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|---------------------------------------|--------|-------------------------|
| $\text{K}_{0.3}\text{Ti}_3\text{S}_4$ | $hP18$ | $(176) P6_3/m - h^2dba$ |
|---------------------------------------|--------|-------------------------|

$\text{K}_{0.6}\text{Ti}_6\text{S}_8$ [1]; $\text{K}_{0.52}\text{Ti}_6\text{Se}_8$ rt [2]

Structural features: Units of three face-linked TiS_6 octahedra share edges to form a 3D-framework; K in channels of hexagonal cross-section parallel to $[001]$ (partial disorder). Filled-up derivative of Nb_3Te_4 .

Schöllhorn R. et al. (1980) [1]

$\text{K}_{0.30}\text{S}_4\text{Ti}_3$

$a = 0.9505$, $c = 0.3414$ nm, $c/a = 0.359$, $V = 0.2671$ nm³, $Z = 2$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|--------|---------------|---------------|---------------|------|-----------------------------------|
| S1 | $6h$ | $m..$ | 0.0491 | 0.3563 | $\frac{1}{4}$ | | 4-vertex polyhedron Ti_4 |
| Ti2 | $6h$ | $m..$ | 0.3546 | 0.4867 | $\frac{1}{4}$ | | octahedron S_6 |
| S3 | $2d$ | $-6..$ | $\frac{2}{3}$ | $\frac{1}{3}$ | $\frac{1}{4}$ | | trigonal prism Ti_6 |
| K4 | $2b$ | $-3..$ | 0 | 0 | 0 | 0.15 | |
| K5 | $2a$ | $-6..$ | 0 | 0 | $\frac{1}{4}$ | 0.15 | |

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.065$

Remarks: We assigned an approximate value to the occupancy of sites K based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Schöllhorn R., Schramm W., Fenske D. (1980), Angew. Chem. Int. Ed. Engl. 19, 492-493 (Angew. Chem. 92, 477-478). [2] Bensch W., Koy J. (1992), Z. Kristallogr. 202, 300-301.