

LiAl₂Cl[OH]₆[H₂O]

hP78

(176) *P*6₃/*m* – ih¹⁰fb**[LiAl₂(OH)₆]Cl·H₂O [1]**

Structural features: Infinite slabs of edge-linked Al(OH)₆ and Li(OH)₆ octahedra alternate with layers containing a disordered arrangement of Cl and H₂O.

Besserguenev A.V. et al. (1997) [1]

Al₂ClH_{8.19}LiO_{7.09}*a* = 0.50963, *c* = 1.52919 nm, *c/a* = 3.001, *V* = 0.3440 nm³, *Z* = 2

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|-------------|-----------------------------|-----------------------------|-----------------------------|-------|--|
| O1 | 12i | 1 | 0.0016 | 0.3576 | 0.0631 | | non-coplanar triangle Al ₂ Li |
| Cl2 | 6h | <i>m</i> .. | 0.0 | 0.35 | ¹ / ₄ | 0.067 | |
| O3 | 6h | <i>m</i> .. | 0.04 | 0.411 | ¹ / ₄ | 0.073 | |
| O4 | 6h | <i>m</i> .. | 0.118 | 0.065 | ¹ / ₄ | 0.073 | |
| O5 | 6h | <i>m</i> .. | 0.125 | 0.388 | ¹ / ₄ | 0.073 | |
| Cl6 | 6h | <i>m</i> .. | 0.162 | 0.242 | ¹ / ₄ | 0.067 | |
| Cl7 | 6h | <i>m</i> .. | 0.191 | 0.561 | ¹ / ₄ | 0.067 | |
| Cl8 | 6h | <i>m</i> .. | 0.24 | 0.16 | ¹ / ₄ | 0.067 | |
| O9 | 6h | <i>m</i> .. | 0.313 | 0.242 | ¹ / ₄ | 0.073 | |
| O10 | 6h | <i>m</i> .. | 0.505 | 0.342 | ¹ / ₄ | 0.073 | |
| Cl11 | 6h | <i>m</i> .. | 0.561 | 0.191 | ¹ / ₄ | 0.067 | |
| Al12 | 4f | 3.. | ¹ / ₃ | ² / ₃ | 0.0 | | octahedron O ₆ |
| Li13 | 2b | -3.. | 0 | 0 | 0 | | octahedron O ₆ |
| H14 | 12i | 1 | 0.342 | 0.035 | 0.129 | | |
| H15 | 6h | <i>m</i> .. | 0.088 | 0.238 | ¹ / ₄ | 0.073 | |
| H16 | 6h | <i>m</i> .. | 0.1 | 0.143 | ¹ / ₄ | 0.073 | |
| H17 | 6h | <i>m</i> .. | 0.109 | 0.12 | ¹ / ₄ | 0.073 | |
| H18 | 6h | <i>m</i> .. | 0.12 | 0.61 | ¹ / ₄ | 0.073 | |
| H19 | 6h | <i>m</i> .. | 0.227 | 0.23 | ¹ / ₄ | 0.073 | |
| H20 | 6h | <i>m</i> .. | 0.24 | 0.37 | ¹ / ₄ | 0.073 | |
| H21 | 6h | <i>m</i> .. | 0.245 | 0.235 | ¹ / ₄ | 0.073 | |
| H22 | 6h | <i>m</i> .. | 0.274 | 0.574 | ¹ / ₄ | 0.073 | |
| H23 | 6h | <i>m</i> .. | 0.36 | 0.49 | ¹ / ₄ | 0.073 | |
| H24 | 6h | <i>m</i> .. | 0.54 | 0.189 | ¹ / ₄ | 0.073 | |

Transformation from published data: origin shift 0 0 ¹/₂Experimental: powder, diffractometer, neutrons, time-of-flight, wR_p = 0.013

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Besserguenev A.V., Fogg A.M., Francis R.J., Price S.J., O'Hare D., Isupov V.P., Tolochko B.P. (1997), Chem. Mater. 9, 241-247.