

$\text{K}_{1.88}\text{Sn}_{5.06}\text{Cl}_{12}$ $hP25$ $(174) P-6 - k^4j^4a$ $\text{K}_{2-2x}\text{Sn}_{5+x}\text{Cl}_{12}$ [1]

Structural features: Infinite chains of vertex-linked SnCl_3 ψ -tetrahedra parallel to [001]; part of Sn replaced by K (disorder, distinct positions for K and Sn), additional (K,Sn) in channels.

Beck H.P., Nau H. (1988) [1]

 $\text{Cl}_{12}\text{K}_{1.88}\text{Sn}_{5.05}$ $a = 1.192$, $c = 0.4289$ nm, $c/a = 0.36$, $V = 0.5278$ nm³, $Z = 1$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	$3k$	$m..$	0.0075	0.2513	$\frac{1}{2}$		single atom Sn
Cl2	$3k$	$m..$	0.1303	0.6148	$\frac{1}{2}$		
K3	$3k$	$m..$	0.4201	0.2418	$\frac{1}{2}$	0.167	
Sn4	$3k$	$m..$	0.4234	0.3126	$\frac{1}{2}$	0.833	
Sn5	$3j$	$m..$	0.1165	0.4217	0	0.833	
K6	$3j$	$m..$	0.164	0.3971	0	0.167	
Cl7	$3j$	$m..$	0.247	0.2346	0		
Cl8	$3j$	$m..$	0.5166	0.1319	0		single atom Sn
M9	$1a$	$-6..$	0	0	0	0.935	coplanar triangle Cl_3

 $\text{M9} = 0.94\text{K} + 0.06\text{Sn}$ Experimental: single crystal, diffractometer, X-rays, $wR = 0.080$

Remarks: Short interatomic distances for partly occupied site(s). We assigned an approximate value to the K/Sn ratio of site M9 based on the nominal composition.

References: [1] Beck H.P., Nau H. (1988), Z. Anorg. Allg. Chem. 558, 193-200.