

$\text{CaAl}_2[\text{OH}]_8[\text{H}_2\text{O}]_{3.84}$ 
*hP96*

(176)  $P6_3/m - i^6h^4$ 
 **$\text{CaAl}_2(\text{OH})_8(\text{H}_2\text{O})_2 \cdot 1.84\text{H}_2\text{O}$**  [1], cement  $\text{CAH}_{10}$ 

Structural features: Units of three edge-linked  $\text{Ca}(\text{OH})_6(\text{OH}_2)_2$  bicapped trigonal prisms and units of two edge-linked  $\text{Al}(\text{OH})_6$  octahedra share edges to form a 3D-framework; additional  $\text{H}_2\text{O}$  between the units and in large channels parallel to [001].

Guirado F. et al. (1998) [1]

 $\text{Al}_2\text{CaH}_{15.68}\text{O}_{11.84}$ 
 $a = 1.6387$ ,  $c = 0.8279$  nm,  $c/a = 0.505$ ,  $V = 1.9253$  nm<sup>3</sup>,  $Z = 6$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH <sub>2</sub> )1	12 <i>i</i>	1	0.0	0.249	0.079	0.71	non-coplanar triangle (OH)(OH <sub>2</sub> ) <sub>2</sub>
Al2	12 <i>i</i>	1	0.0826	0.5795	0.068		octahedron (OH) <sub>6</sub>
(OH <sub>2</sub> )3	12 <i>i</i>	1	0.168	0.403	0.039		single atom Ca
(OH)4	12 <i>i</i>	1	0.213	0.623	0.072		single atom Al
(OH)5	12 <i>i</i>	1	0.436	0.106	0.09		single atom Al
(OH)6	12 <i>i</i>	1	0.574	0.053	0.072		non-colinear Al <sub>2</sub>
(OH)7	6 <i>h</i>	<i>m..</i>	0.077	0.505	<sup>1</sup> / <sub>4</sub>		non-colinear Al <sub>2</sub>
Ca8	6 <i>h</i>	<i>m..</i>	0.2394	0.5185	<sup>1</sup> / <sub>4</sub>		square antiprism (OH <sub>2</sub> ) <sub>2</sub> (OH) <sub>6</sub>
(OH)9	6 <i>h</i>	<i>m..</i>	0.337	0.435	<sup>1</sup> / <sub>4</sub>		non-colinear Al <sub>2</sub>
(OH <sub>2</sub> )10	6 <i>h</i>	<i>m..</i>	0.567	0.251	<sup>1</sup> / <sub>4</sub>	0.42	tetrahedron (OH <sub>2</sub> ) <sub>2</sub> (OH) <sub>2</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: powder, diffractometer, X-rays,  $R_B = 0.086$ 

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Guirado F., Gali S., Chinchon S., Rius J. (1998), *Angew. Chem. Int. Ed.* 37, 72-75 (*Angew. Chem.* 110, 76-79).