

KLi[SO₄]*hP20*(186) *P6₃mc* – db³a**KLiSO₄ form III** [1]

Structural features: K and Li atoms and SO₄ tetrahedra (partial rotational disorder) in a ZrBeSi-type arrangement.

Solans X. et al. (1999) [1]

KLiO₄S $a = 0.5123$, $c = 0.8639$ nm, $c/a = 1.686$, $V = 0.1964$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>d</i>	1	0.0553	0.3986	0.2604	0.5	non-coplanar triangle O ₂ S
O2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0352		colinear SLi
S3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.2058		7-vertex polyhedron O ₇
Li4	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.8193		7-vertex polyhedron O ₇
K5	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		15-vertex polyhedron O ₁₅

Transformation from published data: origin shift 0 0 0.6815

Experimental: single crystal, diffractometer, X-rays, R = 0.051, T = 260 K

Remarks: Phase stable at 250 < T < 268 K.

References: [1] Solans X., Calvet M.T., Martinez Sarrion M.L., Mestres L., Bakkali A., Bocanegra E., Mata J., Herraiz M. (1999), J. Solid State Chem. 148, 316-324.