

Crystal Structure of Bayerite

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Bayerite, one of aluminumtrihydroxides, was identified by Fricke¹⁾ as a new crystal which has a composition of $\text{Al}(\text{OH})_3$ or $\text{Al}_2\text{O}_3 \cdot 3\text{H}_2\text{O}$. Montoro²⁾ reported for the first time that bayerite has a hexagonal lattice with $c=4.76$ kX and $a=5.01$ kX. Later Milligan³⁾ reported that Montoro's lattice was not correct. We have examined the structure of bayerite and found that Montoro's lattice was essentially correct (See Table I). Assuming that the structure is analogous to that of brucite, $\text{Mg}(\text{OH})_2$, from which one third of columns of the metallic ions are taken out, we have arrived at a satisfactory atomic arrangement based upon the space group D'_{3d} . The calculated and the observed values of spacings and intensities are shown in Table II. As can be seen from this table, calculated values are in good accord with observed values. As a result, bayerite has the following structure.

TABLE I

Crystal Class	Hexagonal (Trigonal)
Unit Cell	$a=5.047 \text{ \AA}$ $c=4.730 \text{ \AA}$
Space Group	D'_{3d}
Atomic Coordinates	Al : 2 (c) O : 6 (k) : 0.340 : 0.210

The structure is shown in Fig. 1 and this structure can be said to be the idealized monolayer structure of hydrargillite⁴⁾.

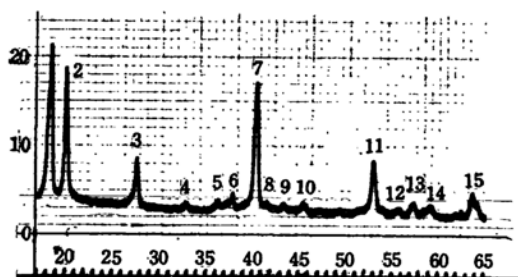


Fig. 1. Diffraction Pattern of Bayerite

- 1) R. Fricke, *Z. anorg. allg. Chem.* **175**, 249 (1928).
- 2) V. Montoro, *Ricerca Sci.* **13**, 565 (1942).
- 3) W. O. Milligan, *J. Phys. Colloid Chem.* **55**, 497 (1951).
- 4) H. Megow, *Z. Krist.* **87**, 185 (1934).

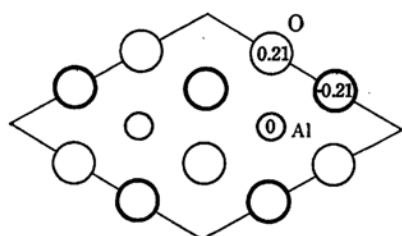


Fig. 2. Crystal Structure of Bayerite.

TABLE II
SPACINGS AND INTENSITIES OF DIFFRACTION
LINES

No.	h k l	Spacings		Intensities	
		obs.	calcd.	obs.	calcd.
1	0 0 1	4.753	4.730	100	100
2	1 0 0	4.385	4.371	60	30
3	1 0 1	3.220	3.210	34	25
4*		2.705			
5*		2.468			
6	0 0 2	2.368	2.365	7	2
7	1 1 1	2.227	2.226	90	99
8	2 0 0	2.171	2.186	2	3
9	1 0 2	2.079	2.080	3	6
10	2 0 1	1.987	1.984	4	6
11	1 1 2	1.725	1.726	45	51
12	1 2 0	1.653	1.653	3	3
13	2 0 2	1.604	1.605	10	6
14	1 2 1	1.560	1.561	15	6
15	3 0 0	1.460	1.457	25	26
16	3 0 1	1.334	1.392	8	14
17	1 1 3	1.333	1.337	21	18
18	2 2 1	1.216	1.219	15	8

* Impurity lines, presumably due to poly-type layer structure of bayerite (to be published later).

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