

The Crystalline Structure of Hambergite, $Be_2BO_3(OH)$.

By

W. H. Zachariasen (Chicago).

(With 5 figures.)

1. Introduction.

The mineral Hambergite was first described by W. C. Brøgger¹⁾ in his monography of the minerals from the nephelite-syenitic pegmatite veins of the Langesundsfjord in Southern Norway. Later on Hambergite has been found in various localities in Madagascar.

Chemical analysis of the mineral lead definitely to the formula $Be_2BO_3(OH)$. The water leaves on strong ignition only, so we must assume it to be present as hydroxyl.

The crystal symmetry is orthorhombic holohedral. According to Brøgger the axial ratio is:

$$a : b : c = 0.7988 : 4 : 0.7268 .$$

There is a perfect cleavage parallel to the b -face and an almost as good one parallel to the a -face. The density is 2.34 and the hardness is $7\frac{1}{2}$. The crystals are optically positive with strong birefringence:

$$\alpha = 4.5595; \beta = 4.5908; \gamma = 4.6344. \quad Ax. \text{ pl. } \parallel b. \quad Bx. \perp c.$$

2. Dimensions and Space Group.

I have worked with the Laue, the oscillation and the ionisation methods. The unit cell has the following dimensions:

$$a = 9.73 \pm 0.04 \text{ \AA}; \quad b = 12.18 \pm 0.02 \text{ \AA}; \quad c = 4.42 \pm 0.04 \text{ \AA}$$

corresponding to $0.7988 : 4 : 0.3629$ ($\frac{1}{2} \times 0,7258$).

There are 8 molecules in this cell. The calculated density is 2.36.

The following reflexions were absent: $h k 0$ if h odd, $h 0 l$ if l odd, $0 k l$ if k odd. Hence the correct space group is $V_h^{15 2}$. The positions of V_h^{15} are:

$$4a. (0 0 0) \left(\frac{1}{2} \frac{1}{2} 0\right) \left(0 \frac{1}{2} \frac{1}{2}\right) \left(\frac{1}{2} 0 \frac{1}{2}\right). \quad 4b. \left(\frac{1}{2} \frac{1}{2} \frac{1}{2}\right) \left(0 0 \frac{1}{2}\right) \left(\frac{1}{2} 0 0\right) \left(0 \frac{1}{2} 0\right). \\ 8c. \pm (x y z) \left(x + \frac{1}{2}, \frac{1}{2} - y, \bar{z}\right) (\bar{x}, y + \frac{1}{2}, \frac{1}{2} - z) \left(\frac{1}{2} - x, \bar{y}, z + \frac{1}{2}\right).$$

1) Z. Krist. **16**, 4890. 2) The possibility that the absent reflexions might be explained by the special positions of the space groups V_h^1 , V_h^5 and V_h^{11} was considered, but had to be rejected.

The symmetry elements of the space group are shown in fig. 4. There are two sets of centres of symmetry, $4a$ and $4b$. There are three sets of glide planes:

$$\begin{array}{l} \text{Gl. pl. } 0 \frac{1}{4} 0 \ 0 \frac{3}{4} 0 \text{ with translation } c/2 \\ \text{Gl. pl. } \frac{1}{4} 0 0 \ \frac{3}{4} 0 0 \text{ " " " } b/2 \\ \text{Gl. pl. } 0 0 \frac{1}{4} \ 0 0 \frac{3}{4} \text{ " " " } a/2 \end{array}$$

Digonal screw axes parallel to the c -axis pass through the points: $\frac{1}{4} 0 0$, $\frac{3}{4} 0 0$, $\frac{1}{4} \frac{1}{2} 0$, $\frac{3}{4} \frac{1}{2} 0 1$.

We cannot expect any atoms to lie in centres of symmetry, as the distance between two atoms then would be 2.21 \AA , which is very small. All atoms are therefore lying in general positions, involving in the whole 24 parameters.

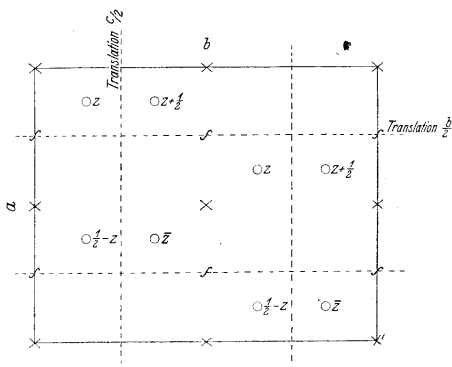


Fig. 4. Projection of the unit cell on (001) with some of the symmetry elements of the space group V_h^{15} . The small circles show the distribution of atoms in general positions.

3. The Deduction of an Ideal Structure for Hambergite.

The determination of a structure with 24 parameters is possible in many cases without great difficulties. In the present case, however, it does not seem to be easy to find a promising way of attacking the structure. Because of the following circumstances the usual ways of attack look hopeless. These complicating circumstances are:

1. All atoms lie in general positions.
2. The space group of Hambergite has neither reflexion planes nor twofold rotation axes.

1) Similarly there are digonal screw axes parallel to the a - and b -axes.

3. The reflexions from the pinacoids are relatively very weak, showing that none of the reflexions $h00$, $0k0$, $00l$ are normal (nor approximately normal) for comparatively low orders.
4. For reflexions occurring at large glancing angles we cannot leave the oxygen influence out of consideration as compared with the cations, nor can we for reflexions at small glancing angles neglect the cation contribution to the intensity of reflexion.

The only method of attacking the structure which I found possible is the following:

On the basis of our experience from other crystal structures we start building up an ideal structure, which is in accordance with the most important empirical rules of crystal structures. Then this ideal structure has to be tested by means of the observed intensities.

Using this method we have to be very careful with the assumptions we make, we must have an intuitive sense in choosing correct assumptions, as otherwise we will never arrive at a correct solution of our problem.

We can assume that Be is surrounded by 4 oxygens in a tetrahedron (we will not make any distinction between O and OH), the distance being of the order $O-O = 2.7 \text{ \AA}$, $Be-O = 1.7-1.8 \text{ \AA}$.

Boron we assume to be surrounded either by 4 oxygens in a tetrahedron as B^{+3} is smaller and also more highly charged than Be^{+2} , or by 3 oxygens in a triangle (the dimensions of this BO_3 -group being somewhat larger than those in the CO_3 -group as B^{+3} is larger and carries a smaller charge than C^{+4}).

In the Danburite¹⁾, $CaB_2Si_2O_8$, we have an example of a BO_4 -tetrahedron, while the rare mineral Nordenskjöldine $CaSn(BO_3)_2$, being isomorphous with Dolomite, shows BO_3 -groups quite analogous to the CO_3 - and NO_3 -groups²⁾.

Beforehand we cannot tell which of the coordination numbers 3 and 4 boron has in Hambergite, we have only to bear in mind that it must be either of these two numbers.

The only kind of anion polyhedra which might be present in the structure are thus tetrahedra and triangles. As the cation-cation distance tends to be as large as possible, the polyhedra will share only corners with each other. If they shared edges it would mean a cation-cation distance of less than 2.0 \AA which must be considered as highly improbable.

1) Compare: W. L. Bragg, *Z. Krist.* **14**, 264, 1930. 2) Deduced from comparison of crystallographical and optical properties of Nordenskjöldine and Dolomite.

There are only 8 boron atoms in the unit cell. Because of their small number compared with the beryllium atoms and because of their high charge we can assume the borons to be distributed in the lattice so that they come far apart from each other. This means that boron polyhedra will not be able to share corners with each other, only with the BeO_4 -tetrahedra.

Fig. 2 represents a projection of the unit cell on the c -face. The line A shows the glide plane $(0 \frac{1}{2} 0)$ with the translation $c/2$. Now $c/2 = 2.21 \text{ \AA}$ so if atoms were situated on these glide planes, the distance between equivalent atoms would be 2.21 \AA . If we take 2.50 \AA as the smallest possible distance between structurally equivalent atoms, we can exclude the striated areas of fig. 2. In these areas no atom can be lying. (A distance $O-O$ less than 2.5 \AA must be expected in a BO_3 -group, so oxygens belonging to such a group might lie within the "forbidden" areas. If they do, however, boron atoms also must lie in these areas. The distance between boron atoms would then also be of the order $2.2-2.5 \text{ \AA}$, which is in disagreement with our assumption stated above.)

Fig. 2. The figure shows one half of the unit cell projected on the c -face. The striated areas represent the parts of the unit cell where no atom can lie if one assumes a minimum distance of 2.50 \AA between structurally equivalent atoms.

arranging BeO_4 -tetrahedra with bonds crossing the glide planes and with no atom inside the "forbidden" area is shown in fig. 3.

As seen in fig. 3 endless chains of BeO_4 -tetrahedra parallel to the c -axis are formed, the composition of these chains being BeO_3 (OH

4) This assumption would not be justifiable if the constituents were highly polarizable, as in that case a layer-lattice might be formed. We cannot expect the Hambergite to have a layer-lattice as the above condition is not present. It is true we have in the OH -groups natural dipoles, but they are small in number compared with the oxygens.

being treated as O), and there are 4 of these chains per unit cell. To build these 4 chains we have used 8 Be and 24 O , so we have left 8 Be , 8 B and 8 O atoms. We will now put the remaining 8 berylliums into the unit cell. They also have to lie inside tetrahedra of oxygens, which share only corners with the tetrahedra in the endless chains. We have only 8 new oxygens to our disposition and we have to build 8 new tetrahedra. It is then obvious that some of the oxygens already present in the cell must form corners of the new tetrahedra; at the same time the new tetrahedra will have to link up the endless chains.

There is only one way of building these new tetrahedra. We have to link the 4 old BeO_3 chains together by means of 4 new congruent BeO_3 chains, the 24 oxygens of

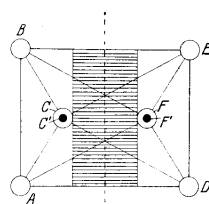


Fig. 3 a.

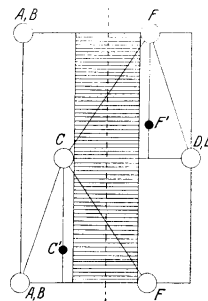


Fig. 3 b.

Fig. 3 a and 3 b. Show the only way by which we can obtain bonds crossing the glide planes with translation $c/2$ without having any atom within the striated areas. Fig. 3 a shows the endless BeO_3 -chains projected on the c -face. Fig. 3 b shows the same chain projected on the a -face. Large open circles represent oxygen atoms (or OH -groups) small black circles represent beryllium atoms. The glide plane A of fig. 2 appears as dotted line.

the new chains being the 8 new oxygens + 16 oxygens belonging to the old chains. The axes of the new chains must be the digonal screw axes $(\frac{1}{2} 0 0)$ $(\frac{2}{3} \frac{1}{2} 0)$ $(\frac{1}{3} \frac{1}{2} 0)$ $(\frac{2}{3} \frac{1}{2} 0)$. The arrangement so obtained is shown in fig. 4.

We have thus got a 3-dimensional network of BeO_4 -tetrahedra, the composition of the network being Be_2O_4 (or more correctly $Be_2O_3(OH)$). All anions are shared between two tetrahedra and two tetrahedra share only one corner, no edge or face.

Into this framework we still have to put 8 boron ions per unit cell. We know that boron can be placed between 3 or between 4 oxygens and we know that only sharing of corners is allowed. No vacant anion tetrahedra satisfying the latter condition can be found in the $Be_2O_3(OH)$

framework, but there are on the other hand triangles of oxygens sharing only corners with the BeO_4 -tetrahedra whose centres can be used as positions for boron. There are two such sets of 8 equivalent positions but we need only one. (Apparently we can choose whichever we like, as the two sets correspond.)

In fig. 4 the BeO_3 -triangles appear as straight lines, the plane of the group being parallel to the c -axis.

Let us consider the binding in our structure. The 32 anions in the cell fall into 4 sets of 8 structurally equivalent anions. Anions belonging to 3 of these sets belong to 2 beryllium tetrahedra and to 1 boron triangle,

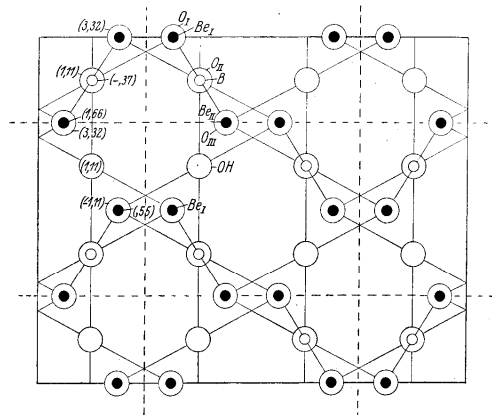


Fig. 4. Represents the ideal structure projected on the c -face. Large open circles are oxygen atoms or OH -groups, small black circles are beryllium atoms, and small open circles are boron atoms.

while the remaining anions belong to 2 beryllium tetrahedra only. The sum of the strength of the valency bonds reaching to each of the former kind of anions is obviously:

$$2 \times \frac{2}{3} + 1 \times \frac{3}{3} = 2$$

while we in the latter case have:

$$2 \times \frac{2}{3} = 1.$$

It then becomes obvious (compare Paulings rule¹⁾) that we have to assume that the anions in the latter case are the 8 OH ions, while the 24 anions connected to 2 Be and one B are the oxygens.

1) L. Pauling, J. Am. chem. Soc. 51, 1010. 1929.

Our structure also satisfies Paulings rule of parsimony¹⁾ as the number of the essentially different kinds of constituents is the smallest possible for the given composition.

With regard to the atomic distances in this ideal structure we calculate:

In the BeO_4 -tetrahedra:

$$O-O = 2.37 \text{ \AA}, 2.43 \text{ \AA}, 2.63 \text{ \AA}, \text{ and } 2.68 \text{ \AA}$$

$$Be-O = 1.63 \text{ \AA}.$$

In the BO_3 -triangles:

$$O-O = 2.63 \text{ \AA} \text{ and } 2.68 \text{ \AA}$$

$$B-O = 1.55 \text{ \AA}.$$

The atomic distances in the former kind of polyhedra are smaller than we ought to expect, in the BO_3 -triangles, however, larger than the probable values. We cannot therefore accept the structure as ultimately correct. That is shown also by the intensity calculations. The atomic coordinates in the ideal structure are:

	x	y	z		x	y	z
Be_I	0°	67,5°	135°	O_I	0°	67,5°	-90°
Be_{II}	90	22,5	135	O_{II}	45	45	90
B	45	45	-30	O_{III}	90	22,5	-90
OH	-45	45	90				

The amplitudes of reflexions $h00$, $0k0$ and $00l$ calculated by means of these figures do not show the slightest agreement with the observed values, as it will be seen from table 4.

Table 4.
Structure Amplitudes Calculated from Ideal Structure.

$h00$	$(F)_{calc}$	$(F)_{obs}$	$0k0$	$(F)_{calc}$	$(F)_{obs}$	$00l$	$(F)_{calc}$	$(F)_{obs}$
200	0	3	020	0	6.5	002	-4.57	34
400	14	16	040	-126	32	004	32	8
600	0	15	060	0	26	006	-4.7	24
800	227	0	080	-43	36	008	2.5	9
10.00	0	14	0.10.0	0	27			
12.00	8	11	0.12.0	-47	0			
14.00	0	18	0.14.0	0	36			
16.00	42	9	0.16.0	62	8			
18.00	0	9						
20.00	4	9						

1) l. c.

This lack of agreement between observed and calculated intensities cannot be considered as an indication of the probability that we have built up a wrong structure. The ideal structure we deduced is so plausible in most respects that the principal correctness of it cannot be doubted. We know, however, from the consideration of the interatomic distances that our structure is not accurate. We will therefore try to distort the ideal structure, and in such a way that agreement between observed and calculated intensities is obtained.

4. The Observations.

I used for my investigation a large crystal of Hambergite from Madagascar. Absolute measurements of the intensities of reflexion were taken from the faces (100), (010), (004) and (140).

The absorption coefficient was measured directly and as result the value $\mu_0 = 1.98$ ($MoK\alpha$) was found. Taking the values for *Be* and *B* given in the paper of Bragg and West¹⁾ as correct we deduce the atomic absorption coefficient 2.86×10^{-6} for oxygen. The value given for oxygen by Bragg and West is 3.3×10^{-6} .

The formula for the reflected intensity is:

Table 2. Absolute Measurements of Reflexions $h00$.

$h00$	$\sin \theta$	$\varrho' \times 10^6$	$\pm F_{\text{corr}}^2)$	F_{calc}	ΣF_{max}
200	.0729	4.5	3	1	330
400	.1458	19.2	16	-7	227
600	.2188	42.0	15	24	163
800	.2947	nil	0	-7	126
10.00	.3646	3.7	14	6	94
12.00	.4375	2.7	14	-5	72
14.00	.5104	5.7	18	-30	52
16.00	.5834	4.3	9	-14	42
18.00	.6563	4.0	9	-3	28
20.00	.7292	4.4	9	-6	23

Table 3. Absolute Measurements of Reflexions $0k0$.

$0k0$	$\sin \theta$	$\varrho' \times 10^6$	$\pm F_{\text{corr}}$	F_{calc}	ΣF_{max}
020	.0581	9.5	6.5	-7	346
040	.1162	93	32	-46	267
060	.1743	43	26	29	196
080	.2324	58	36	-72	156
0.10.0	.2905	29	27	40	126
0.12.0	.3486	0	0	6	100
0.14.0	.4067	33	36	-60	84
0.16.0	.4648	4.2	8	9	62

1) Z. Krist. **69**, 418. 1928.

2) Using $g = 1 \times 10^3$ the agreement seemed to be best.

Table 4. Absolute Measurements of Reflexions $00l$.

$00l$	$\sin \theta$	$\varrho' \times 10^6$	$\pm F_{\text{corr}}$	F_{calc}	ΣF_{max}
002	.1604	64.4	31	-64	240
004	.3202	2.2	8	6	144
006	.4803	9.0	21	29	59
008	.6403	4.2	9	-9	30

Table 5. Absolute Measurements of Reflexions $hkh0$.

$hkh0$	$\sin \theta$	$\varrho' \times 10^6$	$\pm F_{\text{corr}}$	F_{calc}	ΣF_{max}
220	.0933	314	79	-77	300
440	.1867	98	43	35	188
660	.2800	104	56	60	132
880	.3734	0	0	10	92
10.10.0	.4667	4.2	14	6	62
12.12.0	.5600	4.4	9.5	4	42
14.14.0	.6534	2.9	15	14	28

Table 6.

Qualitative Observations from Oscillation Photographs of Reflexions $hkh0$.

$hkh0$	$\sin \theta$	F_{calc}	Int. obs.	$hkh0$	$\sin \theta$	F_{calc}	Int. obs.
200	.0729	1	vwv	600	.2187	21	w
240	.0786	23	m	640	.2308	5	w
220	.0933	-77	s	620	.2264	-34	w
230	.1192	107	vs	630	.2358	-7	w
240	.1376	-38	s	640	.2477	29	w
250	.1628	39	s	650	.2628	22	o
260	.1893	21	vw	660	.2799	60	s
270	.2166	-43	ms	670	.2994	51	s
280	.2443	0	o	680	.3196	-35	m
290	.2708	12	o	690	.3576	13	o
2.10.0	.3004	29	m	800	.2916	-7	o
2.14.0	.3278	26	m	810	.2932	-30	w
400	.1458	-7	w	820	.2974	-2	o
410	.1487	62	vs	830	.3045	-33	m
420	.1574	-12	w	840	.3142	-24	w
430	.1700	-17	w	850	.3261	-5	o
440	.1866	35	m	860	.3400	-27	w
450	.2064	-56	s	870	.3553	5	w
460	.2384	29	w	880	.3732	10	o
470	.2507	-14	o				
480	.2752	-39	s				
490	.2989	-43	s				
4.10.0	.3256	-27	o				

$$g' = \frac{Q}{2\mu} \quad \text{where} \quad Q = \left(\frac{1}{V} \frac{e^2}{mc^2} |F'|^2 \right)^2 \lambda^3 \frac{1 + \cos^2 2\theta}{2 \sin 2\theta}$$

and $\mu = \mu_0 + gQ$, g being the extinction coefficient. Leaving the effect of the extinction out of consideration for the present and inserting the numerical values of the constants, we get:

$$g' = 1.271 \Theta |F'|^2 \times 10^{-8} \quad \text{where} \quad \Theta = \frac{1 + \cos^2 2\theta}{\sin 2\theta}$$

The results of the absolute measurements are compiled in the tables.

5. F -Curves.

The following set of F -curves were used in the calculations.

Table 7.
 F -Curves (MoKa).

$\sin \theta$	0	.1	.2	.3	.4	.5	.6	7.
Be^{+2}	2	4.95	4.75	4.45	4.1	.7	.35	.15
B^{+3}	2	4.95	4.85	4.60	4.25	.85	.50	.25
O^{-2}	4.0	7.5	4.4	2.7	4.75	4.15	.8	.6

The F -curves for beryllium were calculated from data of the electron distribution with which Professor D. R. Hartree kindly provided me. I have tried to account for the temperature effect by letting the F -curve drop a little faster at large values of $\sin \theta$. The F -curve for boron was obtained by extrapolation from the calculations made for beryllium. The oxygen F -curve is essentially the one given by Bragg and West⁴⁾, modified however, to some extent at large glancing angles. For we must assume that the scattering power for large values of $\frac{\sin \theta}{\lambda}$ is chiefly due to the K -electrons. Consequently the values of F_0 for such values must be considerably larger than F_B and F_{Be} . I calculated the F -curves for Be and B also under the assumption of neutral atoms. That of course, means that the F -curves would start at 4 and 5 respectively instead of at 2. For values of $\sin \theta > .2$, however, the F -curve for the neutral atom would almost coincide with the F -curve of the ionized atoms. In the region $\sin \theta < .2$ few observations occur and furthermore the effect of the oxygen lattice is comparatively very great. Thus without introducing serious errors I have used the conception of ionized atoms throughout my calculation.

4) l. c.

6. Determination of the Correct Structure.

Starting from the approximate values of the parameters already given (i. e. parameter values from the ideal structure), I tried to obtain agreement with the observed intensities, through distortion. As there are 7 parameters in the direction of each crystallographic axis this task became rather laborious. I succeeded, however, in deriving a modified set of parameter values, which gave a satisfactory agreement with the observation.

The new set of parameters is given in table 8. The amount of distortion is appreciable as will be seen by comparison with the old set.

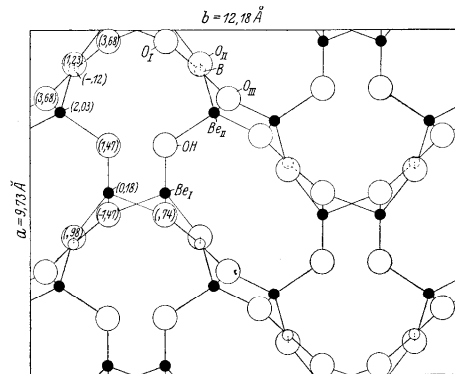


Fig. 5. Gives the projection of the final structure on the c -face. Numbers represent heights in Å. All bonds are given in the figure. Equivalent atoms can be picked out by comparison with fig. 4. The amount of distortion is seen by comparison with fig. 4.

Table 8. Parameter Values.

	Old			New		
	x	y	z	x	y	z
Be_I	0°	67.5°	135°	-44°	66°	165°
Be_{II}	90	22.5	135	85	25	165
B	45	45	-30	42	37	-40
O_I	0	67.5	-90	44	66	-60
O_{II}	45	45	90	35	37	400
O_{III}	90	22.5	-90	70	13.5	-60
OH	-45	45	90	-60	66	60

The calculated and observed structure factors for a number of planes are given in the tables 2-6.

7. Discussion of the Structure.

When trying to distort the ideal structure so as to get agreement with the observed intensities no attention was paid to atomic distances or coordination.

It is therefore all the more satisfactory that our new parameter values lead to a very plausible structure.

The atomic distances are:

Be_I — tetrahedra

$Be_I-O_I = 4.75 \text{ \AA}$	$O_I-O_I = 2.73 \text{ \AA}$
$-O_I = 4.84$	$O_I-O_{II} = 2.72$
$-O_{II} = 4.79$	$O_I-OH = 3.52$
$-OH = 4.85$	$O_I-O_{III} = 2.68$
	$O_I-OH = 2.62$
	$O_{II}-OH = 2.80$

Mean values: $Be_I-(O, OH) = 4.80$

$O_I-(O, OH) = 2.85$

Be_{II} — tetrahedra

$Be_{II}-O_{II} = 4.63 \text{ \AA}$	$O_{II}-O_{III} = 2.75 \text{ \AA}$
$-O_{III} = 4.74$	$O_{II}-O_{III} = 2.63$
$-O_{III} = 4.56$	$O_{II}-OH = 2.48$
$-OH = 4.74$	$O_{III}-O_{III} = 2.64$
	$O_{III}-OH = 3.12$
	$O_{III}-OH = 2.74$

Mean values: $Be_{II}-(O, OH) = 4.68$

Mean values: $Be-(O, OH) = 4.74$

B — triangle

$B-O_I = 4.42 \text{ \AA}$	$O_I-O_{II} = 2.34 \text{ \AA}$
$-O_{II} = 4.36$	$O_I-O_{III} = 2.35$
$-O_{III} = 4.28$	$O_{II}-O_{III} = 2.39$
Mean values: $B-O = 4.35$	$O-O = 2.35$

Boron is lying in the plane of the oxygens.

The linkage is the same as for the ideal structure, namely that the group only share corners and that the oxygen atoms are linked to $2 Be + B$, the hydroxyl groups to the $2 Be$ only. The position of the hydroxyl group with regard to the two neighbouring Be atoms is interesting. The OH -group is not lying on the connection line between the $2 Be$, but moved out from this so that the angle between the $2 OH-Be$ bonds is 146° which is very near the tetrahedral angle. It is interesting to remark that the angle between any two of the three bonds going from OH to the three nearest cations has about the same value in all structures (when OH is not interchangeable with F or O).

The BO_3 groups are situated with their plane parallel to the c -axis. This orientation is in excellent agreement with the optical properties of Hambergite.

8. Summary.

Hambergite, $Be_2BO_3(OH)$, was examined by means of the Laue-method, the oscillation method and the Bragg ionization method with absolute intensity measurements. The crystal used was from Madagascar. As monochromatic X-rays Molybdenum K -radiation was used.

Hambergite is orthorhombic with the space group V_{13}^h . The unit cell which contains 8 molecules has the dimensions:

$$a = 9.73 \pm .01 \text{ \AA} \quad b = 12.18 \pm .02 \text{ \AA} \quad c = 4.42 \pm .01 \text{ \AA}$$

corresponding to

$$a : b : c = .7988 : 4 : .3629.$$

Brögger gives

$$.7988 : 4 : .7268 (2 \times .3634).$$

All atoms are in general positions:

$$\pm (x y z) (x + \frac{1}{2}, \frac{1}{2} - y, \bar{z}) (\bar{x} y + \frac{1}{2}, \frac{1}{2} - x) (\frac{1}{2} - x, \bar{y}, z + \frac{1}{2}).$$

The values of the 24 parameters are:

Be_I	-11°	66°	165°
Be_{II}	85	25	465
B	42	37	-40
O_I	44	66	-60
O_{II}	35	37	400
O_{III}	70	13.5	-60
OH	-60	66	60

The structure was determined in the following way: The structure proved to be too complicated for a direct attack. Therefore an idealized structure was built up from considerations of the empirical rules governing complex structures. The idealized structure did not fit the observed intensities, and was therefore distorted until agreement was obtained. As a result a structure was obtained with parameter values as given above.

The beryllium atoms are all surrounded by 3 oxygens and one HO -group forming nearly regular tetrahedrons. The average distance $Be-O$, OH is 4.74 \AA , and the average distance $O-O$, OH in the tetrahedra is 2.80 \AA . Boron is surrounded by 3 oxygen atoms forming a nearly equilateral triangle with boron in the centre of gravity. The average distances in this group are: $B-O = 4.35 \text{ \AA}$, $O-O = 2.35 \text{ \AA}$.

The tetrahedra and the triangles are linked together so that only corners are shared, no edges or faces. An oxygen atom is linked to two beryllium atoms and one boron atom, an OH -ion to two berylliums only. Paulings principle of the electrostatic valence balance in detail is thus accurately satisfied. The position of the OH -group with regard to the two nearest beryllium atoms indicates the polar nature of the group. The BO_3 -triangles are arranged parallel the to c -axis. The strong positive birefringence of the Hambergite crystals must follow from this orientation.

In conclusion I wish to express my sincere thanks to Professor W. L. Bragg, F.R.S., in whose laboratory the greater part of this work was done, for his kind interest and valuable advice. I am very much indebted to Professor J. Schetelig, Director of Mineralogical-Geological Museum, Oslo, for supplying me with crystals of Hambergite.

Ryerson Physical Laboratory, University of Chicago
August 1930.

Received September 15th 1930.
