

## Inderite: Crystal Structure Refinement and Relationship with Kurnakovite

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The crystal structure of inderite,  $\text{Mg}[\text{B}_3\text{O}_3(\text{OH})_5](\text{H}_2\text{O})_4 \cdot \text{H}_2\text{O}$ , was refined to  $R=0.047$  from 4568 automatic diffractometer reflexions, collected with monochromated Mo  $K$  radiation. The crystals are monoclinic, space group  $P2_1/c$ , with  $a=6.8221$  (3),  $b=13.1145$  (13),  $c=12.0350$  (8) Å,  $\beta=104.552$  (8)°;  $D_m=1.80$  and  $D_x=1.794$  g cm<sup>-3</sup> for  $Z=4$ . The structure consists of  $[\text{B}_3\text{O}_3(\text{OH})_5]^{2-}$  soroborate groups and  $\text{Mg}(\text{OH})_2(\text{H}_2\text{O})_4$  octahedra interconnected into discrete molecules by the sharing of two OH groups. The fifth water molecule is placed in the spaces between the molecules. Both the Mg borate molecules and these 'free' waters are three-dimensionally connected *via* H bonds. Hydrogen atoms were located and their parameters refined.

### Introduction

The discovery of a new borate mineral with the formula  $\text{Mg}_2\text{B}_6\text{O}_{11} \cdot 15\text{H}_2\text{O}$  was reported from the Inder (USSR) deposits by Boldyreva [(1937); in Godlevsky (1940)]. The synthesis of inderite was described by Feigel'son, Grushvitsky & Korobochkina (1940). The same mineral, found in California by Frondel & Morgan (1956) and by Frondel, Morgan & Waugh (1956) was eventually given the new name lesserite; the confusion was also increased by the existence of the triclinic polymorph, kurnakovite, found in the same Inder district by Godlevsky (1940). There were later other findings of both minerals (Heinrich, 1946; Frondel & Morgan, 1956). The confusion around the two minerals was solved by Schaller & Mrose (1960) who showed definitely that the two minerals were polymorphs and that Heinrich's (1946) 'inderite' was the same as Godlevsky's (1940) 'kurnakovite', while Frondel & Morgan's (1956) 'lesserite' corresponded to Boldyreva's (1937) 'inderite'.

The presence of two tetrahedra and one triangle connected into a soroborate ring was postulated by Christ (1960) and by Tennyson (1963) on the basis of Christ's (1960) rules, as well as by Petch, Pennington & Cuthbert (1962) who used the NMR method; these authors, however, did not determine whether the B-O groups were polymerized or discrete. The NMR spectra for inderite were found to be very similar to those of kurnakovite and of colemanite.

A first structure determination of inderite (under the name lesserite) was given by Ashirov, Rumanova & Belov (1962) who solved the structure by direct methods. Virtually the same results, though slightly improved and more detailed, were reported by Rumanova & Ashirov (1963).

The present crystal structure refinement was undertaken with the purpose of investigating the B-O polyion in detail and the hydrogen-bonding system, and of

Table 1. Crystal data for inderite

Monoclinic, $P2_1/c$	$\text{Mg}[\text{B}_3\text{O}_3(\text{OH})_5](\text{H}_2\text{O})_4 \cdot \text{H}_2\text{O}$
$a = 6.8221$ (3) Å	F. W. 289.8
$b = 13.1145$ (13)	$D_m = 1.80$ g cm <sup>-3</sup>
$c = 12.0350$ (9)	$D_x = 1.794$ g cm <sup>-3</sup>
$\beta = 104.552$ (8)°	$Z = 4$
$V = 1073.36$ Å <sup>3</sup>	$\mu(\text{Mo } K\alpha) = 2.51$ cm <sup>-1</sup>
$F(000) = 292$	

making a crystal-chemical comparison with the dimorph kurnakovite.

### Experimental

Crystal data are summarized in Table 1. For the measured density that found by Ashirov *et al.* (1962) was used; it agrees well enough with that calculated in the present work. Lattice constants were refined with the least-squares method applied to a series of 44 independent reflexions at a medium  $\theta$ , collected on a Philips PW 1100 four-circle computer-controlled diffractometer, using the LAT routine. Intensity data were measured on the same diffractometer (Istituto di Mineralogia, Università di Perugia, Italy) and on the same crystal, a colourless transparent splinter from a Californian sample, approximately 0.4 mm in cross dimensions. The  $\omega$ - $2\theta$  scan technique in the range  $3^\circ \leq \theta \leq 35^\circ$  was used, with scan speed  $0.04^\circ$  s<sup>-1</sup> and scan range  $1.2^\circ$ . The background was measured on either side of the peak; the latter was scanned up to three times. Mo  $K$  radiation was monochromated with a graphite crystal; since the corresponding linear absorption coefficient was very low, no allowance was made for it. Reflexions were considered as unobserved if  $(I_{\text{peak}} - 2I_{\text{back}}) \leq I_{\text{back}}$ . 4568 reflexions were collected, 904 of which were unobserved and were assigned an intensity the same as the least intensity actually measured. Intensities were corrected with the Lp factor appropriate for monochromated radiation. No cor-

rection for secondary extinction was applied, but 20 reflexions showing an extinction effect were excluded from the last stages of refinement; they are labelled in the structure factor list.\*

Systematic absences confirmed the  $P2_1/a$  space group found by Ashirov *et al.* (1962), here reported as  $P2_1/c$  in agreement with the standard space groups, after interchanging  $a$  and  $c$ . The solution with the present data confirmed that the previous determination was correct and gave direct information on the hydrogen-atom positions.

Atomic scattering factors for Mg, O and B were taken from Cromer & Waber (1965), while for H the values from *International Tables for X-ray Crystallography* (1962) were used.

### Structure refinement

The previous determination by Rumanova & Ashirov (1963) was used as the starting point with the coordinates of non-hydrogen atoms, tentatively attributing to all of them the same individual  $B$  factor as that obtained by averaging the  $B$ 's found by the same authors for different layer lines. A structure factor calculation with the intensity data of the present work and these atomic parameters, after the correct  $K$  factor was found, yielded an  $R(=\sum||F_o|-|F_c||/\sum|F_o|)$  of 0.208 for reflexions with non-zero weight, thus confirming the previous authors' heavy-atom structure. Two cycles of full-matrix least-squares refinement with isotropic thermal parameters lowered  $R$  to 0.112. From this step on, anisotropic thermal parameters were used for all atoms, and two more cycles of least-squares refinement led to

\* A table of observed and calculated structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31442 (32 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

$R=0.066$ . A three-dimensional difference Fourier synthesis at this stage unambiguously showed peaks corresponding to the 15 missing hydrogen atoms. Their inclusion with rough coordinates and  $B=2.0 \text{ \AA}^2$  reduced  $R$  to 0.056. Two more cycles of block-diagonal least-squares refinement (one block per atom) gave convergence at a final  $R$  index of 0.047 for observed reflexions and of 0.057 if unobserved ones were included. All positional and thermal parameters (anisotropic for non-hydrogen and isotropic for hydrogen atoms), as well as the general scale factor, were allowed to vary at the same time during the last cycles. Refinement continued smoothly even for hydrogen atom parameters; the average ratio between shifts and e.s.d.'s for the heavy-atom coordinates was 0.46 in the last cycle. A difference Fourier map computed with the final parameters showed no relevant residual peaks or troughs. Throughout all refinement cycles a weight of  $1/\sigma$ , with  $\sigma$  derived from counting statistics, was given to all observed reflexions.

Table 2 lists the final positional and anisotropic thermal parameters together with their standard deviations obtained from the inverse of the block-diagonal matrix.

Table 3 gives the final positional and isotropic thermal parameters for hydrogen atoms.

### Results and discussion

The purpose of this work was a more accurate determination of the structure of inderite for a comparison with kurnakovite; the resulting average estimated standard deviations in bond distances (0.005 Å) and bond angles (0.8°) confirm that its reliability is of the same order of magnitude as that for kurnakovite reported by Corazza (1974). The precise positioning (within the limits of the X-ray methods) of hydrogen atoms also affords a better knowledge of the packing attitude of inderite molecules.

Table 2. Final heavy-atom parameters with their standard deviations

Anisotropic thermal parameters ( $\times 10^5$ ) are in the form:  $T = \exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$ .  $B$  equivalent factors ( $\text{\AA}^2$ ) after Hamilton (1959). Standard deviations on the last digits are given in parentheses.

	$x$	$y$	$z$	$B_{\text{eq}}$	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
Mg	0.25554 (6)	0.21593 (3)	0.11712 (4)	1.25	701 (8)	163 (2)	244 (3)	10 (3)	62 (4)	8 (2)
O(1)	0.68846 (13)	0.14513 (7)	0.43446 (7)	1.47	894 (17)	219 (5)	215 (5)	-38 (7)	16 (8)	-28 (4)
O(2)	0.49914 (13)	0.20971 (7)	0.25525 (8)	1.47	756 (16)	163 (4)	319 (6)	-34 (7)	-15 (8)	16 (4)
O(3)	0.76635 (12)	0.08591 (7)	0.25799 (7)	1.38	563 (15)	233 (5)	294 (6)	-79 (7)	143 (8)	-52 (4)
O(4)	0.45422 (12)	0.03518 (6)	0.30389 (7)	1.13	580 (15)	183 (4)	207 (5)	-57 (7)	101 (7)	-11 (4)
O(5)	0.27814 (13)	-0.11030 (6)	0.20271 (8)	1.46	744 (17)	147 (4)	388 (6)	-58 (7)	168 (9)	-4 (4)
O(6)	0.54471 (12)	-0.03606 (7)	0.13879 (8)	1.38	512 (15)	233 (5)	310 (6)	-41 (7)	137 (8)	-73 (4)
O(7)	0.86228 (13)	-0.00752 (8)	0.10960 (8)	2.02	622 (17)	460 (7)	366 (7)	-156 (9)	237 (9)	-154 (6)
O(8)	0.23444 (12)	0.05904 (7)	0.11597 (7)	1.16	576 (15)	173 (4)	255 (5)	5 (6)	58 (7)	1 (4)
O(9)	0.42303 (19)	0.20585 (9)	-0.00794 (11)	3.04	2537 (34)	303 (6)	688 (10)	-358 (12)	1014 (16)	-158 (7)
O(10)	-0.01102 (16)	0.21720 (8)	-0.01379 (10)	2.65	1199 (23)	302 (6)	541 (9)	191 (9)	-306 (12)	-93 (6)
O(11)	0.27596 (16)	0.37071 (7)	0.10495 (9)	2.14	1544 (24)	192 (5)	363 (7)	-70 (9)	-74 (11)	16 (5)
O(12)	0.06975 (16)	0.23179 (9)	0.23651 (10)	2.39	1270 (23)	393 (7)	474 (8)	-119 (10)	398 (11)	-83 (6)
O(13)	0.15545 (15)	0.02048 (8)	0.41014 (9)	2.14	1029 (20)	422 (7)	331 (7)	-8 (9)	210 (10)	24 (6)
B(1)	0.59920 (19)	0.11845 (10)	0.31376 (11)	1.02	496 (21)	157 (6)	196 (7)	-44 (9)	58 (10)	-22 (6)
B(2)	0.37922 (18)	-0.01253 (10)	0.19274 (11)	0.97	443 (21)	138 (6)	219 (7)	-21 (9)	88 (10)	-17 (6)
B(3)	0.72279 (19)	0.01671 (11)	0.17064 (12)	1.19	466 (21)	219 (7)	232 (8)	-4 (10)	98 (10)	-11 (6)

Table 3. *Final hydrogen atom parameters with their standard deviations*

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> (Å <sup>2</sup> )
H(1)	0.730 (3)	0.096 (2)	0.479 (2)	1.8 (5)
H(2)	0.577 (3)	0.263 (2)	0.271 (2)	2.0 (5)
H(3)	0.204 (3)	-0.109 (1)	0.248 (2)	1.4 (5)
H(4)	0.974 (3)	0.025 (2)	0.125 (2)	2.4 (5)
H(5)	0.214 (3)	0.043 (2)	0.041 (2)	2.3 (5)
H(6)	0.493 (3)	0.253 (2)	-0.025 (2)	2.1 (5)
H(7)	0.442 (3)	0.143 (2)	-0.049 (2)	2.2 (5)
H(8)	-0.107 (3)	0.262 (2)	-0.026 (2)	2.0 (5)
H(9)	-0.060 (3)	0.165 (2)	-0.067 (2)	3.1 (6)
H(10)	0.382 (3)	0.412 (2)	0.140 (2)	2.5 (5)
H(11)	0.218 (3)	0.397 (2)	0.034 (2)	2.6 (5)
H(12)	-0.033 (3)	0.192 (2)	0.236 (2)	3.2 (6)
H(13)	0.129 (3)	0.245 (2)	0.306 (2)	2.3 (6)
H(14)	0.036 (3)	0.033 (2)	0.366 (2)	2.6 (5)
H(15)	0.250 (3)	0.030 (2)	0.372 (2)	1.9 (5)

Table 4 reports interatomic distances and bond angles along with their standard deviations, for non-hydrogen atoms. The MgO<sub>6</sub> octahedron is fairly regular, Mg-O distances falling in a range of 0.116 Å with a mean value of 2.081 Å, very close to that reported for kurnakovite (2.074 Å) and to those given in the literature. An interesting feature is the slight elongation of the O(9)-O(12) diagonal of the Mg octahedron, the Mg-O bonds along which have an average length of 2.131 Å compared with 2.057 Å for the other four.

As in kurnakovite, there are no differences in bond distances involving O atoms belonging to hydroxyl groups or water molecules. The shape of the Mg coordination is very regular, the average deviation from 90° being only ±2°. In kurnakovite the OH groups bound to Mg are at opposite corners of the octahedron (because of the chain-like alternation of Mg-O and B-O groups) but in inderite they are at adjacent corners, and shared with the same boroxol group. All other oxygens coordinated to Mg belong to water molecules; they exhibit a thermal motion distinctly higher than that of the OH groups.

The oxygen atoms coordinated by the boron atoms are arranged in two tetrahedra (mean B-O distance 1.476 Å) and one triangle (mean B-O distance 1.479 Å). The boron coordination is very regular both in the tetrahedra (where one distance is, as usual, slightly longer than the three others) and in the triangle [almost perfectly planar, B(3) being 0.01 Å off the plane of the O atoms]. From the sharing of three corners between the two tetrahedra and the triangle a hexagonal borate ring [B<sub>3</sub>O<sub>3</sub>(OH)<sub>3</sub>]<sup>2-</sup> results, of the same kind as that found in kurnakovite (Razmanova, Rumanova & Belov, 1969; Corazza, 1974), the anhydrous borate BaB<sub>4</sub>O (Block & Perloff, 1965) as part of a bigger anion, meyerhofferite (Christ & Clark, 1956, 1960), inderborite (Kurkutova, Rumanova & Belov, 1965),

Table 4. *Mg-O, B-O and B-B distances (Å) and bond angles (°) in inderite*

In parentheses are the estimated standard deviations referred to the last digits.

Mg-O(2)	2.036 (11)	B(2)-O(4)	1.449 (4)	O(2)-Mg-O(8)	90.39 (4)	O(1)-B(1)-O(2)	107.91 (10)
Mg-O(8)	2.062 (1)	B(2)-O(5)	1.475 (2)	O(2)-Mg-O(9)	95.89 (5)	O(1)-B(1)-O(3)	109.42 (8)
Mg-O(9)	2.110 (7)	B(2)-O(6)	1.470 (4)	O(2)-Mg-O(10)	174.39 (15)	O(1)-B(1)-O(4)	111.29 (10)
Mg-O(10)	2.086 (11)	B(2)-O(8)	1.501 (5)	O(2)-Mg-O(11)	92.41 (4)	O(2)-B(1)-O(3)	109.07 (10)
Mg-O(11)	2.042 (1)	Mean	1.474	O(2)-Mg-O(12)	87.46 (4)	O(2)-B(1)-O(4)	110.34 (9)
Mg-O(12)	2.152 (7)			O(8)-Mg-O(9)	88.97 (5)	O(3)-B(1)-O(4)	108.79 (9)
Mean	2.081	B(3)-O(3)	1.364 (3)	O(8)-Mg-O(10)	87.52 (4)	O(4)-B(2)-O(5)	111.36 (10)
		B(3)-O(6)	1.367 (3)	O(8)-Mg-O(11)	175.52 (16)	O(4)-B(2)-O(6)	111.50 (9)
B(1)-O(1)	1.469 (5)	B(3)-O(7)	1.377 (5)	O(8)-Mg-O(12)	92.81 (4)	O(4)-B(2)-O(8)	108.87 (10)
B(1)-O(2)	1.467 (3)	Mean	1.369	O(9)-Mg-O(10)	89.27 (6)	O(5)-B(2)-O(6)	106.26 (10)
B(1)-O(3)	1.522 (4)			O(9)-Mg-O(11)	87.26 (5)	O(5)-B(2)-O(8)	110.19 (8)
B(1)-O(4)	1.458 (2)	B(1)-B(2)	2.495 (7)	O(9)-Mg-O(12)	176.20 (28)	O(6)-B(2)-O(8)	108.61 (10)
Mean	1.479	B(1)-B(3)	2.488 (5)	O(10)-Mg-O(11)	90.01 (4)	O(3)-B(3)-O(6)	124.01 (12)
		B(2)-B(3)	2.454 (3)	O(10)-Mg-O(12)	87.45 (5)	O(3)-B(3)-O(7)	121.24 (11)
		Mean	2.479	O(11)-Mg-O(12)	90.81 (5)	O(6)-B(3)-O(7)	114.71 (12)

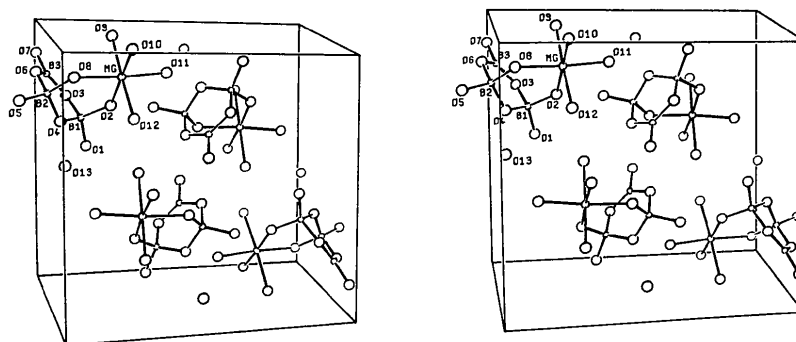


Fig. 1. ORTEP (Johnson, 1965) stereoscopic drawing of the structure of inderite, viewed along the positive *x* direction. Origin of the unit cell in the upper left close corner, *y* axis to the right and *z* axis downward. The atoms in the asymmetric unit have been labelled, and their coordinates are given in Table 2. The size of the spheres is on an arbitrary scale. Hydrogen atoms and related bonds are omitted.

Table 5. Displacements of other atoms from the plane of the atoms in the  $B_2O_3$  ring, and angle between the  $BO_3$  triangle and the ring plane

Ring oxygen atoms	O(3)O(4)O(6)	
Associated atoms	B(1)	0.41 Å
	B(2)	0.33
	B(3)	-0.09
	O(1)	-0.21
	O(2)	1.87
	O(5)	-0.44
	O(7)	-0.32
	O(8)	1.80
Oxygen atoms of the $BO_3$ triangle	O(3) O(6) O(7)	
Triangle-to-ring angle $9.2^\circ$		

inoite (Clark, 1959), synthetic  $CaB_3O_3(OH)_5 \cdot 2H_2O$  (Clark & Christ, 1959). The hexagonal ring in inderite is more nearly planar than in kurnakovite, as pointed out by Razmanova *et al.* (1969).

This evidence is more remarkable if one considers also the OH groups [O(1), O(5) and O(7)] not bound to Mg, all of which are on the side opposite to Mg and close to the ring plane (Table 5). As a consequence the angle between the triangle and the ring is less than in kurnakovite. This general flattening on one side of the boroxol group can be regarded as deriving from the rigid coordination of Mg which keeps the two shared oxygens [O(2) and O(8)] almost at a right angle to

Table 6. Hydrogen-bond system

E.s.d.'s are given on the last digits.

D	H atom	A	D-A (Å)	D-H (Å)	H-A (Å)	$\angle DHA(^\circ)$	$\angle HDH(^\circ)$	$\angle ADA(^\circ)$
O(1)	H(1)	O(13 <sup>l</sup> )	2.889 (6)	0.84 (2)	2.05 (2)	178 (2)		
O(2)	H(2)	O(5 <sup>ii</sup> )	2.784 (3)	0.87 (2)	1.92 (2)	173 (2)		
O(5)	H(3)	O(7 <sup>iii</sup> )	3.086 (8)	0.83 (2)	2.83 (2)	100 (1)		
O(7)	H(4)	O(8 <sup>iv</sup> )	2.667 (1)	0.85 (2)	1.86 (2)	157 (2)		
O(8)	H(5)	O(7 <sup>v</sup> )	2.713 (5)	0.91 (2)	1.81 (2)	172 (2)		
O(9)	H(6)	O(1 <sup>vi</sup> )	2.865 (4)	0.84 (2)	2.03 (2)	173 (2)	110 (2)	105.41 (6)
O(9)	H(7)	O(6 <sup>v</sup> )	2.768 (2)	0.98 (2)	1.79 (2)	173 (2)		
O(10)	H(8)	O(1 <sup>vii</sup> )	2.684 (4)	0.86 (2)	1.82 (2)	174 (2)	105 (2)	81.39 (4)
O(10)	H(9)	O(5 <sup>viii</sup> )	2.893 (12)	0.94 (2)	2.04 (2)	150 (2)		
O(11)	H(10)	O(4 <sup>ix</sup> )	2.868 (6)	0.92 (2)	1.98 (2)	162 (2)	108 (2)	87.74 (4)
O(11)	H(11)	O(13 <sup>vi</sup> )	2.690 (6)	0.92 (2)	1.80 (2)	163 (2)		
O(12)	H(12)	O(3 <sup>xiii</sup> )	2.877 (2)	0.87 (2)	2.02 (2)	169 (2)	108 (2)	76.20 (4)
O(12)	H(13)	O(10 <sup>xv</sup> )	3.258 (4)	0.85 (2)	2.62 (2)	132 (2)		
O(13)	H(14)	O(3 <sup>xiii</sup> )	2.947 (13)	0.87 (2)	2.08 (2)	171 (2)	111 (2)	110.95 (5)
O(13)	H(15)	O(4)	2.671 (8)	0.89 (2)	1.79 (2)	173 (2)		

Key to symmetry operations

Superscript

None	$x$	$y$	$z$	$v$	$1-x$	$-y$	$-z$
i	$1-x$	$-y$	$1-z$	vi	$x$	$\frac{1}{2}-y$	$-\frac{1}{2}+z$
ii	$1-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$	vii	$-1+x$	$\frac{1}{2}-y$	$-\frac{1}{2}+z$
iii	$-1+x$	$y$	$z$	viii	$-x$	$-y$	$-z$
iv	$1+x$	$y$	$z$	ix	$x$	$\frac{1}{2}-y$	$\frac{1}{2}+z$

Table 7. Electrostatic valence balance (*v.u.*)

Atom	Mg	B(1)	B(2)	B(3)	H-	$\cdots H$	Sums
O(1)	-	0.77	-	-	0.83	0.17	1.99
						0.22	
O(2)	0.37	0.77	-	-	0.82	-	1.96
O(3)	-	0.67	-	1.01	-	0.17	2.00
						0.15	
O(4)	-	0.79	0.80	-	-	0.17	1.99
						0.23	
O(5)	-	-	0.75	-	0.87	0.18	1.97
						0.17	
O(6)	-	-	0.75	1.01	-	0.19	1.95
O(7)	-	-	-	0.98	0.77	0.13	2.09
						0.21	
O(8)	0.35	-	0.70	-	0.79	0.23	2.07
O(9)	0.31	-	-	-	0.83	-	1.95
					0.81		
O(10)	0.33	-	-	-	0.78	0.10	2.04
					0.83		
O(11)	0.36	-	-	-	0.83	-	1.97
					0.78		
O(12)	0.28	-	-	-	0.83	-	2.01
					0.90		
O(13)	-	-	-	-	0.85	0.17	2.01
					0.77	0.22	
Sums	2.00	3.00	3.00	3.00	12.29	2.71	26.00

itself, therefore forcing the related B–O bonds toward a right angle with the B–O ring. The equation of the least-squares plane through the nine atoms forming the flat side of the B–O group, that is omitting O(2) and O(8), is:

$$-2.2974x + 9.3938y - 6.1010z = -2.5467.$$

On the other hand, the borate group can also be considered as less regular in inderite if the 'ideal' regular group is defined as one in which the ring plane is a plane of symmetry. In this respect the kurnakovite B–O group, though distorted, is closer to this condition, being bound to Mg almost symmetrically on either side.

As just shown, the relationship between Mg and the B–O group occurs in inderite in a way quite different from kurnakovite as well as from the other borates mentioned above. The result is a molecular structure with isolated  $\text{Mg}(\text{H}_2\text{O})_4\text{B}_3\text{O}_3(\text{OH})_5$  groups interconnected only by H bonds in all directions. The additional 'free' water molecule [O(13) oxygen, not directly coordinated to Mg] provides further hydrogen bonds with its surrounding Mg borate molecules, just in the same manner as in kurnakovite. The complete crystal-chemical formula is then:  $\text{Mg}[\text{B}_3\text{O}_3(\text{OH})_5] \cdot (\text{H}_2\text{O})_4 \cdot \text{H}_2\text{O}$ .

The molecular structure (Fig. 1) accounts for the lower hardness, poorer cleavage (Fron del *et al.*, 1956), and lower density in comparison with kurnakovite.

The hydrogen-bonding system is summarized in Table 6. In inderite no hydrogen bonding takes place within the molecule, all 15 hydrogen bonds being intermolecular or with the free water molecule. Even though interatomic distances in this work are different from those quoted in Rumanova & Ashirov (1963) and more reliable, there is still a very long distance O(12)–O(10<sup>ix</sup>) = 3.258 (4) Å which does not definitely correspond to a real H bond, because of the unusual O–H···O angle (132°). Inspection of the surroundings of O(12) excluded any other possibility other than the Mg polyhedron edges and confirmed the positioning of H(13).

An electrostatic valence balance, given in Table 7, was computed according to the method of Brown & Shannon (1973), using data from their Table 1 and their hydrogen-bond curve reported by Donnay & Donnay (1973). This calculation favours the existence of a weak O(12)–O(10<sup>ix</sup>) hydrogen bond.

The CII 10070 computer was employed for all calculations, using some local programs; extensive use was made of *ORFLS* (Busing, Martin & Levy, 1962) with a block-diagonal modification, of *ORTEP* (John-

son, 1965), of *LSQPL* and *BONDLA* from the X-RAY system (Stewart, Kruger, Ammon, Dickinson & Hall, 1972).

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