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The Crystal Structure of the Isomorphous Orthoborates of Cobalt and Magnesium

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Crystals of orthoborates of cobalt and magnesium have been described by Ebelmen [1], Mallard [2], le Chatelier [3], Ouvrard [4], Guertler [5] and Hofmann-Höschele [6] among others. They are reported to be isomorphous and orthorhombic with a rather perfect cleavage parallel to (110). Those of $Mg_3(BO_3)_2$ are further described to have the axial ratios 0.641 : 1 : 0.549 and to be insoluble in dilute acetic acid.

The crystals used in the present investigation were prepared by melting together in a ZrO_2-crucible 3CoO (3MgO) with 1 B_2O_3. They form thin needles parallel to the axis, which was chosen as *c*-axis. By means of crystals picked out, the crystallographic information given above could be confirmed. Of each substance one needle, suitable for taking single crystal photographs, was examined by the rotation and Weissenberg methods, and the ground crystals by the powder method. Mo-K-radiation was used for the single crystal and Cr-K-radiation for the powder exposures. The parameters of the atoms were determined by Fourier-methods [7].

THE UNIT CELL AND THE SPACE GROUP

The Laue-symmetry is D_{2h}-*mmm*. Rotation and Weissenberg photographs were taken about the *b* and *c* (needle) directions. In the first case only the 0-layer line was registered. By rotation around the needle axis, layer lines with $l = 0 - 6$ were obtained. The dimensions of the unit cell were determined by means of powder photographs from a focusing camera. A list of the observed diffraction lines is given in the Table 1.

Table 1. Powder diffraction data for the orthorhombic borates of cobalt and magnesium.

	$Co_3(BO_3)_2$			$Mg_3(BO_3)_2$		
hkl	Int.	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$	Int.	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$
020 α	w —	0.0719	0.0736	w	0.0731	0.0740
011 α	w —	.0803	.0823	w —	.0817	.0829
101 α	w	.1076	.1078	s	.1088	.1097
111 α	vw	.1255	.1263	m	.1273	.1283
121 α	s	.1814	.1815	vs	.1839	.1838
130 α	m	.2094	.2096	m	.2113	.2114
031 α	w	.2299	.2296	m —	.2296	.2310
201 α	m	.2402	.2397	s	.2454	.2449
220 α	w +	.2498	.2495	m —	.2544	.2540
211 α	s	.2588	.2581	vs	.2633	.2633
131 α	m	.2739	.2736	vs	.2762	.2762
102 α	w +	.2999	.2995	m —	.3039	.3041
221 α	w —	.3139	.3133	w —	.3191	.3189
112 α	w —	.3189	.3181	w —	.3228	.3225
022 α	w —	.3298	.3292	w —	.3328	.3330
141 α	w	.4024	.4024	w	.4059	.4058
231 α	w	.4056	.4053	vw	.4112	.4112
202 α	s	.4317	.4311	vs	.4389	.4390
132 α	s	.4656	.4654	vs	.4710	.4707
311 α	vw	.4776	.4775	w —	.4884	.4881
150 α	w —	.5044	.5042	w —	.5075	.5075
051 α_1	m	.5248	.5242	w +	.5270	.5272
α_2	vw	.5264	.5260	vw	.5286	.5289
321 α_1	s	.5330	.5330	m	.5436	.5436
α_2	w	.5347	.5345	w	.5451	.5454
042 α_1	w —	.5500	.5500	w	.5549	.5550
α_2				vw	.5562	.5567
330 α_1	s	.5608	.5608	vs	.5713	.5713
α_2	m	.5627	.5626	m +	.5733	.5732
013 α_1	m —	.5935	.5932	m	.6002	.6009
α_2	w —	.5955	.5952	w	.6024	.6028
331 α_1	vw	.6248	.6248	w —	.6362	.6360
α_2				vw	.6386	.6382
302 α_1	w	.6510	.6508	vw	.6636	.6638
060 α_1	m —	.6622	.6622	m	.6661	.6660
α_2	w	.6645	.6647	w	.6684	.6683
123 α_1	s	.6922	.6923	s —	.7012	.7019
α_2	m	.6946	.6948	m —	.7035	.7039
251 α_1	s	.6996	.6999	s	.7070	.7070
α_2	m	.7024	.7023	m	.7096	.7094
400 α_1	m —	.7024	.7025	m	.7196	.7193
α_2	w +	.7050	.7051	w	.7220	.7220

		$Co_3(BO_3)_2$			$Mg_3(BO_3)_2$	
hkl	Int.	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$	Int.	$\sin^2\Theta_{obs}$	$\sin^2\Theta_{calc}$
033 α_1	w	0.7400	0.7403	w	0.7492	0.7498
α_2	vw	.7435	.7432	vw	.7520	.7521
203 α_1				w —	.7619	.7627
α_2				vw	.7655	.7656
401 α_1	w +	.7674	.7665	m	.7846	.7846
α_2	vw	.7700	.7692	w	.7869	.7870
420 α_1				m	.7935	.7937
α_2				w	.7958	.7961
411 α_1	m	.7850	.7848	m	.8032	.8031
α_2	w	.7857	.7878	w	.8060	.8059
332 α_1	m	.8161	.8162	w +	.8300	.8302
α_2	w	.8189	.8190	vw	.8330	.8332
260 α_1	w —	.8380	.8382	vw	.8465	.8461
421 α_1				vw	.8578	.8580
350 α_1				vw	.8647	.8648
261 α_1	w —	.9041	.9021	vw	.9104	.9104
143 α_1	w —	.9131	.9133	w	.9238	.9241
α_2				vw	.9274	.9272
233 α_1	vw	.9157	.9159	vw	.9288	.9291
062 α_1	w +	.9178	.9180			
α_2	vw	.9208	.9210			
431 α_1	m —	.9319	.9322			
α_2	w —	.9352	.9356			
170 α_1				vw	.9513	.9512
402 α_1	m	.9580	.9582	w	.9781	.9784
α_2	w —	.9615	.9618	vw	.9815	.9819

vs = very strong, s = strong, m = medium, w = weak and vw = very weak.

Measurements in the reflection region of the highest $\sin^2\Theta$ led to the following axial lengths (referred to wave lengths of Cr-Kα_1 = 2.28962 Å and Cr-Kα_2 = 2.29352 Å)

	$Co_3(BO_3)_2$	$Mg_3(BO_3)_2$
a	5.462 ± 0.002 Å	5.398 ± 0.002 Å
b	8.436 ± 0.002	8.416 ± 0.002
c	4.529 ± 0.002	4.497 ± 0.002

The values given above correspond to the axial ratios — values for the Mg-compound within parentheses — 0.648 : 1 : 0.537 (0.642 : 1 : 0.535). The unit

cell containing 2 $Me_3(BO_3)_2$ has the volume 208.7 (204.3) Å^3, and the calculated density is 4.69 (3.10) g · cm^{-3}. The observed densities are 4.66 (3.04) g · cm^{-3}.

The observed powder and Weissenberg reflections correspond to a simple orthorhombic translation lattice since general planes *hkl* show no regular absences. However, planes *hk*0 and 0*kl* reflect only if $h + k$ and $k + l$ are even. These conditions, and the fact that no piezoelectric effect could be detected, led to D_{2h}^{12} - *Pnmn* as the most probable space group.

INTENSITY MEASUREMENTS

For Mo-K-radiation the observed intensities are based on the relation $I_\beta : I_{\alpha 2} : I_{\alpha 1} = 1 : 2 : 4$ for a given reflection and the relative $|F|$-values are determined according to

$$I = C \cdot \lambda^3 \cdot \frac{1 + \cos^2 2\Theta}{\cos^2 \mu \cdot \sin v} \cdot |F|^2$$

where μ = the angle between the primary beam and the equatorial plane, and

v = the azimute of the reflection from the plane through the primary beam and the rotation axis.

In the present case, where crystals containing light atoms were exposed with Mo-K-radiation, no corrections for absorption are performed. The graphs given by Lu [8] for the inversed value of $\frac{1 + \cos^2 2\Theta}{\cos^2 \mu \cdot \sin v}$ have been used.

The Weissenberg photographs were taken with the equi-inclination method. The connection between intensities of reflections from different layer lines was obtained by changing rotation axis and by Weissenberg oscillation photographs [9].

PATTERSON-HARKER-ANALYSIS

There are about 250 reflections available for the structure determination. By means of the $|F|^2$-values from the reflections *hk*0 and 0*kl* the Patterson-projections $p(xy)$ and $p(yz)$ were calculated. In the case of $Mg_3(BO_3)_2$ the result of these calculations is given in the Figs. 1 and 2.

On account of the symmetry elements existing in the space group D_{2h}^{12}-*Pnmn* it is advisable to develop the function $p(xyz)$ in the cuts $P(xy0)$ and $P(xy\,\frac{1}{2})$ to get the sites of the different kind of atoms. In the Figs. 3 and 4 these sections are reproduced in the case of $Mg_3(BO_3)_2$.

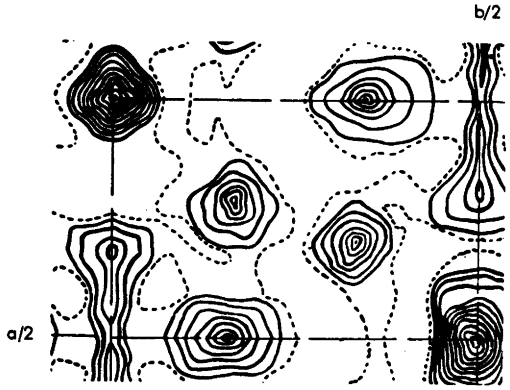

Fig. 1. Projection of the Patterson-function of $Mg_3(BO_3)_2$ on the ab-plane, p(xy). The dotted line corresponds to the 0-level.

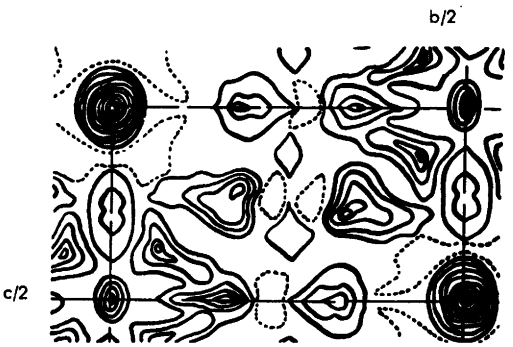

Fig. 2. Projection of the Patterson-function of $Mg_3(BO_3)_2$ on the bc-plane, p(yz).

By combining the different vectors found in the above projections and cuts the atomic arrangement given below will be the only one possible from space reasons. The (4g)-position of the boron-ions is based on the fact that it permits the placing of the boron ions in the centres of gravity of the nearly equilateral triangles formed by the oxygen ions. As will be shown below the dimensions of these triangles are nearly the same as the dimensions of $(BO)_3^{3-}$-triangles, which have been determined in other borates. The denomination is in accordance with the International tables for the determination of crystal structure, Berlin (1935).

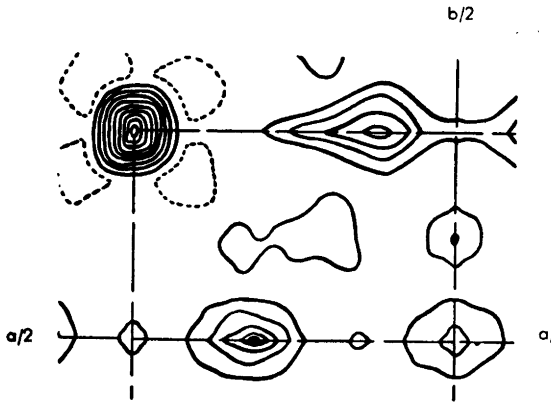

Fig. 3. The Harker-section P(xy0) of $Mg_3(BO_3)_2$.

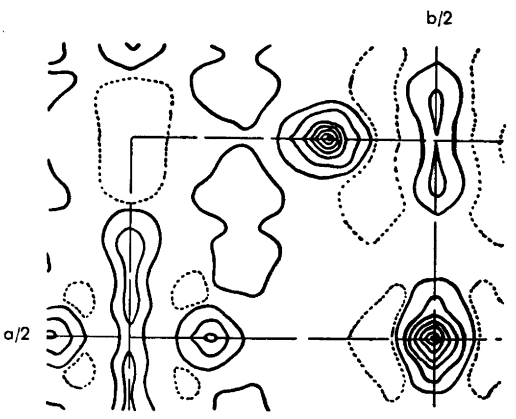

Fig. 4. The Harker-section P(xy1/2) of $Mg_3(BO_3)_2$.

2 Me^{2+} in (2a) = MeI
4 Me^{2+} » (4f) = MeII
4 B^{3+} » (4g) = B
4 O^{2-} » (4g) = OI
8 O^{2-} » (8h) = OII

The result of the above calculations are registered in Table 2 pointing out the different maxima arising from the reported vectors. The relative heights of the peaks are assigned to a common scale based on the calculated heights of the maxima in the origin. The coordinates given are not differentiated for the two compounds because of the nearly equal values found. Reference is also made to Fig. 5.

Table 2. The interatomic vectors of the function p(xyz).

Coordinates			Relative heights		Interatomic vectors
a/60	b/60	c/60	$Co_3(BO_3)_2$	$Mg_3(BO_3)_2$	
0	0	0	4 966	1 816	6 Me — Me 12 O — O 4 B — B
18	0	14	1 250	593	4 MeI — OI 8 MeII — OII 4 MeI — B 2 OI — OI 4 OII — OII 4 OI —B
12	10	14	1 386	655	4 MeI — OII 4 MeII — OI 4 MeII — OII 4 MeII — B 4 OI — OII 2 OII — OII 4 OII — B
30	10	0	3 420	1 042	4 MeI — MeII 2 MeII — MeII 8 OI — OII 4 OII — OII 8 OII — B

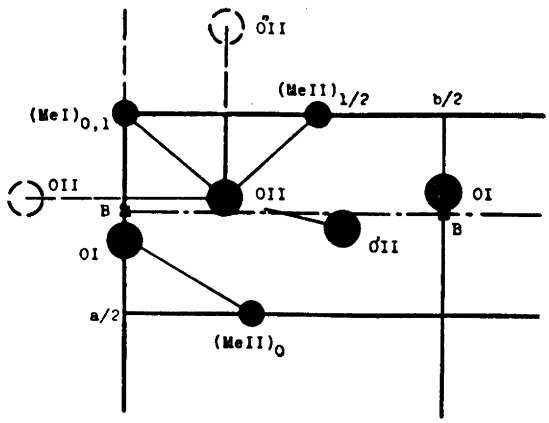

Fig. 5. Projection of the structure parallel to (001). The subscripts correspond to the z-coordinates.

The coordinates of the maxima given in Table 2 lead to the following approximate parameters.

MeII		$y = 0.327$	
OI	$x = 0.317$		$z = 0.273$
OII	$x = 0.202$	$y = 0.139$	$z = 0.702$

Thereby the parameter of the metal-ions is obtained from $Co_3(BO_3)_2$ and the oxygen-parameters from $Mg_3(BO_3)_2$. By means of these parameters the signs necessary for calculating the electron density function are known.

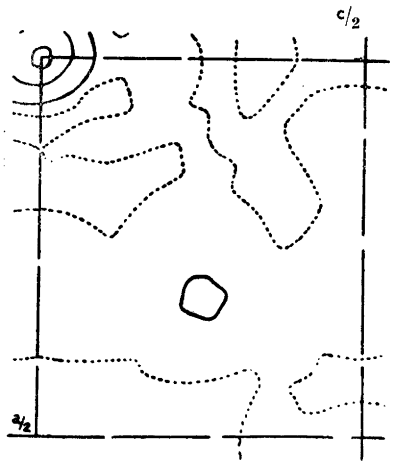

Fig. 6. The section ϱ (x0z) of the electron density of $Mg_3(BO_3)_2$. The height difference = 100. The dotted line = 0-level.

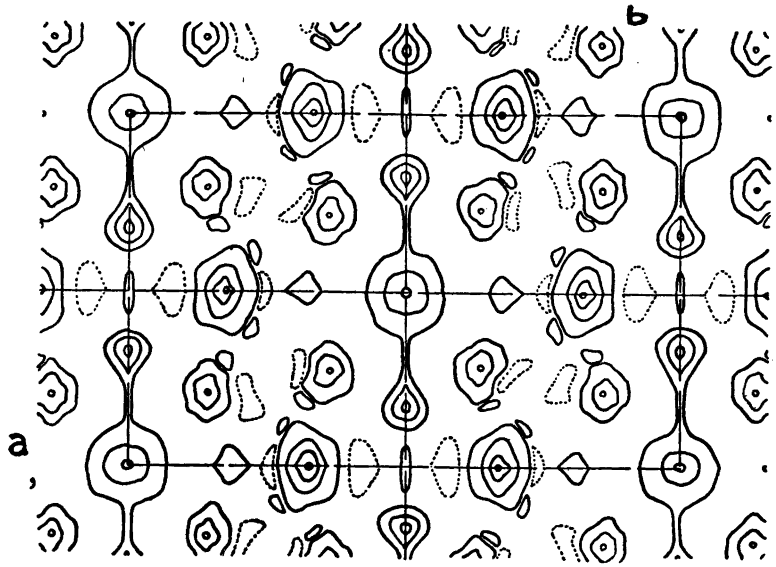

Fig. 7. $Mg_3(BO_3)_2$. *Projection of the electron density parallel to [001].*
The height-difference = 10.
The dotted line = −10-level.

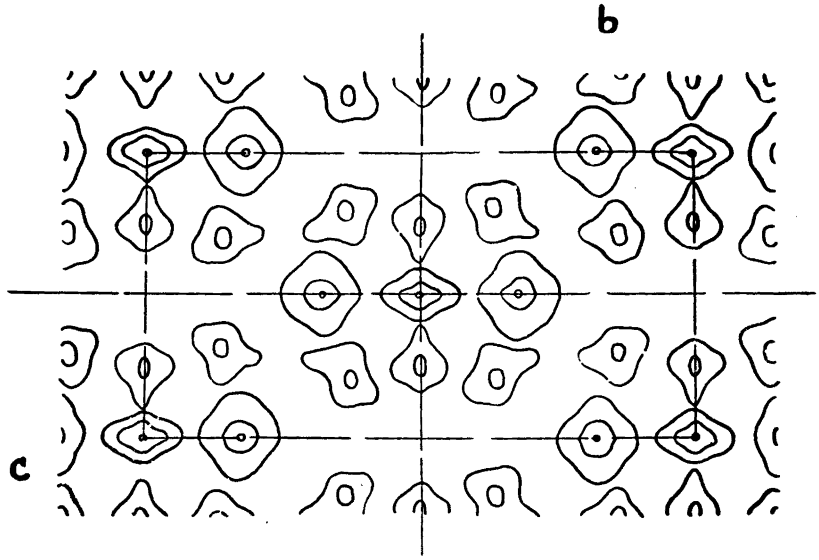

Fig. 8. $Mg_3(BO_3)_2$. *Projection of the electron density parallel to [100].*

DETERMINATION OF THE FINAL PARAMETERS

The practically equal coordinate values for the Patterson maxima of $Co_3(BO_3)_2$ and $Mg_3(BO_3)_2$ respectively, together with the fact that the ionic radii of Co^{2+} and Mg^{2+} are nearly the same — which is also evident from the close agreement between unit dimensions and axial ratios of the two compounds — makes it highly probable that the parameter values of the two cells are nearly equal. Thus, the approximate parameter values, derived from the Patterson syntheses, have been used for determining the signs of the F-values in calculating the electron density. For both compounds the electron density was calculated in the section ϱ $(x0z)$ and the projections ϱ (xy) and ϱ (yz). The results are shown for $Mg_3(BO_3)_2$ in the Figs. 6—8. The final parameter values are given below and proved to be identical for the two compounds. The boron values have been calculated on the asumption that the boron ions occupy the centres of gravity of the practically equilateral oxygen triangles.

The structure of $Co_3(BO_3)_2$ and $Mg_3(BO_3)_2$ in D_{2h}^{12} - *Pnmn* will then be characterized by the positions

2 Me^{2+} in (2a) = MeI				
4 Me^{2+} in (4f) = MeII		$y = 0.321$		
4 B^{3+} in (4g) = B	$x = 0.25$		$z = 0.56$	
4 O^{2-} in (4g) = OI	$x = 0.316$		$z = 0.258$	
8 O^{2-} in (8h) = OII	$x = 0.218$	$y = 0.139$	$z = 0.705$	

DISCUSSION OF THE STRUCTURE

The structure in question is projected in the Figures 9 and 10.

$(BO_3)^{3-}$-*triangle*. The most characteristic feature of the atomic arrangement is formed by the rather equilateral $(BO_3)^{3-}$-triangles, with their very short co-planar bonds found to be

	$Co_3(BO_3)_2$	$Mg_3(BO_3)_2$
OI — OII	2.399 Å	2.383 Å
OII — OII	2.346	2.339
B — OI	1.44	1.42
B — OII	1.35	1.34

Analogous distances within $(BO_3)^{3-}$-triangles have been proved by

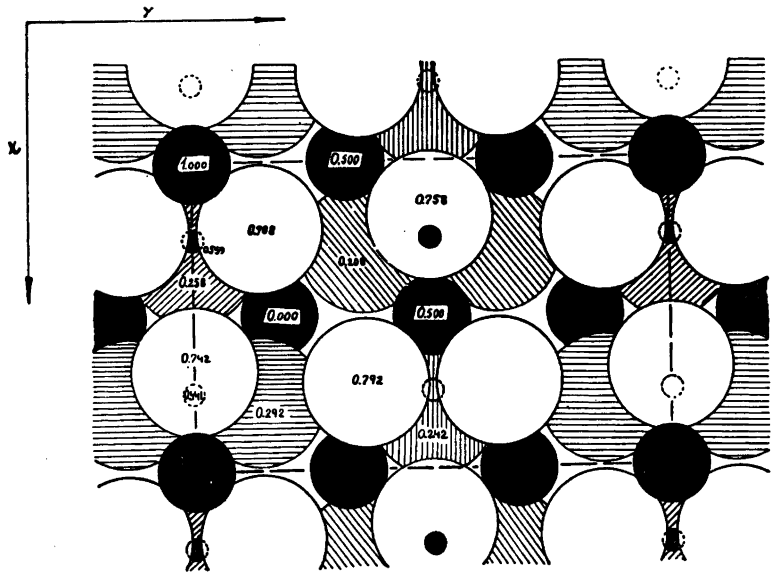

Fig. 9. Projection of the structure parallel to [001].

The large black spheres represent the metal-ions,
» small » » » » boron- »
» large white » » » oxygen- »

***Equal** heights over the planes in question are similarely marked, and the heights over the base-plane are given by numbers within the spheres in the cell.*

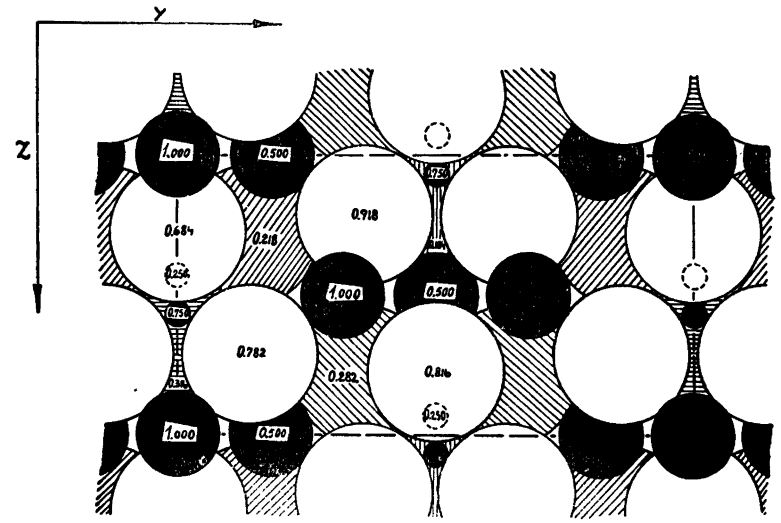

Fig. 10. Projection of the structure parallel to [100].

Author	Substance	Oxygen-oxygen-distances	Boron-oxygen-distances
Zachariasen [11]	Hambergite	2.31—2.35—2.39 Å	1.42—1.35—1.28 Å
Zachariasen and Ziegler [12]	CaB_2O_4	2.35—2.36—2.37	1.38—1.37—1.34
Fang [13]	NaB_2O_4	2.32—2.37	1.34—1.38

Wells [14] reports the boron-oxygen distance within the triangles to be 1.35 Å.

As will be seen from the projection of the structure on the *ab*-plane — Fig. 9 — the oxygen-ions form layers including the $(BO_3)^{3-}$-triangles, with the boron-ions situated in the *n*-planes at right angles to the *x*-axis.

$(MeO_6)^{10-}$-*octahedron*. Moreover, it is obvious from the Figs. 9 and 10 that the metal-ions connecting the layers have the coordination number six. Within the octahedrons formed, the following interionic distances are found

		$Co_3(BO_3)_2$	$Mg_3(BO_3)_2$
$(MeI)_1$	— OII	2.141 Å	2.108 Å
$(MeI)_0$	— OI	2.086	2.063
$(MeII)_0$	— OI	2.157	2.146
$(MeII)_{1/2}$	— OII	2.152	2.164

The remaining interionic distances in the structure are

OII	— O'II	2.958 Å	2.945 Å
OII	— O''II	3.020	2.988

These distances show that the binding within the $(BO_3)^{3-}$-triangles undoubtedly are much stronger than the other bonds. There is, in other words direct evidence for the existance of $(BO_3)^{3-}$-groups in the structure. Accordingly the chemical formula of the compounds under investigation must be written as $Me_3(BO_3)_2$.

By using the above parameters and atomic scattering factors according to the *International tables for the determination of crystal structure* (Berlin, 1935), the following agreement between calculated and observed F-values was obtained:

0k0-reflections

	$Co_3(BO_3)_2$		$Mg_3(BO_3)_2$	
hkl	$\|F\|_{obs}$	$F_{calc.}$	$\|F\|_{obs}$	$F_{calc.}$
020	15.8	10.1	23.0	13.9
040	10.1	2.5	5.5	— 7.6
060	110.0	108.7	59.5	61.7
080	—	2.0	18.8	13.8
0 10 0	20.3	28.8	12.6	7.8
0 12 0	16.3	39.2	10.9	14.3
0 14 0	—	0.6	6.1	11.8
0 16 0	15.9	40.7	9.1	17.0
		hk0-reflections		
110	—	1.7	—	— 1.5
130	114.7	98.3	36.7	34.0
150	34.8	— 27.4	20.1	— 16.1
170	33.9	28.0	16.2	11.8
190	42.2	54.8	16.8	18.9
1 11 0	12.7	— 24.3	7.3	— 11.8
1 13 0	20.2	30.8	1.9	8.8
200	62.8	62.6	16.5	— 6.6
220	28.5	— 17.4	20.1	— 11.4
240	42.3	35.4	24.0	23.8
260	53.3	62.0	10.5	21.7
280	40.5	— 36.7	31.1	— 24.8
2 10 0	38.8	35.7	14.7	16.3
2 12 0	32.2	41.5	2.9	15.4
2 14 0	8.1	— 28.9	10.1	— 18.7
310	—	7.9	—	— 5.5
330	115.2	121.4	64.1	64.1
350	6.2	— 1.4	9.2	7.4
370	33.1	23.6	12.6	8.5
390	52.8	59.8	26.3	26.6
3 11 0	5.1	— 4.1	2.7	7.2
3 13 0	21.2	34.4	6.8	12.7
400	104.8	103.1	54.9	52.7
420	10.1	— 11.5	—	— 6.8
440	1.0	1.7	5.5	— 7.3
460	65.1	70.7	35.7	30.0
480	8.4	— 10.5	—	0.8
4 10 0	13.0	20.6	—	1.8

	$Co_3(BO_3)_2$		$Mg_3(BO_3)_2$	
hkl	$\|F\|_{obs}$	$F_{calc.}$	$\|F\|_{obs}$	$F_{calc.}$
510	—	5.9	—	3.3
530	47.7	52.7	vw	8.1
550	10.9	− 24.7	19.4	− 16.0
570	26.6	27.2	17.0	13.2
590	31.7	41.9	vw	9.7
5 11 0	12.0	− 31.0	16.9	− 20.2
600	56.1	69.3	35.4	25.5
620	—	− 0.4	—	4.8
640	16.3	25.8	4.1	14.8
660	48.5	58.4	25.2	21.7
710	—	− 5.0	—	− 5.9
730	61.0	69.5	32.1	31.9
750	—	− 5.1	—	2.3
770	7.2	7.1	vw	− 4.6
800	37.2	46.3	9.2	11.8
820	vw	− 10.4	vw	− 7.5
840	8.3	14.4	—	− 2.4
860	33.8	39.3	—	2.6
910	vw	13.3	3.3	11.2
930	31.8	40.5	2.7	7.2
950	11.2	− 9.0	—	− 3.2
10 00	22.1	51.1	14.2	20.8
		0kl-reflections		
002	44.8	59.4	vw	− 5.4
004	78.4	97.2	42.5	51.0
006	40.8	52.6	5.7	13.9
008	35.3	44.4	vw	12.9
022	28.0	− 21.6	16.5	− 16.3
024	—	3.7	2.9	7.7
026	vw	− 10.6	5.8	− 7.3
031	34.6	− 28.9	17.4	− 7.8
033	55.0	− 40.7	33.0	− 24.5
035	12.6	− 10.1	—	2.9

0kl-reflections

	$Co_3(BO_3)_2$		$Mg_3(BO_3)_2$	
hkl	$\|F\|_{obs}$	$F_{calc.}$	$\|F\|_{obs}$	$F_{calc.}$
042	49.4	27.7	25.9	16.7
044	23.0	14.3	18.8	5.6
046	vw	7.0	4.6	− 0.3
051	76.3	85.3	38.0	38.1
053	61.5	64.5	26.6	24.8
055	51.5	55.4	19.4	21.4
062	53.4	57.6	13.7	12.8
064	64.5	72.6	35.2	34.0
066	22.3	42.9	10.1	9.9
071	15.9	20.0	—	5.1
073	24.1	34.9	10.3	21.1
075	—	4.1	vw	− 4.9
082	39.3	− 37.5	26.6	− 26.0
084	vw	− 4.3	—	6.2
091	10.9	− 12.6	vw	− 5.1
0 10 2	38.3	32.7	19.2	13.2
0 10 4	21.5	27.7	5.2	9.9
0 11 1	31.3	60.4	10.1	23.1

h0l-reflections

101	38.5	− 44.7	17.1	− 21.0
102	26.5	− 17.1	16.8	− 17.1
103	26.5	− 28.1	9.4	− 10.6
104	—	13.9	9.4	13.9
105	8.7	− 24.4	5.5	− 10.5
201	28.0	32.9	39.9	32.9
202	112.0	136.7	65.9	70.0
203	19.4	− 14.6	21.6	− 14.6
204	56.2	65.2	25.3	20.6
205	—	6.6	5.5	6.6
206	26.4	60.5	25.8	23.0

	$Co_3(BO_3)_2$		$Mg_3(BO_3)_2$	
hkl	$\|F\|_{obs}$	$F_{cala.}$	$\|F\|_{obs}$	$F_{calc.}$
301	27.2	− 30.0	13.3	− 18.0
302	vw	9.7	12.2	9.7
303	38.1	− 33.2	27.8	− 17.4
304	—	− 11.0	vw	− 11.0
305	vw	− 14.4	—	− 1.2
306	—	9.6	12.5	9.6
401	27.5	− 26.4	35.5	− 26.4
402	59.2	70.3	27.4	22.3
403	19.8	16.7	14.6	16.7
404	62.1	69.7	33.7	28.3
405	—	− 8.6	—	− 8.6
406	30.1	52.2	26.2	16.8
501	22.5	− 24.8	19.5	− 9.5
502	—	− 4.8	—	− 4.8
503	vw	− 14.1	—	− 0.3
504	—	7.0	vw	7.0
505	12.7	− 27.0	14.3	− 14.8
601	10.9	18.5	25.1	18.5
602	51.0	55.3	8.3	13.9
603	—	− 13.1	5.1	− 13.1
604	50.1	57.8	21.4	20.6
701	vw	− 16.4	—	− 3.4
702	—	1.1	—	1.1
801	—	− 10.5	3.4	− 10.5
802	50.7	57.3	22.9	22.2

SUMMARY

The crystal structure of the isomorphous orthoborates of cobalt and magnesium is found to be orthorhombic with $2Me_3(BO_3)_2$ in the unit cell. The dimensions of the orthorhombic unit are determined. From the interatomic bond lengths found, it is clear that the most characteristic part of the structure is the nearly equilateral $(BO_3)^{3-}$-triangles and that in consequence of this the formula must be written as $Me_3(BO_3)_2$. The oxygen lattice forms layers parallell to [100] including the triangles and connected by the metal ions with coordination number six. The parameters have been determined by means of Fourier-methods.

The present study was carried out at the Institute of Inorganic Chemistry of the University of Uppsala. To the Head of this Institute Professor G. Hägg, who has not only suggested the problem but even stimulated the interest by many discussions and helpful criticism, I wish to express my sincere gratitude.

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After having finished the present study a copy of a japanese paper by R. Sadanaga[15] 'The crystal structure of Kotoite, $Mg_3B_2O_6$' — up to this day not yet reported in literature — has been received in this Institute.

This structure determination which is based on the asumption of a structural analogy between Mg_2SiO_4 and $Mg_3B_2O_6$ and performed by means of trial and error methods, has resulted in a structure, which is practically identical with the above. The parameter values show slight differences but the present author is of the opinion that his values, derived by Fourier-methods, give a slightly better agreement between observed and calculated intensities. It is also worth mentioning that the dimensions of the $(BO_3)^{3-}$-triangles obtained with Sadanaga's values do not agree very well with those reported by earlier authors.

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