

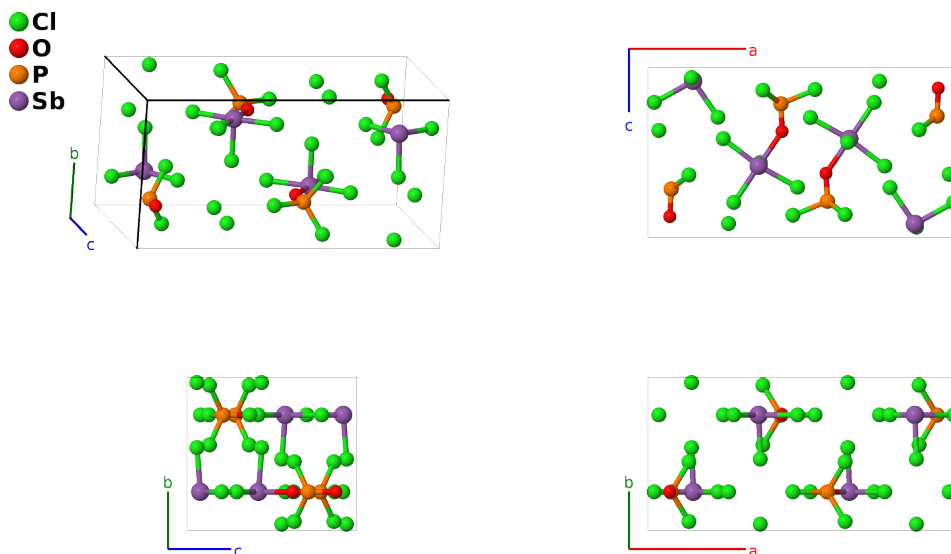
SbCl₅·POCl₃ Structure: A8BCD_oP44_62_4c2d_c_c_c-001

This structure originally had the label A8BCD_oP44_62_4c2d_c_c_c. Calls to that address will be redirected here.

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<https://aflow.org/p/XAT4>

https://aflow.org/p/A8BCD_oP44_62_4c2d_c_c_c-001



Prototype	Cl ₈ OPSb
AFLOW prototype label	A8BCD_oP44_62_4c2d_c_c_c-001
ICSD	26493
Pearson symbol	oP44
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<pre>aflow --proto=A8BCD_oP44_62_4c2d_c_c_c-001 --params=a, b/a, c/a, x₁, z₁, x₂, z₂, x₃, z₃, x₄, z₄, x₅, z₅, x₆, z₆, x₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉</pre>

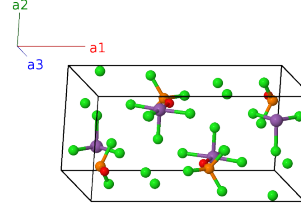
Other compounds with this structure

SbCl₅·POCl₃(CH₃)₃

- (Lindqvist, 1959) give the data for this structure in setting *Pmnb* of space group #62. We used FINDSYM to exchange the *a*- and *b*-axes so that the structure is now in the standard *Pnma* orientation.

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)	Cl III
\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)	Cl III
\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)	Cl III
\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)	Cl III
\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)	Cl IV
\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)	Cl IV
\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)	Cl IV
\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)	Cl IV
\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)	P 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)	P 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)	P 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)	P I
\mathbf{B}_{25}	$= x_7 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4c)	Sb I

$$\begin{aligned}
\mathbf{B}_{26} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} + c \left(z_7 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{Sb I} \\
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -ax_7 \hat{\mathbf{x}} + \frac{3}{4} b \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} &(4c) & \text{Sb I} \\
\mathbf{B}_{28} &= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + \frac{1}{4} b \hat{\mathbf{y}} - c \left(z_7 - \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) & \text{Sb I} \\
\mathbf{B}_{29} &= 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{Cl V} \\
\mathbf{B}_{30} &= -\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{Cl V} \\
\mathbf{B}_{31} &= -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{Cl V} \\
\mathbf{B}_{32} &= \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{Cl V} \\
\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{Cl V} \\
\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{Cl V} \\
\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{Cl V} \\
\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{Cl V} \\
\mathbf{B}_{37} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{38} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{39} &= -x_9 \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{40} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{41} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{42} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c \left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{43} &= x_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - b \left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(8d) & \text{Cl VI} \\
\mathbf{B}_{44} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8d) & \text{Cl VI}
\end{aligned}$$

References

- [1] I. Lindqvist and C.-I. Brändén, *The Crystal Structure of $\text{SbCl}_5 \cdot \text{POCl}_3$* , *Acta Cryst.* **12**, 642–645 (1959), doi:10.1107/S0365110X5900189X.

Found in

- [1] C.-I. Brändén and I. Lindqvist, *The Crystal Structure of $\text{SbCl}_5 \cdot \text{PO}(\text{CH}_3)_3$* , *Acta Chem. Scand.* **15**, 167–174 (1961), doi:10.3891/acta.chem.scand.15-0167.