

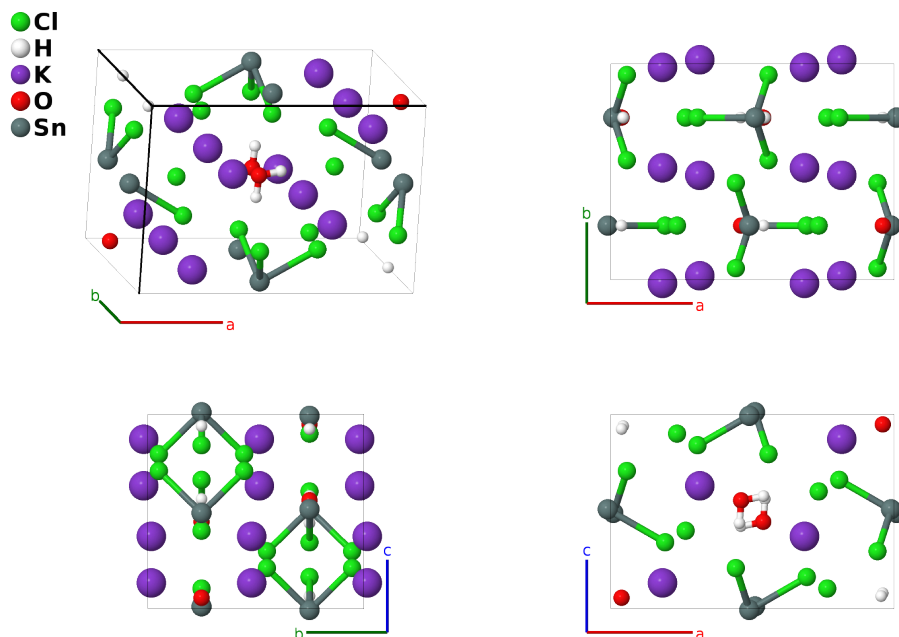
K₂SnCl₄·H₂O Structure:

A4B2C2DE_oP40_62_2cd_2c_d_c_c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/AZ89>

https://aflow.org/p/A4B2C2DE_oP40_62_2cd_2c_d_c_c-001

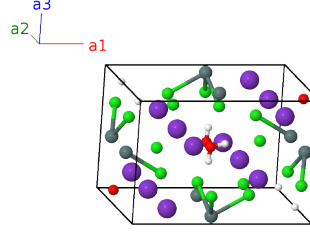


Prototype	Cl ₄ H ₂ K ₂ OSn
AFLOW prototype label	A4B2C2DE_oP40_62_2cd_2c_d_c_c-001
ICSD	290298
Pearson symbol	oP40
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=A4B2C2DE_oP40_62_2cd_2c_d_c_c-001 --params=a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</code>

- Various structures have been proposed for K₂SnCl₄·H₂O:
 - The original determination of this structure was made by (Brasseur, 1939) and given the *Strukturbericht* label *E3*₅ by (Herrmann, 1943).
 - (Kamenar, 1962) proposed an alternative structure. Neither of these experiments located the hydrogen atoms.
 - This was finally accomplished by (Ye, 2013), shown here. Their structure refined that of (Kamenar, 1962).

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	Cl I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cl I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	Cl I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cl I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Cl II
\mathbf{B}_6	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cl II
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Cl II
\mathbf{B}_8	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cl II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_{10}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_{12}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{14}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{16}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	H II
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{18}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{20}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O I
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Sn I
\mathbf{B}_{22}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Sn I
\mathbf{B}_{23}	$= -x_6 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4c)	Sn I
\mathbf{B}_{24}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Sn I
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8d)	Cl III

$$\begin{aligned}
\mathbf{B}_{26} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 - y_7 \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{29} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{30} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + y_7 \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{31} &= x_7 \mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= ax_7 \hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{32} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl III} \\
\mathbf{B}_{33} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{34} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{35} &= -x_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{36} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{37} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{38} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + y_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{39} &= x_8 \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= ax_8 \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} &(8d) & \text{K I} \\
\mathbf{B}_{40} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{K I}
\end{aligned}$$

References

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Found in

- [1] ICSD, Inorganic Crystal Structure Database. ID 290298.