	(14)	0.7023	(8)
	Ueq	0.0379	(131)	0.0460	(131)	0.0370	(144)	0.0391	(152)	0.0380	(113)

		CT16		CT17		CT18		CT19		CT20	
H3	x	0.1320	(14)	0.1311	(13)	0.1335	(15)	0.1348	(18)	0.1281	(23)
	y	0.8680	(14)	0.8689	(13)	0.8665	(15)	0.8652	(18)	0.8719	(23)
	z	0.7048	(6)	0.7045	(6)	0.7055	(5)	0.7054	(5)	0.7034	(17)
	Ueq	0.0173	(102)	0.0166	(94)	0.0252	(109)	0.0240	(128)	0.5327	(359)

		CT21		CT22		CT23		CT24		CT25	
H3	x	0.1373	(20)	0.1343	(20)	0.1298	(16)	0.1329	(16)	0.1365	(16)
	y	0.8627	(20)	0.8657	(20)	0.8702	(16)	0.8671	(16)	0.8636	(16)
	z	0.7056	(8)	0.7041	(7)	0.7041	(10)	0.7049	(6)	0.7045	(8)
	Ueq	0.0390	(151)	0.0227	(146)	0.0134	(106)	0.0240	(116)	0.0280	(116)

		CT26		CT27		CT28		CT29		CT30	
H3	x	0.1338	(17)	0.1268	(16)	0.1308	(16)	0.1317	(16)	0.1303	(13)
	y	0.8662	(17)	0.8732	(16)	0.8692	(16)	0.8683	(16)	0.8697	(13)
	z	0.7059	(5)	0.7032	(12)	0.7062	(7)	0.7044	(6)	0.7037	(7)
	Ueq	0.0402	(133)	0.0392	(129)	0.0222	(117)	0.0133	(106)	0.0229	(98)

		CT31		CT32		CT33		CT34		CT35	
H3	x	0.1281	(18)	0.1356	(14)	0.1362	(19)	0.1177	(17)	0.1346	(17)
	y	0.8719	(18)	0.8644	(14)	0.8638	(19)	0.8823	(17)	0.8654	(17)
	z	0.7033	(11)	0.7028	(5)	0.6959	(13)	0.6829	(24)	0.7032	(6)
	Ueq	0.0518	(147)	0.0186	(100)	0.0614	(153)	0.0778	(183)	0.0350	(134)

		CT36		CT37		CT38		CT39		CT40	
H3	x	0.1328	(15)	0.1232	(18)	0.1257	(17)	0.1281	(25)	0.1240	(14)
	y	0.8672	(15)	0.8769	(18)	0.8743	(17)	0.8720	(25)	0.8760	(14)
	z	0.7030	(5)	0.6871	(21)	0.6954	(11)	0.6953	(10)	0.6900	(10)
	Ueq	0.0325	(118)	0.0497	(158)	0.0354	(138)	0.0338	(190)	0.0457	(122)

		CT41		CT42		CT43		CT44		CT45	
H3	x	0.1289	(33)	0.1300	(16)	0.1249	(13)	0.1295	(14)	0.1344	(18)
	y	0.8711	(33)	0.8700	(16)	0.8751	(13)	0.8705	(14)	0.8656	(18)
	z	0.6961	(9)	0.6960	(6)	0.6977	(9)	0.6900	(8)	0.6946	(4)
	Ueq	0.0688	(314)	0.0269	(125)	0.0527	(117)	0.0508	(121)	0.0398	(144)

		CT46		CT47		CT48		CT49		CT50	
H3	x	0.1330	(18)	0.1311	(14)	0.1296	(19)	0.1310	(14)	0.1295	(15)
	y	0.8670	(18)	0.8689	(14)	0.8704	(19)	0.8690	(14)	0.8705	(15)
	z	0.6975	(5)	0.6923	(5)	0.6917	(9)	0.6959	(7)	0.6945	(10)
	Ueq	0.0372	(144)	0.0362	(109)	0.0433	(154)	0.05		0.0483	(130)

		CT51		CT52		CT53		CT54		CT55	
H3	x	0.1300	(14)	0.1281	(15)	0.1312	(17)	0.1342	(29)	0.1281	(13)
	y	0.8700	(14)	0.8719	(15)	0.8689	(17)	0.8658	(29)	0.8719	(13)
	z	0.6937	(9)	0.6884	(11)	0.6911	(8)	0.6952	(7)	0.6974	(11)
	Ueq	0.0412	(116)	0.0328	(117)	0.0444	(134)	0.0681	(253)	0.0159	(94)

		CT56		CT57		CT58		CT59		CT60	
H3	x	0.1257	(22)	0.1326	(16)	0.1318	(33)	0.1307	(18)	0.1326	(16)
	y	0.8743	(22)	0.8674	(16)	0.8682	(33)	0.8693	(18)	0.8674	(16)
	z	0.6908	(22)	0.6915	(5)	0.6929	(16)	0.7027	(10)	0.7045	(6)
	Ueq	0.0590	(194)	0.05		0.0397	(267)	0.0317	(140)	0.0236	(115)

		CT61		CT62		CT63		CT64		CT65	
H3	x	0.1303	(14)	0.1311	(14)	0.1282	(14)	0.1328	(16)	0.1228	(19)
	y	0.8698	(14)	0.8689	(14)	0.8718	(14)	0.8672	(16)	0.8772	(19)
	z	0.7040	(8)	0.6999	(7)	0.6985	(11)	0.6937	(3)	0.6867	(24)
	Ueq	0.0181	(103)	0.0236	(108)	0.0260	(113)	0.0441	(134)	0.0660	(167)

		CT66		CT67		CT68		CT69		CT70	
H3	x	0.1331	(16)	0.1306	(14)	0.1280	(15)	0.1180	(21)	0.1384	(15)
	y	0.8670	(16)	0.8694	(14)	0.8720	(15)	0.8820	(21)	0.8616	(15)
	z	0.6944	(4)	0.6913	(5)	0.6904	(11)	0.6785	(40)	0.6925	(9)
	Ueq	0.0269	(116)	0.0451	(114)	0.0606	(133)	0.0658	(205)	0.0242	(110)

		CT71		CT72		CT73		CT74		CT75	
H3	x	0.1283	(16)	0.1271	(15)	0.1346	(33)	0.1369	(16)	0.1346	(16)
	y	0.8717	(16)	0.8730	(15)	0.8654	(33)	0.8631	(16)	0.8654	(16)
	z	0.6904	(9)	0.6936	(9)	0.6921	(6)	0.6919	(6)	0.6940	(4)
	Ueq	0.0595	(140)	0.0645	(137)	0.0714	(318)	0.0384	(140)	0.0456	(136)

		CT76		CT77		CT78		CT79		CT80	
H3	x	0.1269	(16)	0.1288	(20)	0.1163	(19)	0.1284	(15)	0.1307	(17)
	y	0.8731	(16)	0.8712	(20)	0.8838	(19)	0.8716	(15)	0.8693	(17)
	z	0.6885	(12)	0.6899	(11)	0.6760	(34)	0.6911	(7)	0.6881	(5)
	Ueq	0.0385	(133)	0.0708	(191)	0.0787	(208)	0.0522	(132)	0.05	

		CT81	CT82	CT83	CT84	CT85
H3	x	0.1329 (19)	0.1307 (19)	0.1359 (19)	0.1286 (19)	0.1341 (17)
	y	0.8671 (19)	0.8693 (19)	0.8641 (19)	0.8714 (19)	0.8659 (17)
	z	0.7078 (5)	0.7066 (9)	0.7088 (4)	0.7057 (13)	0.7034 (14)
	Ueq	0.0582 (157)	0.0501 (153)	0.0341 (144)	0.0440 (154)	0.0585 (206)

		CT86	CT87	CT88	CT89	CT90
H3	x	0.1346 (25)	0.1319 (27)	0.1245 (17)		0.1556 (38)
	y	0.8654 (25)	0.8681 (27)	0.8756 (17)		0.8444 (38)
	z	0.7013 (20)	0.6998 (20)	0.6915 (21)		0.6507 (162)
	Ueq	0.0395 (191)	0.0464 (221)	0.0482 (142)		0.2922 (1094)

		CT91	CT92	CT93	CT94	CT95
H3	x	0.1268 (14)	0.1201 (28)	0.1227 (18)	0.1185 (20)	0.1213 (12)
	y	0.8732 (14)	0.8800 (28)	0.8773 (18)	0.8815 (20)	0.8788 (12)
	z	0.6994 (7)	0.6865 (30)	0.6928 (15)	0.6875 (25)	0.6868 (10)
	Ueq	0.0208 (109)	0.0169 (239)	0.0451 (164)	0.0590 (204)	0.01

		CT96	CT97	CT98	CT99
H3	x			0.1212 (42)	0.1127 (24)
	y			0.8788 (42)	0.8873 (24)
	z			0.6920 (33)	0.6681 (26)
	Ueq			0.01	0.0643 (230)

Section C.3

		CT79
H1	x	0
	y	0
	z	0.1588 (5)
	Ueq	0.05

APPENDIX D

Site-scattering (*epfu*) Data

This appendix lists the refined site-scattering at the *X*-, *Y*-, *Z*- and *W*-sites in equivalent electrons per formula unit. Typical standard deviations are between 0.1 – 0.5 *epfu* at each site. The *T*-site was not refined for any sample.

	CT1	CT2	CT3	CT4	CT5	CT6	CT7	CT8
X	7.45	8.92	6.64	7.24	8.40	8.21	7.38	6.62
Y	27.89	32.64	28.54	26.12	24.98	29.37	24.99	29.43
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	8.97	9.30	8.90	9.19	9.42	9.23	9.30	8.83

	CT9	CT10	CT11	CT12	CT13	CT14	CT15	CT16
X	6.09	7.81	8.00	7.03	9.99	6.89	5.81	10.29
Y	28.30	24.95	26.13	30.36	30.25	26.71	30.49	38.96
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	8.64	9.30	9.07	8.78	9.48	9.10	8.00	9.49

	CT17	CT18	CT19	CT20	CT21	CT22	CT23	CT24
X	9.63	10.26	10.86	10.14	11.03	10.12	9.97	9.34
Y	38.52	37.36	39.36	41.95	38.44	44.13	42.26	37.66
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	9.36	9.42	9.66	10.38	9.59	9.48	9.45	9.33

	CT25	CT26	CT27	CT28	CT29	CT30	CT31	CT32
X	8.75	9.99	8.03	8.22	8.38	9.30	8.64	10.76
Y	31.00	32.43	30.08	29.87	27.83	39.87	25.57	39.51
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	9.43	9.47	9.10	9.32	9.53	9.34	9.30	9.84

	CT33	CT34	CT35	CT36	CT37	CT38	CT39	CT40
X	9.71	11.50	12.32	10.76	15.74	9.91	10.84	11.04
Y	42.84	52.06	39.49	37.35	43.68	37.85	37.56	46.09
Z	78.00	79.14	78.00	78.00	78.00	78.00	78.00	78.00
W	8.00	8.90	8.00	8.00	9.26	8.51	8.00	8.00

	CT41	CT42	CT43	CT44	CT45	CT46	CT47	CT48
X	10.42	9.16	8.37	9.60	14.76	11.83	13.36	13.63
Y	42.62	43.19	41.44	45.05	37.46	36.20	36.37	36.22
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	8.00	8.00	8.00	9.33	9.11	9.17	9.42	9.37

	CT49	CT50	CT51	CT52	CT53	CT54	CT55	CT56
X	10.72	10.72	10.73	9.45	9.51	9.36	11.51	6.69
Y	51.37	49.34	53.48	61.19	62.82	63.60	44.59	61.99
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	9.31	9.32	9.12	9.45	9.55	9.34	9.26	9.89

	CT57	CT58	CT59	CT60	CT61	CT62	CT63	CT64
X	11.51	7.26	9.95	10.54	10.38	11.34	11.10	15.87
Y	66.40	62.09	45.25	44.37	44.63	44.42	45.36	37.34
Z	79.98	78.63	78.00	78.00	78.00	78.00	78.00	78.00
W	8.00	9.54	9.64	9.44	9.17	8.85	9.47	8.96

	CT65	CT66	CT67	CT68	CT69	CT70	CT71	CT72
X	19.69	16.20	17.56	18.85	18.72	15.92	17.04	11.83
Y	37.79	36.87	36.73	38.49	37.86	36.57	36.64	46.04
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	9.46	8.89	9.40	9.80	9.99	9.22	9.31	8.42

	CT73	CT74	CT75	CT76	CT77	CT78	CT79	CT80
X	17.48	19.23	16.04	15.66	15.55	16.67	15.10	14.00
Y	36.78	36.77	36.64	49.12	47.73	39.15	41.57	45.19
Z	78.00	78.00	78.00	79.16	78.00	78.00	78.00	78.00
W	9.68	8.00	8.96	9.09	9.03	9.19	8.00	8.00

	CT81	CT82	CT83	CT84	CT85	CT86	CT87	CT88
X	16.03	17.40	17.53	17.00	3.31	3.55	3.82	2.63
Y	23.21	22.28	28.71	20.83	59.77	59.76	58.05	46.37
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
W	9.56	9.35	9.65	9.29	8.00	8.00	8.47	8.00

	CT89	CT90	CT91	CT92	CT93	CT94	CT95	CT96
X	11.09	11.91	11.45	11.83	12.13	12.69	12.47	11.07
Y	66.00	56.60	49.57	64.40	53.48	58.19	64.37	65.15
Z	82.87	92.19	83.55	94.69	85.36	95.62	95.37	114.28
W	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00

	CT97	CT98	CT99
X	11.86	11.25	14.16
Y	61.02	64.20	70.97
Z	112.23	115.03	128.06
W	8.83	8.00	8.00

APPENDIX E

Chemistry (*epfu*) Data

This appendix lists the assigned chemistry from electron-microprobe analysis at the *X*-, *Y*-, *Z*-, *T*- and *W*-sites in equivalent electrons per formula unit (*epfu*).

Section E.1 lists the *epfu* from the standard normalization and site-assignment scheme discussed in Chapter 3.

Section E.2 lists the *epfu* for those samples (marked with * in Section E.1) that were renormalized on 6 Si *apfu* as initial Si *apfu* values exceeded 6 *apfu* (initial *epfu* > 84).

Section E.3 lists the *epfu* for CT96, calculated as described in Chapter 5, and CT99, calculated as described in Chapter 6.

Section E.1:

	CT1	CT2	CT3	CT4	CT5*	CT6	CT7*	CT8
X	6.38	8.58	5.91	7.07	7.49	7.58	7.35	5.81
Y	26.56	32.94	28.07	26.23	24.79	29.31	24.69	27.64
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	83.92	83.99	83.99	83.96	84.64	83.90	85.09	83.96
W	8.22	8.43	8.32	8.44	8.47	8.47	8.46	8.17

	CT9*	CT10*	CT11	CT12	CT13*	CT14	CT15	CT16*
X	5.63	7.12	6.91	6.29	7.88	6.83	6.49	9.75
Y	26.36	24.53	28.87	29.08	28.41	27.63	27.27	38.53
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	84.14	85.76	83.92	83.88	84.11	83.91	83.84	84.83
W	8.21	8.48	8.44	8.30	8.46	8.45	8.28	8.68

	CT17*	CT18*	CT19*	CT20*	CT21*	CT22	CT23*	CT24*
X	9.00	9.33	9.59	9.19	9.95	9.09	9.41	8.82
Y	37.89	36.76	38.89	39.26	38.16	44.64	42.39	37.74
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	84.38	84.92	85.16	85.23	85.09	83.98	84.20	84.06
W	8.58	8.66	8.58	8.65	8.76	8.56	8.68	8.52

	CT25*	CT26*	CT27*	CT28*	CT29*	CT30	CT31*	CT32
X	7.71	8.45	15.12	7.74	9.32	9.15	8.71	10.58
Y	30.91	31.42	29.19	29.12	29.86	40.97	26.57	40.30
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	84.50	84.69	84.66	84.98	84.53	83.92	84.50	83.95
W	8.50	8.61	8.57	8.51	8.59	8.56	8.56	8.79

	CT33*	CT34	CT35*	CT36*	CT37*	CT38	CT39	CT40
X	9.32	11.09	18.68	9.83	15.97	9.44	10.39	11.44
Y	46.18	49.98	36.59	36.00	34.89	35.34	35.16	46.49
Z	78.00	77.10	77.80	78.00	77.39	78.00	78.00	77.35
T	84.36	83.80	84.41	84.07	84.80	83.94	83.92	83.78
W	8.01	8.17	8.00	8.13	8.50	8.10	8.14	8.14

	CT41	CT42	CT43	CT44	CT45	CT46*	CT47	CT48
X	10.49	9.49	7.81	12.09	14.60	11.12	13.21	14.08
Y	43.35	41.65	41.75	46.28	36.76	35.41	36.14	35.91
Z	77.74	77.97	78.00	77.89	77.46	77.96	78.00	78.00
T	83.83	83.82	83.89	83.89	84.00	84.28	83.64	83.67
W	8.05	8.09	8.03	8.10	8.69	8.70	8.64	8.70

	CT49	CT50	CT51	CT52	CT53*	CT54*	CT55	CT56
X	10.73	10.81	10.87	8.95	9.33	6.79	10.99	6.46
Y	51.51	49.75	54.88	63.14	66.12	66.85	45.86	65.34
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	84.00	83.92	83.94	83.95	84.13	84.34	83.96	83.85
W	8.75	8.75	8.77	8.24	8.47	8.10	8.48	8.23

	CT57	CT58	CT59*	CT60*	CT61*	CT62	CT63	CT64
X	11.12	6.90	9.65	9.89	9.77	11.42	10.99	15.57
Y	68.33	66.40	45.14	43.42	45.63	46.09	46.17	36.13
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	77.48
T	83.54	83.71	86.10	84.45	84.39	83.87	83.86	83.97
W	8.14	8.41	8.53	8.73	8.70	8.60	8.56	8.50

	CT65	CT66	CT67	CT68	CT69	CT70	CT71	CT72
X	19.50	16.57	15.78	17.90	18.00	15.84	16.26	16.72
Y	37.09	37.33	38.45	38.78	36.74	36.26	36.46	45.59
Z	77.07	77.27	77.36	77.29	77.28	77.38	77.41	77.31
T	83.93	83.95	83.87	83.88	83.96	84.00	83.93	83.91
W	8.76	8.54	8.71	8.83	8.77	8.73	8.64	8.66

	CT73	CT74	CT75*	CT76*	CT77	CT78	CT79	CT80
X	17.76	18.80	13.77	15.17	15.64	15.69	15.72	13.39
Y	36.92	37.11	36.14	53.59	54.51	36.17	43.06	47.01
Z	77.63	77.28	77.56	77.11	77.12	77.66	77.51	77.21
T	83.52	83.74	84.11	85.02	83.98	83.75	83.93	83.71
W	8.83	8.99	8.43	8.38	8.38	8.20	8.23	8.30

	CT81*	CT82*	CT83*	CT84	CT85*	CT86	CT87	CT88
X	14.84	16.54	14.10	16.72	2.82	3.13	3.63	1.81
Y	23.28	22.55	29.00	21.69	60.63	60.59	59.34	44.60
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	85.01	84.21	84.62	83.97	84.21	83.92	83.95	83.83
W	8.78	8.85	8.76	8.82	8.02	8.02	8.02	8.03

	CT89	CT90	CT91*	CT92	CT93*	CT94	CT95	CT96*
X	10.72	10.54	10.50	11.19	10.57	11.30	11.01	12.62
Y	72.24	60.59	56.13	62.40	55.45	64.57	61.56	78.94
Z	78.00	76.06	76.38	94.24	76.29	89.18	96.29	106.37
T	83.75	84.00	84.18	83.89	84.78	83.95	83.92	84.13
W	8.79	8.21	8.16	8.39	8.13	8.29	8.34	8.43

	CT97*	CT98*	CT99*
X	12.01	12.12	15.40
Y	71.04	72.71	95.88
Z	108.71	105.30	105.63
T	86.35	87.46	91.22
W	8.52	8.40	8.01

Section E.2:

	CT5	CT7	CT9	CT10	CT13	CT16	CT17	CT18
X	7.45	7.73	5.62	6.98	8.08	9.64	8.96	9.38
Y	24.21	31.78	26.23	22.98	30.39	37.64	37.50	35.82
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	84.00	84.00	84.00	84.00	84.00	84.00	84.00	84.00
W	8.47	8.48	8.21	8.47	8.47	8.68	8.58	8.66

	CT19	CT20	CT21	CT23	CT24	CT25	CT26	CT27
X	9.46	9.05	9.83	9.38	8.80	7.67	8.39	7.51
Y	37.68	37.96	37.03	42.17	37.67	30.43	30.73	28.58
Z	78.00	78.00	78.00	78.00	78.00	78.00	78.00	78.00
T	84.00	84.00	84.00	84.00	84.00	84.00	84.00	84.00
W	8.58	8.64	8.75	8.68	8.52	8.50	8.60	8.56

	CT28	CT29	CT31	CT33	CT35	CT36	CT37	CT46
X	7.65	9.25	8.68	9.29	10.52	9.83	14.27	11.10
Y	28.17	29.35	26.10	45.77	36.22	35.92	42.99	35.15
Z	78.00	78.00	78.00	78.00	77.77	78.00	77.34	77.94
T	84.00	84.00	84.00	84.00	84.00	84.00	84.00	84.00
W	8.50	8.59	8.56	8.01	8.00	8.13	8.49	8.70

	CT53	CT54	CT59	CT60	CT61	CT75	CT76	CT81
X	9.32	6.77	9.63	9.83	9.73	13.77	14.99	14.66
Y	65.91	66.37	44.92	40.97	45.16	36.03	51.41	22.38
Z	78.00	78.00	78.00	78.00	78.00	77.55	77.05	78.00
T	84.00	84.00	84.00	84.00	84.00	84.00	84.00	84.00
W	8.46	8.10	8.52	8.72	8.70	8.43	8.38	8.77

	CT82	CT83	CT85	CT91	CT93	CT97	CT98
X	16.50	14.01	2.81	10.48	10.49	11.67	11.64
Y	22.36	28.43	60.33	55.93	54.52	65.93	65.18
Z	78.00	78.00	78.00	76.37	76.25	109.68	106.83
T	84.00	84.00	84.00	84.00	84.00	84.00	84.00
W	8.85	8.76	8.02	8.16	8.13	8.50	8.38

Section E.3:

	CT96	CT99
X	12.43	14.06
Y	73.71	73.52
Z	107.82	110.28
T	83.92	83.97

APPENDIX F

Selected Interatomic Distances and Angles

This appendix lists the values of selected interatomic distances (Å) and angles (°) within the tourmaline structure for each sample. Mean bond-length is indicated by the symbol <*R*-O>, where *R* is a given cation or site and O is oxygen. Symmetry operators for equivalent positions are as follows:

a: 1-*x*+*y*, *y*, *z*
b: *x*, 1+*x*-*y*, *z*
c: 1-*y*, *x*-*y*, *z*
d: 2/3-*y*, 1/3+*x*-*y*, 1/3+*z*
e: 1/3+*y*-*x*, 2/3-*x*, 2/3+*z*
f: 1/3+*y*-*x*, 2/3-*x*, *z*-1/3
g: *x*, 1+*y*, *z*
h: *x*-1, *x*-*y*, *z*
i: 1-*x*+*y*, 1+*y*, *z*
j: -*x*+*y*, 1-*x*, *z*
k: *x*-1, *y*, *z*
l: *x*-1, *x*-*y*-1, *z*
m: *x*-1, *y*, 1+*z*
n: *x*-1, *x*-*y*-1, 1+*z*
o:1-*x*+*y*, *y*, 1+*z*
p: *x*, *y*-1, 1+*z*
q: *x*, 1+*x*-*y*, 1+*z*
r: *x*-*y*-1, -*x*, 1+*z*

	CT1	CT2	CT3	CT4	CT5	CT6	CT7
X-O(2) k,l,a	2.463 (3)	2.446 (3)	2.460 (4)	2.449 (3)	2.434 (3)	2.445 (3)	2.446 (3)
X-O(4) m,n,o	2.815 (2)	2.811 (2)	2.810 (2)	2.808 (2)	2.812 (2)	2.811 (2)	2.806 (2)
X-O(5) p,q,r	2.745 (2)	2.750 (2)	2.748 (2)	2.745 (2)	2.749 (2)	2.749 (2)	2.746 (2)
<*X*-O>	2.674	2.669	2.673	2.667	2.665	2.668	2.666
Y-O(1) g	1.950 (2)	1.997 (3)	1.962 (4)	1.971 (3)	1.981 (3)	1.977 (3)	1.984 (3)
Y-O(2) h,l	1.964 (3)	1.968 (3)	1.962 (4)	1.966 (3)	1.966 (3)	1.964 (3)	1.969 (3)
Y-O(3)	2.135 (2)	2.151 (2)	2.135 (3)	2.140 (2)	2.145 (2)	2.141 (2)	2.154 (2)
Y-O(6) j,b	1.958 (3)	1.990 (2)	1.969 (3)	1.961 (3)	1.965 (3)	1.972 (2)	1.972 (3)
<*Y*-O>	1.988	2.011	1.993	1.994	1.998	1.998	2.003
Z-O(3) b	1.962 (2)	1.959 (2)	1.961 (3)	1.962 (3)	1.953 (3)	1.961 (2)	1.956 (3)
Z-O(6)	1.867 (3)	1.852 (3)	1.859 (4)	1.858 (3)	1.855 (3)	1.855 (3)	1.852 (3)
Z-O(7) d	1.945 (3)	1.946 (2)	1.943 (3)	1.941 (3)	1.946 (3)	1.740 (2)	1.947 (3)
Z-O(7) e	1.888 (4)	1.881 (3)	1.882 (5)	1.882 (4)	1.881 (3)	1.880 (3)	1.885 (4)
Z-O(8)	1.901 (3)	1.906 (3)	1.901 (4)	1.900 (4)	1.898 (3)	1.903 (3)	1.903 (3)
Z-O(8) f	1.887 (3)	1.880 (3)	1.882 (4)	1.884 (3)	1.885 (3)	1.883 (3)	1.883 (3)
<*Z*-O>	1.908	1.904	1.905	1.905	1.903	1.904	1.904
T-O(4) a	1.620 (2)	1.619 (2)	1.620 (2)	1.620 (2)	1.619 (2)	1.619 (2)	1.619 (2)
T-O(5) b	1.635 (3)	1.636 (2)	1.632 (2)	1.633 (3)	1.633 (3)	1.633 (3)	1.633 (3)
T-O(6)	1.611 (5)	1.604 (4)	1.608 (6)	1.608 (5)	1.604 (5)	1.607 (2)	1.604 (5)
T-O(7)	1.609 (2)	1.608 (2)	1.610 (2)	1.609 (2)	1.606 (2)	1.610 (2)	1.606 (2)
<*T*-O>	1.619	1.617	1.618	1.618	1.616	1.617	1.616
O(4)a-*T*-O(5)b	104.8 (2)	104.3 (1)	104.8 (2)	104.4 (2)	104.3 (1)	104.6 (1)	104.4 (1)
O(4)a-*T*-O(6)	111.9 (2)	111.9 (2)	112.0 (2)	111.8 (2)	111.9 (2)	111.8 (2)	111.8 (2)
O(4)a-*T*-O(7)	109.7 (2)	110.0 (1)	109.7 (2)	109.9 (2)	109.8 (1)	109.9 (1)	110.0 (2)
O(5)b-*T*-O(6)	110.6 (2)	110.9 (2)	110.7 (2)	110.7 (2)	110.8 (2)	110.7 (1)	110.7 (2)
O(5)b-*T*-O(7)	109.1 (2)	109.2 (1)	109.0 (2)	109.2 (2)	109.1 (2)	109.2 (1)	109.2 (2)
O(6)-*T*-O(7)	110.5 (2)	110.4 (1)	110.5 (2)	110.6 (2)	110.8 (2)	110.4 (1)	110.6 (2)
<O-*T*-O>	109.4	109.5	109.5	109.4	109.5	109.4	109.5
B-O(2)	1.361 (1)	1.353 (1)	1.355 (1)	1.356 (1)	1.358 (1)	1.357 (1)	1.355 (1)
B-O(8) c,a	1.383 (2)	1.381 (2)	1.383 (2)	1.383 (2)	1.381 (2)	1.380 (2)	1.383 (2)
<*B*-O>	1.376	1.372	1.374	1.374	1.373	1.372	1.374
O(2)-*B*-O(8)c x2	121.4 (1)	121.3 (1)	121.5 (2)	121.5 (2)	121.4 (1)	121.4 (1)	121.5 (1)
O(8)c-*B*-O(8)a	117.1 (2)	117.3 (2)	117.1 (2)	117.0 (2)	117.2 (2)	117.1 (1)	117.1 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT8	CT9	CT10	CT11	CT12	CT13	CT14
X-O(2) k,l,a	2.474 (3)	2.469 (4)	2.446 (3)	2.460 (3)	2.469 (3)	2.432 (3)	2.450 (4)
X-O(4) m,n,o	2.808 (2)	2.813 (2)	2.804 (2)	2.810 (2)	2.815 (2)	2.812 (2)	2.811 (2)
X-O(5) p,q,r	2.737 (2)	2.745 (2)	2.751 (2)	2.743 (2)	2.743 (2)	2.748 (2)	2.753 (2)
<*X*-O>	2.673	2.676	2.667	2.671	2.676	2.664	2.671
Y-O(1) g	1.934 (3)	1.946 (4)	2.000 (4)	1.975 (3)	1.950 (3)	2.011 (3)	1.980 (4)
Y-O(2) h,l	1.953 (3)	1.950 (4)	1.967 (3)	1.959 (3)	1.952 (3)	1.972 (3)	1.962 (3)
Y-O(3)	2.134 (2)	2.138 (3)	2.149 (2)	2.137 (2)	2.136 (2)	2.153 (2)	2.140 (4)
Y-O(6) j,b	1.960 (3)	1.962 (4)	1.977 (3)	1.964 (3)	1.965 (3)	1.998 (3)	1.969 (4)
<*Y*-O>	1.982	1.985	2.006	1.993	1.987	2.017	1.997
Z-O(3) b	1.954 (3)	1.955 (3)	1.953 (3)	1.959 (3)	1.958 (3)	1.957 (3)	1.960 (3)
Z-O(6)	1.866 (4)	1.861 (4)	1.851 (3)	1.857 (3)	1.858 (4)	1.850 (3)	1.855 (4)
Z-O(7) d	1.943 (3)	1.944 (4)	1.948 (3)	1.942 (3)	1.940 (3)	1.953 (3)	1.943 (4)
Z-O(7) e	1.885 (4)	1.883 (5)	1.884 (4)	1.880 (4)	1.879 (4)	1.883 (3)	1.881 (5)
Z-O(8)	1.898 (4)	1.897 (5)	1.904 (4)	1.901 (4)	1.901 (4)	1.906 (3)	1.900 (4)
Z-O(8) f	1.882 (3)	1.886 (4)	1.884 (3)	1.884 (3)	1.881 (3)	1.882 (3)	1.884 (4)
<*Z*-O>	1.905	1.904	1.904	1.904	1.903	1.905	1.904
T-O(4) a	1.614 (2)	1.616 (2)	1.620 (2)	1.619 (2)	1.615 (2)	1.621 (2)	1.620 (2)
T-O(5) b	1.629 (3)	1.631 (3)	1.633 (3)	1.634 (3)	1.633 (3)	1.637 (3)	1.633 (3)
T-O(6)	1.607 (5)	1.606 (7)	1.602 (5)	1.605 (5)	1.607 (5)	1.601 (4)	1.605 (6)
T-O(7)	1.605 (2)	1.607 (3)	1.608 (2)	1.608 (2)	1.609 (2)	1.607 (2)	1.609 (3)
<*T*-O>	1.614	1.615	1.616	1.617	1.616	1.617	1.617
O(4)a-*T*-O(5)b	105.1 (2)	105.1 (2)	104.3 (2)	104.6 (2)	105.0 (2)	104.0 (1)	104.7 (2)
O(4)a-*T*-O(6)	111.8 (2)	112.0 (2)	111.8 (2)	112.0 (2)	111.9 (2)	111.9 (2)	111.9 (2)
O(4)a-*T*-O(7)	109.5 (2)	109.5 (2)	110.0 (2)	109.7 (2)	109.5 (2)	109.9 (1)	109.8 (2)
O(5)b-*T*-O(6)	110.5 (2)	110.5 (2)	110.8 (2)	110.7 (2)	110.7 (2)	111.0 (2)	110.7 (2)
O(5)b-*T*-O(7)	109.1 (2)	109.0 (2)	109.1 (2)	109.2 (2)	109.1 (2)	109.3 (2)	109.0 (2)
O(6)-*T*-O(7)	110.5 (2)	110.6 (2)	110.6 (2)	110.5 (2)	110.4 (2)	110.5 (2)	110.6 (2)
<O-*T*-O>	109.4	109.5	109.4	109.5	109.4	109.4	109.5
B-O(2)	1.357 (1)	1.359 (2)	1.355 (1)	1.363 (1)	1.360 (1)	1.360 (1)	1.356 (1)
B-O(8) c,a	1.380 (2)	1.379 (2)	1.382 (2)	1.377 (2)	1.375 (2)	1.381 (2)	1.382 (2)
<*B*-O>	1.372	1.372	1.373	1.372	1.370	1.374	1.373
O(2)-*B*-O(8)c x2	121.5 (1)	121.5 (2)	121.4 (2)	121.2 (2)	121.3 (1)	121.2 (2)	121.4 (2)
O(8)c-*B*-O(8)a	117.0 (1)	117.0 (2)	117.2 (2)	117.6 (2)	117.3 (2)	117.6 (2)	117.3 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT15	CT16	CT17	CT18	CT19	CT20	CT21
X-O(2) k,l,a	2.479 (3)	2.437 (3)	2.444 (3)	2.433 (3)	2.430 (3)	2.434 (3)	2.429 (3)
X-O(4) m,n,o	2.817 (2)	2.824 (2)	2.824 (2)	2.822 (2)	2.818 (2)	2.823 (2)	2.820 (2)
X-O(5) p,q,r	2.745 (2)	2.766 (2)	2.763 (2)	2.764 (2)	2.758 (2)	2.768 (2)	2.761 (2)
<*X*-O>	2.680	2.682	2.677	2.673	2.669	2.675	2.670
Y-O(1) g	1.929 (3)	2.038 (3)	2.024 (3)	2.034 (3)	2.034 (4)	2.035 (4)	2.039 (4)
Y-O(2) h,l	1.952 (3)	1.983 (3)	1.980 (3)	1.981 (2)	1.979 (3)	1.976 (3)	1.977 (3)
Y-O(3)	2.118 (3)	2.175 (2)	2.613 (2)	2.166 (2)	2.166 (2)	2.159 (2)	2.162 (2)
Y-O(6) j,b	1.955 (3)	2.024 (2)	2.015 (3)	2.021 (2)	2.022 (3)	2.020 (3)	2.022 (3)
<*Y*-O>	1.977	2.038	2.030	2.034	2.034	2.031	2.033
Z-O(3) b	1.960 (3)	1.963 (2)	1.968 (2)	1.964 (2)	1.960 (3)	1.961 (3)	1.960 (3)
Z-O(6)	1.869 (4)	1.846 (3)	1.852 (3)	1.850 (3)	1.845 (3)	1.846 (3)	1.843 (3)
Z-O(7) d	1.941 (3)	1.957 (3)	1.952 (3)	1.955 (2)	1.953 (3)	1.954 (3)	1.955 (3)
Z-O(7) e	1.884 (4)	1.887 (3)	1.885 (3)	1.885 (3)	1.879 (4)	1.879 (4)	1.880 (3)
Z-O(8)	1.901 (4)	1.916 (3)	1.914 (3)	1.913 (3)	1.909 (3)	1.911 (4)	1.910 (3)
Z-O(8) f	1.883 (4)	1.883 (3)	1.885 (3)	1.884 (3)	1.880 (3)	1.878 (3)	1.878 (3)
<*Z*-O>	1.906	1.909	1.909	1.909	1.918	1.905	1.904
T-O(4) a	1.618 (2)	1.624 (2)	1.625 (2)	1.624 (2)	1.622 (2)	1.622 (2)	1.621 (2)
T-O(5) b	1.632 (3)	1.638 (2)	1.640 (2)	1.639 (2)	1.637 (3)	1.635 (3)	1.637 (3)
T-O(6)	1.613 (6)	1.608 (4)	1.609 (4)	1.605 (4)	1.599 (4)	1.603 (5)	1.601 (4)
T-O(7)	1.610 (2)	1.611 (2)	1.615 (2)	1.613 (2)	1.611 (2)	1.610 (2)	1.608 (2)
<*T*-O>	1.618	1.620	1.622	1.620	1.617	1.618	1.617
O(4)a-*T*-O(5)b	105.2 (2)	104.0 (1)	104.3 (1)	104.0 (1)	104.0 (1)	104.3 (2)	104.0 (1)
O(4)a-*T*-O(6)	111.9 (2)	111.8 (2)	111.9 (2)	111.9 (2)	112.0 (2)	112.0 (2)	112.0 (2)
O(4)a-*T*-O(7)	109.4 (2)	110.2 (1)	110.1 (1)	110.2 (1)	110.1 (2)	110.0 (2)	110.1 (2)
O(5)b-*T*-O(6)	110.5 (2)	110.9 (2)	110.9 (2)	110.9 (1)	111.0 (2)	110.8 (2)	111.0 (2)
O(5)b-*T*-O(7)	109.0 (2)	109.5 (1)	109.4 (1)	109.5 (1)	109.5 (2)	109.5 (2)	109.5 (2)
O(6)-*T*-O(7)	110.6 (2)	110.2 (1)	110.1 (1)	110.2 (1)	110.2 (2)	110.2 (2)	110.2 (2)
<O-*T*-O>	109.4	109.4	109.5	109.5	109.5	109.5	109.4
B-O(2)	1.356 (1)	1.353 (1)	1.354 (1)	1.355 (1)	1.351 (1)	1.351 (1)	1.355 (1)
B-O(8) c,a	1.382 (2)	1.386 (2)	1.387 (2)	1.387 (2)	1.385 (3)	1.387 (3)	1.383 (2)
<*B*-O>	1.373	1.375	1.376	1.376	1.374	1.375	1.374
O(2)-*B*-O(8)c x2	121.6 (1)	121.1 (2)	121.2 (1)	121.1 (1)	121.1 (2)	121.2 (2)	121.0 (2)
O(8)c-*B*-O(8)a	116.8 (1)	117.7 (2)	117.6 (2)	117.7 (2)	117.7 (2)	117.6 (2)	118.0 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT22	CT23	CT24	CT25	CT26	CT27	CT28
X-O(2) k,l,a	2.449 (4)	2.444 (3)	2.441 (3)	2.439 (3)	2.430 (3)	2.447 (3)	2.434 (3)
X-O(4) m,n,o	2.822 (2)	2.821 (2)	2.817 (2)	2.816 (2)	2.811 (2)	2.812 (2)	2.809 (2)
X-O(5) p,q,r	2.765 (2)	2.762 (2)	2.755 (2)	2.757 (2)	2.754 (2)	2.754 (2)	2.751 (2)
<*X*-O>	2.679	2.676	2.671	2.671	2.665	2.671	2.665
Y-O(1) g	2.045 (4)	2.045 (3)	2.024 (3)	2.004 (3)	2.017 (3)	1.997 (3)	1.991 (4)
Y-O(2) h,l	1.982 (3)	1.981 (3)	1.976 (3)	1.967 (3)	1.969 (3)	1.967 (3)	1.963 (3)
Y-O(3)	2.158 (2)	2.160 (2)	2.161 (2)	2.152 (2)	2.149 (2)	2.146 (2)	2.148 (2)
Y-O(6) j,b	2.027 (3)	2.026 (3)	2.012 (3)	1.996 (3)	1.999 (3)	1.985 (3)	1.981 (3)
<*Y*-O>	2.037	2.037	2.027	2.014	2.017	2.008	2.005
Z-O(3) b	1.963 (3)	1.967 (3)	1.962 (3)	1.960 (3)	1.956 (2)	1.961 (3)	1.955 (3)
Z-O(6)	1.847 (4)	1.846 (3)	1.847 (3)	1.849 (3)	1.848 (3)	1.854 (3)	1.849 (4)
Z-O(7) d	1.955 (3)	1.955 (3)	1.952 (3)	1.949 (3)	1.950 (2)	1.947 (3)	1.946 (3)
Z-O(7) e	1.878 (4)	1.877 (3)	1.879 (4)	1.884 (4)	1.879 (3)	1.885 (4)	1.881 (4)
Z-O(8)	1.914 (4)	1.912 (3)	1.909 (3)	1.907 (3)	1.904 (3)	1.906 (4)	1.902 (4)
Z-O(8) f	1.877 (4)	1.880 (3)	1.879 (3)	1.882 (3)	1.880 (3)	1.885 (3)	1.879 (3)
<*Z*-O>	1.906	1.906	1.905	1.905	1.903	1.906	1.902
T-O(4) a	1.624 (2)	1.625 (2)	1.622 (2)	1.620 (2)	1.620 (2)	1.621 (2)	1.616 (2)
T-O(5) b	1.639 (3)	1.640 (3)	1.637 (3)	1.635 (3)	1.635 (2)	1.636 (3)	1.631 (3)
T-O(6)	1.603 (6)	1.603 (4)	1.603 (5)	1.607 (5)	1.599 (4)	1.606 (5)	1.605 (5)
T-O(7)	1.612 (2)	1.613 (2)	1.609 (2)	1.607 (2)	1.607 (2)	1.610 (2)	1.603 (2)
<*T*-O>	1.620	1.620	1.618	1.617	1.615	1.618	1.614
O(4)a-*T*-O(5)b	104.2 (2)	104.0 (1)	104.2 (1)	104.5 (1)	104.1 (1)	104.4 (2)	104.5 (2)
O(4)a-*T*-O(6)	112.0 (2)	112.0 (2)	112.0 (2)	111.8 (2)	111.9 (2)	111.9 (2)	111.8 (2)
O(4)a-*T*-O(7)	110.1 (2)	110.0 (1)	110.0 (2)	110.0 (2)	109.9 (1)	110.0 (2)	110.0 (2)
O(5)b-*T*-O(6)	111.0 (2)	111.1 (2)	110.8 (2)	110.8 (2)	111.0 (1)	110.8 (2)	110.8 (2)
O(5)b-*T*-O(7)	109.4 (2)	109.4 (2)	109.4 (2)	109.2 (2)	109.2 (1)	109.0 (2)	109.2 (2)
O(6)-*T*-O(7)	110.0 (2)	110.1 (1)	110.3 (2)	110.4 (2)	110.5 (1)	110.4 (2)	110.5 (2)
<O-*T*-O>	109.5	109.4	109.5	109.5	109.4	109.4	109.5
B-O(2)	1.351 (1)	1.348 (1)	1.354 (1)	1.354 (1)	1.353 (1)	1.360 (1)	1.352 (1)
B-O(8) c,a	1.386 (3)	1.388 (2)	1.384 (2)	1.384 (2)	1.381 (2)	1.381 (2)	1.381 (2)
<*B*-O>	1.374	1.375	1.374	1.374	1.372	1.374	1.371
O(2)-*B*-O(8)c x2	121.0 (2)	121.2 (2)	121.2 (2)	121.4 (2)	121.3 (2)	121.2 (2)	121.5 (2)
O(8)c-*B*-O(8)a	118.0 (2)	117.7 (2)	117.7 (2)	117.2 (2)	117.5 (2)	117.5 (2)	117.0 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT29	CT30	CT31	CT32	CT33	CT34	CT35
X-O(2) k,l,a	2.445 (3)	2.444 (3)	2.440 (3)	2.438 (3)	2.502 (2)	2.528 (2)	2.446 (2)
X-O(4) m,n,o	2.810 (2)	2.820 (2)	2.802 (2)	2.820 (2)	2.838 (2)	2.787 (2)	2.836 (2)
X-O(5) p,q,r	2.751 (2)	2.761 (2)	2.751 (2)	2.759 (2)	2.743 (1)	2.705 (1)	2.746 (2)
<*X*-O>	2.655	2.675	2.664	2.672	2.694	2.673	2.676
Y-O(1) g	1.998 (4)	2.027 (3)	2.010 (3)	2.056 (3)	1.949 (2)	1.942 (2)	2.005 (3)
Y-O(2) h,l	1.969 (3)	1.974 (3)	1.975 (3)	1.986 (2)	2.000 (2)	2.078 (2)	2.016 (2)
Y-O(3)	2.150 (2)	2.157 (2)	2.153 (2)	2.162 (2)	2.117 (2)	1.999 (1)	2.116 (2)
Y-O(6) j,b	1.982 (3)	2.018 (2)	1.986 (3)	2.042 (2)	1.987 (2)	1.970 (2)	2.005 (2)
<*Y*-O>	2.008	2.028	2.014	2.046	2.007	1.993	2.027
Z-O(3) b	1.959 (3)	1.965 (2)	1.953 (2)	1.967 (2)	2.001 (2)	2.007 (2)	1.989 (2)
Z-O(6)	1.853 (3)	1.848 (3)	1.848 (3)	1.848 (3)	1.909 (2)	1.924 (2)	1.883 (3)
Z-O(7) d	1.947 (3)	1.950 (2)	1.952 (3)	1.956 (2)	1.960 (2)	1.951 (2)	1.957 (2)
Z-O(7) e	1.883 (4)	1.881 (3)	1.888 (3)	1.882 (3)	1.910 (3)	1.913 (2)	1.907 (3)
Z-O(8)	1.901 (4)	1.812 (3)	1.907 (3)	1.915 (3)	1.931 (3)	1.929 (2)	1.931 (3)
Z-O(8) f	1.885 (3)	1.882 (3)	1.887 (3)	1.878 (3)	1.899 (2)	1.904 (2)	1.891 (3)
<Z-O>	1.905	1.906	1.906	1.908	1.935	1.938	1.926
T-O(4) a	1.619 (2)	1.622 (2)	1.623 (2)	1.625 (2)	1.625 (1)	1.623 (1)	1.623 (2)
T-O(5) b	1.634 (3)	1.637 (2)	1.636 (3)	1.638 (2)	1.642 (2)	1.640 (2)	1.638 (3)
T-O(6)	1.605 (5)	1.606 (4)	1.601 (4)	1.600 (4)	1.612 (4)	1.609 (3)	1.608 (4)
T-O(7)	1.609 (2)	1.614 (2)	1.605 (2)	1.611 (2)	1.604 (2)	1.601 (2)	1.599 (2)
<*T*-O>	1.617	1.620	1.616	1.619	1.621	1.618	1.617
O(4)a-*T*-O(5)b	104.5 (2)	104.4 (1)	103.8 (1)	104.0 (1)	104.1 (1)	103.1 (1)	102.8 (1)
O(4)a-*T*-O(6)	111.6 (2)	111.9 (2)	111.8 (2)	111.9 (2)	111.5 (1)	111.5 (1)	111.5 (2)
O(4)a-*T*-O(7)	110.1 (2)	110.0 (1)	110.3 (1)	110.0 (1)	109.7 (1)	110.3 (1)	110.4 (1)
O(5)b-*T*-O(6)	110.8 (2)	110.9 (1)	111.0 (2)	111.0 (1)	110.2 (1)	110.3 (1)	110.2 (1)
O(5)b-*T*-O(7)	109.2 (2)	109.3 (1)	109.2 (2)	109.5 (1)	110.0 (1)	110.4 (1)	110.7 (1)
O(6)-*T*-O(7)	110.5 (2)	110.1 (1)	110.6 (2)	110.2 (1)	109.7 (1)	111.0 (1)	111.0 (1)
<O-*T*-O>	109.5	109.4	109.5	109.4	109.4	109.4	109.4
B-O(2)	1.355 (1)	1.355 (1)	1.356 (1)	1.356 (1)	1.375 (1)	1.381 (1)	1.360 (1)
B-O(8) c,a	1.385 (2)	1.383 (2)	1.378 (2)	1.385 (2)	1.376 (2)	1.366 (2)	1.377 (2)
<*B*-O>	1.375	1.374	1.371	1.375	1.376	1.371	1.371
O(2)-*B*-O(8)c x2	121.4 (2)	121.1 (1)	121.2 (2)	120.9 (1)	120.6 (1)	120.5 (1)	120.6 (2)
O(8)c-*B*-O(8)a	117.2 (2)	117.8 (1)	117.6 (2)	118.3 (2)	118.7 (1)	119.0 (1)	118.8 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT36	CT37	CT38	CT39	CT40	CT41	CT42
X-O(2) k,l,a	2.456 (3)	2.461 (2)	2.496 (3)	2.496 (4)	2.517 (2)	2.506 (5)	2.517 (3)
X-O(4) m,n,o	2.835 (2)	2.789 (1)	2.815 (2)	2.812 (3)	2.802 (1)	2.823 (3)	2.814 (2)
X-O(5) p,q,r	2.745 (2)	2.703 (1)	2.723 (2)	2.716 (2)	2.713 (1)	2.732 (3)	2.728 (2)
<*X*-O>	2.679	2.651	2.678	2.675	2.677	2.687	2.686
Y-O(1) g	1.990 (2)	2.017 (2)	1.968 (3)	1.963 (4)	1.954 (2)	1.956 (5)	1.946 (3)
Y-O(2) h,l	1.999 (2)	2.035 (2)	1.990 (3)	1.998 (4)	2.003 (2)	2.001 (5)	1.989 (3)
Y-O(3)	2.095 (2)	2.140 (1)	2.098 (2)	2.107 (3)	2.092 (1)	2.090 (3)	2.081 (2)
Y-O(6) j,b	1.991 (2)	2.018 (2)	1.981 (3)	1.980 (4)	1.979 (2)	1.980 (5)	1.973 (3)
<*Y*-O>	2.011	2.044	2.001	2.004	2.002	2.001	1.992
Z-O(3) b	1.990 (2)	1.985 (2)	1.991 (3)	1.993 (3)	2.004 (2)	2.000 (4)	2.004 (3)
Z-O(6)	1.888 (3)	1.887 (2)	1.890 (3)	1.892 (4)	1.912 (2)	1.905 (5)	1.914 (3)
Z-O(7) d	1.954 (2)	1.962 (2)	1.949 (3)	1.952 (4)	1.954 (2)	1.953 (5)	1.951 (3)
Z-O(7) e	1.903 (3)	1.907 (2)	1.898 (3)	1.905 (4)	1.912 (3)	1.918 (6)	1.913 (4)
Z-O(8)	1.925 (3)	1.927 (2)	1.919 (3)	1.925 (4)	1.927 (3)	1.928 (6)	1.929 (4)
Z-O(8) f	1.893 (3)	1.893 (2)	1.892 (3)	1.892 (4)	1.906 (2)	1.905 (5)	1.900 (3)
<*Z*-O>	1.932	1.927	1.923	1.927	1.936	1.935	1.935
T-O(4) a	1.623 (2)	1.629 (1)	1.622 (2)	1.623 (2)	1.625 (1)	1.622 (3)	1.622 (2)
T-O(5) b	1.639 (2)	1.643 (2)	1.638 (3)	1.640 (4)	1.642 (2)	1.639 (5)	1.639 (3)
T-O(6)	1.604 (4)	1.599 (3)	1.606 (4)	1.610 (6)	1.612 (3)	1.613 (7)	1.611 (5)
T-O(7)	1.602 (2)	1.601 (1)	1.603 (2)	1.601 (3)	1.603 (1)	1.599 (3)	1.603 (2)
<*T*-O>	1.617	1.618	1.617	1.619	1.621	1.618	1.619
O(4)a-*T*-O(5)b	103.4 (1)	101.6 (1)	103.7 (1)	103.4 (2)	103.2 (1)	103.8 (2)	103.8 (2)
O(4)a-*T*-O(6)	111.5 (2)	111.5 (1)	111.6 (2)	111.6 (2)	111.5 (1)	111.2 (3)	111.5 (2)
O(4)a-*T*-O(7)	110.2 (1)	110.8 (1)	109.9 (1)	110.0 (2)	110.2 (1)	110.6 (3)	110.1 (2)
O(5)b-*T*-O(6)	110.3 (1)	110.6 (1)	110.2 (2)	110.1 (2)	110.4 (1)	110.0 (3)	110.1 (2)
O(5)b-*T*-O(7)	110.2 (1)	110.8 (1)	110.1 (2)	110.4 (2)	110.3 (1)	110.3 (3)	110.2 (2)
O(6)-*T*-O(7)	111.0 (1)	111.0 (1)	111.0 (2)	111.1 (2)	110.9 (1)	110.8 (3)	110.9 (2)
<O-*T*-O>	109.4	109.4	109.4	109.4	109.4	109.5	109.4
B-O(2)	1.361 (1)	1.361 (1)	1.362 (1)	1.367 (1)	1.373 (1)	1.366 (2)	1.373 (1)
B-O(8) c,a	1.378 (2)	1.382 (2)	1.376 (2)	1.376 (3)	1.373 (2)	1.372 (4)	1.373 (3)
<*B*-O>	1.372	1.375	1.371	1.373	1.373	1.370	1.373
O(2)-*B*-O(8)c x2	120.8 (1)	120.7 (2)	120.8 (2)	120.9 (2)	120.6 (1)	120.5 (3)	120.8 (2)
O(8)c-*B*-O(8)a	118.4 (2)	118.7 (2)	118.3 (2)	118.2 (2)	118.7 (1)	118.8 (3)	118.3 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT43	CT44	CT45	CT46	CT47	CT48	CT49
X-O(2) k,l,a	2.500 (2)	2.452 (1)	2.454 (2)	2.460 (2)	2.478 (2)	2.473 (2)	2.474 (2)
X-O(4) m,n,o	2.829 (2)	2.775 (1)	2.795 (1)	2.810 (2)	2.790 (1)	2.794 (2)	1.719 (1)
X-O(5) p,q,r	2.743 (1)	2.694 (1)	2.710 (1)	2.734 (2)	2.711 (1)	2.716 (2)	2.758 (1)
<*X*-O>	2.691	2.640	2.653	2.668	2.660	2.661	2.684
Y-O(1) g	1.968 (2)	2.041 (1)	2.023 (2)	2.024 (2)	2.022 (2)	2.029 (2)	2.068 (2)
Y-O(2) h,l	1.989 (2)	2.045 (1)	2.029 (2)	2.012 (2)	2.019 (2)	2.023 (2)	2.017 (2)
Y-O(3)	2.082 (2)	2.147 (1)	2.131 (1)	2.121 (2)	2.132 (1)	2.132 (1)	2.149 (1)
Y-O(6) j,b	1.981 (2)	2.024 (1)	2.019 (2)	2.016 (2)	2.011 (2)	2.014 (2)	2.048 (2)
<*Y*-O>	1.998	2.054	2.042	2.034	2.036	2.039	2.058
Z-O(3) b	1.998 (2)	1.985 (1)	1.984 (2)	1.982 (2)	1.985 (2)	1.985 (2)	1.981 (2)
Z-O(6)	1.901 (3)	1.882 (1)	1.877 (2)	1.866 (3)	1.865 (2)	1.865 (2)	1.859 (2)
Z-O(7) d	1.952 (2)	1.964 (1)	1.963 (2)	1.956 (2)	1.949 (2)	1.952 (2)	1.961 (2)
Z-O(7) e	1.906 (3)	1.905 (2)	1.904 (2)	1.897 (3)	1.891 (2)	1.894 (3)	1.888 (2)
Z-O(8)	1.925 (3)	1.929 (2)	1.926 (2)	1.821 (3)	1.922 (2)	1.924 (3)	1.923 (2)
Z-O(8) f	1.901 (2)	1.894 (1)	1.889 (2)	1.884 (3)	1.889 (2)	1.889 (2)	1.883 (2)
<*Z*-O>	1.931	1.926	1.924	1.918	1.917	1.918	1.916
T-O(4) a	1.621 (1)	1.632 (1)	1.627 (1)	1.623	1.631 (1)	1.631 (1)	1.627 (1)
T-O(5) b	1.637 (2)	1.648 (2)	1.644 (2)	1.638	1.646 (2)	1.647 (2)	1.640 (2)
T-O(6)	1.611 (4)	1.601 (2)	1.600 (3)	1.605	1.611 (2)	1.612 (3)	1.603 (3)
T-O(7)	1.603 (2)	1.603 (1)	1.600 (1)	1.604	1.614 (1)	1.614 (1)	1.614 (1)
<*T*-O>	1.618	1.621	1.618	1.618	1.626	1.626	1.621
O(4)a-*T*-O(5)b	104.2 (1)	101.1 (1)	102.1 (1)	103.4 (1)	102.7 (1)	102.8 (1)	104.0 (1)
O(4)a-*T*-O(6)	111.4 (1)	111.6 (1)	111.6 (1)	111.5 (2)	111.7 (1)	111.5 (1)	111.7 (1)
O(4)a-*T*-O(7)	110.0 (1)	111.1 (1)	110.6 (1)	110.3 (1)	110.6 (1)	110.7 (1)	110.2 (1)
O(5)b-*T*-O(6)	110.1 (1)	110.8 (1)	110.6 (1)	110.5 (1)	110.6 (1)	110.6 (1)	110.8 (1)
O(5)b-*T*-O(7)	110.1 (1)	110.8 (1)	110.6 (1)	110.2 (1)	110.4 (1)	110.3 (1)	110.0 (1)
O(6)-*T*-O(7)	110.8 (1)	111.0 (1)	111.0 (1)	110.7 (1)	110.7 (1)	110.7 (1)	110.0 (1)
<O-*T*-O>	109.4	109.4	109.4	109.4	109.5	109.4	109.5
B-O(2)	1.361 (1)	1.372 (1)	1.363 (1)	1.351 (1)	1.359 (1)	1.360 (1)	1.353 (1)
B-O(8) c,a	1.375 (2)	1.381 (2)	1.380 (2)	1.385 (2)	1.385 (2)	1.386 (2)	1.388 (2)
<*B*-O>	1.370	1.378	1.374	1.374	1.376	1.377	1.376
O(2)-*B*-O(8)c x2	120.8 (1)	120.5 (1)	120.8 (2)	121.1 (2)	120.9 (1)	120.9 (2)	120.7 (1)
O(8)c-*B*-O(8)a	118.4 (1)	119.0 (1)	118.4 (2)	117.9 (2)	118.2 (1)	118.2 (2)	118.7 (1)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT50	CT51	CT52	CT53	CT54	CT55	CT56
X-O(2) k,l,a	2.471 (2)	2.490 (2)	2.526 (3)	2.515 (3)	2.507 (4)	2.458 (2)	2.535 (4)
X-O(4) m,n,o	2.813 (1)	2.814 (1)	2.807 (2)	2.809 (2)	2.821 (2)	2.804 (2)	2.812 (2)
X-O(5) p,q,r	2.747 (1)	2.754 (1)	2.753 (2)	2.758 (2)	2.766 (2)	2.749 (2)	2.766 (2)
<*X*-O>	2.677	2.686	2.695	2.694	2.698	2.670	2.704
Y-O(1) g	2.061 (2)	2.071 (2)	2.019 (3)	2.064 (3)	2.048 (4)	2.041 (3)	2.034 (4)
Y-O(2) h,l	2.014 (2)	2.014 (2)	2.010 (3)	2.017 (3)	2.014 (4)	2.000 (2)	1.989 (4)
Y-O(3)	2.146 (1)	2.146 (1)	2.194 (2)	2.180 (2)	2.172 (2)	2.184 (2)	2.153 (3)
Y-O(6) j,b	2.041 (2)	2.045 (2)	2.042 (3)	2.049 (3)	2.043 (4)	2.033 (2)	2.032 (4)
<*Y*-O>	2.053	2.056	2.053	2.063	2.056	2.158	2.038
Z-O(3) b	1.977 (2)	1.979 (2)	1.981 (2)	1.981 (2)	1.985 (3)	1.964 (2)	1.981 (3)
Z-O(6)	1.858 (2)	1.860 (2)	1.869 (3)	1.868 (3)	1.870 (4)	1.848 (2)	1.865 (5)
Z-O(7) d	1.958 (2)	1.963 (2)	1.963 (3)	1.965 (3)	1.965 (4)	1.957 (2)	1.958 (4)
Z-O(7) e	1.886 (3)	1.888 (3)	1.888 (3)	1.889 (3)	1.890 (5)	1.880 (3)	1.882 (5)
Z-O(8)	1.921 (3)	1.922 (3)	1.926 (3)	1.929 (3)	1.929 (4)	1.915 (3)	1.924 (5)
Z-O(8) f	1.878 (2)	1.883 (2)	1.892 (3)	1.888 (3)	1.893 (4)	1.881 (2)	1.888 (4)
<*Z*-O>	1.913	1.916	1.920	1.920	1.922	1.908	1.916
T-O(4) a	1.625 (1)	1.626 (1)	1.628 (2)	1.628 (2)	1.629 (2)	1.625 (1)	1.625 (2)
T-O(5) b	1.639 (2)	1.639 (2)	1.642 (3)	1.642 (2)	1.642 (3)	1.641 (2)	1.638 (4)
T-O(6)	1.601 (3)	1.603 (3)	1.614 (4)	1.610 (4)	1.608 (6)	1.603 (3)	1.612 (7)
T-O(7)	1.610 (2)	1.609 (2)	1.616 (2)	1.614 (2)	1.615 (3)	1.612 (1)	1.615 (3)
<*T*-O>	1.619	1.619	1.625	1.624	1.624	1.621	1.623
O(4)a-*T*-O(5)b	103.9 (1)	104.1 (1)	104.7 (1)	104.3 (1)	104.2 (2)	103.7 (1)	105.1 (2)
O(4)a-*T*-O(6)	111.6 (1)	111.6 (1)	111.5 (2)	111.7 (2)	111.4 (2)	111.9 (1)	111.6 (3)
O(4)a-*T*-O(7)	110.3 (1)	110.2 (1)	110.4 (1)	110.4 (1)	110.6 (2)	110.4 (1)	110.3 (2)
O(5)b-*T*-O(6)	110.7 (1)	110.8 (1)	110.6 (2)	110.7 (2)	110.5 (2)	111.1 (1)	110.4 (2)
O(5)b-*T*-O(7)	110.0 (1)	110.0 (1)	109.9 (2)	109.9 (1)	110.1 (2)	109.6 (1)	109.7 (2)
O(6)-*T*-O(7)	110.2 (1)	110.0 (1)	109.7 (2)	109.8 (1)	109.8 (2)	110.1 (1)	109.6 (2)
<O-*T*-O>	109.5	109.5	109.5	109.5	109.4	109.5	109.5
B-O(2)	1.351 (1)	1.353 (1)	1.357 (1)	1.357 (1)	1.358 (1)	1.344 (1)	1.351 (1)
B-O(8) c,a	1.388 (2)	1.387 (2)	1.386 (2)	1.385 (2)	1.384 (3)	1.385 (2)	1.383 (3)
<*B*-O>	1.376	1.376	1.376	1.376	1.375	1.371	1.372
O(2)-*B*-O(8)c x2	120.9 (1)	120.6 (1)	120.6 (2)	120.4 (1)	120.4 (2)	120.9 (1)	120.6 (2)
O(8)c-*B*-O(8)a	118.2 (1)	118.9 (1)	118.8 (2)	119.1 (2)	119.3 (2)	118.2 (2)	118.7 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT57	CT58	CT59	CT60	CT61	CT62	CT63
X-O(2) k,l,a	2.507 (2)	2.540 (7)	2.447 (3)	2.445 (3)	2.445 (3)	2.452 (3)	2.452 (3)
X-O(4) m,n,o	2.800 (2)	2.810 (4)	2.821 (2)	2.821 (2)	2.821 (2)	2.811 (2)	2.809 (2)
X-O(5) p,q,r	2.748 (2)	2.764 (4)	2.763 (2)	2.764 (2)	2.763 (2)	2.753 (2)	2.758 (2)
<*X*-O>	2.685	2.705	2.677	2.677	2.676	2.672	2.673
Y-O(1) g	2.005 (3)	2.060 (8)	2.044 (4)	2.050 (3)	2.042 (3)	2.049 (3)	2.040 (3)
Y-O(2) h,l	2.017 (2)	1.989 (6)	1.986 (3)	1.981 (3)	1.980 (3)	1.996 (2)	1.994 (2)
Y-O(3)	2.202 (2)	2.152 (5)	2.173 (2)	2.160 (2)	2.166 (2)	2.179 (2)	2.182 (2)
Y-O(6) j,b	2.029 (2)	2.038 (7)	2.031 (3)	2.027 (3)	2.026 (3)	2.033 (2)	2.035 (2)
<*Y*-O>	2.050	2.044	2.042	2.038	2.037	2.048	2.047
Z-O(3) b	1.981 (2)	1.981 (6)	1.965 (3)	1.965 (2)	1.964 (3)	1.966 (2)	1.964 (2)
Z-O(6)	1.860 (2)	1.860 (8)	1.845 (3)	1.844 (3)	1.846 (3)	1.848 (2)	1.848 (3)
Z-O(7) d	1.952 (2)	1.961 (6)	1.956 (3)	1.953 (3)	1.952 (3)	1.959 (2)	1.961 (2)
Z-O(7) e	1.878 (3)	1.877 (9)	1.883 (4)	1.880 (3)	1.878 (3)	1.881 (3)	1.884 (3)
Z-O(8)	1.925 (3)	1.925 (8)	1.916 (3)	1.914 (3)	1.911 (3)	1.917 (3)	1.918 (3)
Z-O(8) f	1.891 (2)	1.886 (7)	1.881 (3)	1.878 (3)	1.878 (3)	1.883 (2)	1.887 (3)
<*Z*-O>	1.915	1.915	1.908	1.906	1.905	1.909	1.910
T-O(4) a	1.630 (1)	1.626 (4)	1.622 (2)	1.623 (2)	1.623 (2)	1.627 (1)	1.626 (2)
T-O(5) b	1.643 (2)	1.639 (6)	1.637 (3)	1.637 (3)	1.637 (2)	1.642 (2)	1.640 (2)
T-O(6)	1.622 (4)	1.612 (12)	1.607 (5)	1.604 (4)	1.604 (4)	1.605 (4)	1.605 (4)
T-O(7)	1.618 (2)	1.614 (5)	1.610 (2)	1.612 (2)	1.613 (2)	1.614 (2)	1.610 (2)
<*T*-O>	1.628	1.623	1.619	1.618	1.619	1.622	1.620
O(4)a-*T*-O(5)b	104.2 (1)	105.1 (3)	104.2 (1)	104.2 (1)	104.1 (1)	103.7 (1)	103.8 (1)
O(4)a-*T*-O(6)	111.7 (1)	111.5 (4)	111.8 (2)	112.0 (2)	112.0 (2)	111.8 (1)	111.9 (2)
O(4)a-*T*-O(7)	110.5 (1)	110.3 (4)	110.3 (2)	110.2 (1)	110.1 (1)	110.4 (1)	110.5 (1)
O(5)b-*T*-O(6)	110.6 (1)	110.6 (4)	110.9 (2)	110.8 (2)	110.8 (2)	111.0 (1)	110.8 (1)
O(5)b-*T*-O(7)	110.1 (1)	109.7 (4)	109.6 (2)	109.6 (2)	109.6 (1)	109.6 (1)	109.7 (1)
O(6)-*T*-O(7)	109.6 (1)	109.5 (4)	110.0 (2)	109.9 (1)	110.0 (1)	110.1 (1)	110.0 (1)
<O-*T*-O>	109.5	109.5	109.5	109.5	109.4	109.4	109.5
B-O(2)	1.358 (1)	1.354 (2)	1.353 (1)	1.351 (1)	1.354 (1)	1.359 (1)	1.353 (1)
B-O(8) c,a	1.383 (2)	1.384 (4)	1.383 (2)	1.386 (2)	1.384 (2)	1.384 (2)	1.383 (2)
<*B*-O>	1.375	1.374	1.373	1.374	1.374	1.376	1.373
O(2)-*B*-O(8)c x2	120.6 (1)	120.6 (3)	120.9 (2)	121.0 (2)	120.8 (2)	120.7 (2)	120.9 (2)
O(8)c-*B*-O(8)a	118.8 (1)	118.8 (3)	118.1 (2)	117.9 (2)	118.4 (2)	118.6 (2)	118.2 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT64	CT65	CT66	CT67	CT68	CT69	CT70
X-O(2) k,l,a	2.452 (2)	2.419 (2)	2.436 (2)	2.453 (1)	2.432 (1)	2.429 (2)	2.447 (2)
X-O(4) m,n,o	2.787 (2)	2.768 (2)	2.783 (2)	2.780 (1)	2.774 (1)	2.773 (2)	2.789 (1)
X-O(5) p,q,r	2.699 (2)	2.674 (2)	2.691 (2)	2.692 (1)	2.684 (1)	2.680 (1)	2.702 (1)
<*X*-O>	2.646	2.620	2.637	2.642	2.630	2.627	2.654
Y-O(1) g	2.012 (2)	2.037 (2)	2.020 (2)	2.029 (1)	2.051 (1)	2.030 (2)	2.024 (2)
Y-O(2) h,l	2.034 (2)	2.054 (2)	2.044 (2)	2.042 (1)	2.047 (1)	2.045 (2)	2.038 (2)
Y-O(3)	2.133 (1)	2.130 (1)	2.125 (1)	2.124 (1)	2.128 (1)	2.128 (1)	2.130 (1)
Y-O(6) j,b	2.011 (2)	2.013 (2)	2.010 (2)	2.014 (1)	2.022 (1)	2.011 (2)	2.016 (2)
<*Y*-O>	2.039	2.050	2.042	2.044	2.053	2.045	2.044
Z-O(3) b	1.986 (2)	1.987 (2)	1.987 (2)	1.989 (2)	1.984 (1)	1.982 (2)	1.985 (2)
Z-O(6)	1.883 (2)	1.887 (2)	1.885 (2)	1.885 (1)	1.883 (1)	1.885 (2)	1.882 (2)
Z-O(7) d	1.959 (2)	1.966 (2)	1.962 (2)	1.963 (2)	1.865 (1)	1.964 (2)	1.963 (2)
Z-O(7) e	1.904 (2)	1.911 (2)	1.908 (2)	1.910 (2)	1.909 (1)	1.911 (2)	1.907 (2)
Z-O(8)	1.927 (2)	1.931 (2)	1.928 (2)	1.929 (2)	1.929 (2)	1.928 (2)	1.927 (2)
Z-O(8) f	1.893 (2)	1.897 (2)	1.894 (2)	1.898 (1)	1.895 (1)	1.893 (2)	1.891 (2)
<*Z*-O>	1.925	1.930	1.927	1.929	1.928	1.927	1.926
T-O(4) a	1.629 (1)	1.633 (1)	1.628 (1)	1.632 (1)	1.633 (1)	1.631 (1)	1.629 (1)
T-O(5) b	1.645 (2)	1.652 (2)	1.646 (2)	1.649 (2)	1.650 (2)	1.647 (2)	1.646 (2)
T-O(6)	1.600 (2)	1.597 (2)	1.600 (2)	1.603 (2)	1.599 (2)	1.598 (2)	1.601 (2)
T-O(7)	1.603 (1)	1.599 (1)	1.597 (1)	1.605 (1)	1.602 (1)	1.599 (1)	1.602 (1)
<*T*-O>	1.619	1.620	1.618	1.622	1.621	1.619	1.620
O(4)a-*T*-O(5)b	101.5 (1)	99.8 (1)	101.0 (1)	101.1 (1)	100.4 (1)	100.5 (1)	101.6 (1)
O(4)a-*T*-O(6)	111.6 (1)	111.6 (1)	111.6 (1)	111.6 (1)	111.6 (1)	111.7 (1)	111.6 (1)
O(4)a-*T*-O(7)	110.8 (1)	111.5 (1)	111.0 (1)	110.9 (1)	111.2 (1)	111.1 (1)	110.9 (1)
O(5)b-*T*-O(6)	110.6 (1)	110.7 (1)	110.6 (1)	110.7 (1)	110.8 (1)	110.7 (1)	110.6 (1)
O(5)b-*T*-O(7)	110.7 (1)	111.2 (1)	111.0 (1)	110.8 (1)	110.9 (1)	111.0 (1)	110.7 (1)
O(6)-*T*-O(7)	111.2 (1)	111.5 (1)	111.3 (1)	111.3 (1)	111.4 (1)	111.5 (1)	111.2 (1)
<O-*T*-O>	109.4	109.4	109.4	109.4	109.4	109.4	109.4
B-O(2)	1.371 (1)	1.378 (1)	1.366 (1)	1.370 (1)	1.371 (1)	1.371 (1)	1.369 (1)
B-O(8) c,a	1.377 (2)	1.377 (2)	1.376 (2)	1.380 (2)	1.382 (2)	1.379 (2)	1.381 (2)
<*B*-O>	1.375	1.377	1.373	1.377	1.378	1.376	1.377
O(2)-*B*-O(8)c x2	120.5 (1)	120.5 (1)	120.5 (2)	120.6 (1)	120.6 (1)	120.6 (2)	120.6 (1)
O(8)c-*B*-O(8)a	119.0 (1)	119.0 (1)	118.9 (2)	118.9 (1)	118.8 (1)	118.7 (2)	118.8 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT71	CT72	CT73	CT74	CT75	CT76	CT77
X-O(2) k,l,a	2.452 (2)	2.483 (2)	2.445 (3)	2.430 (2)	2.443 (2)	2.469 (2)	2.466 (2)
X-O(4) m,n,o	2.778 (1)	2.807 (1)	2.776 (2)	2.772 (2)	2.786 (2)	2.783 (1)	2.788 (1)
X-O(5) p,q,r	2.689 (1)	2.724 (1)	2.688 (2)	2.682 (2)	2.694 (2)	2.699 (1)	2.705 (1)
<*X*-O>	2.640	2.671	2.636	2.628	2.641	2.650	2.653
Y-O(1) g	2.019 (2)	1.984 (2)	2.042 (3)	2.045 (2)	2.020 (2)	1.991 (2)	2.012 (2)
Y-O(2) h,l	2.036 (2)	2.016 (2)	2.045 (3)	2.050 (2)	2.040 (2)	2.043 (2)	2.047 (2)
Y-O(3)	2.123 (1)	2.137 (1)	2.136 (2)	2.128 (1)	2.126 (1)	2.162 (1)	2.156 (1)
Y-O(6) j,b	2.012 (2)	2.005 (2)	2.014 (3)	2.021 (2)	2.007 (2)	2.016 (2)	2.023 (2)
<*Y*-O>	2.040	2.027	2.049	2.053	2.040	2.045	2.051
Z-O(3) b	1.984 (2)	1.988 (2)	1.986 (3)	1.986 (2)	1.987 (2)	1.988 (2)	1.990 (2)
Z-O(6)	1.885 (2)	1.886 (2)	1.872 (3)	1.875 (2)	1.885 (2)	1.892 (2)	1.894 (2)
Z-O(7) d	1.962 (2)	1.957 (2)	1.956 (3)	1.961 (2)	1.961 (2)	1.966 (2)	1.969 (2)
Z-O(7) e	1.909 (2)	1.902 (2)	1.902 (3)	1.906 (2)	1.909 (2)	1.912 (2)	1.913 (2)
Z-O(8)	1.926 (2)	1.927 (2)	1.930 (4)	1.929 (2)	1.930 (2)	1.930 (2)	1.935 (2)
Z-O(8) f	1.896 (1)	1.894 (2)	1.895 (3)	1.900 (2)	1.894 (2)	1.897 (2)	1.900 (2)
<*Z*-O>	1.927	1.926	1.924	1.926	1.928	1.931	1.935
T-O(4) a	1.630 (1)	1.626 (1)	1.635 (2)	1.635 (1)	1.629 (1)	1.628 (1)	1.631 (1)
T-O(5) b	1.647 (2)	1.642 (2)	1.654 (4)	1.651 (2)	1.646 (2)	1.644 (2)	1.647 (2)
T-O(6)	1.599 (2)	1.608 (3)	1.611 (4)	1.603 (2)	1.602 (2)	1.601 (3)	1.603 (3)
T-O(7)	1.602 (1)	1.605 (1)	1.610 (2)	1.605 (1)	1.600 (1)	1.598 (1)	1.604 (1)
<*T*-O>	1.620	1.620	1.628	1.624	1.619	1.618	1.621
O(4)a-*T*-O(5)b	101.1 (1)	102.9 (1)	101.0 (2)	100.3 (1)	101.2 (1)	101.7 (1)	101.6 (1)
O(4)a-*T*-O(6)	111.7 (1)	111.6 (1)	111.6 (2)	111.7 (1)	111.5 (1)	111.6 (1)	111.6 (1)
O(4)a-*T*-O(7)	110.9 (1)	110.6 (1)	111.5 (2)	111.2 (1)	111.0 (1)	111.0 (1)	111.0 (1)
O(5)b-*T*-O(6)	110.6 (1)	110.3 (1)	110.7 (2)	110.9 (1)	110.5 (1)	110.6 (1)	110.6 (1)
O(5)b-*T*-O(7)	110.8 (1)	110.5 (1)	110.9 (2)	111.0 (1)	110.9 (1)	110.8 (1)	110.8 (1)
O(6)-*T*-O(7)	111.3 (1)	110.8 (1)	110.9 (1)	111.3 (1)	111.3 (1)	110.9 (1)	110.9 (1)
<O-*T*-O>	109.4	109.5	109.4	109.4	109.4	109.4	109.4
B-O(2)	1.366 (1)	1.363 (1)	1.376 (1)	1.369 (1)	1.368 (1)	1.367 (1)	1.370 (1)
B-O(8) c,a	1.380 (2)	1.378 (2)	1.380 (4)	1.379 (2)	1.377 (2)	1.379 (2)	1.379 (2)
<*B*-O>	1.375	1.373	1.379	1.375	1.374	1.375	1.376
O(2)-*B*-O(8)c x2	120.7 (1)	120.6 (1)	120.5 (3)	120.7 (2)	120.6 (1)	120.6 (2)	120.5 (2)
O(8)c-*B*-O(8)a	118.7 (1)	118.8 (1)	119.0 (3)	118.7 (2)	118.7 (1)	118.9 (2)	119.0 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT78	CT79	CT80	CT81	CT82	CT83	CT84
X-O(2) k,l,a	2.492 (2)	2.473 (2)	2.508 (2)	2.374 (2)	2.369 (2)	2.373 (2)	2.371 (2)
X-O(4) m,n,o	2.775 (1)	2.788 (1)	2.783 (2)	2.788 (2)	2.778 (1)	2.802 (2)	2.782 (2)
X-O(5) p,q,r	2.676 (1)	2.696 (1)	2.704 (1)	2.723 (2)	2.715 (1)	2.740 (2)	2.722 (2)
<*X*-O>	2.648	2.652	2.665	2.628	2.621	2.638	2.625
Y-O(1) g	1.961 (2)	1.976 (2)	1.978 (2)	2.016 (3)	2.018 (3)	2.044 (3)	2.022 (3)
Y-O(2) h,l	2.024 (2)	2.036 (2)	2.029 (2)	1.999 (2)	2.006 (2)	1.997 (2)	2.006 (3)
Y-O(3)	2.121 (1)	2.139 (1)	2.130 (1)	2.185 (1)	2.187 (1)	2.174 (1)	2.184 (1)
Y-O(6) j,b	1.980 (2)	2.001 (2)	2.004 (2)	1.984 (2)	1.981 (2)	2.010 (2)	1.981 (2)
<*Y*-O>	2.015	2.032	2.029	2.028	2.030	2.039	2.030
Z-O(3) b	1.993 (2)	1.992 (2)	1.995 (2)	1.943 (2)	1.941 (2)	1.950 (2)	1.940 (2)
Z-O(6)	1.906 (2)	1.896 (2)	1.896 (2)	1.844 (2)	1.842 (2)	1.843 (2)	1.843 (2)
Z-O(7) d	1.959 (2)	1.963 (2)	1.964 (2)	1.960 (2)	1.961 (2)	1.958 (2)	1.960 (2)
Z-O(7) e	1.915 (2)	1.911 (2)	1.908 (2)	1.886 (2)	1.886 (2)	1.884 (2)	1.892 (2)
Z-O(8)	1.931 (2)	1.933 (2)	1.928 (3)	1.905 (2)	1.904 (2)	1.907 (2)	1.905 (2)
Z-O(8) f	1.903 (2)	1.902 (2)	1.906 (2)	1.883 (2)	1.881 (2)	1.879 (2)	1.887 (2)
<*Z*-O>	1.935	1.933	1.933	1.904	1.903	1.904	1.905
T-O(4) a	1.630 (1)	1.629 (1)	1.629 (1)	1.625 (1)	1.625 (1)	1.625 (1)	1.627 (1)
T-O(5) b	1.649 (2)	1.648 (2)	1.646 (2)	1.641 (2)	1.642 (2)	1.639 (2)	1.643 (2)
T-O(6)	1.607 (2)	1.604 (2)	1.610 (3)	1.594 (2)	1.598 (2)	1.597 (3)	1.597 (3)
T-O(7)	1.600 (1)	1.603 (1)	1.607 (1)	1.605 (1)	1.604 (1)	1.605 (1)	1.604 (2)
<*T*-O>	1.622	1.621	1.623	1.616	1.617	1.617	1.618
O(4)a-*T*-O(5)b	101.2 (1)	101.6 (1)	102.5 (1)	101.8 (1)	101.3 (1)	102.3 (1)	101.4 (1)
O(4)a-*T*-O(6)	111.7 (1)	111.6 (1)	111.6 (1)	112.1 (1)	112.2 (1)	112.0 (1)	112.1 (1)
O(4)a-*T*-O(7)	110.8 (1)	110.9 (1)	110.7 (1)	110.7 (1)	110.8 (1)	110.5 (1)	111.0 (1)
O(5)b-*T*-O(6)	110.3 (1)	110.5 (1)	110.4 (1)	111.2 (1)	111.3 (1)	111.2 (1)	111.4 (1)
O(5)b-*T*-O(7)	110.9 (1)	110.8 (1)	110.4 (1)	109.7 (1)	109.6 (1)	109.8 (1)	109.5 (1)
O(6)-*T*-O(7)	111.5 (1)	111.2 (1)	110.9 (1)	111.0 (1)	111.2 (1)	110.8 (1)	111.1 (1)
<O-*T*-O>	109.4	109.4	109.4	109.4	109.4	109.4	109.4
B-O(2)	1.378 (1)	1.372 (1)	1.368 (1)	1.355 (1)	1.355 (1)	1.351 (1)	1.357 (1)
B-O(8) c,a	1.374 (2)	1.374 (2)	1.376 (2)	1.385 (2)	1.384 (2)	1.386 (2)	1.382 (2)
<*B*-O>	1.375	1.373	1.373	1.375	1.374	1.374	1.374
O(2)-*B*-O(8)c x2	120.7 (1)	120.5 (1)	120.4 (2)	121.6 (1)	121.5 (1)	121.3 (2)	121.4 (2)
O(8)c-*B*-O(8)a	118.6 (2)	118.9 (1)	119.1 (2)	116.9 (1)	117.0 (2)	117.4 (2)	117.1 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT85	CT86	CT87	CT88	CT89	CT90	CT91
X-O(2) k,l,a	2.504 (8)	2.512 (11)	2.523 (10)	2.553 (10)	2.558 (3)	2.517 (5)	2.488 (3)
X-O(4) m,n,o	2.850 (4)	2.846 (6)	2.844 (6)	2.822 (5)	2.779 (1)	2.814 (3)	2.831 (2)
X-O(5) p,q,r	2.804 (4)	2.795 (5)	2.792 (5)	2.758 (5)	2.669 (2)	2.748 (3)	2.752 (2)
<*X*-O>	2.719	2.718	2.720	2.711	2.669	2.693	2.690
Y-O(1) g	2.047 (8)	2.045 (11)	2.042 (11)	1.964 (9)	2.115 (2)	1.975 (5)	1.978 (3)
Y-O(2) h,l	1.975 (7)	1.978 (10)	1.981 (10)	1.954 (9)	1.999 (2)	2.025 (5)	2.018 (3)
Y-O(3)	2.155 (6)	2.149 (8)	2.148 (7)	2.082 (8)	1.946 (1)	2.074 (4)	2.080 (2)
Y-O(6) j,b	2.048 (8)	2.049 (11)	2.049 (10)	1.996 (10)	1.984 (2)	1.980 (5)	1.989 (3)
<*Y*-O>	2.041	2.041	2.042	1.991	2.005	2.010	2.012
Z-O(3) b	1.980 (6)	1.978 (8)	1.979 (7)	1.975 (7)	1.902 (2)	2.027 (5)	2.013 (2)
Z-O(6)	1.849 (9)	1.852 (13)	1.853 (12)	1.872 (12)	1.924 (3)	1.953 (5)	1.926 (3)
Z-O(7) d	1.958 (7)	1.961 (10)	1.960 (10)	1.949 (9)	1.977 (2)	1.989 (5)	1.965 (3)
Z-O(7) e	1.875 (11)	1.874 (15)	1.878 (14)	1.882 (14)	1.879 (3)	1.954 (6)	1.929 (3)
Z-O(8)	1.919 (9)	1.917 (13)	1.920 (12)	1.906 (12)	1.924 (3)	1.951 (6)	1.944 (3)
Z-O(8) f	1.878 (9)	1.880 (12)	1.881 (12)	1.884 (11)	1.889 (3)	1.940 (5)	1.920 (3)
<*Z*-O>	1.910	1.910	1.912	1.911	1.916	1.969	1.950
T-O(4) a	1.620 (4)	1.621 (6)	1.621 (6)	1.617 (6)	1.624 (2)	1.625 (3)	1.626 (2)
T-O(5) b	1.634 (6)	1.633 (8)	1.635 (8)	1.630 (8)	1.627 (2)	1.643 (5)	1.641 (3)
T-O(6)	1.610 (14)	1.608 (20)	1.608 (19)	1.616 (18)	1.620 (4)	1.622 (7)	1.609 (4)
T-O(7)	1.612 (5)	1.612 (7)	1.611 (7)	1.610 (6)	1.609 (2)	1.587 (4)	1.600 (2)
<*T*-O>	1.619	1.619	1.619	1.618	1.620	1.619	1.619
O(4)a-*T*-O(5)b	106.4 (4)	106.3 (6)	106.3 (5)	106.7 (5)	103.2 (1)	102.6 (2)	103.1 (1)
O(4)a-*T*-O(6)	111.3 (5)	111.3 (7)	111.2 (7)	111.6 (6)	111.6 (1)	110.7 (3)	111.3 (2)
O(4)a-*T*-O(7)	110.0 (4)	109.9 (6)	109.9 (5)	109.3 (5)	109.7 (1)	111.3 (3)	110.6 (2)
O(5)b-*T*-O(6)	110.3 (5)	110.3 (6)	110.4 (6)	110.2 (6)	109.5 (1)	110.0 (3)	110.2 (2)
O(5)b-*T*-O(7)	109.5 (5)	109.6 (6)	109.5 (6)	109.3 (6)	112.2 (1)	110.8 (3)	110.5 (2)
O(6)-*T*-O(7)	109.3 (5)	109.4 (7)	109.4 (6)	109.8 (6)	110.4 (1)	111.1 (3)	111.0 (2)
<O-*T*-O>	109.5	109.5	109.5	109.5	109.4	109.4	109.5
B-O(2)	1.345 (3)	1.346 (4)	1.345 (4)	1.346 (4)	1.380 (1)	1.377 (2)	1.371 (1)
B-O(8) c,a	1.387 (3)	1.385 (3)	1.382 (4)	1.385 (3)	1.374 (2)	1.368 (5)	1.366 (3)
<*B*-O>	1.373	1.372	1.370	1.372	1.376	1.371	1.368
O(2)-*B*-O(8)c x2	120.8 (2)	120.6 (3)	120.5 (3)	121.2 (2)	120.5 (1)	120.7 (4)	120.3 (2)
O(8)c-*B*-O(8)a	118.4 (2)	118.8 (3)	119.0 (3)	117.5 (3)	118.9 (1)	118.5 (4)	119.3 (2)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT92	CT93	CT94	CT95	CT96	CT97	CT98
X-O(2) k,l,a	2.543 (6)	2.515 (3)	2.529 (3)	2.565 (2)	2.590 (5)	2.610 (8)	2.582 (10)
X-O(4) m,n,o	2.803 (4)	2.822 (2)	2.817 (2)	2.801 (2)	2.819 (4)	2.797 (5)	2.821 (7)
X-O(5) p,q,r	2.729 (4)	2.736 (2)	2.736 (2)	2.723 (2)	2.763 (3)	2.753 (5)	2.763 (6)
<*X*-O>	2.692	2.691	2.694	2.696	2.724	2.720	2.722
Y-O(1) g	1.949 (6)	1.965 (3)	1.972 (3)	1.947 (2)	1.966 (5)	1.978 (7)	1.967 (9)
Y-O(2) h,l	2.011 (5)	2.013 (3)	2.025 (3)	2.012 (2)	2.040 (5)	2.049 (7)	2.038 (9)
Y-O(3)	2.086 (4)	2.084 (2)	2.080 (2)	2.074 (2)	2.073 (4)	2.058 (6)	2.087 (7)
Y-O(6) j,b	1.973 (5)	1.985 (3)	1.984 (3)	1.977 (2)	1.983 (5)	1.996 (8)	1.991 (9)
<*Y*-O>	2.001	2.008	2.012	2.000	2.014	2.021	2.019
Z-O(3) b	2.023 (5)	2.016 (3)	2.025 (3)	2.034 (2)	2.053 (4)	2.061 (6)	2.060 (8)
Z-O(6)	1.980 (6)	1.939 (3)	1.962 (3)	1.979 (3)	2.012 (6)	2.033 (9)	2.024 (11)
Z-O(7) d	1.989 (6)	1.971 (3)	1.984 (3)	1.987 (2)	2.014 (5)	2.008 (7)	2.013 (9)
Z-O(7) e	1.957 (7)	1.935 (4)	1.953 (4)	1.955 (3)	1.981 (6)	1.973 (10)	1.981 (12)
Z-O(8)	1.950 (7)	1.943 (4)	1.951 (4)	1.951 (3)	1.991 (6)	1.985 (9)	1.986 (11)
Z-O(8) f	1.940 (6)	1.926 (3)	1.941 (3)	1.945 (3)	1.985 (5)	1.978 (8)	1.978 (10)
<*Z*-O>	1.973	1.955	1.969	1.975	2.006	2.006	2.007
T-O(4) a	1.628 (4)	1.626 (2)	1.627 (2)	1.628 (2)	1.628 (3)	1.638 (5)	1.636 (7)
T-O(5) b	1.645 (6)	1.643 (3)	1.643 (3)	1.641 (2)	1.639 (5)	1.645 (7)	1.650 (10)
T-O(6)	1.613 (8)	1.609 (5)	1.612 (5)	1.612 (4)	1.610 (8)	1.586 (12)	1.596 (15)
T-O(7)	1.593 (4)	1.598 (2)	1.596 (2)	1.596 (2)	1.599 (4)	1.618 (5)	1.606 (7)
<*T*-O>	1.620	1.619	1.620	1.619	1.619	1.622	1.622
O(4)a-*T*-O(5)b	102.9 (3)	103.0 (2)	102.6 (2)	103.1 (1)	103.3 (3)	102.4 (4)	102.8 (5)
O(4)a-*T*-O(6)	111.5 (4)	111.4 (2)	111.2 (2)	111.3 (2)	110.8 (3)	111.8 (5)	111.7 (6)
O(4)a-*T*-O(7)	110.6 (3)	110.5 (2)	110.9 (2)	110.5 (1)	110.6 (3)	110.4 (4)	110.4 (5)
O(5)b-*T*-O(6)	110.1 (4)	110.3 (2)	109.9 (2)	109.9 (1)	109.9 (3)	110.2 (5)	109.9 (6)
O(5)b-*T*-O(7)	110.4 (3)	110.5 (2)	110.9 (2)	110.8 (1)	110.8 (3)	110.6 (4)	110.4 (5)
O(6)-*T*-O(7)	111.1 (3)	111.0 (2)	111.1 (2)	111.0 (1)	111.2 (3)	111.0 (4)	111.3 (5)
<O-*T*-O>	109.4	109.5	109.4	109.4	109.4	109.4	109.4
B-O(2)	1.402 (2)	1.384 (1)	1.372 (1)	1.386 (1)	1.350 (2)	1.305 (3)	1.369 (4)
B-O(8) c,a	1.366 (6)	1.365 (3)	1.371 (3)	1.368 (3)	1.358 (5)	1.391 (7)	1.366 (10)
<*B*-O>	1.378	1.371	1.371	1.374	1.355	1.362	1.367
O(2)-*B*-O(8)c x2	120.4 (5)	120.3 (2)	120.7 (2)	120.5 (2)	120.9 (3)	121.9 (5)	120.8 (7)
O(8)c-*B*-O(8)a	119.2 (4)	119.4 (2)	118.6 (2)	119.0 (2)	118.2 (3)	116.1 (5)	118.4 (7)
<O-*B*-O>	120.0	120.0	120.0	120.0	120.0	120.0	120.0

	CT99
X-O(2) k,l,a	2.660 (2)
X-O(4) m,n,o	2.838 (2)
X-O(5) p,q,r	2.768 (2)
<*X*-O>	2.755
Y-O(1) g	1.969 (2)
Y-O(2) h,l	2.059 (2)
Y-O(3)	2.134 (2)
Y-O(6) j,b	2.017 (2)
<*Y*-O>	2.043
Z-O(3) b	2.073 (2)
Z-O(6)	2.024 (2)
Z-O(7) d	2.036 (2)
Z-O(7) e	1.998 (3)
Z-O(8)	2.001 (3)
Z-O(8) f	1.977 (2)
<Z-O>	2.018
T-O(4) a	1.633 (2)
T-O(5) b	1.648 (2)
T-O(6)	1.617 (3)
T-O(7)	1.607 (2)
<*T*-O>	1.626
O(4)a-*T*-O(5)b	103.9 (1)
O(4)a-*T*-O(6)	111.3 (1)
O(4)a-*T*-O(7)	109.9 (1)
O(5)b-*T*-O(6)	109.9 (1)
O(5)b-*T*-O(7)	110.4 (1)
O(6)-*T*-O(7)	111.2 (1)
<O-*T*-O>	109.4
B-O(2)	1.388 (1)
B-O(8) c,a	1.367 (2)
<*B*-O>	1.374
O(2)-*B*-O(8)c x2	120.0 (2)
O(8)c-*B*-O(8)a	119.9 (2)
<O-*B*-O>	120.0

APPENDIX G

Chemical Analyses

This appendix lists chemical analyses in terms of weight percent oxide. Chemical analyses were done on a CAMECA SX-50 microprobe. Asterisks indicate that the chemical component was determined by stoichiometry (Li_2O, B_2O_3, and H_2O).

Section G.1 includes the recalculated formulae, determined as discussed in the text under Experimental Methods. The term 'vacancy' stands for the amount of vacancy present at the *X*-site.

Section G.2 includes recalculated formulae, normalized on Si = 6 *apfu*. The only samples in this section are those that had Si > 6 *apfu* in section G.1.

Section G.3 includes recalculated formulae for CT96 (as discussed in Chapter 5) and CT99 (as discussed in Chapter 6).

Section G.1

	CT1	CT2	CT3	CT4	CT5	CT6	CT7	CT8	CT9
SiO2	38.26	37.19	37.91	37.97	38.42	37.16	38.57	38.38	38.45
TiO2	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Al2O3	42.92	39.17	41.38	41.78	40.72	41.23	40.29	42.48	41.91
V2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MgO	0.00	0.06	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	0.23	0.29	0.04	0.50	0.44	0.46	0.46	0.04	0.00
MnO	0.03	0.55	0.74	0.13	0.09	0.53	0.29	0.12	0.05
FeO	0.00	2.51	0.01	0.01	0.00	0.88	0.00	0.33	0.00
ZnO	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CuO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na2O	1.69	2.01	1.71	1.61	1.78	1.77	1.72	1.71	1.69
K2O	0.01	0.02	0.02	0.00	0.01	0.01	0.00	0.00	0.00
F	0.44	0.85	0.63	0.88	0.95	0.94	0.93	0.34	0.42
Li2O*	2.01	1.76	1.91	2.06	2.28	1.90	2.34	1.94	2.02
B2O3*	11.23	10.79	11.01	11.08	11.04	10.95	11.03	11.20	11.12
H2O*	3.67	3.32	3.50	3.40	3.36	3.33	3.36	3.70	3.64
O=F	-0.19	-0.36	-0.27	-0.37	-0.40	-0.40	-0.39	-0.14	-0.18
Total	100.31	98.20	98.59	99.05	98.69	98.77	98.60	100.09	99.12
Na	0.507	0.682	0.523	0.490	0.543	0.544	0.526	0.515	0.512
K	0.002	0.004	0.001	0.000	0.002	0.002	0.000	0.000	0.000
Ca	0.038	0.050	0.007	0.084	0.074	0.078	0.078	0.007	0.000
Vacancy	0.453	0.264	0.469	0.426	0.381	0.376	0.396	0.478	0.488
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.250	1.143	1.213	1.299	1.435	1.206	1.478	1.211	1.272
Mg	0.000	0.014	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Ti4+	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
V3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cr3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mn2+	0.004	0.075	0.099	0.017	0.012	0.071	0.039	0.016	0.007
Fe2+	0.000	0.338	0.001	0.001	0.000	0.117	0.000	0.043	0.000
Cu	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Zn	0.000	0.005	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	1.745	1.425	1.687	1.683	1.553	1.606	1.483	1.730	1.721
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.081	0.010	0.014	0.043	0.000	0.104	0.000	0.042	0.000
Si	5.919	5.990	5.986	5.957	6.046	5.896	6.078	5.958	6.010
T Total	6.000	6.000	6.000	6.000	6.046	6.000	6.078	6.000	6.010
OH	3.785	3.567	3.685	3.563	3.527	3.528	3.537	3.833	3.792
F	0.215	0.433	0.315	0.437	0.473	0.472	0.463	0.167	0.208

	CT10	CT11	CT12	CT13	CT14	CT15	CT16	CT17	CT18
SiO2	38.95	37.15	37.20	37.43	38.42	38.20	37.57	37.48	37.69
TiO2	0.00	0.00	0.00	0.00	0.01	0.00	0.30	0.00	0.03
Al2O3	39.82	41.20	41.97	40.86	42.94	43.98	36.52	37.72	37.11
V2O3	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00
Cr2O3	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
MgO	0.00	0.00	0.00	0.00	0.00	0.00	0.18	0.08	0.11
CaO	0.29	0.28	0.08	0.49	0.07	0.24	0.20	0.25	0.29
MnO	0.48	0.27	0.62	1.22	0.36	0.18	0.89	0.53	1.39
FeO	0.10	0.00	0.00	0.18	0.18	0.01	5.27	5.06	4.17
ZnO	0.00	0.00	0.00	0.00	0.03	0.02	0.00	0.00	0.00
CuO	0.00	0.81	0.38	0.00	---	---	0.00	0.00	0.00
Na2O	1.83	1.75	1.78	1.86	2.00	1.74	2.61	2.35	2.44
K2O	0.00	0.00	0.00	0.01	0.01	0.01	0.02	0.02	0.03
F	0.96	0.88	0.60	0.93	0.93	0.58	1.34	1.14	1.30
Li2O*	2.43	1.88	1.83	2.03	1.99	1.96	1.77	1.67	1.83
B2O3*	11.05	10.91	10.99	11.12	11.30	11.37	10.78	10.81	10.80
H2O*	3.36	3.35	3.51	3.39	3.46	3.65	3.08	3.19	3.11
O=F	-0.40	-0.37	-0.25	-0.39	-0.39	-0.24	-0.56	-0.48	-0.55
Total	98.87	98.11	98.70	100.13	101.33	101.70	99.97	99.82	99.75
Na	0.558	0.541	0.546	0.564	0.596	0.516	0.816	0.733	0.761
K	0.000	0.000	0.000	0.002	0.002	0.002	0.004	0.004	0.006
Ca	0.049	0.048	0.014	0.082	0.012	0.039	0.035	0.043	0.042
Vacancy	0.393	0.411	0.440	0.352	0.390	0.443	0.145	0.220	0.158
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.541	1.211	1.164	1.285	1.231	1.206	1.146	1.080	1.181
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.043	0.019	0.026
Ti4+	0.000	0.000	0.000	0.000	0.001	0.000	0.036	0.000	0.004
V3+	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.000
Cr3+	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000
Mn2+	0.064	0.036	0.083	0.162	0.047	0.023	0.122	0.072	0.189
Fe2+	0.013	0.000	0.000	0.024	0.023	0.001	0.711	0.680	0.561
Cu	0.000	0.097	0.045	0.000	---	---	0.000	0.000	0.000
Zn	0.000	0.000	0.000	0.000	0.003	0.002	0.000	0.000	0.000
Al	1.382	1.656	1.708	1.529	1.693	1.767	0.942	1.149	1.039
Y Total	3.000	3.000	3.000	3.000	3.000	2.999	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.081	0.116	0.000	0.091	0.159	0.000	0.000	0.000
Si	6.126	5.919	5.884	6.008	5.909	5.841	6.059	6.027	6.066
T Total	6.126	6.000	6.000	6.008	6.000	6.000	6.059	6.027	6.066
OH	3.522	3.557	3.700	3.540	3.548	3.720	3.316	3.420	3.338
F	0.478	0.443	0.300	0.460	0.452	0.280	0.684	0.580	0.662

	CT19	CT20	CT21	CT22	CT23	CT24	CT25	CT26	CT27
SiO2	37.65	37.37	37.54	36.11	36.72	36.78	37.56	37.72	38.58
TiO2	0.06	0.02	0.01	0.01	0.02	0.01	0.00	0.00	0.00
Al2O3	36.38	36.14	36.51	36.18	36.44	37.54	39.07	38.69	40.19
V2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.02
MgO	0.12	0.12	0.00	0.11	0.06	0.03	0.00	0.00	0.04
CaO	0.30	0.13	0.19	0.09	0.12	0.16	0.09	0.32	0.25
MnO	1.26	0.60	1.44	0.60	0.55	1.08	1.69	0.72	0.15
FeO	5.29	5.98	4.86	7.19	6.64	4.15	0.87	2.31	1.65
ZnO	0.00	0.00	0.00	0.07	0.09	0.03	0.05	0.00	0.13
CuO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na2O	2.45	2.48	2.67	2.46	2.55	2.36	2.14	2.15	2.01
K2O	0.03	0.03	0.02	0.02	0.02	0.01	0.02	0.00	0.00
F	1.14	1.26	1.49	1.06	1.31	1.00	0.99	1.20	1.14
Li2O*	1.77	1.73	1.79	1.27	1.45	1.60	1.93	1.97	2.08
B2O3*	10.76	10.67	10.74	10.50	10.61	10.65	10.82	10.84	11.09
H2O*	3.17	3.08	3.00	3.12	3.04	3.20	3.26	3.17	3.29
O=F	-0.48	-0.53	-0.63	-0.45	-0.55	-0.42	-0.42	-0.51	-0.48
Total	99.90	99.08	99.63	98.34	99.07	98.18	98.07	98.59	100.14
Na	0.767	0.783	0.838	0.790	0.810	0.747	0.667	0.668	0.611
K	0.006	0.006	0.004	0.004	0.004	0.002	0.004	0.000	0.000
Ca	0.052	0.023	0.033	0.016	0.021	0.028	0.015	0.055	0.420
Vacancy	0.175	0.188	0.125	0.190	0.165	0.223	0.314	0.277	0.347
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.150	1.132	1.177	0.845	0.953	1.049	1.247	1.279	1.313
Mg	0.029	0.029	0.000	0.027	0.015	0.007	0.000	0.000	0.009
Ti4+	0.007	0.002	0.001	0.001	0.002	0.001	0.000	0.000	0.000
V3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cr3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002
Mn2+	0.172	0.083	0.197	0.084	0.076	0.149	0.230	0.098	0.020
Fe2+	0.715	0.815	0.658	0.996	0.909	0.567	0.117	0.310	0.216
Cu	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Zn	0.000	0.000	0.000	0.009	0.011	0.004	0.006	0.000	0.015
Al	0.927	0.939	0.967	1.038	1.034	1.223	1.400	1.313	1.425
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.000	0.022	0.000	0.000	0.000	0.000	0.000
Si	6.083	6.088	6.078	5.978	6.014	6.004	6.036	6.049	6.047
T Total	6.083	6.088	6.078	6.000	6.014	6.004	6.036	6.049	6.047
OH	3.418	3.351	3.237	3.445	3.321	3.484	3.497	3.391	3.435
F	0.582	0.649	0.763	0.555	0.679	0.516	0.503	0.609	0.565

	CT28	CT29	CT30	CT31	CT32	CT33	CT34	CT35	CT36
SiO2	38.18	38.38	37.27	38.44	36.74	37.19	34.86	37.59	37.57
TiO2	0.00	0.00	0.04	0.01	0.02	0.25	0.01	1.03	0.23
Al2O3	39.31	39.48	38.83	40.26	37.35	31.53	27.04	30.66	32.57
V2O3	0.00	0.00	0.01	0.02	0.01	0.00	0.00	0.00	0.00
Cr2O3	0.00	0.00	0.00	0.00	0.01	0.05	10.80	0.00	0.00
MgO	0.00	0.00	0.00	0.00	0.00	9.07	8.41	12.21	11.25
CaO	0.21	0.77	0.19	0.71	0.13	0.05	0.98	0.26	0.42
MnO	0.16	2.06	1.27	0.97	6.38	0.02	0.01	0.00	0.00
FeO	1.82	0.49	4.10	0.04	0.36	5.29	0.05	0.26	0.32
ZnO	0.13	0.04	1.16	0.01	0.03	0.00	0.00	0.00	0.00
CuO	0.00	0.00	---	---	---	0.00	0.00	0.00	0.00
Na2O	2.06	1.99	2.50	1.88	2.91	2.57	2.05	2.83	2.44
K2O	0.01	0.01	0.01	0.01	0.02	0.07	0.08	0.00	0.02
F	1.01	1.19	1.11	1.13	1.54	0.01	0.33	0.00	0.25
Li2O*	2.12	2.10	1.49	2.23	1.53	0.05	0.55	0.19	0.18
B2O3*	10.93	11.05	10.94	11.07	10.74	10.78	10.45	10.84	10.87
H2O*	3.29	3.25	3.25	3.28	2.97	3.72	3.45	3.74	3.63
O=F	-0.43	-0.50	-0.47	-0.48	-0.65	-0.01	-0.14	0.00	-0.11
Total	98.81	100.31	101.70	99.59	100.09	100.58	99.06	99.61	99.65
Na	0.635	0.607	0.770	0.572	0.913	0.807	0.661	0.880	0.756
K	0.002	0.002	0.002	0.002	0.004	0.014	0.017	0.000	0.004
Ca	0.036	0.130	0.032	0.119	0.023	0.009	0.175	0.045	0.072
Vacancy	0.327	0.261	0.196	0.307	0.060	0.170	0.147	0.075	0.168
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.355	1.336	0.953	1.410	0.994	0.032	0.372	0.127	0.113
Mg	0.000	0.000	0.000	0.000	0.000	2.191	1.182	2.714	2.681
Ti4+	0.000	0.000	0.005	0.001	0.002	0.030	0.018	0.124	0.028
V3+	0.000	0.000	0.001	0.003	0.001	0.000	0.000	0.000	0.000
Cr3+	0.000	0.000	0.000	0.000	0.001	0.006	1.420	0.000	0.000
Mn2+	0.022	0.275	0.171	0.129	0.875	0.003	0.001	0.000	0.000
Fe2+	0.242	0.064	0.545	0.005	0.049	0.717	0.007	0.035	0.043
Cu	0.000	0.000	---	---	---	0.000	0.000	0.000	0.000
Zn	0.015	0.005	0.136	0.001	0.004	0.000	0.000	0.000	0.000
Al	1.366	1.320	1.189	1.451	1.074	0.021	0.000	0.000	0.135
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.903	0.205	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	5.097	5.795	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.080	0.000	0.052	0.000	0.203	0.000	0.000
Si	6.070	6.038	5.920	6.036	5.948	6.026	5.797	6.029	6.005
T Total	6.070	6.038	6.000	6.036	6.000	6.026	6.000	6.029	6.005
OH	3.492	3.408	3.442	3.439	3.212	3.995	3.826	4.000	3.874
F	0.508	0.592	0.558	0.561	0.788	0.005	0.174	0.000	0.126

	CT37	CT38	CT39	CT40	CT41	CT42	CT43	CT44	CT45
SiO2	36.26	37.18	37.66	35.98	36.32	36.41	37.28	36.46	37.01
TiO2	1.38	0.48	0.04	0.07	0.11	0.02	0.02	0.56	2.05
Al2O3	27.38	33.89	34.03	29.49	31.27	32.68	32.95	31.50	28.59
V2O3	0.08	0.00	0.25	0.29	0.13	0.06	0.08	0.12	0.00
Cr2O3	0.25	0.00	0.06	8.21	5.35	4.74	4.03	0.02	0.00
MgO	12.01	9.85	10.44	9.41	9.22	8.78	9.63	9.18	13.39
CaO	2.43	0.67	1.05	1.18	0.71	0.31	0.18	1.45	2.55
MnO	0.02	0.03	0.02	0.01	0.00	0.00	0.02	0.00	0.00
FeO	2.83	0.30	0.05	0.06	0.65	0.42	0.42	5.34	0.34
ZnO	0.00	0.00	0.00	0.02	0.00	0.00	0.01	0.02	0.00
CuO	0.00	0.00	0.00	---	---	---	---	---	0.00
Na2O	1.56	2.05	2.00	2.08	2.33	2.45	2.13	2.04	1.66
K2O	0.04	0.04	0.04	0.07	0.02	0.02	0.01	0.01	0.00
F	0.94	0.20	0.28	0.28	0.09	0.18	0.05	0.19	1.35
Li2O*	0.57	0.38	0.36	0.46	0.40	0.42	0.22	0.13	0.20
B2O3*	10.40	10.89	11.06	10.83	10.83	10.88	11.01	10.75	10.72
H2O*	3.14	3.66	3.68	3.60	3.70	3.67	3.77	3.62	3.06
O=F	-0.40	-0.08	-0.12	-0.12	-0.04	-0.08	-0.02	-0.08	-0.57
Total	96.13	99.53	101.29	101.92	101.09	100.96	101.79	101.31	99.36
Na	0.505	0.635	0.609	0.647	0.725	0.759	0.652	0.639	0.522
K	0.090	0.008	0.008	0.014	0.004	0.004	0.002	0.002	0.000
Ca	0.435	0.115	0.177	0.203	0.122	0.053	0.030	0.251	0.443
Vacancy	0.051	0.242	0.206	0.136	0.149	0.184	0.316	0.108	0.035
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	0.390	0.241	0.236	0.296	0.259	0.270	0.140	0.084	0.129
Mg	2.382	2.344	2.446	1.606	1.945	2.065	2.267	2.105	2.697
Ti4+	0.173	0.058	0.050	0.008	0.013	0.002	0.002	0.068	0.128
V3+	0.011	0.000	0.031	0.037	0.017	0.008	0.010	0.016	0.000
Cr3+	0.033	0.000	0.007	1.042	0.679	0.599	0.503	0.003	0.000
Mn2+	0.003	0.004	0.003	0.001	0.000	0.000	0.003	0.000	0.000
Fe2+	0.008	0.040	0.007	0.008	0.087	0.056	0.055	0.722	0.046
Cu	0.000	0.000	0.000	---	---	---	---	---	0.000
Zn	0.000	0.000	0.000	0.002	0.000	0.000	0.001	0.002	0.000
Al	0.000	0.313	0.220	0.000	0.000	0.000	0.019	0.000	0.000
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.609	0.000	0.000	0.646	0.260	0.027	0.000	0.107	0.539
Al	5.391	6.000	6.000	5.354	5.740	5.973	6.000	5.893	5.461
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.064	0.082	0.225	0.173	0.182	0.113	0.107	0.001
Si	6.057	5.936	5.918	5.775	5.827	5.818	5.887	5.893	5.999
T Total	6.057	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
OH	3.503	3.899	3.861	3.858	3.954	3.909	3.975	3.903	3.308
F	0.497	0.101	0.139	0.142	0.046	0.091	0.025	0.097	0.692

	CT46	CT47	CT48	CT49	CT50	CT51	CT52	CT53	CT54
SiO2	37.38	35.79	36.07	36.67	36.02	35.83	34.58	34.74	35.05
TiO2	0.15	0.10	0.06	0.25	0.25	0.08	0.21	0.35	0.08
Al2O3	31.38	34.83	34.24	31.32	31.69	31.57	31.77	30.39	31.44
V2O3	0.00	0.38	0.49	0.03	0.02	0.01	0.00	0.00	0.00
Cr2O3	0.03	0.14	0.10	0.04	0.01	0.02	0.00	0.00	0.01
MgO	12.08	11.50	11.90	7.14	7.71	6.14	1.31	1.47	1.07
CaO	0.87	2.05	2.43	0.18	0.25	0.09	0.27	0.10	0.14
MnO	0.00	0.01	0.02	0.45	0.67	0.03	0.70	1.22	0.14
FeO	0.09	0.03	0.02	7.73	6.41	9.69	13.43	14.11	15.33
ZnO	0.00	0.02	0.00	0.03	0.05	0.01	0.00	0.00	0.10
CuO	0.00	---	---	---	---	---	0.00	0.00	0.00
Na2O	2.31	1.85	1.75	2.87	2.80	2.77	2.11	2.36	1.69
K2O	0.05	0.02	0.01	0.02	0.03	0.19	0.05	0.06	0.02
F	1.38	1.29	1.41	1.44	1.45	1.47	0.44	0.85	0.18
Li2O*	0.17	0.16	0.19	0.10	0.05	0.04	0.30	0.23	0.16
B2O3*	10.79	11.03	11.06	10.63	10.57	10.49	10.10	10.05	10.11
H2O*	3.07	3.19	3.15	2.99	2.96	2.92	3.28	3.06	3.40
O=F	-0.58	-0.54	-0.59	-0.61	-0.61	-0.62	-0.19	-0.36	-0.08
Total	99.17	101.85	102.31	101.28	100.33	100.74	98.37	98.63	98.85
Na	0.721	0.565	0.533	0.910	0.892	0.890	0.704	0.791	0.563
K	0.010	0.004	0.002	0.004	0.006	0.040	0.011	0.013	0.004
Ca	0.150	0.346	0.409	0.032	0.044	0.016	0.050	0.019	0.026
Vacancy	0.119	0.085	0.056	0.054	0.058	0.054	0.235	0.177	0.407
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	0.110	0.103	0.119	0.068	0.035	0.025	0.211	0.160	0.109
Mg	2.856	2.702	2.787	1.740	1.889	1.516	0.336	0.379	0.274
Ti4+	0.018	0.012	0.007	0.031	0.031	0.010	0.027	0.046	0.010
V3+	0.000	0.048	0.062	0.004	0.003	0.001	0.000	0.000	0.000
Cr3+	0.004	0.017	0.012	0.005	0.001	0.003	0.000	0.000	0.001
Mn2+	0.000	0.001	0.003	0.062	0.093	0.004	0.102	0.179	0.020
Fe2+	0.012	0.004	0.003	1.057	0.881	1.342	1.932	2.041	2.204
Cu	0.000	---	---	---	---	---	0.000	0.000	0.000
Zn	0.000	0.002	0.000	0.004	0.006	0.001	0.000	0.000	0.013
Al	0.000	0.111	0.007	0.029	0.061	0.098	0.392	0.195	0.369
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.044	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	5.956	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.359	0.333	0.005	0.079	0.065	0.050	0.000	0.000
Si	6.020	5.641	5.667	5.995	5.921	5.935	5.950	6.009	6.024
T Total	6.020	6.000	6.000	6.000	6.000	6.000	6.000	6.009	6.024
OH	3.297	3.357	3.299	3.255	3.246	3.230	3.761	3.535	3.902
F	0.703	0.643	0.701	0.745	0.754	0.770	0.239	0.465	0.098

	CT55	CT56	CT57	CT58	CT59	CT60	CT61	CT62	CT63
SiO2	36.04	34.61	32.60	33.72	36.56	36.95	36.21	35.80	35.89
TiO2	1.12	0.09	0.07	0.41	0.24	0.03	0.06	0.60	0.77
Al2O3	34.51	34.27	34.87	34.75	35.50	35.02	35.05	35.78	35.80
V2O3	0.00	0.01	0.01	0.01	0.00	0.00	0.00	0.02	0.02
Cr2O3	0.00	0.01	0.01	0.02	0.00	0.00	0.02	0.00	0.01
MgO	0.35	0.13	0.17	0.25	0.20	0.07	0.14	0.43	0.63
CaO	1.06	0.10	0.09	0.07	0.25	0.03	0.00	1.14	0.96
MnO	0.91	0.36	0.13	0.32	1.10	0.67	0.58	1.13	0.65
FeO	7.52	14.55	16.14	14.70	7.25	7.27	7.83	7.43	7.71
ZnO	0.00	0.16	0.08	0.11	0.00	0.00	0.14	0.01	0.03
CuO	0.00	0.00	---	---	0.00	0.00	0.00	---	---
Na2O	2.03	1.66	2.90	1.79	2.49	2.79	2.72	2.09	2.17
K2O	0.02	0.03	0.07	0.04	0.01	0.02	0.03	0.03	0.02
F	0.91	0.42	0.26	0.77	1.01	1.41	1.33	1.16	1.08
Li2O*	1.40	0.21	0.14	0.13	1.34	1.47	1.33	1.31	1.28
B2O3*	10.52	10.28	10.22	10.26	10.56	10.65	10.44	10.61	10.64
H2O*	3.20	3.35	3.40	3.18	3.17	3.00	2.97	3.11	3.16
O=F	-0.38	-0.18	-0.11	-0.32	-0.43	-0.59	-0.56	-0.49	-0.45
Total	99.20	100.06	101.06	100.20	99.26	99.78	98.29	100.16	100.36
Na	0.650	0.544	0.956	0.588	0.794	0.883	0.878	0.664	0.687
K	0.004	0.006	0.015	0.009	0.002	0.004	0.006	0.006	0.004
Ca	0.188	0.018	0.016	0.013	0.044	0.005	0.000	0.200	0.168
Vacancy	0.158	0.432	0.013	0.390	0.160	0.108	0.116	0.130	0.141
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	0.934	0.145	0.095	0.090	0.888	0.962	0.888	0.864	0.842
Mg	0.086	0.033	0.043	0.063	0.049	0.017	0.035	0.105	0.153
Ti4+	0.139	0.011	0.009	0.052	0.030	0.004	0.008	0.074	0.095
V3+	0.000	0.001	0.001	0.001	0.000	0.000	0.000	0.003	0.003
Cr3+	0.000	0.001	0.001	0.003	0.000	0.000	0.003	0.000	0.001
Mn2+	0.127	0.052	0.019	0.046	0.153	0.093	0.082	0.157	0.090
Fe2+	1.039	2.057	2.294	2.082	0.997	0.993	1.090	1.018	1.054
Cu	0.000	0.000	---	---	0.000	0.000	0.000	---	---
Zn	0.000	0.020	0.010	0.014	0.000	0.000	0.017	0.001	0.004
Al	0.675	0.680	0.528	0.649	0.883	0.931	0.877	0.778	0.758
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.045	0.149	0.458	0.288	0.000	0.000	0.000	0.133	0.136
Si	5.955	5.851	5.542	5.712	6.150	6.032	6.028	5.867	5.864
T Total	6.000	6.000	6.000	6.000	6.150	6.032	6.028	6.000	6.000
OH	3.524	3.775	3.860	3.588	3.474	3.272	3.300	3.399	3.442
F	0.476	0.225	0.140	0.412	0.526	0.728	0.700	0.601	0.558

	CT64	CT65	CT66	CT67	CT68	CT69	CT70	CT71	CT72
SiO2	36.80	36.33	36.28	36.57	36.46	36.27	37.21	37.44	36.41
TiO2	0.93	0.06	0.75	0.09	0.29	0.31	0.87	0.47	0.89
Al2O3	28.80	26.72	27.54	29.06	28.43	27.44	28.31	29.37	28.27
V2O3	0.00	0.00	0.16	1.35	0.03	0.00	0.00	0.36	0.06
Cr2O3	0.00	0.02	0.09	0.23	0.04	0.00	0.00	0.08	0.03
MgO	13.04	15.17	14.25	14.32	14.42	14.33	14.00	14.29	11.71
CaO	3.15	5.44	3.94	3.71	4.60	4.56	3.26	3.62	3.79
MnO	0.00	0.00	0.00	0.01	0.02	0.00	0.00	0.01	0.02
FeO	0.39	0.58	0.36	0.01	1.29	0.61	0.19	0.01	4.76
ZnO	0.00	0.00	0.00	0.02	0.02	0.00	0.00	0.04	0.02
CuO	0.00	0.00	0.00	---	---	0.00	0.00	---	---
Na2O	1.30	0.14	0.78	0.87	0.57	0.50	1.30	1.11	1.00
K2O	0.03	0.00	0.00	0.01	0.01	0.05	0.03	0.06	0.02
F	0.98	1.48	1.04	1.40	1.63	1.49	1.44	1.27	1.29
Li2O*	0.30	0.14	0.11	0.00	0.03	0.14	0.20	0.15	0.13
B2O3*	10.71	10.65	10.60	10.84	10.77	10.57	10.78	10.97	10.71
H2O*	3.23	2.97	3.16	3.07	2.94	2.94	3.04	3.18	3.08
O=F	-0.41	-0.62	-0.44	-0.59	-0.69	-0.63	-0.61	-0.53	-0.54
Total	99.24	99.63	98.62	100.97	100.87	98.59	100.02	101.90	101.65
Na	0.409	0.044	0.248	0.271	0.178	0.159	0.406	0.341	0.315
K	0.006	0.000	0.000	0.002	0.002	0.010	0.006	0.012	0.004
Ca	0.548	0.951	0.692	0.638	0.795	0.803	0.563	0.614	0.659
Vacancy	0.037	0.005	0.060	0.089	0.025	0.028	0.025	0.033	0.022
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	0.195	0.089	0.072	0.000	0.021	0.091	0.128	0.094	0.084
Mg	2.638	2.754	2.754	2.783	2.756	2.787	2.741	2.787	2.144
Ti4+	0.114	0.075	0.092	0.011	0.035	0.038	0.105	0.056	0.109
V3+	0.000	0.000	0.021	0.174	0.004	0.000	0.000	0.046	0.008
Cr3+	0.000	0.003	0.012	0.029	0.005	0.000	0.000	0.010	0.004
Mn2+	0.000	0.000	0.000	0.001	0.003	0.000	0.000	0.001	0.003
Fe2+	0.053	0.079	0.049	0.001	0.174	0.084	0.026	0.001	0.646
Cu	0.000	0.000	0.000	---	---	0.000	0.000	---	---
Zn	0.000	0.000	0.000	0.002	0.002	0.000	0.000	0.005	0.002
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Y Total	3.000	3.000	3.000	3.001	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.517	0.935	0.729	0.641	0.712	0.724	0.623	0.587	0.688
Al	5.483	5.065	5.271	5.359	5.288	5.276	5.377	5.413	5.312
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.027	0.073	0.051	0.134	0.118	0.039	0.002	0.070	0.093
Si	5.973	5.927	5.949	5.866	5.882	5.961	5.998	5.930	5.907
T Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
OH	3.497	3.236	3.461	3.290	3.168	3.226	3.266	3.364	3.338
F	0.503	0.764	0.539	0.710	0.832	0.774	0.734	0.636	0.662

	CT73	CT74	CT75	CT76	CT77	CT78	CT79	CT80	CT81
SiO2	34.69	35.79	37.24	35.53	35.74	36.34	35.77	35.54	38.28
TiO2	0.19	0.35	0.57	0.05	0.73	0.85	0.40	0.68	0.08
Al2O3	32.55	29.31	29.25	25.35	26.06	31.66	28.55	29.08	37.48
V2O3	0.56	0.07	0.22	0.00	0.04	0.09	0.01	5.25	0.00
Cr2O3	0.20	0.03	0.09	0.00	0.00	0.66	0.03	1.80	0.00
MgO	13.47	15.22	13.30	10.37	10.89	12.36	11.52	9.88	0.34
CaO	4.57	5.22	2.97	2.69	2.90	3.44	3.30	2.60	3.30
MnO	0.01	0.02	0.00	0.02	0.01	0.00	0.02	0.03	0.21
FeO	0.03	0.22	0.06	8.41	8.32	0.03	3.67	1.25	0.88
ZnO	0.00	0.00	0.00	0.00	0.01	0.00	0.01	0.02	0.00
CuO	---	---	0.00	0.00	---	---	---	---	0.00
Na2O	0.64	0.25	1.02	1.40	1.40	1.07	1.12	1.20	1.07
K2O	0.00	0.00	0.00	0.05	0.06	0.11	0.01	0.09	0.00
F	1.64	1.95	0.85	0.71	0.72	0.39	0.43	0.59	1.56
Li2O*	0.08	0.00	0.19	0.00	0.00	0.35	0.11	0.42	2.75
B2O3*	10.92	10.84	10.77	10.17	10.39	10.98	10.48	10.83	10.96
H2O*	2.99	2.81	3.31	3.17	3.24	3.60	3.41	3.46	3.04
O=F	-0.69	-0.82	-0.36	-0.30	-0.30	-0.16	-0.18	-0.25	-0.66
Total	101.85	101.26	99.49	98.02	100.20	101.77	98.67	102.46	99.29
Na	0.198	0.078	0.319	0.464	0.454	0.328	0.360	0.373	0.329
K	0.000	0.000	0.000	0.011	0.013	0.022	0.002	0.018	0.000
Ca	0.779	0.897	0.513	0.493	0.520	0.583	0.586	0.447	0.561
Vacancy	0.023	0.025	0.168	0.032	0.013	0.067	0.052	0.162	0.110
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	0.051	0.000	0.123	0.000	0.000	0.224	0.076	0.269	1.759
Mg	2.825	2.919	2.761	1.749	1.838	2.577	2.356	1.571	0.080
Ti4+	0.023	0.042	0.069	0.058	0.092	0.101	0.050	0.082	0.010
V3+	0.071	0.009	0.028	0.000	0.005	0.011	0.001	0.676	0.000
Cr3+	0.025	0.004	0.011	0.000	0.000	0.083	0.004	0.228	0.000
Mn2+	0.001	0.003	0.000	0.003	0.001	0.000	0.003	0.004	0.028
Fe2+	0.004	0.030	0.008	1.202	1.164	0.004	0.509	0.168	0.117
Cu	---	---	0.000	0.000	---	---	---	---	0.000
Zn	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.002	0.000
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.006
Y Total	3.000	3.007	3.000	3.012	3.101	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.371	0.720	0.438	0.893	0.879	0.340	0.491	0.793	0.000
Al	5.629	5.280	5.562	5.107	5.121	5.660	5.509	5.207	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.478	0.260	0.000	0.000	0.019	0.247	0.070	0.295	0.000
Si	5.522	5.740	6.008	6.073	5.981	5.753	5.930	5.705	6.072
T Total	6.000	6.000	6.008	6.073	6.000	6.000	6.000	6.000	6.072
OH	3.174	3.011	3.566	3.616	3.619	3.805	3.775	3.700	3.217
F	0.826	0.989	0.434	0.384	0.381	0.195	0.225	0.300	0.783

	CT82	CT83	CT84	CT85	CT86	CT87	CT88	CT89	CT90
SiO2	37.44	37.79	38.18	35.90	36.04	36.38	37.26	33.52	35.20
TiO2	0.21	0.00	0.04	0.00	0.04	0.07	0.02	0.42	0.08
Al2O3	37.24	37.08	38.96	34.90	36.07	35.98	41.07	32.21	20.21
V2O3	0.00	0.00	0.02	0.00	0.02	0.01	0.00	0.02	0.04
Cr2O3	0.02	0.00	0.02	0.00	0.01	0.01	0.00	0.01	15.80
MgO	0.09	0.00	0.00	0.21	0.69	0.71	1.94	0.12	10.13
CaO	4.16	2.82	4.30	0.03	0.02	0.03	0.01	0.38	0.21
MnO	0.12	3.35	0.17	1.71	1.62	1.63	0.02	0.18	0.05
FeO	0.63	0.04	0.12	11.45	11.30	10.92	5.80	17.68	0.18
ZnO	0.00	0.00	0.02	0.00	0.04	0.10	0.02	0.14	0.04
CuO	0.00	0.00	---	0.00	---	---	---	---	---
Na2O	0.65	1.29	0.69	0.75	0.86	1.00	0.53	2.47	2.67
K2O	0.00	0.01	0.00	0.01	0.01	0.01	0.00	0.07	0.02
F	1.68	1.51	1.66	0.03	0.03	0.03	0.06	1.45	0.39
Li2O*	2.79	2.43	2.85	0.31	0.20	0.29	0.62	0.12	0.27
B2O3*	10.82	10.87	11.11	10.37	10.58	10.62	11.12	10.14	10.20
H2O*	2.94	3.03	3.05	3.56	3.63	3.65	3.81	2.81	3.33
O=F	-0.71	-0.64	-0.70	-0.01	-0.01	-0.01	-0.03	-0.61	-0.16
Total	98.07	99.59	100.49	99.22	101.15	101.43	102.25	101.13	98.65
Na	0.202	0.400	0.209	0.244	0.274	0.317	0.161	0.821	0.882
K	0.000	0.002	0.000	0.002	0.002	0.002	0.000	0.015	0.004
Ca	0.716	0.483	0.721	0.005	0.004	0.005	0.002	0.070	0.038
Vacancy	0.082	0.115	0.070	0.749	0.720	0.676	0.837	0.094	0.076
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.798	1.551	1.793	0.209	0.130	0.193	0.389	0.082	0.184
Mg	0.022	0.000	0.000	0.052	0.169	0.173	0.452	0.031	0.634
Ti4+	0.025	0.000	0.005	0.000	0.005	0.009	0.002	0.054	0.010
V3+	0.000	0.000	0.003	0.000	0.003	0.001	0.000	0.003	0.005
Cr3+	0.003	0.000	0.002	0.000	0.001	0.001	0.000	0.001	2.129
Mn2+	0.016	0.454	0.023	0.243	0.225	0.226	0.003	0.026	0.007
Fe2+	0.085	0.005	0.016	1.604	1.553	1.494	0.758	2.534	0.026
Cu	0.000	0.000	---	0.000	---	---	---	---	---
Zn	0.000	0.000	0.002	0.000	0.005	0.012	0.002	0.018	0.005
Al	1.051	0.990	1.156	0.892	0.909	0.891	1.394	0.251	0.000
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.940
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	4.060
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.027	0.000	0.077	0.047	0.174	0.255	0.000
Si	6.015	6.044	5.973	6.015	5.923	5.953	5.826	5.745	6.000
T Total	6.015	6.044	6.000	6.015	6.000	6.000	6.000	6.000	6.000
OH	3.146	3.236	3.179	3.984	3.984	3.984	3.970	3.214	3.790
F	0.854	0.764	0.821	0.016	0.016	0.016	0.030	0.786	0.210

	CT91	CT92	CT93	CT94	CT95	CT96	CT97	CT98	CT99
SiO2	35.55	33.25	36.05	33.68	33.01	31.10	32.40	32.28	32.04
TiO2	0.10	0.15	0.12	0.19	0.11	0.09	0.08	0.08	2.49
Al2O3	21.98	11.72	21.68	12.25	11.00	1.25	0.65	2.33	6.36
V2O3	0.06	0.04	0.07	0.06	0.05	0.02	0.02	0.00	0.09
Cr2O3	13.30	29.68	13.27	27.25	30.36	33.54	34.77	29.24	0.01
MgO	10.26	7.57	10.37	8.64	7.19	9.98	9.89	9.49	7.20
CaO	0.20	0.23	0.19	0.38	0.21	0.00	0.01	0.00	0.01
MnO	0.02	0.01	0.01	0.03	0.03	0.51	0.45	0.32	0.03
FeO	0.18	0.07	0.26	0.17	0.05	5.09	3.84	6.88	33.13
ZnO	0.01	0.03	0.03	0.01	0.02	0.07	0.05	0.03	0.02
CuO	---	---	---	---	---	---	---	---	---
Na2O	2.68	2.67	2.73	2.56	2.60	2.72	2.56	2.62	1.96
K2O	0.03	0.05	0.03	0.05	0.06	0.30	0.34	0.28	1.39
F	0.29	0.69	0.25	0.52	0.59	0.71	0.86	0.65	0.01
Li2O*	0.29	0.64	0.42	0.50	0.69	0.00	0.14	0.10	0.00
B2O3*	10.28	9.81	10.35	9.84	9.70	9.00	9.13	8.98	8.55
H2O*	3.41	3.06	3.45	3.15	3.07	2.77	2.74	2.79	2.94
O=F	-0.12	-0.29	-0.11	-0.22	-0.25	-0.30	-0.36	-0.27	0.00
Total	98.52	99.37	99.17	99.06	98.48	96.84	97.57	95.80	96.23
Na	0.879	0.918	0.889	0.877	0.904	1.019	0.945	0.983	0.773
K	0.006	0.011	0.006	0.011	0.014	0.074	0.083	0.069	0.361
Ca	0.036	0.044	0.034	0.072	0.040	0.000	0.002	0.000	0.002
Vacancy	0.079	0.027	0.071	0.040	0.042	0.000	0.000	0.000	0.000
X Total	1.000	1.000	1.000	1.000	1.000	1.093	1.030	1.052	1.136
Li	0.204	0.457	0.283	0.354	0.497	0.000	0.108	0.075	0.000
Mg	0.968	0.000	0.889	0.000	0.000	0.000	0.000	0.000	0.000
Ti4+	0.013	0.020	0.015	0.025	0.015	0.013	0.011	0.012	0.381
V3+	0.008	0.006	0.009	0.008	0.007	0.003	0.003	0.000	0.015
Cr3+	1.778	2.501	1.762	2.583	2.466	2.284	2.187	1.743	0.002
Mn2+	0.003	0.002	0.001	0.004	0.005	0.083	0.073	0.052	0.005
Fe2+	0.025	0.010	0.037	0.025	0.007	0.823	0.611	1.114	3.342
Cu	---	---	---	---	---	---	---	---	---
Zn	0.001	0.004	0.004	0.001	0.003	0.010	0.007	0.004	0.003
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Y Total	3.000	3.000	3.000	3.000	3.000	3.216	3.000	3.000	3.748
Cr/Fe	0.000 Cr	1.658	0.000 Cr	1.223 Cr	1.837 Cr	2.840 Cr	3.047 Cr	2.731 Fe	2.293
Mg	1.619	2.000	1.708	2.276	1.921	2.875	2.807	2.738	2.183
Al	4.381	2.342	4.292	2.501	2.242	0.285	0.146	0.531	1.524
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.106	0.000	0.050	0.082	0.000	0.000	0.000	0.000
Si	6.013	5.894	6.056	5.950	5.918	6.009	6.168	6.247	6.516
T Total	6.013	6.000	6.056	6.000	6.000	6.009	6.168	6.247	6.516
OH	3.845	3.613	3.867	3.709	3.665	3.566	3.482	3.602	3.994
F	0.155	0.387	0.133	0.291	0.335	0.434	0.518	0.398	0.006

Section G.2

	CT5	CT7	CT9	CT10	CT13	CT16	CT17	CT18	CT19
SiO2	38.42	37.16	38.45	38.95	37.43	37.57	37.48	37.69	37.65
TiO2	0.00	0.00	0.00	0.00	0.00	0.30	0.00	0.03	0.06
Al2O3	40.72	41.23	41.91	39.82	40.86	36.52	37.72	37.11	36.38
V2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MgO	0.00	0.00	0.00	0.00	0.00	0.18	0.08	0.11	0.12
CaO	0.44	0.46	0.00	0.29	0.49	0.20	0.25	0.29	0.30
MnO	0.09	0.53	0.05	0.48	1.22	0.89	0.53	1.39	1.26
FeO	0.00	0.88	0.00	0.10	0.18	5.27	5.06	4.17	5.29
ZnO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na2O	1.78	1.77	1.69	1.83	1.86	2.61	2.35	2.44	2.45
K2O	0.01	0.01	0.00	0.00	0.01	0.02	0.02	0.03	0.03
F	0.95	0.94	0.42	0.96	0.93	1.34	1.14	1.30	1.14
Li2O*	2.38	1.48	2.05	2.74	1.69	1.90	1.73	1.98	1.96
B2O3*	11.13	10.76	11.14	11.28	10.84	10.88	10.86	10.92	10.91
H2O*	3.39	3.27	3.64	3.44	3.30	3.12	3.21	3.15	3.22
O=F	-0.40	-0.40	-0.18	-0.40	-0.39	-0.56	-0.48	-0.55	-0.48
Total	98.91	98.10	99.17	99.49	98.42	100.24	99.94	100.06	100.29
Na	0.539	0.554	0.511	0.547	0.578	0.808	0.729	0.753	0.757
K	0.002	0.002	0.000	0.000	0.002	0.004	0.004	0.006	0.006
Ca	0.074	0.080	0.000	0.048	0.084	0.034	0.043	0.049	0.051
Vacancy	0.385	0.364	0.489	0.405	0.336	0.154	0.224	0.192	0.186
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.493	0.963	1.285	1.695	1.091	1.223	1.115	1.265	1.256
Mg	0.000	0.000	0.000	0.000	0.000	0.043	0.019	0.026	0.029
Ti4+	0.000	0.000	0.000	0.000	0.000	0.036	0.000	0.004	0.007
V3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cr3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mn2+	0.012	0.072	0.007	0.063	0.166	0.120	0.072	0.187	0.170
Fe2+	0.000	0.119	0.000	0.013	0.024	0.704	0.677	0.555	0.705
Zn	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	1.495	1.846	1.708	1.229	1.719	0.874	1.117	0.963	0.833
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Si	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
T Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
OH	3.531	3.520	3.793	3.532	3.529	3.323	3.423	3.345	3.425
F	0.469	0.480	0.207	0.468	0.471	0.677	0.577	0.655	0.575
Anions	30.845	31.298	30.967	30.589	31.188	30.800	30.910	30.783	30.728

	CT20	CT21	CT23	CT24	CT25	CT26	CT27	CT28	CT29
SiO2	37.37	37.54	36.72	36.78	37.56	37.72	38.58	38.18	38.38
TiO2	0.02	0.01	0.02	0.01	0.00	0.00	0.00	0.00	0.00
Al2O3	36.14	36.51	36.44	37.54	39.07	38.69	40.19	39.31	39.48
V2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cr2O3	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00
MgO	0.12	0.00	0.06	0.03	0.00	0.00	0.04	0.00	0.00
CaO	0.13	0.19	0.12	0.16	0.09	0.32	0.25	0.21	0.77
MnO	0.60	1.44	0.55	1.08	1.69	0.72	0.15	0.16	2.06
FeO	5.98	4.86	6.64	4.15	0.87	2.31	1.65	1.82	0.49
ZnO	0.00	0.00	0.09	0.03	0.05	0.00	0.13	0.13	0.04
Na2O	2.48	2.67	2.55	2.36	2.14	2.15	2.01	2.06	1.99
K2O	0.03	0.02	0.02	0.01	0.02	0.00	0.00	0.01	0.01
F	1.26	1.49	1.31	1.00	0.99	1.20	1.14	1.01	1.19
Li2O*	1.93	1.99	1.48	1.61	2.01	2.10	2.19	2.28	2.20
B2O3*	10.82	10.87	10.64	10.65	10.88	10.93	11.18	11.06	11.12
H2O*	3.14	3.05	3.05	3.20	3.28	3.20	3.32	3.34	3.27
O=F	-0.53	-0.63	-0.55	-0.42	-0.42	-0.51	-0.48	-0.43	-0.50
Total	99.49	100.01	99.13	98.19	98.24	98.83	100.36	99.14	100.50
Na	0.77	0.827	0.808	0.746	0.663	0.663	0.606	0.628	0.603
K	0.006	0.004	0.004	0.002	0.004	0.000	0.000	0.002	0.002
Ca	0.022	0.033	0.021	0.028	0.015	0.055	0.042	0.035	0.129
Vacancy	0.200	0.136	0.167	0.224	0.318	0.282	0.352	0.335	0.266
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.245	1.277	0.972	1.055	1.293	1.343	1.372	1.444	1.384
Mg	0.029	0.000	0.015	0.007	0.000	0.000	0.009	0.000	0.000
Ti4+	0.002	0.001	0.002	0.001	0.000	0.000	0.000	0.000	0.000
V3+	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Cr3+	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000
Mn2+	0.082	0.195	0.076	0.149	0.229	0.097	0.020	0.021	0.273
Fe2+	0.803	0.650	0.907	0.566	0.116	0.307	0.215	0.239	0.064
Zn	0.000	0.000	0.011	0.004	0.006	0.000	0.015	0.015	0.005
Al	0.839	0.877	1.017	1.218	1.356	1.253	1.367	1.281	1.274
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Al	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Si	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
T Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
OH	3.360	3.247	3.323	3.484	3.500	3.396	3.439	3.498	3.412
F	0.640	0.753	0.677	0.516	0.500	0.604	0.561	0.502	0.588
Anions	30.711	30.751	30.953	30.985	30.879	30.842	30.842	30.767	30.876

	CT31	CT33	CT35	CT36	CT37	CT46	CT53	CT54	CT59
SiO2	38.44	37.19	37.59	37.57	36.26	37.38	34.74	35.05	36.56
TiO2	0.01	0.25	1.03	0.23	1.38	0.15	0.35	0.08	0.24
Al2O3	40.26	31.53	30.66	32.57	27.38	31.38	30.39	31.44	35.50
V2O3	0.02	0.00	0.00	0.00	0.08	0	0.00	0.00	0.00
Cr2O3	0.00	0.05	0.00	0.00	0.25	0.03	0.00	0.01	0.00
MgO	0.00	9.07	12.21	11.25	12.01	12.08	1.47	1.07	0.20
CaO	0.71	0.05	0.26	0.42	2.43	0.87	0.10	0.14	0.25
MnO	0.97	0.02	0.00	0.00	0.02	0	1.22	0.14	1.10
FeO	0.04	5.29	0.26	0.32	2.83	0.09	14.11	15.33	7.25
ZnO	0.01	0.00	0.00	0.00	0.00	0	0.00	0.10	0.00
Na2O	1.88	2.57	2.83	2.44	1.56	2.31	2.36	1.69	2.49
K2O	0.01	0.07	0.00	0.02	0.04	0.05	0.06	0.02	0.01
F	1.13	0.01	0.00	0.25	0.94	1.38	0.85	0.18	1.01
Li2O*	2.32	0.11	0.26	0.19	0.13	0.22	0.25	0.21	1.37
B2O3*	11.13	10.77	10.89	10.88	10.50	10.83	10.06	10.15	10.59
H2O*	3.31	3.71	3.76	3.64	3.18	3.08	3.07	3.42	3.18
O=F	-0.48	0.00	0.00	-0.11	-0.40	-0.58	-0.36	-0.08	-0.43
Total	99.76	100.69	99.75	99.67	98.60	99.27	98.67	98.95	99.32
Na	0.56	0.804	0.876	0.756	0.500	0.719	0.790	0.561	0.792
K	0.002	0.014	0.000	0.004	0.008	0.010	0.013	0.004	0.002
Ca	0.119	0.009	0.044	0.072	0.431	0.150	0.019	0.026	0.044
Vacancy	0.310	0.173	0.080	0.168	0.061	0.121	0.178	0.409	0.162
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.456	0.071	0.168	0.121	0.086	0.139	0.175	0.145	0.907
Mg	0.000	2.176	2.673	2.678	2.303	2.827	0.378	0.273	0.049
Ti4+	0.001	0.030	0.124	0.028	0.172	0.018	0.045	0.010	0.030
V3+	0.003	0.000	0.000	0.000	0.011	0.000	0.000	0.000	0.000
Cr3+	0.000	0.006	0.000	0.000	0.033	0.004	0.000	0.001	0.000
Mn2+	0.128	0.003	0.000	0.000	0.003	0.000	0.178	0.020	0.153
Fe2+	0.005	0.714	0.035	0.043	0.392	0.012	2.038	2.195	0.995
Zn	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.013	0.000
Al	1.406	0.000	0.000	0.130	0.000	0.000	0.186	0.343	0.866
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.005	0.232	0.000	0.660	0.064	0.000	0.000	0.000
Al	6.000	5.995	5.768	6.000	5.340	5.936	6.000	6.000	6.000
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Si	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
T Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
OH	3.442	3.995	4.000	3.874	3.508	3.299	3.536	3.903	3.476
F	0.558	0.005	0.000	0.126	0.492	0.701	0.464	0.097	0.524
Anions	30.882	30.914	30.905	30.985	31.003	30.934	30.972	30.919	30.949

	CT60	CT61	CT75	CT76	CT81	CT82	CT83	CT85	CT91
SiO2	36.95	36.21	37.24	35.53	38.28	37.44	37.79	35.90	35.55
TiO2	0.03	0.06	0.57	0.05	0.08	0.21	0.00	0.00	0.10
Al2O3	35.02	35.05	29.25	25.35	37.48	37.24	37.08	34.90	21.98
V2O3	0.00	0.00	0.22	0.00	0.00	0.00	0.00	0.00	0.06
Cr2O3	0.00	0.02	0.09	0.00	0.00	0.02	0.00	0.00	13.30
MgO	0.07	0.14	13.30	10.37	0.34	0.09	0.00	0.21	10.26
CaO	0.03	0.00	2.97	2.69	3.30	4.16	2.82	0.03	0.20
MnO	0.67	0.58	0.00	0.02	0.21	0.12	3.35	1.71	0.02
FeO	7.27	7.83	0.06	8.41	0.88	0.63	0.04	11.45	0.18
ZnO	0.00	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.01
Na2O	2.79	2.72	1.02	1.40	1.07	0.65	1.29	0.75	2.68
K2O	0.02	0.03	0.00	0.05	0.00	0.00	0.01	0.01	0.03
F	1.41	1.33	0.85	0.71	1.56	1.68	1.51	0.03	0.29
Li2O*	1.83	1.39	0.21	0.22	2.93	2.82	2.51	0.34	0.33
B2O3*	10.70	10.49	10.79	10.29	11.09	10.85	10.95	10.40	10.30
H2O*	3.02	2.99	3.32	3.21	3.09	2.95	3.06	3.57	3.42
O=F	-0.59	-0.56	-0.36	-0.30	-0.66	-0.71	-0.64	-0.01	-0.12
Total	99.22	98.42	99.53	98.01	99.65	98.14	99.77	99.29	98.58
Na	0.878	0.874	0.319	0.458	0.325	0.202	0.397	0.243	0.877
K	0.004	0.006	0.000	0.011	0.000	0.000	0.002	0.002	0.006
Ca	0.005	0.000	0.513	0.487	0.554	0.714	0.480	0.005	0.036
Vacancy	0.113	0.120	0.168	0.044	0.121	0.084	0.121	0.750	0.081
X Total	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Li	1.198	0.927	0.135	0.147	1.845	1.816	1.605	0.232	0.222
Mg	0.017	0.035	2.749	1.656	0.079	0.022	0.000	0.052	0.953
Ti4+	0.004	0.007	0.069	0.006	0.009	0.025	0.000	0.000	0.013
V3+	0.000	0.000	0.028	0.000	0.000	0.000	0.000	0.000	0.008
Cr3+	0.000	0.003	0.011	0.000	0.000	0.003	0.000	0.000	1.775
Mn2+	0.092	0.081	0.000	0.003	0.028	0.016	0.451	0.242	0.003
Fe2+	0.987	1.085	0.008	1.188	0.115	0.084	0.005	1.600	0.025
Zn	0.000	0.017	0.000	0.000	0.000	0.000	0.000	0.000	0.001
Al	0.702	0.845	0.000	0.000	0.924	1.034	0.939	0.874	0.000
Y Total	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000	3.000
Cr/Fe	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Mg	0.000	0.000	0.446	0.955	0.000	0.000	0.000	0.000	1.628
Al	6.000	6.000	5.554	5.045	6.000	6.000	6.000	6.000	4.372
Z Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
Al	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Si	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
T Total	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000	6.000
OH	3.276	3.303	3.567	3.621	3.227	3.149	3.242	3.984	3.845
F	0.724	0.697	0.433	0.379	0.773	0.851	0.758	0.016	0.155
Anions	30.701	30.908	30.972	30.678	30.767	30.951	30.844	30.949	30.959

Section G.3

	CT93	CT97	CT98
SiO2	36.05	32.40	32.28
TiO2	0.12	0.08	0.08
Al2O3	21.68	0.65	2.33
V2O3	0.07	0.02	0.00
Cr2O3	13.27	34.77	29.24
MgO	10.37	9.89	9.49
CaO	0.19	0.01	0.00
MnO	0.01	0.45	0.32
FeO	0.26	3.84	6.88
ZnO	0.03	0.05	0.03
Na2O	2.73	2.56	2.62
K2O	0.03	0.34	0.28
F	0.25	0.86	0.65
Li2O*	0.54	0.47	0.57
B2O3*	10.44	9.39	9.35
H2O*	3.48	2.83	2.92
O=F	-0.11	-0.36	-0.27
Total	99.42	98.24	96.76
Na	0.881	0.919	0.944
K	0.006	0.080	0.066
Ca	0.034	0.002	0.000
Vacancy	0.079	-0.001	-0.010
X Total	1.000	1.000	1.000
Li	0.363	0.350	0.429
Mg	0.826	0.000	0.000
Ti4+	0.015	0.011	0.011
V3+	0.009	0.003	0.000
Cr3+	1.746	1.963	1.437
Mn2+	0.001	0.071	0.050
Fe2+	0.036	0.595	1.069
Zn	0.004	0.007	0.004
Al	0.000	0.000	0.000
Y Total	3.000	3.000	3.000
Cr/Fe	0.000	3.128	2.860
Mg	1.747	2.730	2.630
Al	4.253	0.142	0.510
Z Total	6.000	6.000	6.000
Al	0.000	0.000	0.000
Si	6.000	6.000	6.000
T Total	6.000	6.000	6.000
OH	3.868	3.496	3.618
F	0.132	0.504	0.382
Anions	30.815	30.455	30.206

	CT96		CT99
SiO2	31.10		32.04
TiO2	0.09		2.49
Al2O3	1.25		6.36
V2O3	0.02		0.09
Cr2O3	33.54		0.00
Fe2O3	5.06		36.81
MgO	9.98		7.21
CaO	0.00		0.00
MnO	0.51		0.00
FeO	0.54		0.00
ZnO	0.07		0.00
Na2O	2.72		1.96
K2O	0.30		1.39
F	0.71		0.00
B2O3*	9.13		9.33
H2O*	2.81		2.42
O=F	-0.30		-----
Total	97.53		100.10
Na	1.004		0.708
K	0.073		0.330
Ca	0.000		0.000
Vacancy	-0.077		-0.038
X Total	1.000		1.000
Mg	0.000		0.000
Ti4+	0.013		0.349
V3+	0.003		0.013
Cr3+	2.080		0.000
Mn2+	0.082		0.000
Fe3+	0.725		1.795
Fe2+	0.086		0.000
Zn	0.010		0.000
Al	0.000		0.000
Y Total	3.000		2.157
Cr/Fe Cr	2.968	Fe3+	3.363
Mg	2.832		2.001
Al	0.200		1.362
Z Total	6.000		6.000
Al	0.080		0.034
Si	5.920		5.966
T Total	6.000		6.000
OH	3.573		3.000
F	0.427		0.000
OH + F	4.000		3.000