Phase II K_2SnCl_6 Structure: A6B2C_tP18_128_eh_d_a-001

This structure previously used the label(s) `A6B2C_tP18_128_eh_d_a`. Calls to these addresses will be redirected here.

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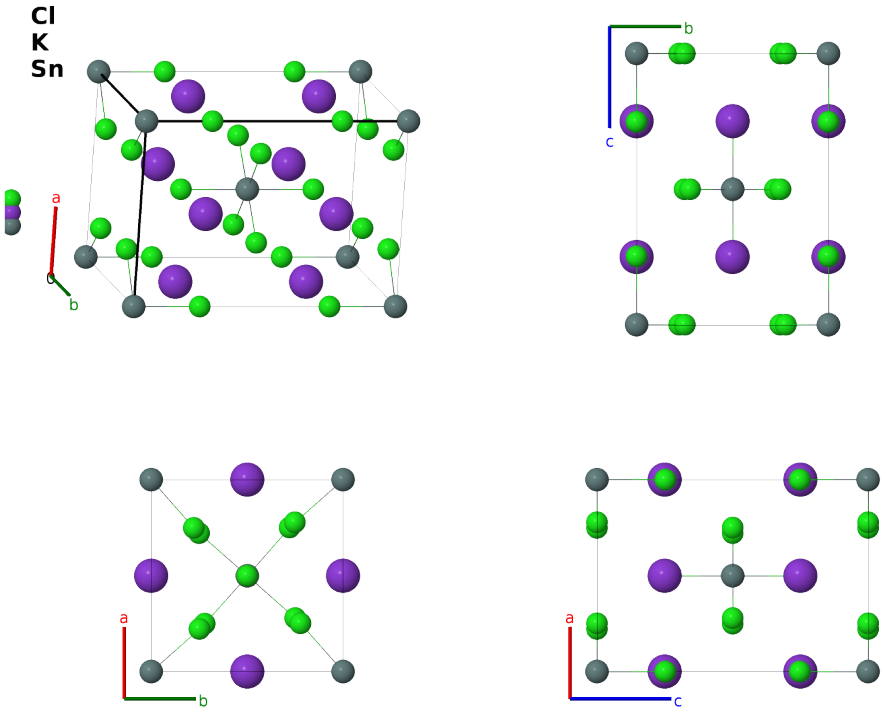
https://aflow.org/prototype-encyclopedia/AD9M

https://aflow.org/prototype-encyclopedia/A6B2C_tP18_128_eh_d_a-001

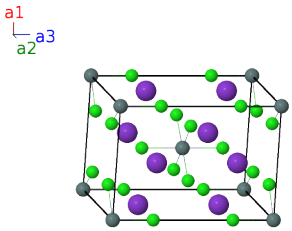


Prototype	Cl_6K_2Sn
AFLOW prototype label	A6B2C_tP18_128_eh_d_a-001
ICSD	1669
CCDC	1591736
Pearson symbol	tP18
Space group number	128
Space group symbol	$P4/mnc$
AFLOW prototype command	`aflow --proto=A6B2C_tP18_128_eh_d_a-001 --params=`$a, c/a, z_3, x_4, y_4$

- K_2SnCl_6 is found in three forms, depending on the temperature:
  - Below 255K it is in the monoclinic Phase I structure.
  - In the range 255-261K it is in the tetragonal Phase II structure (this structure).
  - Above 261K it transforms to Phase III, which has the K_2PtCl_6 ($J1_1$) structure.
- Data for Phase II was taken at 265K.

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= a\,\hat{\mathbf{x}}\\ \mathbf{a_2} &= a\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Sn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	Sn I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	K I
$\mathbf{B_7}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_9}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_{11}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}$	(8h)	Cl II
$\mathbf{B_{12}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}$	(8h)	Cl II
$\mathbf{B_{13}}$	=	$-y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}$	(8h)	Cl II
$\mathbf{B_{14}}$	=	$y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}$	(8h)	Cl II
$\mathbf{B_{15}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cl II
$\mathbf{B_{16}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cl II
$\mathbf{B_{17}}$	=	$\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cl II
$\mathbf{B_{18}}$	=	$-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Cl II

References

[1] H. Boysen and A. W. Hewat, *A neutron powder investigation of the structural changes in K_2SnCl_6*, Acta Crystallogr. Sect. B **34**, 1412–1418 (1978), doi:10.1107/S0567740878005816.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

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