THE DETERMINATION OF THE CRYSTAL STRUCTURE OF INDERITE

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The crystal structure of the hydrated magnesium borate, inderite $Mg[B_3O_3(OH)_5] \cdot 5H_2O$, is solved by a direct determination of the signs of F_{hkl}. The structure is monoclinic; a = 12.02, b = 13.12, c = 6.84 A, β = 104°40', space group $C_{2h}^5 = P2_1/a$, Z = 4. The reference group of signs with the greatest $|U_{hkl}|$ are determined by the comparison method, the majority of the remaining signs are found statistically. The coordinates of all the atoms (among them those that overlap in the usual projections) are refined with the help of the phase and zonal weighted projections of the electron density. On the basis of various phase projections, the objective values of the average errors in the coordinates are found. The hydrogen bonds are fixed by an analysis of the interatomic distances between the oxygen atoms.

The structure of inderite is composed of separate neutral complexes $MgB_3O_3 \cdot (OH)_5 \cdot 4H_2O$, bound together by hydrogen bonds. The Mg-octahedron enters into the composition of each complex, two neighboring apices of which adjoint the polyion $[B_3O_3(OH)_5]^{-2}$. Another H_2O molecule is not connected with any cation and only participates in the hydrogen bond system.

The colorless, transparent crystals of the hydrated borate inderite $Mg_2B_6O_{11} \cdot 15H_2O$ were first discovered by Boldyreva in 1937 [1]. In 1956 the same mineral was found in California and was described as a new one under the name of lesserite [2]. In [2], the parameters of a monclinic cell are given and the space group (a = 12.11 A; b = 13.18 A; c = 6.83 A; β = 104°49'; $P2_1/a$). The confusion in the nomenclature was caused by the American article of 1946 [3], in which a triclinic kurnakovite of the same chemical composition (see [9]) was erroneously called inderite. An analysis of the first Soviet articles on kurnakovite [4,5], inderite [1, 6, 7], and of the American articles on "inderite" [3, 8] and "lesserite" [2] leaves no doubts that the American "lesserite" is the Soviet inderite, and that the American "inderite" is the Soviet kurnakovite. The confirmation of this can be found in Table 1, where the results of the measurements of the specific gravity and of the indices of refraction of samples of different authors are collected, and are published in [1-8].

The small crystals that we analyzed under the name of "lesserite" were obtained from Professor Frondel of Harvard (USA). We repeated the determination of the cell parameters (camera RKV, CuK-radiation), and also the symmetry group of the crystal: a = 12.02 ± 0.03 A; b = 13.12 ± 0.04 A; c = 6.84 ± 0.02 A; β = 104°40'; $C_{2h}^5 = P2_1/a$. In a cell of these dimensions is contained $2[Mg_2B_6O_{11} \cdot 15H_2O]$; the specific gravity of the samples, $d_{exp} = 1.80$; $d_{theor} = 1.82$.

TABLE 1

Sample	Density	Indices of refraction		
		N_p	N_m	N_g
Inderite [1]	1.79	–	1.488	1.504
Inderite [6]	1.78	–	1.489	1.505
Inderite [7]	–	–	1.487	1.505
Lesserite [2]	1.785	1.488	1.491	1.505
Kurnakovite [4]	1.85	1.489	1.510	1.525
Kurnakovite [5]	–	1.492	–	1.519
Inderite [3]	1.86	1.488	1.508	1.515
Inderite [8]	1.861	1.490	1.511	1.520

Using MoK_α-radiation and a small crystal ground into a sphere, Weissenberg patterns were obtained of the zero and first, second, and third lines about the c axis, and also the zero and first layer line around the a axis. The intensities of the reflections were evaluated visually by comparison with a blackening scale (with the step $\sqrt[4]{2}$).

The unit cell of inderite contains a considerable number of atoms (68, not counting the hydrogens) with atomic numbers close together. Therefore, a direct determination of the signs of F_{hkl} was the basis of the interpretation of the structure [11-13], in agreement with the statistical relationships of Sayre and Zachariasen [14, 15]. To interpret and refine the structure, all the observed nonzero reflections were used: 144 F_{hk0}, 283 F_{hk1}, 289 F_{hk2}, 192 F_{hk3}, 114 F_{0kl} and 247 F_{1kl}.* The reference group, into which entered about 37% of the nonzero reflections of the types hk0, hk1, and hk2 with the greatest unitary amplitudes (263 U_{hkl} in all), it was possible to obtain by the comparison method [11] 127 sign correlations between pairs of hk0 reflections. Through common reflections a considerable number of these correlations were connected into 14 sign chains [12]. In this way, 50 of the S_{hk0} that occurred obtained a sign characteristic as one of 14 letters. To decrease the number of letters, statistical relationships [14, 15], $S_H = S(\overline{S_{K_i} \cdot S_{H+K_i}})$, were set up for each fundamental S_{hk0}, in which one letter (S_H) was in turn made equal to the product of two others ($S_{K_i} \cdot S_{H+K_i}$). Carefully selecting the frequently recurring relationships, connections were established between the products of different letters ($S_{K_i} \cdot S_{H+K_i}$ and $S_{K_j} \cdot S_{H+K_j}$), also between separate letters and their products (S_H and $S_{K_i} \cdot S_{H+K_i}$). As a result, the number of letters decreases to three and, with their aid, "securely" (with a probability of $w \geq 0.70$) the signs 44 S_{hk0} were stated, composing a new fundamental group; using it, we covered the large tract of the remaining S_{hk0}, among which (under the condition that $w \geq 0.60$), 41 S_{hk0} were determined (i.e., were expressed by three letters). To enlarge the groups of the S_{hk0} that were determined, the signs S_{hk1} were used, and the procedure for determining S_{hk1} was analogous to the one described for S_{hk0}. In conclusion, the signs S_{hk1} were expressed by four letters (among them the three mentioned above), one of which was reduced to a plus, and of the three remaining ones we took advantage of the right to assign them arbitrarily which, as is well known, fixes the origin of the cell at one of the eight centers of symmetry in the unit cell [16]. From the S_{hk1} that were found, the signs of 41 F_{hk0} ($w \geq 0.60$) were also determined and, in this way, from 144 S_{hk0}, 126 turned out to be determined; likewise, of 283 F_{hk1}, 232 signs were determined.

From the signs assigned to the structure factors, projections of the electron density, $\sigma(x,y)$, were constructed, and the two "basic" modulated projections $C_1(x,y)$ and $S_1(x,y)$. From the analysis of these three projections it was possible to assign the (x, y, z) coordinates of the atoms which make up the oxygen octahedron around the Mg and around boron tetrahedron. The remaining atoms (2B and 4O) were not discovered on these syntheses, due to numerous parasite peaks, with heights comparable to and sometimes even exceeding those of the peaks taken for O atoms. The latter circumstance, and especially the excessively high Mg peaks, indicated the effect on the syntheses, not only the significance of the termination of the series, but also the errors in some of the S_{hk0}. After calculating the signs of the F_{hk0} from the coordinates of the 11 atoms (out of the 17 basic ones), it was found that some S_{hk0} of the reference group, and which were determinable statistically with great probability, did not coincide with those calculated from the coordinates; on the other hand, a series of such $(S_{hk0})_{calc}$, because of the large values of F_{calc}, definitely cannot undergo any change through the insertion of missing atoms. This was explained by analyzing the Mg contributions to F_{hk0}. It was found that all the $(S_{hk0})_{stat}$ that were established coincided, almost without exception, with the signs of the contributions of this light cation; in the case of a considerable $Mg(S_{hk0})_{stat}$ contribution they were fixed, almost without contradiction, by the large number of determining pairs, but if the Mg contribution was small, then the probability of a determination, and the number of determining pairs, declined sharply. Thus, the remaining atoms of the structure had very little effect on the statistical result. (This fact was brought to light after the final interpretation of the structure. Having calculated F_{hk0} and F_{hk1} from the coordinates found, and having compared them with the signs of the Mg contributions, we discovered that they were 74% identical.)

Having substituted in the reference group $(S_{hk0})_{stat}$ for $(S_{hk0})_{calc}$† in those reflections the signs of which appeared to be certain (i.e., could not be changed by the contributions of missing atoms), and having included as reference signs the newly determines ones and having discarded the doubtful ones, the signs of all the F_{hk1} were determined anew statistically. A series of signs was changed. For some reflections with large U the probability of determining S_{hk1} fell sharply, which proved the unreliability of the first result. Such signs were reversed (this procedure was justified by its consequences). From the $(S_{hk0})_{calc}$ and $(S_{hk1})_{stat}$, a second set of syntheses was constructed: $\sigma(x,y)$, $C_1(x,y)$, and $S_1(x,y)$. The peaks for the atoms already known stood out more clearly on the new maps, three new distinct maxima appeared corresponding to the second B-tetrahedron (O_5, O_6, B_2) and a peak was noticed which did not enter into the polyhedra (subsequently identified as a molecule of water). The two missing atoms of the borate triangle (O_7 and B_3) were determined by the subsequent recalculation of the signs of S_{hk0} and the construction of a difference synthesis of the electron density $\Delta\sigma(x,y)$,

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*To refine the structure, the hk0 and hk1 patterns were taken repeatedly, and 184 nonzero F_{hk0} and 406 F_{hk1} were fixed.

†The signs of F_{hk1} were not calculated, since the z coordinates of atoms were determined very roughly from a pair of modulated projections, according to the formula

$$\frac{2\pi z_n}{c} = \operatorname{arc\,tg} \frac{S_1(x_n, y_n)}{C_1(x_n, y_n)}.$$

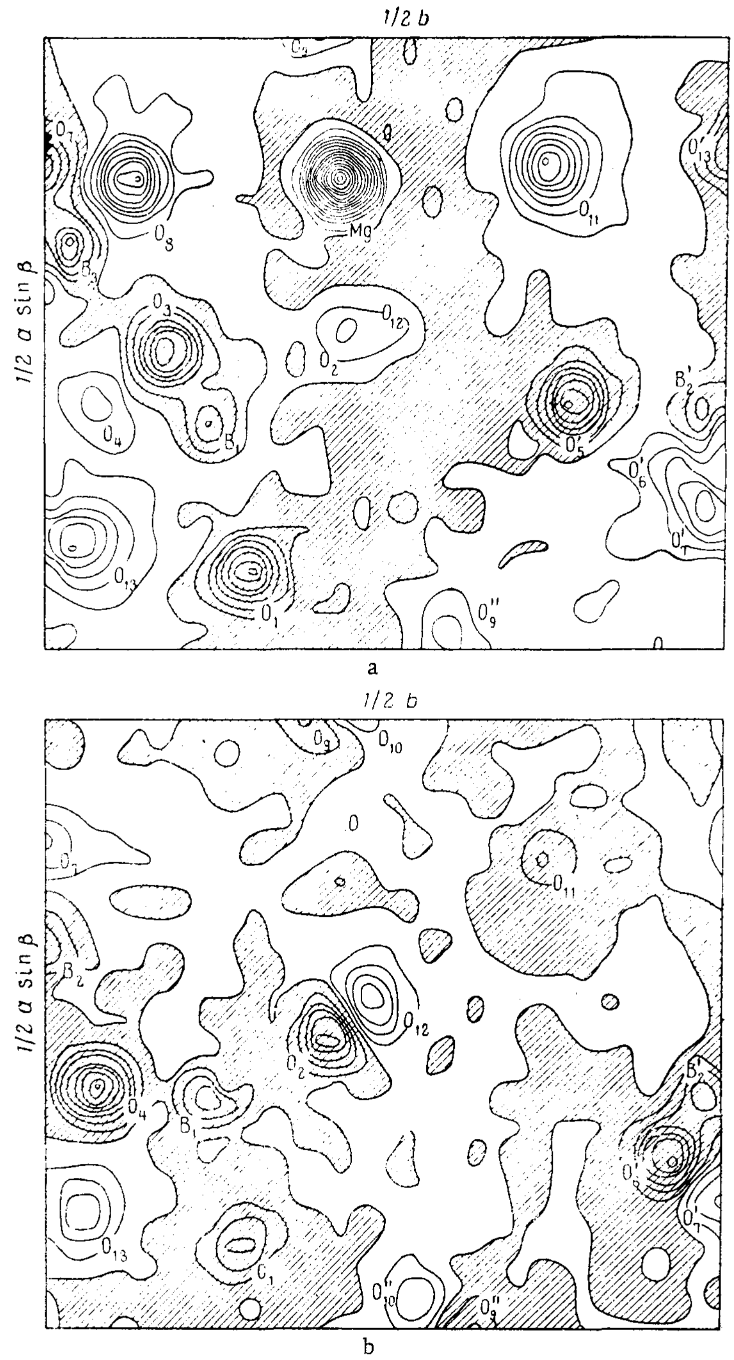

Fig. 1. Modulated projections of the electron density: a) $S_1(x, y)$; b) $C_1(x, y)$. Contours are drawn at intervals of 2 electrons/A^2, negative regions are cross-hatched.

from which all contributions of the previously found atoms had been removed; it was found that O_7 and B_3 overlap in the xy projection with B_2 and O_6, which hampered their detection.

For confirmation and refinement of the z-coordinates of the atoms, a Fourier synthesis $\sigma(y,z)$ was constructed. The necessary signs of F_{0kl} were determined in the following manner: on the basis of the existing S_{hk0} and S_{hk1} from the Sayre-Zachariasen relationships, groups of the reference signs of S_{hk2} and S_{hk3} were known; then, from all the reference signs S_{hk0}-S_{hk3}, the signs of S_{0k0} to S_{0k6} were analyzed, and, further, from the new reference group S_{0k0}-S_{0k6}, the whole large collection of S_{0kl} were found, with a subsequent final recalculation

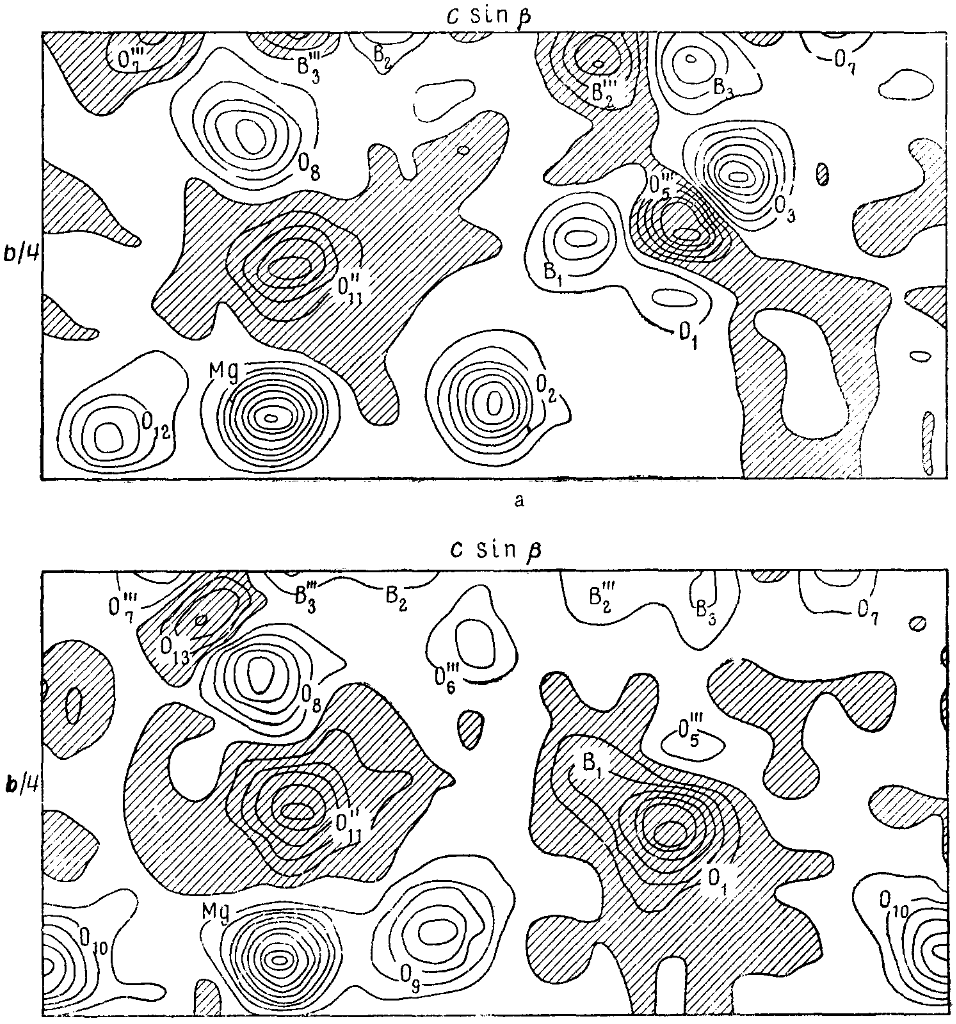

Fig. 2. Modulated projections of the electron density: a) $S_1(y, z)$; b) $C_1(y, z)$. Contours are drawn at intervals of 2 electrons/A^2, negative regions are cross-hatched.

from the group S_{0k0}-$S_{0.k.12}$; 87 S_{0kl} in all were fixed (out of 114). From the coordinates found from this synthesis, a cycle of refinement as carried out using the usual projections σ(x,y) and σ(y,z), and also the modulated $C_1(y,z)$ and $S_1(y,z)$; these were especially important due to the mutual overlappings of the majority of atoms in projection along the a axis.

In the conclusive stage, the signs of hk0-hk3, 0k*l*, and 1k*l* were recalculated (and partially were established anew); syntheses σ(x,y), $C_l(x,y)$, $S_l(x,y)$ ($l = 1,2,3$), σ(y,z), $C_1(y,z)$, and $S_1(y,z)$ were constructed from these (see Figs. 1 and 2). Combining them with phase projections [17], we were able to refine the locations of the atoms. The coordinates of nonoverlapping atoms were averaged from the collections of phase projections.

$$C_l(x, y, Z_a) = \int_0^c \rho(x, y, z) \cos \frac{2\pi l}{c}(z - Z_a)\, dz$$

and, correspondingly, $C_h(X_a, y, z)$, where $Z_a(X_a)$ is the coordinate of the atom under refinement. The coordinates of the overlapping atoms were determined from the projections

$$S_l(x, y, Z_a) = \int_0^c \rho(x, y, z) \sin \frac{2\pi l}{c}(z - Z_a)\, dz,$$

and also $S_h(X_a, y, z)$, where Z_a (X_a) is the coordinate of the interfering atom. To refine (x,y) – the coordinates O_2, O_{12} and O_9, O_{10}, overlapping in pairs in the xy projection when the difference $z_1 - z_2$, close to c/2,‡ in addition to the syntheses $S_3(x, y, Z_a)$, zonal modulated projections [18], $\sigma_L^{[z_1,z_2]}(x,y)$ were constructed using the large mass of reflections $F_{hk0} - F_{hk3}$:

$$C_{0.5}^{[-c/2,\, c/2]}(x, y) = \int_{-c/2}^{c/2} \rho(x, y, z) \cos \pi z\, dz$$

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‡When the condition is exact, $z_1 - z_2 = c/2$; then the coordinates cannot be made accurate from phase projections [17].

$$= \frac{2}{\pi A_c} \sum_{h}^{\infty} \sum_{-\infty k} \left(F_{hk0} + \frac{F_{hk1}}{1.5} - \frac{F_{hk2}}{7.5} + \frac{F_{hk3}}{17.5} + \ldots + \frac{(-1)^l 2F_{hkl}}{1-4l^2} + \ldots + \right) \times \cos 2\pi \left(\frac{hx}{a} + \frac{ky}{b} \right)$$

$$= \frac{2}{\pi A_c} \left[\sigma(x, y) + \frac{C_1(x, y)}{1.5} - \frac{C_2(x, y)}{7.5} + \frac{C_3(x, y)}{17.5} + \ldots + \frac{(-1)^l \cdot 2C_l(x, y)}{1-4l^2} + \ldots \right]$$

for the determination of O_{12},

$$C_1^{[c/4,\, 3c/4]}(x, y) = \int_{c/4}^{3c/4} \rho(x, y, z) \cos 2\pi z \, dz \, [^{18}]$$

for the determination of O_2

$$S_{0,5}^{[0,\, c]}(x, y) = \int_{0}^{c} \rho(x, y, z) \sin \pi z \, dz \, [^{18}]$$

for O_9 and

$$C_1^{[-c/4,\, c/4]}(x,y) = \int_{-c/4}^{c/4} \rho(x, y, z) \cos 2\pi z \, dz \, [^{18}]$$

for O_{10}.

The choice of the projections shown was conditioned, on the one hand, by the best exposure of the atom sought and the removal of the hindering one and, on the other hand, by the rate of convergence of the Fourier series.

The (y,z) coordinates of the atoms O_7''', O_8, which overlap in the yz projection with O_{13}, and O_1 and O_3, overlap with O_5''',** were refined from the zonal projections.

$$C_{2/3}^{[-3a/8,\, 3a/8]}(y, z) = \int_{-3a/8}^{3a/8} \rho(x, y, z) \cos \frac{4\pi x}{3} \, dx$$

$$= \frac{1{,}7}{\pi A_a} \left[\frac{\sigma(y, z)}{1{,}13} + C_1(y, z) - \frac{C_3(y, z)}{15{,}4} + \ldots + \frac{10 \cos \frac{3\pi h}{4} C_h(y,z)}{\sqrt{2}\,(4-9h^2)} + \ldots \right]$$

and, correspondingly, $S_{2/3}^{[0,3a/4]}(y,z)$ [18] for the construction of which the experimental data for F_{0kl} and F_{1kl} were sufficient. Figure 3 shows a comparison of these syntheses with the corresponding sections σ(y,z). It is ap-

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** Due to the triple overlapping, the coordinates of these atoms cannot be accurately fixed from modulated projections.

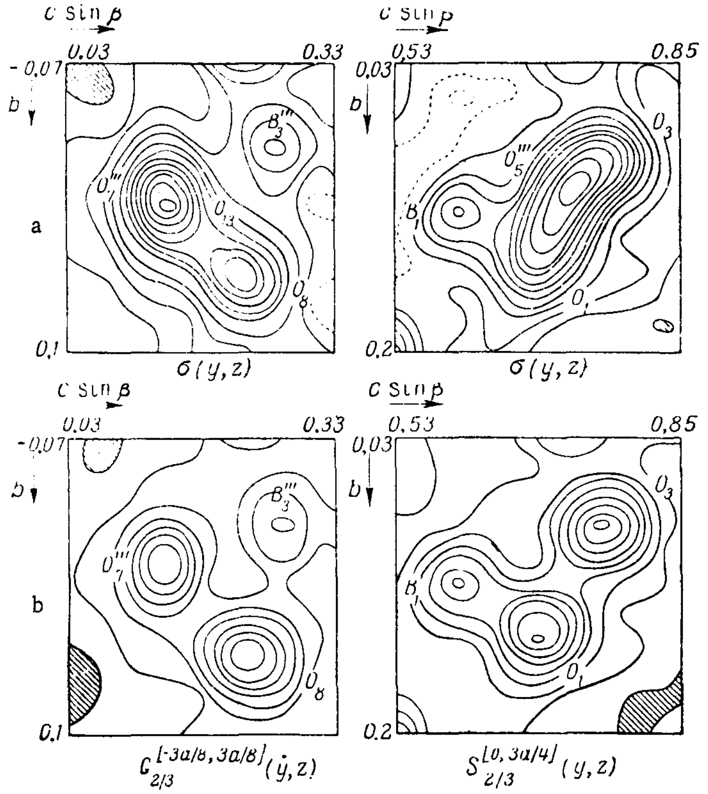

Fig. 3. Projections of electron density: a) $\sigma(y, z)$; b) $C_{2/3}^{[-3a/8,\, 3a/8]}(y, z)$ and $S_{2/3}^{[0,3a/4]}(y, z)$. Contour lines are drawn at intervals of 2 electrons per A^2, dotted ones indicate depressions.

parent that the atoms O_{13} and O_5''' are absent from the zonal projections, and that the remaining ones are fixed quite clearly.

The coordinates of the atoms of the inderite structure obtained from the totality of the usual, modulated, and zonal projections, are collected in Table 2. From the coordinates definitely accepted, the structure factors of F_{hk0}, F_{hk1}, F_{0kl}, F_{1kl} were recomputed. They are given in Tables 3-6, together with F_{exp}; the convergence factors calculated from all nonzero reflections with isotropic temperature corrections were also calculated.

The basic characteristics of the inderite structure are shown in Fig. 4. Mg cations are located within the octahedra formed by two OH groups and four H_2O groups. The atoms B_1 and B_2 are in tetrahedra, and B_3 in triangles of O atoms and OH groups. The structure can be described as an arrangement of isolated neutral groups of a "molecular" type [10], into the composition of which enters an Mg-octahedron and its two neighboring (OH) peaks, one trinucleic borate anion $[B_3O_3(OH)_5]^{-2}$ in the shape of a ring of two $BO_2(OH)_2$ tetrahedra and one $BO_2(OH)$ triangle, connected by the common O-vertices. Such a radical has been found earlier in Ca-borates: Inyoite [20], synthetic $Ca[B_3O_3(OH)_5] \cdot 2H_2O$ [21], and in meyerhofferite [22]. "Molecular" complexes $MgB_3O_3(OH)_5 \cdot 4H_2O$ are joined directly into a single structure by numerous hydrogen bonds and, through a buffer water molecule (O_{13}) which does not take part in coordinational polyhedra, but merely participates in the redistribution of hydrogen bonds; in addition, each such molecule is joined with four O atoms by hydrogen bonds.

The basic interatomic distances are assembled in Table 7. They are in good agreement with the results obtained for other borates [15, 19-23]. The three angles of the triangle O – B – O $BO_2(OH)$ total 359° which, within the limits of error, indicates a strict localization of the boron atom in the plane of the triangle. The distribution of protons between the oxygen atoms to produce OH and H_2O was made on the basis of the balance of valences.

Hydrogen bonds were assigned after finding the lengths of the O – O vectors which did not coincide with the edges of the coordination polyhedra, on the condition that at least one end of such a vector terminates on an atom of an OH or H_2O group. The shortest such distances are enumerated in Table 8. Thirteen O – O distances do not exceed 3.00 A. Since there are 15 H atoms per asymmetric unit, these distances can be interpreted as hydrogen bonds. Table 8 shows that in each concrete case there is an OH or H_2O proton donor. Six more distances $H_2O(OH)$ – $H_2O(OH)$, in which a proton bond is possible, are within the limits 3.17-3.31 A, and the remainder exceed 3.43 A. It is doubtful whether the last six distances correspond to hydrogen bonds, although there are indications in the literature of such elongated H-bonds (3.11, 3.12, 3.17 A [23]).

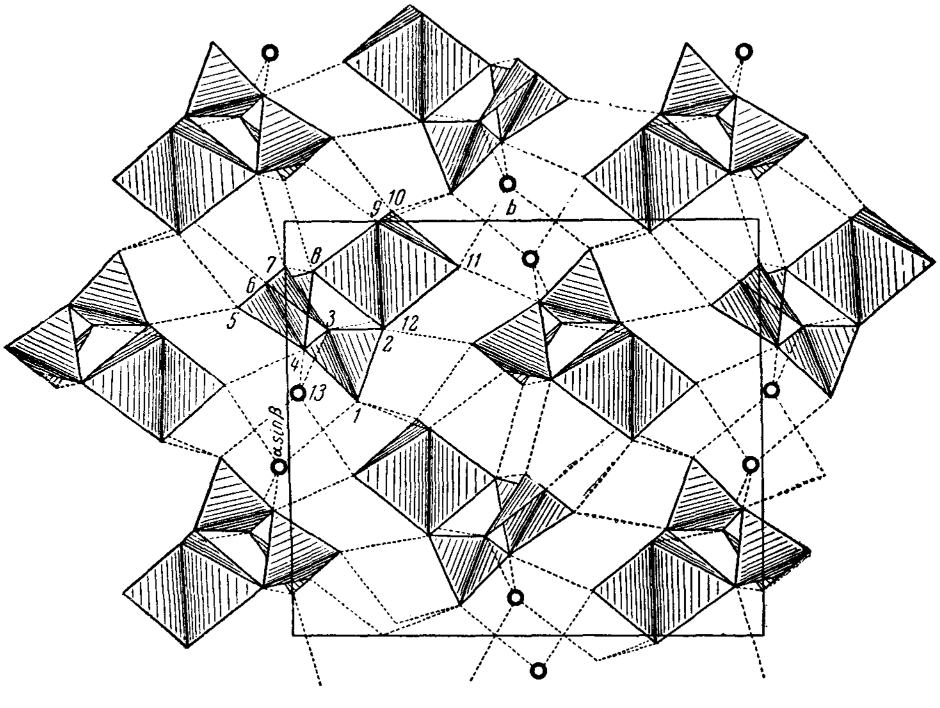

Fig. 4. Structure of inderite in polyhedra. Projection along the c axis. Circles indicate the H_2O molecules that do not form polyhedra. Dotted lines correspond to hydrogen bonds.

TABLE 2. Coordinates of the Basic Atoms of the Inderite Structure

Atoms	Co-ordinates	Syntheses from which the coordinates were obtained						Average values of coordinates and average errors
		$\sigma(x, y)$ (I) $\sigma_l^{[z_1;\, z_2]}(x, y)$ (II)	$C_1(x, y, Z_j)$ (I) $S_1(x, y, Z_j)$ (II—j)	$C_2(x, y, Z_j)$ (I) $S_2(x, y, Z_j)$ (II—j)	$C_3(x, y, Z_j)$ (I) $S_3(x, y, Z_j)$ (II—j)	$\sigma(y, z)$ (I) $C_{2/3}^{[-3a/8,\, 3a/8]}(y, z)$ (II) $S_{2/3}^{[0, 3a/4]}(y, z)$ (III)	$C_1(X_j, y, z)$ (I) $S_1(X_j, y, z)$ (II—j)	
Mg	x/a	0.117 (I)	0.117 (I)	0.118 (I)	0.118 (I)			0.118±0.001
	y/b	0.216 (I)	0.216 (I)	0.215 (I)	0.216 ()	0.215 (I)	0.216 (I)	0.216±0.001
	z/c					0.258 (I)	0.256 (I)	0.257
O_1^*	x/a	0.436 (I)	0.435 (I)	0.437 (I)	0.435 (I)			0.436±0.001
	y/b	0.146 (I)	0.146 (I)	0.146 (I)	0.145 (I)	0.143 (III)	0.144 (I)	0.145±0.001
	z/c					0.692 (III)	0.684 (I)	0.688
O_2^*	x/a	0.255 (II)			0.257 (II — O_{12})			0.256
	y/b	0.212 (II)			0.213 (II — O_{12})		0.210 (I)	0.212±0.001
	z/c						0.497 (I)	0.497
O_3	x/a	0.257 (I)	0.256 (I, II — B_1)	0.260 (I, II — B_1)				0.258±0.002
	y/b	0.084 (I)	0.087 (I, II — B_1)	0.085 (I, II — B_1)		0.087 (III)		0.086±0.001
	z/c					0.764 (III)		0.764
O_4	x/a	0.304 (I)	0.304 (I)	0.306 (I)				0.305±0.001
	y/b	0.037 (I)	0.035 (I)	0.035 (I)				0.036±0.001
	z/c					0.453 (I)		0.453
O_5^*	x/a	0.204 (I)	0.202 (I)	0.204 (I)	0.203 (I)			0.203±0.001
	y/b	—0.110 (I)	—0.111 (I)	—0.111 (I)	—0.109 (I)		—0.110 (I)	—0.110±0.001
	z/c						0.290 (I)	0.290
O_6	x/a		0.140 (I, II — O_7)	0.139 (I, II — O_7)				0.140
	y/b		—0.037 (I, II — O_7)	—0.036 (I, II — O_7)				—0.037
	z/c					0.547 (I)		0.547
O_7^*	x/a		0.107 (I, II — O_6, B_3)	0.108 (II — O_6, O_8)				0.108
	y/b		—0.007 (I, II — O_6, B_3)	—0.005 (II — O_6, O_8)		—0.006 (II)		—0.006±0.001
	z/c					0.861 (II)		0.861
O_8^*	x/a		0.117 (II — O_7)	0.116 (I)				0.117
	y/b		0.062 (II — O_7)	0.062 (I)		0.057 (II)	0.058 (II — O_{13})	0.060±0.002
	z/c					0.231 (II)	0.230 (II — O_{13})	0.231
O_9^{**}	x/a	—0.006 (II)			—0.011 (II — O_{10})			—0.009
	y/b	0.206 (II)			0.206 (II — O_{10})		0.204 (I)	0.205±0.001
	z/c						0.426 (I)	0.426

TABLE 2 (continued)

Atoms	Co-ordinates	Syntheses from which the coordinates were obtained						Average values of coordinates and average errors
		σ (x, y) (I) $\sigma_l^{[z_1,\, z_2]}(z, y)$ (II)	C_1 (x, y, Z_j) (I) S_1 (x, y, Z_j) (II − j)	C_2 (x, y, Z_j) (I) S_2 (x, y, Z_j) (II − j)	C_3 (x, y, Z_j) (I) S_3(x, y, Z_j) (II−j)	σ (y, z) (I) $C_{2/3}^{[-3a/8,\, 3a/8]}$ (y,z) (II) $S_{2/3}^{[0, 3a/4]}$ (y, z) (III)	C_1 (X_j, y, z) (I) S_1 (X_j, y, z) (II−j)	
O_{10}^{**}	x/a	−0,016 (II)			−0,020 (II − O_9)			−0,018
	y/b	0,217 (II)			0.215 (II − O_9)		0.220 (II − O_{12})	0,217±0.002
	z/c						−0,008 (II − O_{12})	−0.008
O_{11}^{**}	x/a	0.106 (I)	0.106 (I)	0.109 (I)	0,108 (I)			0,107±0.001
	y/b	0.369 (I)	0.371 (I)	0,370 (I)	0,369 (I)	0.367 (I)	0,369 (I)	0,369±0.001
	z/c					0.275 (I)	0,274 (I)	0.275
O_{12}^{**}	x/a	0.236 (II)			0.239 (II − O_2)			0.238
	y/b	0.231 (II)			0.234 (II − O_2)			0.233
	z/c						0,074 (II − O_{10})	0,074
O_{13}^{**}	x/a	0.411 (I)	0,409 (I)	0.410 (I)	0.412 (I)			0.411±0.001
	y/b	0.022 (I)	0.021 (I)	0,020 (I)	0,019 (I)	0,022 (III)		0,021±0.001
	z/c					0.162 (III)		0.162
B_1	x/a		0.313 (II − O_3)	0.312 (II − O_3)	0.314 (I)			0.313±0.001·
	y/b		0.118 (II − O_3)	0.116 (II − O_3)	0.118 (I)	0,118 (III)	0,117 (I)	0.117±0.001
	z/c					0.601 (III)	0,597 (I)	0.599
B_2	x/a		0.196 (I)	0,195 (I. II − O_6B_3)				0,196
	y/b		−0.015 (I)	−0.014 (I, II − O_6, B_3)			−0.011 (I)	−0,013±0.002
	z/c						0.383 (I)	0,383
B_3	x/a		0.170 (I, II − O_6, B_2)	0.170 (I, II − B_2)				0.170
	y/b		0.015 (I, II − O_6, B_2)	0.019 (I, II − B_2)		0,019 (I)	0,018 (I)	0,018±0.001
	z/c					0.732 (I)	0.724 (I)	0.728

TABLE 3. Experimental and Calculated Values of the Structure Factors F_{hk0} of Inderite. A Temperature Factor $\exp\left[-1.3A^2\left(\frac{\sin\theta}{\lambda}\right)^2\right]$ is Introduced into F_{calc}. $R_{hk0} = 12.9\%$ $\left(\text{for } F_{exp} \neq 0;\ \frac{\sin\theta}{\lambda} \leqslant 0.93\ \text{A}^{-1}\right)$

h \ k	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0	— +524		32.2 +32.7		91.5 +95.4		<3.0 −0.1		33.7 +31.2		30.0 +31.8		49.6 −45.8		24.8 +27.0		18.5 −19.4		9.4 +4.6		<7.7 +4.5
1		30.2 +32.5	52.8 −55.9	11.1 +11.7	12.5 +10.0	86.5 +81.1	84.0 −77.6	79.0 −80.9	32.3 +34.9	31.1 +33.5	12.5 −12.8	<5.1 −0.9	20.8 +19.8	7.4 +5.1	7.4 −10.7	<6.3 +5.4	7.6 −5.5	<6.9 +1.2	8.9 +4.8	14.6 +16.9	<7.7 −0.6
2	55.0 −63.8	10.9 −15.3	48.7 −47.8	49.2 +54.5	<3.1 −1.5	4.4 +5.6	42.9 +44.5	30.2 +29.3	10.8 −12.6	27.8 +35.1	14.9 −6.2	11.7 +16.7	<5.4 −7.9	32.9 +32.3	17.4 +20.0	<6.3 −2.1	<6.7 +2.5	<6.9 +0.9	<7.2 −1.6	10.0 −7.1	<7.8 +4.3
3		39.7 −42.9	12.8 +12.2	48.3 −51.0	6.3 −4.1	<3.6 −0.1	6.3 +9.3	16.8 −18.7	17.3 −19.9	<5.0 −2.1	<5.0 +5.0	5.2 −5.3	7.4 +1.7	10.9 −11.6	<6.1 +2.1	<6.3 +2.9	<6.7 −3.4	<7.0 −6.1	<7.3 +1.3	<7.6 −2.4	13.3 −12.3
4	13.9 −14.9	7.1 −6.7	104 −101.0	51.1 −50.5	16.1 −11.7	15.9 −12.2	44.2 −45.7	9.2 +12.1	14.5 −14.1	<4.9 +5.0	20.9 +17.8	21.2 −14.7	9.3 +8.0	6.8 +1.2	<6.2 −3.3	15.7 +18.1	8.0 −9.1	<7.0 +7.9	<7.3 −2.8	<7.6 −1.0	11.1 +2.8
5		<3.5 −1.1	33.2 −32.1	45.2 −45.8	7.9 −10.2	12.6 −5.9	<4.3 +5.8	32.8 +27.9	9.3 −11.3	20.7 +20.6	<5.3 −3.2	7.9 +2.8	<5.8 +3.5	<6.0 −0.7	8.4 −11.2	<6.6 +1.2	<6.9 −2.6	<7.2 −4.0	<7.4 +2.1	<7.7 −7.0	10.1 +12.7
6	44.7 −44.0	74.2 +79.8	9.3 +4.5	21.0 +18.5	11.0 +6.0	<4.4 −0.5	8.4 +8.0	17.4 −12.5	6.6 −12.5	<5.2 −8.5	<5.4 +5.1	16.7 +20.0	8.2 −13.5	25.1 −26.7	16.5 −15.4	8.0 +7.1	<7.0 −0.1	<7.3 −6.8	<7.6 +3.3	9.5 +5.0	<8.0 +0.8
7		49.2 +49.8	22.8 +23.4	<4.4 −3.4	19.3 −22.2	38.7 +41.2	52.2 +58.1	13.7 −17.7	52.3 −56.1	<5.4 −0.2	<5.6 +4.0	22.7 −20.2	16.1 −13.7	<6.3 −3.7	9.1 +9.0	<6.9 +3.3	<7.2 +3.4	17.1 −19.0	<7.5 −7.7	<7.9 +2.0	12.7 +9.5
8	50.4 +58.7	22.6 +24.4	39.7 −47.6	23.4 −26.9	40.0 +41.4	<4.9 +3.2	27.6 −28.7	6.7 −6.7	27.6 −25.2	<5.6 −5.9	16.4 +15.8	8.3 −8.0	13.6 −12.9	20.7 −24.5	22.2 +25.2	<7.0 −4.6	9.5 −7.2	<7.5 −7.2	<7.8 +5.3	<8.0 −2.5	
9		14.7 +17.3	<4.9 −4.4	21.0 −20.0	13.3 +10.1	23.3 +27.0	8.3 +11.5	25.7 −26.0	36.2 +34.1	15.3 +16.6	9.1 +10.2	13.6 −12.0	<6.5 +6.9	8.0 +8.9	<7.0 −4.5	<7.2 +5.1	<7.5 −0.9	<7.7 +3.6	<7.9 −4.8	11.4 +13.4	
10	32.8 +34.7	20.1 −17.0	14.2 +16.6	<5.3 −0.2	9.3 +8.0	<5.5 +0.3	10.4 +12.9	<5.8 +4.7	13.2 +13.5	<6.1 −10.5	10.1 +14.6	<6.4 +5.1	11.9 −12.7	12.8 +9.9	<7.2 +11.0	<7.4 +2.2	10.0 +7.5	<7.9 −6.8	9.8 +7.5		
11		10.2 −9.8	15.1 +20.5	<5.6 −8.1	6.0 −10.1	<5.8 +2.8	19.4 −15.4	<6.0 −3.0	<6.2 −5.8	<6.3 +3.3	8.8 +11.5	15.7 +15.6	7.9 +5.4	9.4 +9.2	9.5 +9.3	10.0 +10.7	10.8 +10.9	<8.0 −3.5			
12	<5.8 −2.3	7.1 −2.1	<5.9 −6.0	<5.8 −10.4	<6.0 +5.5	6.4 +9.7	<6.2 +2.5	<6.3 −1.7	<6.5 +0.3	<6.7 +2.0	<6.8 +5.6	10.0 +11.8	<7.2 +6.9	12.9 +11.3	<7.6 +3.5	<7.8 −1.6					
13		11.0 −10.5	<6.2 −2.5	<6.2 −3.4	11.0 −17.8	8.8 −7.4	9.5 −4.8	9.3 +5.5	<6.8 −1.4	<6.9 −6.2	<7.1 −3.1	<7.3 −9.1	13.2 −13.4	13.5 −11.3	<7.8 −7.7	<8.0 −7.0					
14	19.0 −20.4	<6.6 +9.1	<6.6 −1.3	12.7 −13.8	9.9 −7.6	<6.8 +7.8	<6.8 +3.5	<6.9 +3.4	<7.1 −5.6	18.3 −18.3	11.4 −8.1	<7.6 +2.3	<7.7 −1.6	21.7 −11.9	11.7 −9.4						
15		<6.9 +4.3	14.2 +17.7	<7.0 −4.4	<7.0 −6.7	<7.1 −3.9	13.7 +19.2	<7.3 −6.5	16.4 −18.7	<7.5 +4.7	<7.6 +7.1	9.2 +3.4	10.0 −7.4						10.3 −8.4		
16	21.2 +22.4	14.9 +19.5	<7.2 −7.4	<7.3 +0.5	<7.3 0.0	10.7 +11.0	<7.4 −4.9	<7.6 +4.0	<7.7 −3.4	10.9 +10.1	<8.0 +2.0	10.4 +11.3			10.0 +6.0						
17		<7.5 +1.3	<7.5 −5.8	<7.5 +7.4	<7.5 −1.5	15.3 +16.0	<7.7 +8.8	<7.8 −7.5	<7.9 −0.7												
18	<7.8 −1.8	<7.9 +2.9	<7.9 −6.2	<7.9 +0.7	<7.9 −2.0	10.4 −7.6									12.1 +9.3						
19													9.5 +2.8								
20						10.0 −6.1															

TABLE 4. Experimental and Calculated Values of the Structure Factors F_{0kl} of Inderite. A Temperature Factor $\exp\left[-0.9A^2\left(\frac{\sin\theta}{\lambda}\right)^2\right]$ is Introduced into F_{calc}. $R_{0kl} = 16.1\%$ $\left(\text{for } F_{\text{exp}} \neq 0;\ \frac{\sin\theta}{\lambda} \leqslant 0.91A^{-1}\right)$

l k	0	1	2	3	4	5	6	7	8	9	10	11	12
0	— +524	— −71.8	56.6 −51.9	23.2 −18.5	88.2 +77.8	24.6 −17.2	34.4 −30.6	24.3 +31.0	21.5 +14.7	<7.6 −8.5	<8.3 −7.1		
1		— −43.1	14.1 −17.9	10.0 −12.5	14.8 +17.6	40.5 −43.8	7.8 +8.9	12.8 +16.5	<7.0 +2.4	9.1 −6.7	<8.3 +9.5	8.8 +15.2	
2	30.5 +32.8	25.1 −28.6	64.6 −52.2	60.8 −62.5	39.0 −38.8	11.3 +13.6	6.7 +10.6	14.0 +9.7	<7.0 −4.7	<7.7 +3.6	12.7 −13.4	<9.1 +1.0	11.8 −16.1
3		61.0 +60.5	14.1 −19.2	27.8 −16.1	34.6 +34.8	17.6 +18.6	<5.9 +1.7	24.8 −23.5	10.9 +8.8	<7.8 −9.0	<8.3 −3.8		
4	91.6 +96.2	29.6 +25.8	93.7 +79.7	57.0 −60.9	<4.8 −4.9	5.9 +11.2	<7.0 +1.6	<7.4 +1.6	12.0 +11.5	<7.8 −0.7	12.8 −15.1		
5		73.6 −64.7	4.9 +4.6	23.4 −24.9	13.7 +16.0	26.1 −19.6	15.5 +15.1	8.0 −13.1	<7.2 +10.3	<7.9 +3.0	<8.4 −1.7		
6	<3.0 −0.1	23.2 −19.3	18.4 +7.8	11.2 −14.2	42.7 −38.5	11.7 −6.0	26.8 +23.2	16.2 +19.7	<7.3 −3.7	<8.0 −7.3	<8.6 −2.6		
7		45.0 −41.0	14.2 +16.7	8.5 −9.4	43.0 +42.2	16.3 −12.7	16.8 +15.3	<6.9 −11.9	<7.5 +1.1	<8.1 −4.0			
8	32.3 +32.4	16.7 +20.0	23.8 −20.9	24.6 +20.9	26.4 −26.5	13.4 −18.8	<6.6 +4.9	16.3 +16.8	7.7 −1.4	15.5 −20.4			
9		9.0 −9.3	29.0 −28.8	12.6 −9.1	15.1 +16.0	12.1 −8.2	<6.7 +7.5	10.5 −11.2	<7.7 +6.9	8.3 −9.1			
10	33.9 +33.7	<5.2 −0.4	<5.4 −6.9	<5.7 −4.7	<6.0 +3.3	<6.4 +6.8	<6.9 −3.3	<7.3 +12.4	18.8 +19.6	13.2 −12.3			
11		12.9 −15.2	<5.7 −2.2	<6.2 −2.7	15.5 +20.5	<7.2 −6.0	16.3 +18.4	8.6 −10.3	9.6 +1.6				
12	52.8 −49.9	32.4 +34.8	9.2 −14.1	<6.2 −1.7	28.0 −31.8	7.2 +3.7	<7.3 +7.3	8.7 −14.7					
13		36.8 +32.6	14.1 −18.4	34.2 −31.0	<6.8 +1.6	23.8 +31.5	<7.6 +0.2	20.4 −25.4					
14	25.7 +30.3	6.5 +10.6	17.2 −17.9	7.6 +7.1	12.0 +16.9	<7.3 −1.3	<7.8 +0.2	<8.2 +0.3	11.1 +18.6				
15		<6.8 −4.6	<6.9 −6.6	<7.1 −3.0	<7.3 +6.1	<7.7 +4.1	8.3 +7.0	8.7 +3.0	8.7 −10.7				
16	18.4 −22.5	<7.0 +7.4	8.7 −9.8	<7.3 +2.5	15.4 −20.0	<7.9 +2.6	<8.3 −3.1						
17		8.4 +3.7	8.7 −11.3	<7.7 +0.8	<7.9 −2.9	<8.2 +12.7	<8.4 +9.8						
18	<7.7 +5.6	7.3 +9.2	8.0 −0.8	<8.0 +5.7	<8.2 +2.7								
19		<8.0 −7.0	11.4 −17.5	14.6 +17.0	<8.3 −8.0								
20													
21			8.8 −11.3										

TABLE 5. Experimental and Calculated Values of the Structure Factors F_{hkl} of Inderite. A Temperature Factor $\exp\left[-1.0\,A^2\left(\frac{\sin\theta}{\lambda}\right)^2\right]$ is Introduced into F_{calc}. $R_{hkl} = 14.7\%$ (for $F_{exp} \neq 0$; $\frac{\sin\theta}{\lambda} \leqslant 1.06\ A^{-1}$)

h \ k	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	24	26	27
24	9.8 +10.4																									
20	9.7 −12.8	<8.2 +8.1																								
19		<7.9 +6.5	<7.9 +6.7	9.0 +11.2	<8.0 +4.0	<8.0 +0.9	<8.0 −7.2	15.7 +21.5																		
18	<7.6 −1.4	8.8 −14.2	8.5 +9.6	<7.7 −0.3	<7.7 +0.8	<7.8 −1.1	<7.8 +4.4	<7.9 +7.1																		
17		<7.3 +3.8	8.1 −10.2	<7.4 −3.2	<7.5 −3.1	<7.5 −2.5	<7.5 −6.9	<7.6 −4.8																		
16	<7.0 −6.4	<7.1 +2.2	10.2 −10.1	<7.0 −1.1	<7.2 −5.0	10.2 −8.0	13.9 −13.7	10.4 −11.1	12.1 −10.1																	
15		<6.7 −8.5	<6.7 −8.7	<6.7 −2.5	<6.9 +4.7	<7.0 +1.7	<7.0 +4.2	12.0 −12.2	11.3 −13.7	7.8 −11.8	9.6 −10.8	9.9 −8.0														
14	18.2 +16.8	14.1 +11.6	<6.4 −4.7	7.5 +12.3	<6.5 −0.8	<6.6 −0.7	<6.7 +2.9	<6.8 +4.3	6.9 +4.3	13.1 +15.6	9.5 +9.0	<7.3 +6.6	8.9 −10.7	9.0 −6.9	8.6 +6.6	<7.9 +1.4	<8.1 −3.7	<8.2 −1.2	8.7 +6.2							
13		<6.6 −0.7	<6.1 −0.8	7.7 −9.4	6.2 −3.2	<6.3 −4.3	23.6 +24.1	7.0 −7.3	11.3 −9.3	15.2 −15.4	8.2 +6.9	7.8 +6.6	<7.2 −2.3	7.4 +8.5	<7.5 −3.1	<7.7 +2.7	<7.9 −0.9	<8.0 +5.6	<8.2 −3.0	<8.3 +1.9	9.7 +13.9					
12	<5.8 +2.3	20.1 +20.3	15.8 +17.0	10.3 −11.1	6.9 +10.6	15.3 +16.4	6.1 +6.9	<6.2 +3.6	7.0 +8.0	<6.5 −1.3	7.9 −7.8	<6.9 −5.0	12.0 +15.3	10.7 −12.0	<7.4 −7.0	14.6 +15.3	8.1 −7.5	<7.9 −3.5	<8.0 −7.5	<8.2 +1.3	<8.3 −0.5					
11		14.9 −14.6	11.1 +9.8	11.6 +13.9	15.5 +14.6	8.8 −10.0	16.4 +16.8	18.4 +23.2	8.2 +7.6	7.1 −9.7	13.0 +16.1	<6.6 +0.1	<6.7 −0.3	14.2 −12.1	9.0 +14.8	<7.3 −1.5	<7.5 −2.4	<7.7 +7.0	<7.9 +4.6	<8.0 +6.5	<8.3 −6.1					
10	26.2 −29.8	17.8 −17.9	<5.1 +6.2	<5.2 −2.0	9.1 −8.3	13.6 −14.4	19.5 +20.1	11.2 −14.9	<5.8 +2.7	<5.9 −1.5	<6.1 −4.1	<6.3 +0.5	<6.5 +6.7	8.1 +5.9	<7.0 +2.2	9.6 −12.6	<7.4 +0.8	<7.5 −8.2	<7.8 −1.8	<8.0 +5.8	<8.2 +6.8					
9		21.1 +21.6	6.7 −5.7	25.5 +26.5	16.7 −15.7	<5.1 +2.6	40.2 −44.2	<5.4 +0.3	6.1 +5.8	6.6 +7.9	<5.9 −2.1	9.7 +11.3	<6.3 +2.6	<6.5 +2.3	<6.7 −3.0	8.8 −9.4	<7.2 +7.1	<7.5 0.0	<7.6 +2.5	<7.9 −3.2	<8.0 +2.7					
8	53.5 +47.9	33.4 −36.5	<4.5 +0.8	13.2 −9.6	14.1 −15.1	<4.9 +1.7	11.8 −17.4	10.0 −11.4	19.6 +20.4	18.1 −17.1	<5.7 −5.4	19.3 −20.0	<6.1 −1.1	17.9 +13.9	<6.7 −0.1	<6.8 −4.5	<7.1 +3.1	<7.3 −4.9	<7.5 +6.8	10.7 −6.7	<7.9 −4.4	<8.1 −10.1				
7		20.9 −20.8	<4.2 +1.2	<4.3 −3.5	5.6 +7.9	24.8 +23.1	23.6 −23.4	27.5 −22.1	17.1 +15.3	10.8 +7.5	<5.4 −2.3	6.3 −6.0	11.4 −16.1	13.0 +10.8	<6.4 +7.4	7.9 +2.6	<7.0 −8.2	<7.2 +5.5	<7.4 +4.9	9.0 +7.6	15.2 −16.7	8.9 −11.5			10.1 −2.0	
6	29.8 −28.0	10.9 −9.8	60.8 −66.1	11.4 −9.9	<4.2 −6.8	12.3 +15.5	23.8 −20.6	4.9 +7.0	35.9 −37.3	6.4 +11.9	5.8 −6.3	9.8 +9.1	21.6 −23.8	<6.0 −0.2	30.5 +28.0	<6.5 −0.9	<6.7 −6.0	<6.6 +2.0	<7.3 +6.1	10.2 +14.0	<7.7 −3.6					11.3 −2.7
5		27.5 +21.1	34.4 +31.0	21.2 −22.3	<3.9 −1.3	6.3 −7.7	46.3 +44.0	39.0 −39.3	5.6 −6.7	5.1 −7.3	13.3 +11.5	23.4 −23.7	7.3 −6.1	<5.8 +1.7	<6.1 −1.6	8.3 −10.3	<6.6 +3.7	10.9 −12.8	13.9 −16.2	<7.3 −0.1	14.7 +15.4					
4	8.8 −0.9	69.2 +78.0	7.1 +8.9	59.8 +64.0	6.1 +8.4	56.2 +57.6	33.5 −34.2	8.0 +9.2	17.3 +18.3	14.1 +14.8	<4.9 +1.3	34.0 +34.8	9.5 +7.6	8.5 −6.3	20.6 −21.6	7.2 +11.9	<6.5 −2.1	<6.8 −3.7	9.3 +8.0	9.3 +11.3	<7.5 −8.9					
3		<2.7 −1.4	31.6 −26.0	22.2 −17.7	18.5 −14.0	12.6 −10.9	<3.8 +3.4	60.5 +66.5	30.3 −31.7	6.6 +5.7	16.3 −13.0	<5.1 −8.9	28.1 −28.4	<5.6 +4.2	<5.9 +7.7	7.2 −2.1	7.4 −9.6	<6.7 +6.0	<7.0 +5.2	<7.3 −3.2	<7.5 +0.4	<7.7 +9.2				
2	28.3 −21.3	42.1 −46.1	86.0 +110.0	71.7 −78.3	87.5 +89.8	29.4 −28.5	58.3 +52.9	<3.9 −0.3	5.0 +7.7	<4.4 +4.7	16.3 +19.0	26.9 −26.5	10.9 +11.3	6.6 −8.8	12.0 −20.5	<6.1 +3.3	8.3 −8.7	<6.7 +1.7	8.3 −3.7	<7.2 +0.2	<7.5 −4.4	<7.7 −1.0				

TABLE 5 (continued)

k h	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	24	26	27
1		5.1 +7.3	17.6 −15.5	21.8 −16.7	8.1 +9.0	38.0 −36.5	35.1 −30.7	43.3 +43.7	17.6 +17.9	5.6 −3.4	<4.7 +4.6	11.2 +10.3	28.0 +25.1	14.3 +18.0	7.4 −5.8	<6.0 +9.0	<6.3 +2.6	<6.6 +0.4	<6.9 +2.6	13.9 −7.4	<7.5 +0.4	<7.7 +7.6	<7.9 −7.2			
0	— −71.7	— −43.1	24.3 −28.5	50.5 +60.4	31.4 +25.7	70.0 −64.5	24.0 −19.2	40.8 −40.8	15.2 +19.8	10.0 −9.2	<4.6 −0.4	13.1 −14.9	32.2 +34.0	38.6 +31.8	<5.7 +10.3	<6.0 −4.5	6.9 +7.1	7.2 +3.5	6.9 +8.8	<7.2 −6.7	<7.5 −4.9	<7.7 +3.6	<8.1 +7.2			
$\bar{1}$		— −6.6	33.1 −37.9	18.9 −17.5	46.5 +47.5	24.1 +23.7	44.8 −42.0	34.6 −33.8	27.6 +27.1	22.6 +21.1	<4.6 +3.4	25.5 −24.4	25.2 +21.7	<5.4 +6.9	14.2 +16.9	<6.0 −5.3	7.0 −7.5	10.7 +13.0	20.5 +21.1	15.1 +13.1	8.9 −11.2	<7.4 −5.1	<7.7 +5.2			
$\bar{2}$	74.7 +136.0	10.3 −5.4	34.6 −36.9	30.2 −21.8	46.7 −47.1	5.0 +6.0	36.8 −32.2	30.8 +26.7	<4.1 −6.5	34.0 +31.4	<4.7 +4.8	17.5 −19.0	45.7 −44.6	9.8 −12.8	21.2 +19.8	7.2 −13.1	6.3 −8.0	8.1 −12.1	17.9 +15.8	13.4 −13.0	<7.5 −4.3	<7.7 −8.7	<7.9 −2.1			
$\bar{3}$		6.1 −1.7	5.5 −4.4	47.0 +39.2	20.2 +14.8	20.9 +11.7	59.5 +57.2	66.6 −65.7	<4.2 −7.5	7.3 −5.2	<4.7 −2.8	<5.0 +3.6	8.9 −5.7	17.3 +10.4	15.7 −15.3	<6.1 −8.8	<6.4 −2.6	6.7 −10.8	13.7 −12.8	<7.2 +2.3	<7.5 +2.9	<7.7 −12.6	12.3 −13.7			
$\bar{4}$	6.2 −12.0	39.0 +30.8	24.3 −32.3	43.7 +36.6	17.2 −12.2	3.8 −11.6	13.9 −13.8	19.6 −13.9	<4.3 −4.0	29.7 −23.5	50.5 −51.5	6.4 −8.5	<5.4 −7.0	22.8 −20.6	<5.9 +2.2	13.5 +13.0	9.6 −10.5	<6.7 +2.6	7.8 −7.4	<7.2 +1.5	<7.5 −4.8	<7.8 +0.8	12.2 +12.4			
$\bar{5}$		<3.2 −3.6	7.5 +3.1	48.2 +41.2	10.1 +14.0	23.6 +20.4	16.4 +12.6	12.1 +9.7	18.3 −17.6	<4.7 +4.1	6.1 +1.5	15.9 −19.1	<5.4 −12.8	22.6 −18.8	12.2 +9.6	20.4 −24.1	<6.6 −7.8	<6.8 +6.9	<7.2 +6.0	10.0 −11.1	13.5 +11.3	<7.9 +7.2	<8.0 +11.2			
$\bar{6}$	38.1 −39.1	27.2 +25.7	4.2 −6.0	<3.7 −0.1	42.4 −40.6	17.0 +13.1	9.7 +8.5	<4.5 +2.1	19.8 +18.7	33.1 +32.6	7.7 +8.9	31.1 +29.0	18.5 +8.9	<5.8 +8.1	<6.1 −1.6	<6.4 +2.0	<6.7 −1.1	8.7 +11.4	<7.2 +1.7	19.6 +19.6	<7.7 +5.5	<7.9 +9.1				
$\bar{7}$		20.9 −13.6	27.3 −23.0	10.1 +9.2	28.3 −23.2	49.2 −48.6	27.3 −28.3	39.0 +38.0	<4.9 +1.7	<5.1 +5.5	27.2 −25.1	37.7 +34.2	7.6 −6.0	<6.0 +8.5	<6.2 +0.8	<6.5 +5.6	15.7 +13.3	<7.1 +8.3	<7.3 −1.8	8.3 −4.1	<7.7 −1.6	<8.0 +5.4				
$\bar{8}$	14.1 −14.6	67.8 −68.8	37.5 +32.4	21.8 +21.9	21.9 +20.9	7.6 −5.3	19.7 +17.0	5.6 +12.6	18.8 +21.1	13.8 −9.7	9.3 −7.6	16.3 −15.2	18.5 +19.5	21.9 +25.5	7.7 −7.0	8.4 −7.6	<6.9 +3.3	<7.2 +6.4	<7.4 +3.7	14.2 −14.0	<7.9 −2.2	8.8 −8.1		10.2 −2.8		
$\bar{9}$		15.3 −16.7	10.5 +8.9	12.9 −11.0	20.1 +20.3	18.0 +17.7	45.8 −47.2	7.4 −5.9	36.1 +38.9	<5.5 +6.1	<5.7 +1.9	18.5 −17.7	<6.1 +3.3	12.8 +15.5	11.1 −10.5	7.2 +5.6	16.3 −15.1	9.3 +12.0	<7.5 −0.9	<7.7 +2.6	20.6 −22.7					
$\overline{10}$	34.1 +33.2	14.4 −17.7	5.6 −0.5	12.9 −12.3	27.9 +25.0	6.0 +4.4	12.7 −6.8	8.4 −16.6	13.9 −9.3	<5.8 −2.0	9.2 +7.1	<6.0 −0.5	7.6 −6.3	12.2 +11.7	16.7 −14.1	12.0 −16.4	<7.2 −9.0	<7.5 −6.8	<7.7 +4.2							
$\overline{11}$		35.7 +31.1	15.5 +16.6	<5.2 +2.2	<5.3 −0.1	6.8 −10.0	<5.5 +3.4	14.8 −4.4	<5.8 +3.9	<6.0 −3.9	8.4 +5.8	13.4 −8.5	<6.6 +3.0	<6.8 −5.9	<7.0 +4.4	7.2 −8.5	15.6 +14.3	<7.6 −6.6								
$\overline{12}$	13.5 +8.9	<5.4 +0.4	<5.5 +6.7	+12.1 12.1	<5.7 −3.4	11.0 +4.0	9.5 −9.5	<5.9 +4.4	<6.1 +5.7	<6.3 −11.1	<6.5 −7.3	<6.6 −1.8	14.9 −12.0	<7.0 −5.9	8.6 −10.9	<7.4 +0.1	<7.5 +2.1									
$\overline{13}$		23.0 −23.2	<5.8 −8.1	7.3 −7.1	<5.9 −3.1	8.5 +5.0	14.6 +11.3	<6.2 −0.8	<6.5 −0.7	7.2 −7.8	<6.7 −5.2	<6.9 −7.8	7.8 −5.3	11.2 +12.7	<7.4 −0.7	<7.5 −4.3										
$\overline{14}$	27.9 −33.9	12.8 +12.8	8.8 −8.4	16.3 −15.2	11.1 −12.2	7.2 −8.4	<6.5 −10.2	9.8 −10.1	<6.7 −5.6	<6.8 −3.5	<7.0 −4.2	8.5 −8.0	<7.3 +6.4	20.3 −15.9	<7.5 −4.4											
$\overline{15}$		<6.5 +2.1	<6.4 +3.9	<6.9 +6.1	7.9 +9.1	17.3 −21.7	<6.7 +5.0	19.5 +25.3	<7.0 −6.4	<7.2 −6.5	<7.2 −0.6	9.1 +9.4	8.3 +11.4	<7.7 −3.4												
$\overline{16}$	24.5 −27.8	<6.7 −6.4	10.9 +8.2	21.8 +24.8	<7.0 −4.0	8.4 −8.4	<7.0 +5.1	<7.2 +7.4	<7.2 +7.8	11.5 +13.0	<7.5 +2.0	<7.6 +5.1	12.5 +16.1	9.4 +12.6												
$\overline{17}$		8.5 +11.9	20.2 −20.0	<7.2 +7.7	<7.2 +2.8	<7.2 +8.2	<7.3 −8.3	<7.4 +11.0	8.6 +12.8	<7.6 +10.1	9.3 −9.9															
$\overline{18}$	23.0 +20.9	<7.4 −3.3	7.5 +9.0	<7.4 −4.7	8.5 +10.5	<7.4 −0.1	<7.6 +0.5	<7.7 +6.8	<8.2 −0.2	<7.9 +8.5																
$\overline{19}$		<7.6 −4.8	<7.7 +6.6	<7.7 +4.1				9.5 −7.8	<7.7 −8.3	<8.0 −8.8																
$\overline{20}$										9.0 −12.5																

TABLE 6. Experimental and Calculated Values of the Structure Factors F_{1kl} of Inderite. A Temperature Factor $\exp\left[-1.2A^2\left(\frac{\sin\theta}{\lambda}\right)^2\right]$ is Introduced into F_{calc}. $R_{1kl} = 16.5\%$ $\left(F_{exp} \neq 0;\ \frac{\sin\theta}{\lambda} \leqslant 0.97A^{-1}\right)$

l \ k	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23
12								9.0 +7.5															
11	<7.6 −2.9	9.6 +9.9	<7.6 −6.1	<7.7 −3.7	<7.7 +5.6	<7.7 +1.4	<7.8 −4.2	9.7 −10.9															
10	<7.1 +1.1	<7.1 −5.3	<7.1 +0.6	<7.2 +1.5	<7.2 +1.9	<7.3 +3.4	<7.4 −3.6	8.1 −7.1	<7.6 +7.7														
9	<6.6 +8.4	<6.6 −1.0	<6.6 +3.5	10.9 −13.2	<6.7 −2.3	<6.9 +5.2	<6.9 −1.0	<7.0 −0.5	<7.1 +3.2	<7.2 +7.8													
8	11.4 +11.3	<6.1 −1.8	<6.1 +0.7	9.7 +10.3	15.4 +12.9	<6.3 −5.3	<6.4 +3.6	20.2 +20.3	6.5 +4.9	<6.8 +6.2	10.6 −10.2	7.4 −0.4	6.8 +9.5										
7	<5.5 −5.7	14.8 +15.1	<5.6 −6.0	5.3 −3.9	22.0 +20.4	15.4 +15.3	13.3 −17.3	29.0 −28.0	9.7 +11.6	<6.4 +5.8	<6.5 −2.1	8.1 −5.6	6.2 +5.8	6.4 −2.0									
6	17.9 −17.6	7.9 +7.7	9.9 −10.0	<5.1 −5.4	29.0 −31.2	16.0 +17.8	5.3 −2.9	9.8 −14.8	5.4 +2.5	<5.9 +4.6	6.4 +5.9	7.8 −5.9	12.0 −9.6	8.5 +10.3	8.9 −9.1	<7.1 −0.6							
5	5.3 +8.4	17.0 −19.0	6.3 −10.9	24.0 −20.8	9.5 −12.0	4.5 −5.4	12.6 +10.5	7.7 +10.2	10.1 −9.7	<5.5 +2.5	<5.7 +1.7	<5.9 −7.4	6.0 +1.0	8.8 +10.2	7.8 +8.0	9.8 +6.3	8.0 −12.9	<7.2 +2.4	7.2 −6.1				
4	14.9 +12.0	5.4 −3.8	4.1 +5.8	3.9 +2.8	25.9 +25.0	37.0 −33.5	16.5 −17.8	4.7 +1.7	5.9 −10.4	4.8 +0.7	17.2 −16.3	11.2 +6.8	<5.8 −0.9	20.2 −19.9	<6.3 +2.2	17.4 −17.1	7.0 −11.1	<7.0 +4.2	<7.2 +2.9	<7.4 −3.7			
3	13.5 −15.9	19.1 +19.2	5.5 −3.3	3.7 +7.8	19.1 +19.0	35.0 +30.7	37.4 −35.5	21.6 −19.8	23.3 +18.3	<4.5 +2.0	7.9 −4.1	11.3 −9.5	13.1 −16.6	<5.8 +2.8	6.2 −3.2	<6.3 +0.8	7.7 +3.1	6.9 −5.7	14.8 +14.8	8.0 +7.8	11.9 −15.1		
2	14.2 +16.6	20.8 +22.3	7.8 −6.1	8.6 +7.3	8.9 +10.5	40.1 +43.5	30.0 +29.5	5.2 +4.1	<4.4 +5.4	9.0 −6.1	12.8 +10.4	12.5 −4.3	<5.4 −0.5	11.4 +9.5	<5.8 +5.8	13.4 +18.0	8.4 −10.1	6.8 −8.6	7.1 +0.2	<7.1 +0.7	<7.4 +3.4		
1	5.9 +7.3	15.0 −15.5	20.3 −16.6	9.2 +9.0	35.8 −36.2	35.7 −30.3	38.4 +43.0	17.8 +17.6	6.7 −3.3	4.3 +4.5	9.8 +10.0	27.4 +24.0	12.9 +17.1	5.4 −5.4	5.8 +8.4	<6.0 +2.4	<6.3 +0.4	<6.5 +2.3	12.0 −6.7	<7.1 +0.3	<7.3 +6.7	<7.5 −6.3	
0	28.4 +32.6	49.6 −55.9	11.8 +11.8	12.9 +10.0	78.5 +81.4	81.2 −78.0	80.0 −81.5	30.8 +35.3	29.7 +33.9	13.1 −13.0	<4.6 −0.9	20.9 +20.2	<5.2 +5.2	7.3 −10.9	<5.7 +5.6	9.1 −5.6	7.0 +1.2	8.9 +5.0	15.2 +17.8	<7.0 −0.7	8.0 −6.2	6.9 +4.6	
$\bar{1}$	— −6.6	25.8 +37.9	16.8 −17.5	43.6 −47.2	23.5 +23.5	30.5 +41.4	32.2 −33.3	25.8 −25.6	22.6 +20.6	<4.4 −3.3	25.4 −23.5	22.7 −20.8	<5.2 +6.6	12.7 −16.0	5.9 −4.9	5.6 +6.9	9.7 +11.8	18.4 −19.1	12.3 +11.8	8.6 +9.9	<7.3 −4.5	<7.6 −4.5	8.1 −1.4
$\bar{2}$	11.8 +4.6	27.6 −23.7	60.0 −59.1	47.5 +50.3	<3.4 +4.1	16.2 +14.4	21.8 +15.9	4.2 +1.3	<4.3 −1.3	24.7 −24.6	20.0 −27.2	8.7 −4.4	5.6 −2.7	15.0 +12.9	<5.8 −3.1	7.1 +7.6	<6.4 −7.1	6.0 +5.5	10.8 −13.1	7.0 +2.1	<7.3 +1.2	<7.6 +2.0	
$\bar{3}$	10.8 −3.6	24.4 +33.1	22.0 +18.3	<3.6 +3.9	20.8 +17.0	10.0 −6.8	9.3 −10.5	4.7 −3.4	10.5 +10.5	10.7 +13.4	11.8 +5.7	21.6 +22.6	13.4 +10.7	6.9 −6.7	19.1 −14.5	<6.2 +3.6	9.7 −8.7	<6.8 +1.2	13.0 −16.0	<7.2 +0.9	<7.4 −1.8		
$\bar{4}$	11.6 +6.9	22.2 −21.8	21.7 −24.8	<4.1 +2.0	8.0 +8.1	53.5 −55.5	45.0 −52.5	25.5 +31.0	22.0 +27.2	<5.1 −0.8	12.1 −12.9	<5.4 −1.3	<5.7 +0.7	<6.0 +0.7	8.7 −13.3	15.0 −13.6	<6.7 +4.0	6.0 +5.1	8.5 +7.3	9.5 −10.6	7.9 −7.5		
$\bar{5}$	7.9 +3.9	4.8 −6.5	30.8 −34.7	24.8 −29.2	17.9 +23.7	50.0 +62.2	21.2 −24.9	9.7 −13.2	7.4 +5.4	11.3 +12.7	24.8 −26.3	9.1 −8.7	5.5 +7.8	8.6 +8.4	5.9 +8.3	10.7 +9.5	<6.9 +1.5	7.5 −7.5	10.0 +10.7				
$\bar{6}$	7.8 −6.9	8.0 +10.6	17.5 +15.8	15.7 +16.8	<5.1 −0.2	<5.2 −0.9	20.9 +22.5	13.0 −15.6	<5.7 −3.3	<5.8 −1.7	5.8 +2.3	6.2 −3.9	6.3 +9.4	<6.6 +1.1	7.4 +5.3	7.0 −10.0	8.1 +10.1						
$\bar{7}$	<5.4 +6.7	9.8 +12.6	<5.5 +0.2	<5.5 +1.8	<5.6 +4.8	15.5 −16.3	<5.8 −5.1	<5.9 −2.0	11.0 +15.6	<6.2 −2.3	7.9 +10.5	<6.6 −6.8	<6.8 −4.2	<6.9 −1.9	<7.1 −2.1								
$\bar{8}$	7.6 +7.2	12.4 −13.6	6.2 −0.9	<6.0 −7.0	<6.1 +8.1	11.2 −6.6	9.9 −4.5	7.2 +7.1	6.8 +7.0	<6.7 −2.0	<6.8 +1.8	<7.0 −0.7	9.2 +8.1										
$\bar{9}$	<6.5 +4.2	7.0 −7.4	<6.5 −5.5	8.0 −6.0	<6.6 +6.4	14.6 +13.6	<6.7 −5.8	<6.9 −6.0	<7.0 −1.6	8.3 +6.2	8.7 −10.3												
$\overline{10}$									10.1 −8.2														

TABLE 7. Interatomic Distances in the Structure of Inderite

B_1-tetrahedron	
$B_1 — O_1^*$	1.50 A
$B_1 — O_2^*$	1.50 A
$B_1 — O_3$	1.50 A
$B_1 — O_4$	1.44 A
$O_1^* — O_2^*$	2.39 A
$O_1^* — O_3$	2.45 A
$O_1^* — O_4$	2.41 A
$O_2^* — O_3$	2.45 A
$O_2^* — O_4$	2.41 A
$O_3 — O_4$	2.43 A
B_2-tetrahedron	
$B_2 — O_4$	1.44 A
$B_2 — O_5^*$	1.44 A
$B_2 — O_6$	1.46 A
$B_2 — O_8^*$	1.55 A
$O_4 — O_5^*$	2.39 A
$O_4 — O_6$	2.42 A
$O_4 — O_8^*$	2.41 A
$O_5^* — O_6$	2.29 A
$O_5^* — O_8^*$	2.45 A
$O_6 — O_8^*$	2.46 A
B_3-triangle	
$B_3 — O_3$	1.37 A
$B_3 — O_6$	1.39 A
$B_3 — O_7^*$	1.35 A
$O_5 — O_7$	2.39 A
$O_3 — O_7^*$	2.40 A
$O_6 — O_7^*$	2.32 A
Mg-octahedron	
$Mg — O_2^*$	2.02 A
$Mg — O_8^*$	2.04 A
$Mg — O_9^{**}$	2.14 A
$Mg — O_{10}^{**}$	2.10 A
$Mg — O_{11}^{**}$	2.03 A
$Mg — O_{12}^{**}$	2.14 A
$O_2^* — O_8^*$	2.92 A
$O_2^* — O_9^{**}$	3.10 A
$O_2^* — O_{11}^{**}$	2.91 A
$O_2^* — O_{12}^{**}$	2.86 A
$O_8^* — O_9^{**}$	2.95 A
$O_8^* — O_{10}^{**}$	2.85 A
$O_8^* — O_{12}^{**}$	3.03 A
$O_9^{**} — O_{10}^{**}$	2.95 A
$O_9^{**} — O_{11}^{**}$	2.90 A
$O_{10}^{**} — O_{11}^{**}$	2.91 A
$O_{10}^{**} — O_{12}^{**}$	2.97 A
$O_{11}^{**} — O_{12}^{**}$	2.93 A

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* Atom O in the OH group.

** Atom O in the H_2O molecule.

TABLE 8. The Shortest Distances between Oxygen Atoms Which Do Not Coincide with the Edges of Coordinational Polyhedra. For O–O Taken for Lengths of Hydrogen Bonds, $OH(H_2O)$ – Proton Donors – Are Indicated

O – O vector	Length of O – O vector in A	$OH(H_2O)$ - proton donors
$O_4 — O_{13}^{**}$	2.62	O_{13}^{**}
$O_7^* — O_8^*$	2.65	O_7^* or O_8^*
$O_7^* — O_8^{\prime\prime\prime *}$	2.70	O_8^* or O_7^*
$O_1^* — O_{10}^{\prime\prime **}$	2.71	$O_{10}^{\prime\prime **}$
$O_{11}^{**} — O_{13}^{\prime\prime **}$	2.71	O_{11}^{**}
$O_2^* — O_5^{\prime *}$	2.74	$O_5^{\prime *}$ or O_2^*
$O_6^{\prime\prime\prime} — O_9^{**}$	2.75	O_9^{**}
$O_1^* — O_9^{\prime\prime **}$	2.85	$O_9^{\prime\prime **}$
$O_1^* — O_{13}^{\prime\prime\prime **}$	2.87	O_1^*
$O_4 — O_{11}^{\prime **}$	2.90	$O_{11}^{\prime **}$
$O_3 — O_{12}^*$	2.92	O_{12}^{**}
$O_5^{\prime\prime\prime *} — O_{10}^{**}$	2.92	O_{10}^{**} or $O_5^{\prime\prime\prime *}$
$O_3 — O_{13}^{**}$	3.00	O_{13}^{**}
$O_5^* — O_7^*$	3.17	
$O_2^* — O_9^{\prime\prime **}$	3.18	
$O_{10}^{**} — O_{12}^{\prime\prime **}$	3.21	
$O_7^* — O_{10}^{\prime\prime\prime **}$	3.23	
$O_5^{\prime *} — O_{11}^{**}$	3.28	
$O_5^* — O_{13}^{**}$	3.31	

* Atom O in the OH group.

** Atom O in a molecule of water.

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All abbreviations of periodicals in the above bibliography are letter-by-letter transliterations of the abbreviations as given in the original Russian journal. ***Some or all of this periodical literature may well be available in English translation.*** **A complete list of the cover-to-cover English translations appears at the back of this issue.**