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The unit cell and space group of $4CaO.3Al_2O_3.3H_2O$.

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The compound $4\,CaO.3\,Al_2O_3.3\,H_2O$ was first described by Johnson & Thorvaldson (1943), and has also been reported by Peppler & Wells (1954) and Majumdar & Roy (1956). It forms slightly elongated, rectangular plates. These appear to be orthorhombic, but no crystallographic data except optical properties and the X-ray powder pattern have been reported.

A sample was prepared hydrothermally from $CaAl_2O_4$, $Ca(OH)_2$, and water at 350 °C., and yielded crystals up to 80μ long. From X-ray oscillation and rotation photographs about a and c, together with indexed powder data, the unit cell was found to be orthorhombic with

$$a = 12{\cdot}78,\ b = 12{\cdot}42,\ c = 8{\cdot}90\ \text{Å}.$$

The prism axis is c, the cleavage (010), and the optic orientation $X=a$, $Y=b$, $Z=c$. hkl reflections are present only for $h+l=2n$, $hk0$ for $k=2n$, and $h0l$ for $h=2n$ and $l=2n$. The space group could therefore be either $B2cb$ (C_{2v}^{17}; non-centrosymmetric) or $Bmab$ (D_{2h}^{18}; centrosymmetric). No attempt was made to find which was correct. The calculated density, for cell contents $4\,[4\,CaO.3\,Al_2O_3.3\,H_2O]$, is 2·74 g.cm.$^{-3}$; Johnson & Thorvaldson reported 2·71 g.cm.$^{-3}$. The ionic constitution is probably $4\,[Ca_4Al_6O_{10}(OH)_6]$.

X-ray powder data (Table 1) were obtained with filtered copper radiation ($\lambda = 1{\cdot}542$ Å), using 6 and 11·46 cm. diameter cameras, and also a diffractometer. Indexing was effected by superimposing powder and single crystal patterns made on the same camera, care being taken to match relative intensities as well as spacings.

The work was carried out as part of a programme of research on the system CaO–Al_2O_3–H_2O, supported by the Lafarge Aluminous Cement Company, Ltd., whose generous assistance is gratefully acknowledged. We are not planning to do any further work on the crystal structure of this compound.

References

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Table 1. *X-ray powder data*

Observed			Calculated	Observed			Calculated
Spacing (Å)	Relative intensity	Indices	spacing (Å)	Spacing (Å)	Relative intensity	Indices	spacing (Å)
3·61	*vs*	131	3·601	2·085	*ms*	351	2·086
3·50	*vw*	212	3·503	2·070	*w*	214	2·072
3·27	*s*	321	3·268			060	2·070
3·02	*m*	032	3·034	1·984	*vw*	260	1·969
2·85	*w*	420	2·842	1·913	*w*	343	1·916
2·80	*vvs*	331	2·817			513	1·914
		113	2·815	1·870	*vvw*	602	1·877
		240	2·793			612	1·856
2·74	*vvw*	232	2·739	1·834	*vw*	622	1·836
2·60	*mw*	123	2·620	1·799	*w*	262	1·801
		402	2·596			452	1·795
2·54	*mw*	042	2·546	1·773	*vvw*	?	
		412	2·542	1·740	*vw*	353	1·739
2·42–2·38	*w/b*	341	2·415	1·688	*vw*	163	1·682
		422	2·395	1·663	*vw*	434	1·671
		313	2·389			054	1·657
2·35	*w*	151	2·351	1·642	*vvw*	?	
2·29	*mw*	521	2·285	1·616	*vvw*	?	
2·23	*mw*	440	2·227	1·598	*mw*	800	1·598
		004	2·225	1·572	*ms*	444	1·574
2·13	*w*	600	2·131	1·552	*w*	080	1·552
2·100	*vvw*	204	2·101	1·537	*w*		
		333	2·099	1·514	*vvw*		
		024	2·094	1·508	*w*		

s = strong, *m* = moderate, *w* = weak, *v* = very, *b* = broad.