

KAl[SiO<sub>4</sub>]*hP*24(186) *P*6<sub>3</sub>*mc* – *dc*b<sup>2</sup>*a***KAlSiO<sub>4</sub> ht1** [1], kalsilite-1H highStructural features: AlO<sub>4</sub> and SiO<sub>4</sub> tetrahedra share vertices (splitting of one O site) to form a tridymite-type framework; K in channels delimited by 6-rings parallel to [001].

Kawahara A. et al. (1987) [1]

AlKO<sub>4</sub>Si*a* = 0.53, *c* = 0.865 nm, *c/a* = 1.632, *V* = 0.2104 nm<sup>3</sup>, *Z* = 2

| site | Wyck.       | sym.         | <i>x</i>                    | <i>y</i>                    | <i>z</i> | occ.  | atomic environment |
|------|-------------|--------------|-----------------------------|-----------------------------|----------|-------|--------------------|
| O1   | 12 <i>d</i> | 1            | 0.593                       | 0.259                       | 0.0      | 0.167 | non-colinear SiAl  |
| O2   | 6 <i>c</i>  | . <i>m</i> . | 0.506                       | 0.494                       | 0.234    |       |                    |
| Al3  | 2 <i>b</i>  | 3 <i>m</i> . | <sup>1</sup> / <sub>3</sub> | <sup>2</sup> / <sub>3</sub> | 0.308    |       |                    |
| Si4  | 2 <i>b</i>  | 3 <i>m</i> . | <sup>1</sup> / <sub>3</sub> | <sup>2</sup> / <sub>3</sub> | 0.689    |       |                    |
| K5   | 2 <i>a</i>  | 3 <i>m</i> . | 0                           | 0                           | 0.0      |       |                    |

Transformation from published data: origin shift 0 0 0.75

Experimental: single crystal, diffractometer, X-rays, *R* = 0.095, *T* = 1223 KRemarks: Phase stable at *T* > 1138 K. Short interatomic distances for partly occupied site(s). In table 2 of [1] the *x*-coordinate of former O(1) is misprinted as 0.056 instead of 0.506 (checked on interatomic distances).

References: [1] Kawahara A., Andou Y., Marumo F., Okuno M. (1987), Mineral. J. 13, 260-270.