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Crystal-Structure Refinement of Cubic Boracite

SHIGEHO SUENO
Department of Earth and Space Sciences, State University of New York at Stony Brook, New York 11790

JOAN R. CLARK
U. S. Geological Survey, Washington, D. C. 20242

J. J. PAPIKE
Department of Earth and Space Sciences, State University of New York at Stony Brook, New York 11790

JUDITH A. KONNERT
U. S. Geological Survey, Washington, D. C. 20242

Abstract

Single-crystal data for boracite, $Mg_3ClB_7O_{13}$, have been collected above the transition point (268 ± 7°C) for refinement of the cubic structure originally determined by Ito, Morimoto, and Sadanaga in 1951. The space group is confirmed as $F\bar{4}3c$; at 400°C, $a = 12.0986 \pm 0.0002$ Å. The cubic structure can be considered in three ways: as a true, high-temperature "point-atom" array; as a disordered space-time average of the various ferroelectric orientations of the orthorhombic structure; and as a combination of these two possibilities. Thermal data and least-squares refinements of split-atom models indicate that the combination model is the most likely. In it, the borate framework at high temperature appears to be reasonably ordered and consists entirely of corner-linked tetrahedra. One of the two crystallographically distinct oxygen atoms is surrounded tetrahedrally by four boron atoms, each at 1.693 Å. The improved residual factors for split-atom refinements of Cl and Mg atomic positions, together with the high thermal parameters, especially for Mg atoms, suggest that these atoms are disordered within the cavities of the framework.

Introduction

Boracite, $Mg_3ClB_7O_{13}$, is orthorhombic at room temperature, but the symmetry changes to cubic above a temperature of about 265°C, as determined by Mehmel (1934a). The two forms are referred to in the literature as α and β, or as high and low, corresponding, respectively, to cubic and orthorhombic. Mehmel (1934a) considered possible arrangements of the atoms in some cubic space groups without detailed experimental confirmation. The structure of the cubic form was solved by Ito, Morimoto, and Sadanaga in 1951 with data taken from powder photographs. They also solved the structure of the orthorhombic form by analogy to that of the cubic form, using single-crystal photographic data obtained from a twinned crystal and corrected appropriately. Twinning is common in boracite crystals and has been described by Mehmel (1934b) and by Palache *et al* (1951). Recently Dowty and Clark (1973) refined the structure of low boracite, using single-crystal diffractometer data obtained with an untwinned crystal. The same crystal has now been used for collection of data above the transition point, and the results of the refinement are reported here. A preliminary account was presented orally at the Ninth International Congress of Crystallography, Kyoto, Japan (August 30, 1972).

Experimental Work

Crystallographic and X-ray diffraction data

The crystal of boracite used for this study was described by Dowty and Clark (1973) as "an irregular fragment with trapezoidal shape from a specimen originating at Solvayshall, Roschwitz, Germany (U. S. National Museum No. B12325); the size of the fragment was 0.23 × 0.16 × 0.10 mm. It was verified optically to be a single domain." Precession photographs were taken both at room temperature and at 400°C for the crystal mounted along the orthorhombic a^* axis; the effects of the transition on the diffraction patterns are apparent from the disappearance of a large number of reflections above the transition point. The transition temperature was measured by a thermocouple calibrated with the melting points of $NaNO_3$ and NH_4NO_3, 306.8°C and 169.6°C, respectively, and was monitored by observation of the orthorhombic 331 reflection and its equivalents while the crystal was heated to the data-collection temperature of 400 ± 10°C. These reflections disappear abruptly when the symmetry change occurs at 268 ± 7°C, a value in agreement, within the error, with that reported by Mehmel (1934a). The transition point is sharp and reproducible over repeated runs.

The space group $F\bar{4}3c$ (no. 219, Henry and Lonsdale, 1952) is verified both by absence of all hkl reflections with $h + k$, $k + l$, $l + h$ odd and all hhl reflections with l, (h) odd, and also by the failure of attempts to refine the structure in other cubic space groups such as $F\bar{4}3m$ and $F23$. The cubic cell constant was obtained by least-squares refinement of twelve crystallographically independent reflections measured at 400°C: $a = 12.0986 \pm 0.0002$ Å. This value can be compared with the orthorhombic c dimension at room temperature, 12.0910 ± 0.0009 Å (Dowty and Clark, 1973). The orthorhombic c may coincide with any of the three cubic axes, and the orthorhombic a and b directions must lie along the cubic [110]. There are thus six possible orientations which account for the twinning of low boracite and are important in considering the ferroelectricity and ferroelasticity of boracite (*e.g.* Ascher *et al*, 1966; Dowty and Clark, 1972; Torre *et al*, 1972).

The data were collected on a Picker single-crystal automatic diffractometer using Mo$K\alpha$ radiation monochromatized by a graphite crystal. Brown *et al* (1973) have described the modification of the apparatus for high-temperature work, and the special method used for mounting the crystal. A total of 834 data were collected; these included many equivalents, all of which agreed within the errors of observation that were derived from the counting statistics. The data were corrected for Lorentz and polarization factors but not for absorption which was considered negligible ($\mu = 7.6$ cm^{-1}). The strong 400 reflection appeared to suffer from extinction effects and was removed from the final cycles of refinement. The values for all equivalent reflections were averaged to reduce the final data set to 148; only eight of this number had values below the statistical threshold of observation.

Refinement procedures

The least-squares program RFINE written by L. W. Finger, Geophysical Laboratory, Washington, D. C., was used initially, including all 724 observed data. The scattering factors were calculated from a nine-coefficient analytical function (Cromer and Waber, 1965) using the coefficients given by Cromer and Mann (1968) for neutral atoms. The initial atomic parameters were obtained from the structure of low boracite (Dowty and Clark, 1972) after appropriate transformation to the cubic space group. In $F\bar{4}3c$

TABLE 1. Atomic Parameters in Cubic Boracite[1]

Space group $F\bar{4}3c$ (no. 219)[2]						
Atom	Cl	Mg	B(1)	B(2)	O(1)	O(2)
Position[2]	8b	24c	24d	32e	8a	96h
Point symmetry	23	$\bar{4}$	$\bar{4}$	3	23	1
x	0.250	0.	0.250	0.0808(2)	0.	0.0987(2)
y	0.250	0.250	0.	0.0808	0.	0.0214(2)
z	0.250	0.250	0.	0.0808	0.	0.1821(2)
Equivalent isotropic B (Å)^2	3.2(1)	2.75(8)	0.6(1)	1.1(1)	1.1(1)	0.72(4)
β_{11}	0.0054(2)	0.0111(4)	0.0007(4)	0.0019(2)	0.0018(3)	0.0011(2)
β_{22}	0.0054	0.0015(1)	0.0011(3)	0.0019	0.0018	0.0016(2)
β_{33}	0.0054	0.0015	0.0011	0.0019	0.0018	0.0011(1)
β_{12}	0.	0.	0.	0.0010(2)	0.	0.0005(1)
β_{13}	0.	0.	0.	0.0010	0.	0.0003(1)
β_{23}	0.	0.	0.	0.0010	0.	0.0004(1)

[1] *Error in parentheses is one standard deviation; for 0.0808(2) read 0.0808±0.0002, etc.*

The β_{ij} *are in the temperature factor form:* $\exp\{-\sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_j \beta_{ij}\}$.

[2] *Henry and Lonsdale (1952).*

there are four positional parameters plus seven isotropic or 14 anisotropic temperature factors to refine, in addition to the scale factor. The conventional $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ was initially 0.16; it dropped to 0.063 after three cycles of refinement using anisotropic temperature factors. When the data set was reduced to 140, the corresponding R was 0.053. Split-atom models for Cl, Mg, O(1), and B(1) were refined with anisotropic temperature factors; the results are discussed in a following section. Using only the 140 non-equivalent data above threshold value, an electron-density map and a difference Fourier map were calculated at the end of anisotropic refinement, using *X-Ray 67, Program System for X-Ray Crystallography*, written by J. M. Stewart, University of Maryland (modified for the IBM 360/65 by Daniel E. Appleman, U. S. Geological Survey, Washington, D. C.). The maps showed no anomalous features, and the largest peaks on the difference Fourier were only about $1/3\ e/\text{Å}^3$. The atomic parameters are listed in Table 1, and the structure factors are compared for observed and calculated data in Table 2. The thermal ellipsoids are given in Table 3. The results for the split-atom models are shown in Table 4.

Description of Structure

Structure of orthorhombic boracite

In order to consider the cubic structure, it is necessary to review the features of the orthorhombic structure. Its borate framework consists of linked tetrahedra, including a ring system with three boron atoms attached to one O(1) oxygen atom; corner-linked triangles complete the framework. The arrangement in space is such that a boron atom of one triangle approaches an O(1) oxygen atom at 2.303 Å (Fig. 1). During the polarity changes, as shown by Dowty and Clark (1972), a bond from O(1) shifts from a tetrahedrally to a triangularly coordinated boron atom, the two boron atoms thereby switching coordination type from tetrahedral to triangular and vice versa. These shifts involve displacements of about 0.5 Å. The Mg cations, in addition to four oxygen neighbors, have one close Cl anion at about 2.6 Å and one distant one at about 3.5 Å. The polarity changes also shift some of these bonds from the close Cl anions to those that were previously distant. These displacements are about 0.4 Å. The structure remains the same before and after the polarity changes; only the orientation is different (Dowty and Clark, 1973).

TABLE 2. Comparison of Observed and Calculated Structure Factors for Cubic Boracite

h	k	ℓ	F_o	F_c	h	k	ℓ	F_o	F_c	h	k	ℓ	F_o	F_c
2	0	0	112	106	17,	5,	1	42	44	15,	9,	3	18	21
4	0		E	365	9	7		60	59	13,	11,		17	16
6	0		61	63	11,	7,		50	50	4	4	4	323	331
8	0		202	195	13,	7,		39	36	6	4		121	114
10,	0,		85	80	15,	7,		39	37	8	4		260	251
12,	0,		241	243	11,	9,		32	36	10,	4,		117	112
14,	0,		135	138	13,	9,		16	17	12,	4,		125	121
16,	0,		58	56	15,	9,		22	20	14,	4,		32	28
2	2		26	13	13,	11,		10	8	16,	4,		52	53
2	4		180	171	2	2	2	196	190	6	6		105	98
2	6		61	55	4	2		130	118	8	6		48	46
2	8		139	126	6	2		180	166	10,	6,		38	40
2,	10,		74	69	8	2		81	79	12,	6,		9	8
2,	12,		35	34	10,	2,		*	5	14,	6,		47	44
2,	14,		*	8	12,	2,		73	70	16,	6,		30	35
2,	16,		28	21	14,	2,		62	64	8	8		171	162
4	4		253	252	16,	2,		34	33	10,	8,		75	71
4	6		131	124	4	4		31	25	12,	8,		90	87
4	8		226	218	6	4		75	67	14,	8,		*	5
4,	10,		59	53	8	4		50	46	10,	10,		32	28
4,	12,		135	129	10,	4,		71	70	12,	10,		19	24
4,	14,		58	55	12,	4,		30	31	14,	10,		44	44
4,	16,		82	86	14,	4,		30	31	12,	12,		60	59
6	6		14	15	16,	4,		14	10	9	7	5	26	23
6	8		*	5	6	6		74	65	11,	7,		34	35
6,	10,		68	65	8	6		61	58	13,	7,		45	47
6,	12,		27	33	10,	6,		38	34	15,	7,		16	18
6,	14,		23	24	12,	6,		50	48	11,	9,		47	44
6,	16,		23	25	14,	6,		*	6	13,	9,		18	19
8	8		144	132	16,	6,		45	40	13,	11,		*	3
8,	10,		56	53	8	8		34	30	6	6	6	146	142
8,	12,		91	90	10,	8,		34	33	8	6		53	54
8,	14,		46	40	12,	8,		22	22	10,	6,		40	41
8,	16,		89	91	14,	8,		20	21	12,	6,		22	26
10,	10,		71	71	10,	10,		17	33	14,	6,		37	34
10,	12,		14	17	12,	10,		19	18	8	8		50	49
10,	14,		24	25	14,	10,		38	38	10,	8,		17	16
12,	12		112	113	12,	12,		86	85	12,	8,		28	25
5	3	1	228	211	7	5	3	50	49	14,	8,		27	22
7	3		98	97	9	5		41	41	10,	10,		30	30
9	3		86	85	11,	5,		70	68	10,	12,		*	6
11,	3,		30	24	13,	5,		33	35	11,	9,	7	54	54
13,	3,		24	20	15,	5,		47	51	13,	9,		61	61
15,	3,		28	28	17,	5,		21	20	8	8	8	106	102
17,	3,		32	33	9	7		66	64	10,	8,		32	31
7	5		87	79	11,	7,		22	21	12,	8,		89	85
9	5		50	46	13,	7,		20	22	10,	10,		21	18
11,	5,		66	66	15,	7,		37	38	12,	10,		20	13
13,	5,		28	26	11,	9,		19	34	10,	10,	10	15	17
15,	5,		*	11	13,	9,		40	40					

* *marks reflections for which the values were statistically below background.*
E *designates reflection affected by extinction.*

TABLE 3. Thermal Ellipsoids in Cubic Boracite

Atom	Axis	RMS Amplitude (Å)			
Cl	1 = 2 = 3	0.201(3)			
Mg	1 = 2	0.105(4)			
	3	0.287(6)	parallel to a		
B(1)	1	0.07(2)	parallel to a		
	2 = 3	0.089(2)			
B(2)	1 = 2	0.08(2)			
	3	0.17(1)	parallel to 3-axis direction		
O(1)	1 = 2 = 3	0.12(1)			
			angle of axis with		
			a	b	c
O(2)	1	0.075(8)	150(23)°	72(38)°	67(57)°
	2	0.081(7)	100(56)	57(25)	145(45)
	3	0.124(6)	62(6)	39(7)	65(6)

TABLE 4. Results of Split-Atom Model Refinements*

Atom split	O(1)	O(1)	Cl	Mg	(Cl + Mg)†	
Cubic coordinates						
x	0.	0.	0.250	0.	0.250	0.
y	0.	0.	0.250	0.250	0.250	0.250
z	0.	0.	0.250	0.250	0.250	0.250
Initial coordinates						
x	0.050	0.030	0.265	0.015	0.268	0.018
y	0.	0.030	0.265	0.250	0.250	0.250
z	0.	0.030	0.265	0.250	0.250	0.250
Refined coordinates						
x	0.018	0.002	0.252	0.017	0.265	0.017
y	0.	0.002	0.252	0.250	0.250	0.250
z	0.	0.002	0.252	0.250	0.250	0.250
R	0.067	0.050	0.041	0.041	0.044	

* 3 cycles, anisotropic temperature factors. Increased R factors resulted for split B(1) and various combinations.

† Refinement carried out with 781 data, including equivalents.

Possible models for the cubic structure

The cubic structure is necessarily an "average" of the orthorhombic structure. Three models can be considered. First, the cubic structure might be a true, high-temperature structure, *i.e.*, point atoms with high thermal motion which stabilizes the new coordination. Second, the cubic structure might be a disordered space-time average of the various ferroelectric orientations of the orthorhombic structure. Third, it might be a combination of these two possibilities, considering the borate framework separately from the Mg and Cl atoms. We describe first the structure on the basis of point atoms, and then consider the other two possibilities.

"Point-atom" cubic structure

The Cl anions are located at the point symmetry 23 and are each surrounded octahedrally by magnesium cations located at point symmetries $\bar{4}$ (Fig. 2). The angles are, of course, exactly octahedral and the Mg–Cl distance is $1/4\ a = 3.025$ Å. Each Mg cation is in turn coordinated octahedrally by two chlorine anions and four of the O(2) oxygen atoms that are located in the general position of the space group (Table 1). The Mg–O(2) distances are 2.023 ± 0.003 Å, and the O(2)–Mg–O(2) angles are 90.94 ± 0.02° and 165.3 ± 0.2°. The Cl–Mg–O(2) angles are 82.7 ± 0.1° and 97.3 ± 0.1°. The thermal ellipsoids of the Mg cations are appreciably elongated parallel to the Cl–Mg–Cl bonding (Table 3, Fig. 2).

The configuration of the borate framework differs from the description given by Ito *et al* (1951), who refer to the presence of BO_3 triangles, further described as flat trigonal pyramids. The present refinement shows that only borate tetrahedra occur. The unique feature of the arrangement (corner-linked tetrahedra) is that one oxygen atom, O(1), serves as a corner point for four borate tetrahedra (Fig. 3). Returning to the orthorhombic structure (Fig. 1), this feature results from establishment, for example, of a B(3)–O(1) bond by pulling in the borate triangle of the orthorhombic borate framework without releasing one of the other three tetrahedral bonds to O(1). In the

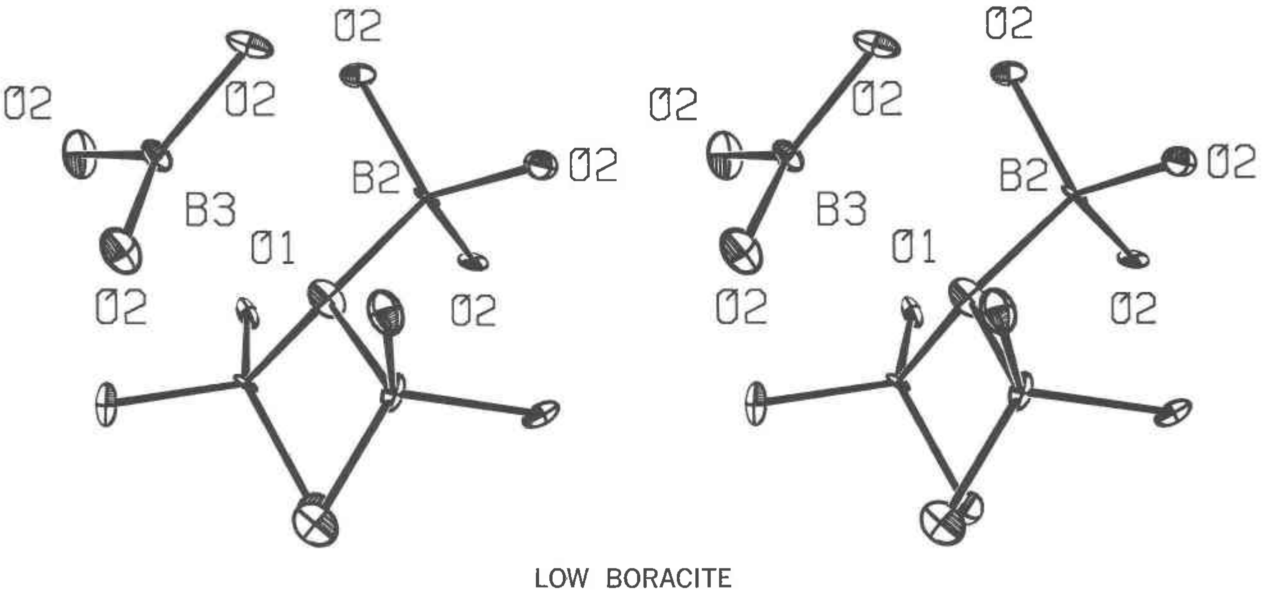

FIG. 1. Stereographic-pair view of the coordination around O(1) in the orthorhombic structure, looking approximately along *b* but rotated +30° around *c*. The approach, B(3)–O(1), is 2.303 Å. Thermal ellipsoids are for 50 percent probability. Drawing produced by ORTEP (Johnson, 1965).

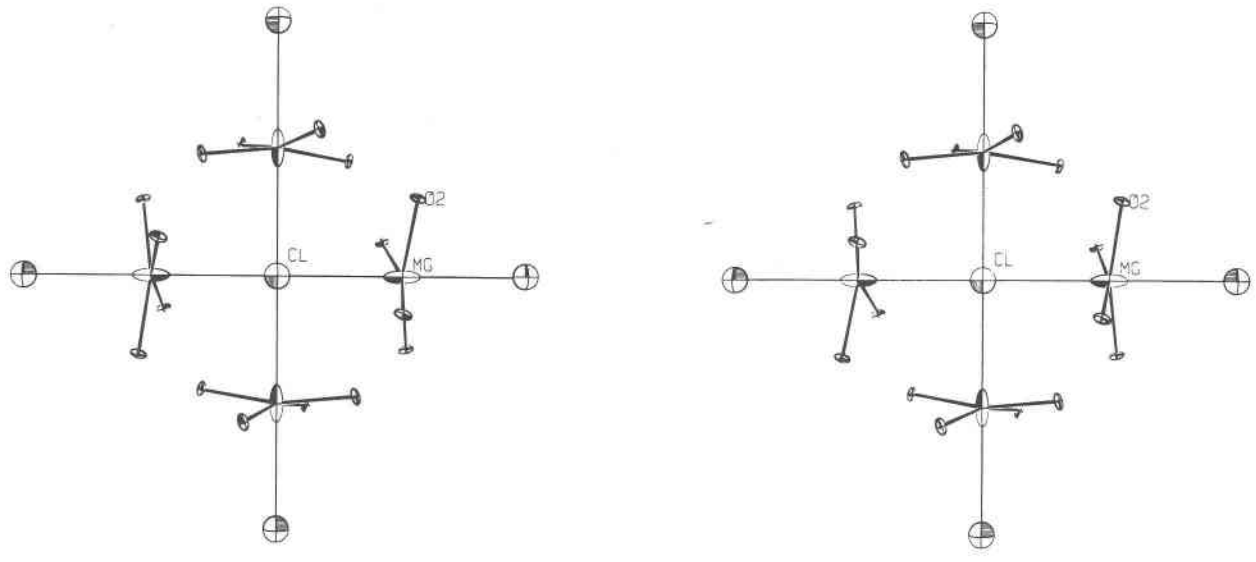

FIG. 2. Stereographic-pair view of the chlorine coordination looking along a cubic axis. Thermal ellipsoids for 50 percent probability. Drawing produced by ORTEP (Johnson, 1965).

cubic arrangement, the O(1) oxygen atoms are located at point symmetry 23, and four B(2) atoms located at point symmetry 3 surround each O(1) tetrahedrally at distances of 1.693 ± 0.005 Å. The B(2) tetrahedron is completed by three O(2) atoms at distances of 1.437 ± 0.003 Å, so the average B–O distance for the tetrahedron is 1.501 Å. The three O(2)–B(2)–O(2) angles are 111.9 ± 0.2°, and the three O(1)–B(2)–O(2) angles are 106.9 ± 0.2°. The remaining tetrahedra of the framework are made up of the B(1) atoms, located at point symmetry $\bar{4}$, linked to four O(2) oxygen atoms at 1.472 ± 0.003 Å. Three of the O(2)–B(1)–O(2) angles are 108.1 ± 0.1°, and the other three are 112.2 ± 0.2°. The B(1)–O(2)–B(2) angles are 116.2 ± 0.2°, the B(1)–B(2) distances are 2.470 ± 0.001 Å, and the B(2)–B(2) distances are 2.765 ± 0.008 Å.

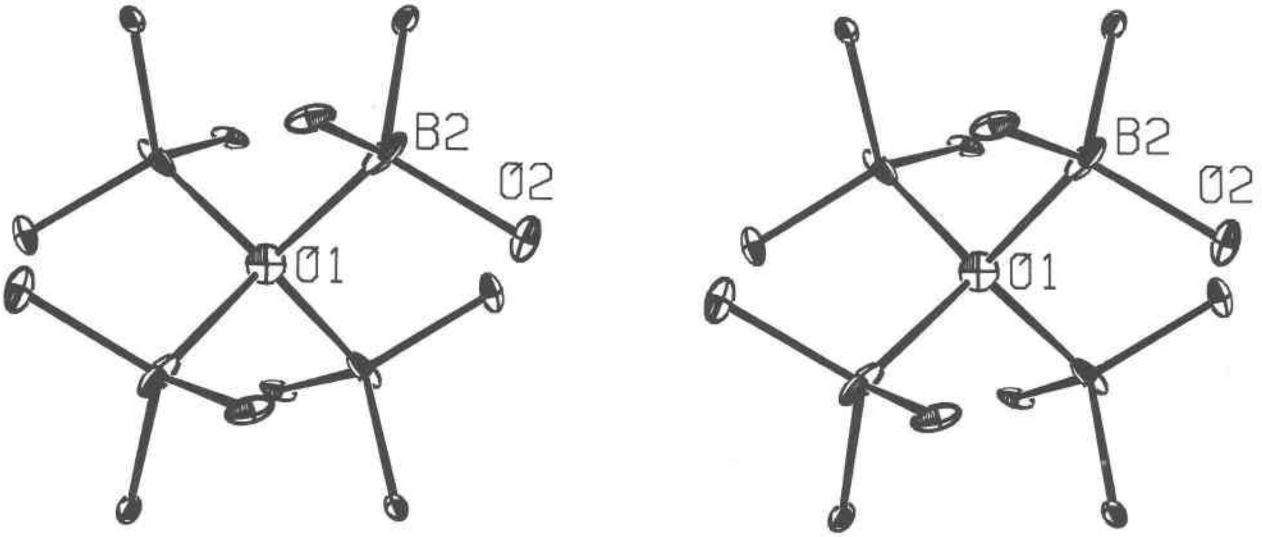

FIG. 3. Stereographic-pair view of the coordination around O(1) in the cubic structure, looking along a cubic axis. Thermal ellipsoids for 50 percent probability. Drawing produced by ORTEP (Johnson, 1965).

Disordered structure model

This model is a space-time average of the various ferroelectric orientations of the orthorhombic structure. Although it is a plausible possibility, we believe there is cogent evidence against it. First, the transition point is, as previously mentioned, sharp and reproducible. Second, above the transition point, there is no diffraction evidence for disorder. The reflections are sharp; no streaking or diffuseness were observed. Third, the observed thermal parameters for the cubic structure are not high enough to include the necessary displacements, 0.4 to 0.5 Å in most cases. A comparison of the thermal parameters for the orthorhombic and cubic structures given in Table 5 shows that no increases are that large. Fourth, the electron-density map and difference Fourier provide no evidence for such extreme disordering (in line with the observed character of the diffraction data). Fifth, the bond distances would be expected in this model to be close to an average of those for the various orthorhombic orientations. However, this is not true for the critical B–O(1) distance: average, cubic, 1.693 Å, compared with average, orthorhombic, 1.745 Å. This same argument does point to the possibility of disorder in Mg and Cl locations, because the average Mg–Cl distance in the orthorhombic structure is exactly what is found in the cubic structure. This argument is subject, also, to the errors attached to the bond distances and the thermal motion. Nevertheless, for the borate framework, it provides an additional point to consider.

TABLE 5. Comparison of Thermal Motion in Orthorhombic and Cubic Boracites for Similar Atoms

		Amplitude (Å)		Amplitude (Å)	
		Orthorhombic	Cubic	Orthorhombic	Cubic
		Dowty and Clark (1973)	This paper	Dowty and Clark (1973)	This paper
Atom		O(1)		O(2)	
Ellipsoid axis	1	0.05	0.12	0.05	0.075
	2	0.07	0.12	0.07	0.081
	3	0.09	0.12	0.09	0.124
Equiv. isotropic	B (Å^2)	0.40	1.1	0.40	0.72
Atom		B(1)		B(2)	
Ellipsoid axis	1	0.05	0.07	0.05	0.08
	2	0.06	0.089	0.07	0.08
	3	0.09	0.089	0.10	0.17
Equiv. isotropic	B (Å^2)	0.38	0.6	0.60	1.1
Atom		Mg		Cl	
Ellipsoid axis	1	0.07	0.105	0.10	0.201
	2	0.08	0.105	0.11	0.201
	3	0.11	0.287	0.11	0.201
Equiv. isotropic	B (Å^2)	0.60	2.75	0.92	3.2

Equivalent isotropic B for split Mg (Table 4), 1.4 Å^2, and for split Cl, 1.6 Å^2.

Combination model

This model assumes the borate framework to be a reasonable "point-atom" one, subject to thermal parameters compatible to the temperature at which data were taken. However, within the cavities of the framework, the Mg and Cl atoms are affected by disordering. We prefer this model for the reasons given in connection with the discussion on the fully disordered model, considered together with the following results. First, refinements of various split-atom models were carried out as given in Table 4. The only appreciable drop in the residual factor comes with splitting the Cl and Mg atoms. Second, even in these refinements, movement of the atoms is negligible except for Mg, which shows movement of about 0.1 Å. In all the other refinements, the tendency was for the split atoms to return to the exact cubic parameters, but for the Mg atoms the tendency was to diverge away from the fixed cubic parameter. Third, the thermal ellipsoids for all atoms, when compared with the averages found in the orthorhombic structure for like atoms, are reasonably increased for oxygen and boron atoms at 400°C. But the increase for Mg is the largest of all, and Cl is second (Table 5). Combining all available evidence, therefore, strongly suggests that some kind of space-time averaging may well be going on for Mg and Cl atoms within the cavities of the framework, while the framework itself has the normal elevated-temperature vibrations associated with a stable configuration. This configuration, although truly distinct from that of the orthorhombic borate framework, is reasonably obtained from it.

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