

KSnAs	<i>hP6</i>	(186) $P6_3mc - b^2a$
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KSnAs [2]

Structural features: :SnAs_3 ψ -tetrahedra share vertices to form infinite layers; K in trigonal prismatic voids. Ordering variant of 2H-CaGe₂.

Klein J., Eisenmann B. (1988) [1]

AsKSn

$a = 0.4102$, $c = 1.2816$ nm, $c/a = 3.124$, $V = 0.1868$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
K1	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.2823		16-vertex polyhedron $\text{As}_4\text{Sn}_6\text{K}_6$
As2	$2b$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.6028		octahedron Sn_3K_3
Sn3	$2a$	$3m.$	0	0	0.0		non-coplanar triangle As_3

Transformation from published data: $-x, -y, -z$; origin shift 0 0 0.2177

Experimental: single crystal, diffractometer, X-rays, $R = 0.042$

References: [1] Klein J., Eisenmann B. (1988), Mater. Res. Bull. 23, 587-594. [2] Lii K.H., Haushalter R.C. (1987), J. Solid State Chem. 67, 374-378.