

$\text{K}_{0.72}\text{In}_{0.72}\text{Sn}_{0.28}\text{O}_2$ $hP12$ $(187) P-6m2 - \text{ihg}^2\text{fcba}$ **$\text{K}_{0.72}(\text{In}_{0.72}\text{Sn}_{0.28})\text{O}_2$ [1]**

Structural features: Close-packed O layers in BBCC stacking; In and Sn in octahedral voids (substitutional disorder, Sn displaced towards a face), K in trigonal voids (partial disorder). $(\text{In},\text{Sn})\text{O}_6$ octahedra (distinct positions for In and Sn) share edges to form infinite slabs.

Delmas C., Werner P.E. (1978) [1]

 $\text{In}_{0.72}\text{K}_{0.72}\text{O}_2\text{Sn}_{0.28}$ $a = 0.32314$, $c = 1.282$ nm, $c/a = 3.967$, $V = 0.1159$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$2i$	$3m.$	$\frac{2}{3}$	$\frac{1}{3}$	0.184		non-coplanar triangle Sn_3
O2	$2h$	$3m.$	$\frac{1}{3}$	$\frac{2}{3}$	0.392		
Sn3	$2g$	$3m.$	0	0	0.205	0.28	
In4	$2g$	$3m.$	0	0	0.261	0.72	
K5	$1f$	$-6m2$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{2}$	0.486	
K6	$1c$	$-6m2$	$\frac{1}{3}$	$\frac{2}{3}$	0	0.486	
K7	$1b$	$-6m2$	0	0	$\frac{1}{2}$	0.234	
K8	$1a$	$-6m2$	0	0	0	0.234	

Transformation from published data: origin shift $\frac{1}{3} \frac{2}{3} \frac{1}{2}$ Experimental: powder, film, X-rays, $R_p = 0.128$, $T = 298$ K

Remarks: O could not be located with certainty. Short interatomic distances for partly occupied site(s).

References: [1] Delmas C., Werner P.E. (1978), Acta Chem. Scand. A 32, 329-332.