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TWO CRYSTAL STRUCTURE REFINEMENTS OF A *P*2/*n* TITANIAN FERRO-OMPHACITE

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ABSTRACT

A unique titanian ferro-omphacite has been found in the regionally metamorphosed peralkaline (agpaitic) rocks of the Red Wine alkalic province of Central Labrador. The mineral is characterized by its brilliant blue pleochroism and by its unusual composition, which is richer in Ti and Fe, and lower in Mg and Ca than previously decribed omphacites.

The mineral may be represented by the simplified formula $(Na_{.52}Ca_{.48})$ $(Al_{.46}Fe_{.47}Ti_{.07})$ Si_2O_6; it is monoclinic and crystallizes in space group *P*2/*n*, with cell dimensions $a = 9.622(2)$, $b = 8.826(2)$, $c = 5.279(1)$ Å, $\beta = 106.92(2)°$, $Z = 4$. Two independent structure refinements carried out on three-dimensional Mo*Kα* counter data gave unweighted residuals of 0.047 and 0.041. Ordering of the cations in the *M* sites is similar to that reported for *P*2 omphacite, with Fe enriched in *M*1 (and *M*1(1)*H*), Al in *M*1(1) (and *M*1*H*), Na in *M*2 (and *M*2(1)*H*) and Ca in *M*2(1) (and *M*2*H*).

INTRODUCTION

During geological investigations of a metamorphosed alkaline complex in central Labrador, an unusual blue pyroxene was encountered (Curtis *et al.* 1974). Subsequent chemical analysis indicated that the clinopyroxene was an iron-titanian-omphacite, conforming to the definition proposed by Clark & Papike (1968) *viz.* $Al/Al+Fe^{3+})>0.5$, and $0.2 \leqslant Na/(Na+Ca) \leqslant 0.8$ (Table 1). The omphacite is notably higher in Ti, Fe and Na, and correspondingly low in Mg and Ca compared to other omphacites described in the literature.

The blue pyroxene occurs in alkaline gneisses and metamorphosed syenites and malignites, and coexists with alkali feldspar, arfvedsonite, nepheline and aluminous pyroxenes. The omphacite occurs either as a single pyroxene phase, or else it coexists with aluminous aegirines (chloromelanites, see Essene & Fyfe 1967, Onuki & Ernst 1969) or aegirine-jadeites, within the same hand specimen, or more rarely within a single grain. Textural relationships suggest that the pyroxenes are metamorphic with the increase in the Jd component resulting from the lower Si in the undersaturated environment (Coleman & Clark 1967, Bell & Kalb 1969, Currie & Curtis in prep.). Similar aluminous pyroxenes are common in blueschist facies rocks in Japan, California and elsewhere. Two of the occurrences from the blueschist Sanbagawa region occur in metamorphosed derivatives of alkalic rocks (Iwasaki 1960), thus supporting the proposed metamorphic origin for these Labrador pyroxenes.

Recently an omphacite from a "hornblende bearing eclogite" described by Matsumoto & Banno (1970) was found to have *P*2/*n* symmetry, in contrast to the *P*2 symmetry ascribed to omphacites by Clark, Appleman & Papike (1969). A structural determination of the Labrador omphacite was undertaken in order to assign a structure type to this unique composition, and also to attempt to resolve the apparent conflict in the structural definition of omphacites.

EXPERIMENTAL

This paper describes structural refinements on two different crystals of the blue omphacite carried out independently at the University of Toronto and at the University of Manitoba, hereafter designated as (T) and (W).

Several representative grains of the material were analyzed by electron microprobe prior to the final analysis of the actual crystals used in the data collection. The University of Toronto ARL-EMX microprobe was used for determination of the elements under operating conditions of 15kv and 0.03μa sample current, using the method described by Rucklidge *et al.* (1970). Analysed sodic amphibole and aenigmatite were used as an internal standard. The ferric to ferrous iron ratio was determined by wet chemical methods on a bulk separate from the same sample. The analyses and crystal data are presented in Table 1. Optical parameters, determined by D. Sturman at the Royal Ontario Museum are also presented in Table 1.

Although the formulae derived from the analyses in Table 1 indicate a slight excess in the *Y* group cations, and a slight deficiency in the *X* group, the sum of the two groups is almost exactly 2.00. As the division of some of the minor elements between these groups is somewhat arbitrary, we have assumed for the purposes of crystal structure refinement that the total occupancy of the sites associated with each group is unity. We have thus been able to calculate binary combinations of elements which possess the same mean atomic number (*Z*) as the more complex real groups, and these pairs have been used in the site occupancy refinement process. The equivalent binary combination are:

	X Group	*Y* Group
Toronto	.508 Na, .492 Ca	.475 Fe, .525 Al
Winnipeg	.534 Na, .466 Ca	.518 Fe, .482 Al

TABLE 1. CRYSTAL AND CHEMICAL DATA FOR TITANIAN FERRO-OMPHACITE

Crystal data (T and W)

a=9.622(2), b=8.826(2), c=5.279(1)Å, β=106.92(2)°

V=428.85Å^3 D_m=3.42 g/cm^3 D_c=3.46 g/cm^3 Z=4

Space group *P*2/*n* (from structure determination)

Optical data (T and W)

X - dark blue	γ=1.723	Absorption *X*>*Y*>>*Z*
Y - azure blue	β=1.712	
Z - colourless	α=1.701	2V_z=84°

O.A.P. (010) $c \wedge Z$ =74° (in obtuse β)

Electron probe analyses

	TORONTO				*WINNIPEG*				
	Wt. %	Cation proportions*		$\bar{Z}$	Wt. %	Cation proportions		$\bar{Z}$	Cation group
SiO_2	52.8	1.973	2.00	13.98	52.5	1.952	2.00	13.98	*Z*
		0.027				0.048			
Al_2O_3	11.5	0.480	1.02	19.17	10.2	0.399	1.01	19.74	*Y*
TiO_2	0.88	0.025			2.60	0.073			
Fe_2O_3†	4.98	0.140			5.05	0.141			
FeO	10.5	0.332			10.8	0.334			
MgO	0.84	0.047			1.04	0.058			
MnO	0.64	0.020	0.98	15.43	0.57	0.018	0.99	15.19	*X*
CaO	11.2	0.448			10.7	0.426			
K_2O	0.05	0.002			0.05	0.002			
Na_2O	6.99	0.507			7.60	0.548			
	100.4				101.1				

Chemical formulae*

Toronto:
$(Na_{.52}Ca_{.46}Mn_{.02})_{0.98}(Al_{.47}Fe^{2+}_{.33}Fe^{3+}_{.14}Mg_{.04}Ti_{.02})_{1.02}(Si_{.97}Al_{.03})_{2.0}O_6$

Winnipeg:
$(Na_{.55}Ca_{.43}Mn_{.02})_{1.00}(Al_{.40}Fe^{2+}_{.33}Fe^{3+}_{.14}Mg_{.06}Ti_{.07})_{1.00}(Si_{.98}Al_{.02})_{2.0}O_6$

*Cation proportions and formulae calculated on the basis of 6 oxygens. The sum of the partial atoms within the brackets has been scaled to unity.

†Fe^{3+}/Fe^{2+} determined by wet chemical analysis. Assumed equal for both samples.

It became apparent from the microprobe scans and microscopic observations that the dark blue—pale blue pleochroism which characterizes this pyroxene could be correlated with the changes in the Ti content, which may in turn be dependent on Fe. The dark blue zones were found to be higher in Ti and lower in Ca and Al relative to the pale blue zones. It is interesting to note that the cell dimensions of both forms (dark blue and blue) determined independently at (W) and (T) were virtually identical (within 2σ). It was concluded, therefore, that the small variations in the Ti content between (W) and (T) crystals (See Table 1) did not substantially affect the cell dimensions.

The material used for the *x*-ray study was selected from crushed fragments of some of the larger blue crystals. The common heterogeneous association of pyroxene crystals in these rocks rendered difficult the selection of a suitable homogeneous crystal, but the quality of the crystals finally chosen was assessed using the polarizing microscope, and Weissenberg and precession photographs taken with Cu$K\alpha$ and Mo$K\alpha$ radiation.

All tested crystals showed violation of *C*-centring and *c* glide extinctions in space group *C*2/*c*, but $h0l$ reflections with $h + l = 2n + 1$ remained systematically absent. These systematic absences were confirmed by long (80-120 hrs) exposure of the $h0l$ level taken on a precession camera with both Cu$K\alpha$ and Mo$K\alpha$ radiations and by slow 2θ scans carried out on a four circle diffractometer with Mo$K\alpha$ radiation. These observations indicated that the space group symmetry of this omphacite is lowered from *C*2/*c* to *Pn* or *P*2/*n* rather than to *P*2 as previously reported for other omphacites from California and Venezuela localities (Clark & Papike 1968; Clark, Appleman & Papike 1969).

The refinements of both structures were initiated using modified jadeite coordinates (Prewitt & Burnham, 1966) in the centrosymmetric space group *P*2/*n*. A shift of origin from *C*2/*c*

TABLE 2. SUMMARY OF EXPERIMENTAL METHODS EMPLOYED IN THE DATA COLLECTION AND FINAL RESIDUALS FROM THE LEAST-SQUARES REFINEMENT

	Toronto	Winnipeg
Crystal size	0.03 x 0.06 x 0.3 mm	0.04 x 0.11 x 0.23 mm
Radiation used	Zr-filtered Mo$K\alpha$	graphite-monochromated Mo
2θ-θ scan speed	0.5°/min.	variable, 2-24°/min.
Diffractometer used	Picker FACS-1	Syntex P $\bar{1}$
Background	2 x 40 sec.	variable with scan speed
Standard reflections measured	2 every 60 refl.	2 every 50 refl.
sin θ/λ max.	0.70	0.756
Absorp. corrections	not applied	Gaussian quadrature
Number of independent reflections measured	1269	1335
Number of reflections "observed"	843(3σ)	922(4σ)
Weighting scheme	unit weights	unit weights
Final *R*-value on "observed" data	0.047	0.041
Final R_w-value on "observed data"	0.045	0.040

TABLE 3. POSITIONAL PARAMETERS AND ISOTROPIC TEMPERATURE FACTORS

	TORONTO					*WINNIPEG*				
Atom	Site Occupancy	x	y	z	B(Å^2)	Site Occupancy	x	y	z	B(Å^2)
*M*1	Fe 0.779 Al 0.221	0.75	0.6570(2)	0.25	0.61	Fe 0.786 Al 0.214	0.75	0.6560(1)	0.25	0.56
*M*1(1)	Fe 0.171 Al 0.829	0.75	0.8499(2)	0.75	0.41	Fe 0.251 Al 0.749	0.75	0.8499(2)	0.75	0.44
*M*2	Ca 0.285 Na 0.715	0.75	0.0524(4)	0.25	1.50	Ca 0.260 Na 0.740	0.75	0.0520(3)	0.25	1.40
*M*2(1)	Ca 0.699 Na 0.301	0.75	0.4530(2)	0.75	1.19	Ca 0.672 Na 0.328	0.75	0.4526(2)	0.75	1.15
Si 1	1.0	0.0402(2)	0.8472(2)	0.2298(3)	0.57	1.0	0.0402(2)	0.8464(1)	0.2305(3)	0.51
Si 2	1.0	0.0381(2)	0.6651(2)	0.7354(3)	0.54	1.0	0.0382(2)	0.6647(1)	0.7353(3)	0.49
O 1(1)	1.0	0.8655(4)	0.8410(5)	0.1223(8)	0.83	1.0	0.8646(4)	0.8400(4)	0.1227(7)	0.68
O 1(2)	1.0	0.8622(5)	0.6804(5)	0.6561(8)	0.89	1.0	0.8632(4)	0.6798(4)	0.6559(7)	0.66
O 2(1)	1.0	0.1154(4)	0.0091(4)	0.3095(5)	0.93	1.0	0.1156(4)	0.0088(4)	0.3088(7)	0.73
O 2(2)	1.0	0.1039(5)	0.5007(5)	0.8052(8)	1.12	1.0	0.1041(4)	0.5002(4)	0.8058(7)	0.90
O 3(1)	1.0	0.1077(5)	0.7660(5)	0.0082(8)	0.93	1.0	0.1072(4)	0.7661(4)	0.0102(7)	0.70
O 3(2)	1.0	0.0969(4)	0.7430(5)	0.5019(8)	0.87	1.0	0.0972(4)	0.7428(4)	0.5024(7)	0.61

e.s.d.'s in parentheses refer to last decimal place.

Origin at $\bar{1}$. Equivalent positions: x,y,z; $\bar{x},\bar{y},\bar{z}$; $\frac{1}{2}-x,\bar{y},\frac{1}{2}-z$; $\frac{1}{2}+x,\bar{y},\frac{1}{2}+z$.

to *P*2/*n* requires a change of +¼ or –¼ in both the *x* and *y* coordinates). For both refinements initial *R*-values were about 0.30 - 0.35, but the structures converged rapidly after several cycles of least squares refinement to 0.06 (T) and 0.051 (W) using refined individual isotropic temperature factors. Conversion to anisotropic temperature factors resulted in final unweighted *R*-values (observed data) of 0.047 (T) and 0.041 (W). Neutral scattering factors of Cromer & Mann (1968) (T) and Doyle & Turner (1968) (W), and anomalous dispersion corrections of Cromer & Lieberman (1970) (T) and Cromer (1965) (W) were used in the refinements. The results of the refinement confirm the choice of *P*2/*n*, the higher symmetry of the two possible space groups.

TABLE 4. ANISOTROPIC TEMPERATURE FACTORS (x 10^4)

	TORONTO						*WINNIPEG*					
Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
*M*1	21(2)	22(2)	39(5)	0	9(2)	0	17(1)	21(1)	53(4)	0	5(2)	0
*M*1(1)	16(2)	13(2)	37(8)	0	16(3)	0	13(2)	16(2)	38(6)	0	8(3)	0
*M*2	56(4)	36(4)	119(12)	0	15(5)	0	52(3)	35(2)	106(10)	0	5(4)	0
*M*2(1)	52(3)	29(3)	82(8)	0	3(3)	0	45(2)	33(2)	95(7)	0	-3(3)	0
Si1	23(2)	16(2)	52(5)	1(1)	20(2)	-2(2)	15(1)	20(1)	46(4)	0(1)	11(2)	1(2)
Si2	19(2)	19(2)	45(5)	0(1)	15(2)	0(2)	17(1)	18(1)	35(4)	1(1)	10(2)	1(2)
O1(1)	19(4)	31(5)	98(14)	1(3)	25(6)	-3(6)	17(3)	30(4)	53(12)	-1(3)	12(5)	-1(5)
O1(2)	27(4)	28(5)	102(14)	4(4)	25(6)	-6(6)	12(3)	30(4)	61(21)	-3(3)	12(5)	-3(5)
O2(1)	36(5)	27(5)	74(14)	-7(4)	18(6)	0(5)	22(3)	19(3)	77(13)	-3(3)	7(5)	-4(5)
O2(2)	43(5)	31(5)	113(15)	16(4)	34(7)	18(7)	33(4)	22(4)	89(13)	8(3)	19(6)	7(6)
O3(1)	38(5)	32(4)	60(14)	1(4)	21(6)	-13(7)	18(3)	27(3)	67(13)	3(3)	10(5)	-12(5)
O3(2)	24(4)	34(5)	82(15)	2(4)	21(6)	7(7)	20(4)	27(3)	33(12)	-1(3)	17(5)	8(5)

e.s.d.'s in parentheses refer to last decimal place

TABLE 5. IMPORTANT INTERATOMIC DISTANCES AND ANGLES

			TORONTO	*WINNIPEG*
Si1	- O1(1)		1.611(5)Å	1.619(4)
	- O2(1)		1.602(5)	1.606(4)
	- O3(1)		1.656(5)	1.646(4)
	- O3(2)		1.659(4)	1.655(4)
		Mean	1.632	1.631
		Q.E.	1.0049	1.0049
Si2	- O1(2)		1.627(5)	1.618(4)
	- O2(2)		1.584(5)	1.584(4)
	- O3(1)		1.660(4)	1.670(4)
	- O3(2)		1.649(4)	1.648(4)
		Mean	1.630	1.630
		Q.E.	1.0046	1.0047
*M*1	- O1(1)	(2x)	2.182(4)	2.177(4)
	- O1(2)	(2x)	2.112(4)	2.113(4)
	- O2(2)	(2x)	2.058(5)	2.050(4)
		Mean	2.117	2.113
		Q.E.	1.0151	1.0153
Site occupancy		Fe	0.78(1)	0.79(1)
		Al	0.22	0.21
*M*1(1)	- O1(1)	(2x)	1.958(4)	1.957(4)
	- O1(2)	(2x)	1.990(5)	2.000(4)
	- O2(1)	(2x)	1.887(5)	1.886(4)
		Mean	1.945	1.948
		Q.E.	1.0060	1.0059
Site occupancy		Fe	0.17	0.25
		Al	0.83	0.75
*M*2	- O1(1)	(2x)	2.368(5)	2.367(4)
	- O2(1)	(2x)	2.373(4)	2.372(4)
	- O3(2)	(2x)	2.455(5)	2.456(4)
	- O3(1)	(2x)	2.718(5)	2.729(4)
		Mean	2.479	2.481
Site occupancy		Ca	0.29(2)	0.26
		Na	0.71	0.74(2)
*M*2(1)	- O1(2)	(2x)	2.398(4)	2.402(4)
	- O2(2)	(2x)	2.396(4)	2.393(4)
	- O3(1)	(2x)	2.495(5)	2.491(4)
	- O3(2)	(2x)	2.841(4)	2.838(4)
		Mean	2.533	2.531
Site occupancy		Ca	0.70	0.67
		Na	0.30	0.33

Angles(°)	*TORONTO*	*WINNIPEG*
O1(1)-Si1-O2(1)	117.9	117.8
O1(1)- -O3(1)	108.6	108.7
O1(1)- -O3(2)	109.5	109.5
O2(1)- -O3(1)	109.4	108.9
O2(1)- -O3(2)	104.9	105.0
O3(1)- -O3(2)	105.9	106.0
Mean	109.4	109.3
O1(1)-Si2-O2(2)	116.9	116.9
O1(2)- -O3(1)	107.8	107.6
O1(2)- -O3(2)	109.3	109.3
O2(2)- -O3(1)	104.9	104.9
O2(2)- -O3(2)	110.8	111.7
O3(1)- -O3(2)	106.9	106.7
Mean	109.4	109.5

e.s.d.'s in parentheses refer to last decimal place

Q.E. is the quadratic elongation parameter (Robinson *et al.* 1971)

For O1(1)-Si2-O2(2): read O1(2)-Si2-O2(2)

A summary of the experimental methods employed in the data collections at (T) and (W) is given in Table 2. Both refinements were carried out using the full-matrix least squares program RFINE (Finger 1969) which permits multiple site occupancy refinement with chemical constraints. Table 3 lists positional parameters and individual isotropic temperature factors for both structures. Nomenclature for the atoms follow the scheme set out by Burnham *et al.* (1967). Anisotropic temperature factors are given in Table 4, and some of the more important interatomic distances and angles in Table 5. Table 6, which contains observed and calculated structure factors for the two refinements, has been deposited with the National Science Library Ottawa*.

DISCUSSION

The titanium content of this omphacite is clearly variable, as the microprobe analyses have

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*This table has been deposited with the Depository of Unpublished Data. Copies may be obtained on request to: Depository of Unpublished Data, National Science Library, National Research Council of Canada, Ottawa, Ontario, Canada.

shown, and the intensity of the blue colouring can be correlated with TiO_2. The two crystals chosen for structure determination had widely differing TiO_2 contents, namely .88 and 2.60 wt. %. The former is not unusual but the latter greatly exceeds the TiO_2 content of most omphacites which rarely rises above 0.5%. However, this work shows that the two specimens have virtually identical crystal structures, so the presence or absence of Ti does not seem to be an important structural consideration.

This omphacite can be seen to differ from others in a more dramatic way when one considers its extremely low Mg content (~1% MgO) and its rather high Fe (15% FeO equivalent). Both these quantities lie well outside the normal range reported for omphacites, and it may be that the substitution of Fe for Mg has some bearing on the more restricted ordering pattern over 2 cation sites in *P*2/*n* as observed in this study compared with the *P*2 omphacites, where there are 4 independent disordered cation sites. Fig. 1a illustrates the omphacite compositional field within the aluminous and ferric clinopyroxenes (Clark & Papike 1968). When plotted on this diagram (Fig. 1b) the compositions of the two crystals analysed in this study fall right in the middle of the omphacite field as defined by those authors. Also plotted in Fig. 1b are individual analyses of other clinopyroxenes from the Red Wine province, and it is seen that a continuous range exists right across to aegirine. The colour also varies across this range, and crystals can broadly be classed into 3 groups on this basis: 1) blue, in the omphacite field, 2) pale blue or colourless in the circled area, and 3) green towards aegirine.

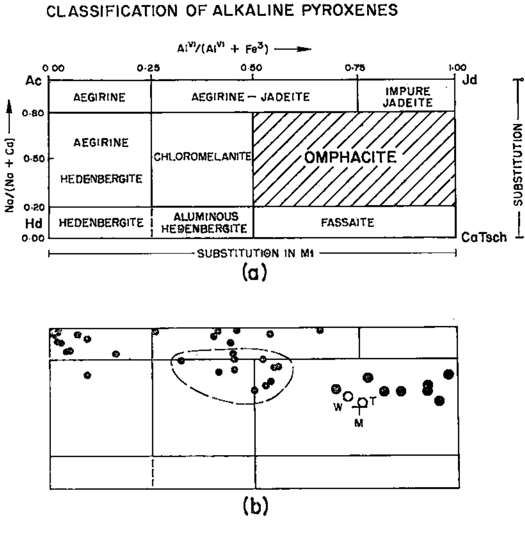

FIG 1. (a) Classification proposed for alkaline pyroxenes, incorporating the field of omphacite as defined by Clark & Papike (1968).

(b) Analyses of pyroxenes from the Red Wine complex covering the range omphacite to aegirine. The dashed area represents pyroxenes distinguished optically as chloromelanites. The *P*2/*n* samples are designated W and T, the *P*2/*n* specimen of Matsumoto and Banno (1970) is designated M.

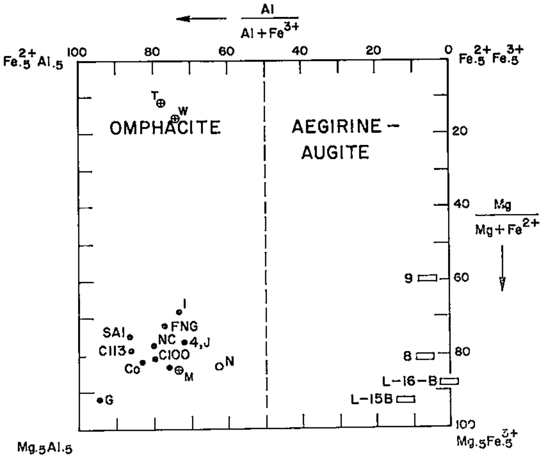

FIG. 2. Diagram of Al/(Al + Fe^{3+}) versus Mg/(Mg + Fe^{2+}) showing previously studied omphacites (Clark & Papike 1968) and the *P*2/*n* omphacites of this study as T. W, and of Matsumoto & Banno (1970) as M.

The compositions of the analysed samples as plotted in Fig. 1. are unremarkable. However, when the same compositions are presented on a Mg/(Mg+Fe^{2+}) vs Al/(Al+Fe^{3+}) diagram, as in Fig. 2, it is clear that these specimens lie far outside the normal range.

The existence of *P*2/*n* omphacite has already been noted (Matsumoto & Banno 1970, 1971; Matsumoto *et al.* 1972) although no structure refinement of this crystal appears to have been published. The composition of their sample plots in the normal range for omphacites as seen in figs. 1, and 2, so it becomes less tenable to attribute the existence of this new pyroxene space group to a high Fe/Mg ratio.

The crystal structure of our *P*2/*n* omphacite bears close resemblance to that of the *P*2 omphacite described by Clark & Papike (1968). However, whereas in their structure the absence of a centre of symmetry and *n* glide) demand the existence of two independent tetrahedral chains, *A* and *C*, in *P*2/*n* all chains are equivalent. Each chain still contains two independent Si atoms Si1 and Si2 linked through O3(1) and O3(2). Similarly the number of independent *M* sites is reduced from 8 to 4, namely *M*1, *M*1(1), *M*2 and *M*2(1) to which *M*1(1)*H*, *M*1*H*, *M*2(1)*H* and *M*2*H* are respectively equivalent.

Close similarities also exist in the site occupancies which in the *P*2 model were described with nearly identical occupancies in *M*- and *M*-(1)*H*, and *M*-(1) and *M*-*H*, though this is not required by *P*2 symmetry. In *P*2/*n* these pairs are symmetry related, and hence constrained to be equal in the refinement. In two refined *P*2 omphacites (Clark *et al.* 1969) the ratio Mg/(Mg+Fe) is about 0.8 while in our *P*2/*n* sample, this ratio is about 0.1. Hence we cannot directly compare site occupancies beyond saying that in both structures Al is concentrated in *M*1(1) and *(M*1 *H)*, Fe and Mg in *M*1 (and *M*1(1)*H)*; for *M*2 the similarity persists with Na enriched in *M*2 (and *M*2(1)*H)* and Ca in *M*2(1) (and *M*2*H)*. Thus the *P*2/*n* structure is seen to offer an ordering pattern for the 4 different non-tetrahedrally coordinated cation species (Mg,Fe), Al, Na and Ca, which is simpler than in the *P*2 structure model. In the latter, 8 sites are available for occupancy by 4 groups while the former has a one to one correspondence. However, only in this minor respect do the structures differ, and the geometrical structural details described by Clark & Papike (1968) for *P*2 apply almost equally to the *P*2/*n* arrangement.

Champness (1973) has speculated on the possibility of an order-disorder transformation existing in the omphacite field, whereby disordered *C*2/*c* jadeite-diopside solid solution would order into *P*2 or *P*2/*n* on cooling. An omphacite which has experienced this ordering would consist of two sets of domains in which the origins of the primitive cells on opposite sides of an antiphase boundary would differ by ½(a±b). If the crystal originally formed as an ordered phase, one would expect the anti-phase domains to be absent, but these can only be detected by electron microscope studies, which have not been attempted here. The attractive possibility exists, however, of defining more precisely the conditions of formation by this approach.

As a final point it is worth noting that the quadratic elongation distortion parameters (Robinson *et al.* 1971) for the two *M*1 octahedra differ markedly. The octahedron enriched in Fe has a distortion of 1.015 in contrast to the Al-enriched octahedron, *M*1(1), where the distortion is only 1.005. This result bears out the fairly general observation that Fe-bearing octahedra are often more distorted than Fe-free ones. This compares with corresponding values of 1.015, 1.017, 1.010, and 1.016 for *M*1, *M*1 (1)*H*, *M*1(1) and *M*1*H* in the *P*2 omphacite of Clark & Papike (1968). The distortion in the first two, which contain mainly Mg with minor Fe, is interestingly similar to the Fe-rich ones of our structure. Even when the Clark & Papike (1968) data are refined in *P*2/*n* (when a residual of 0.046 can be obtained) the distortions of *M*1 and *M*1(1) octahedra become 1.014 and 1.006. This result would appear to indicate that the structure, rather than the Fe content, is responsible for the distortion.

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