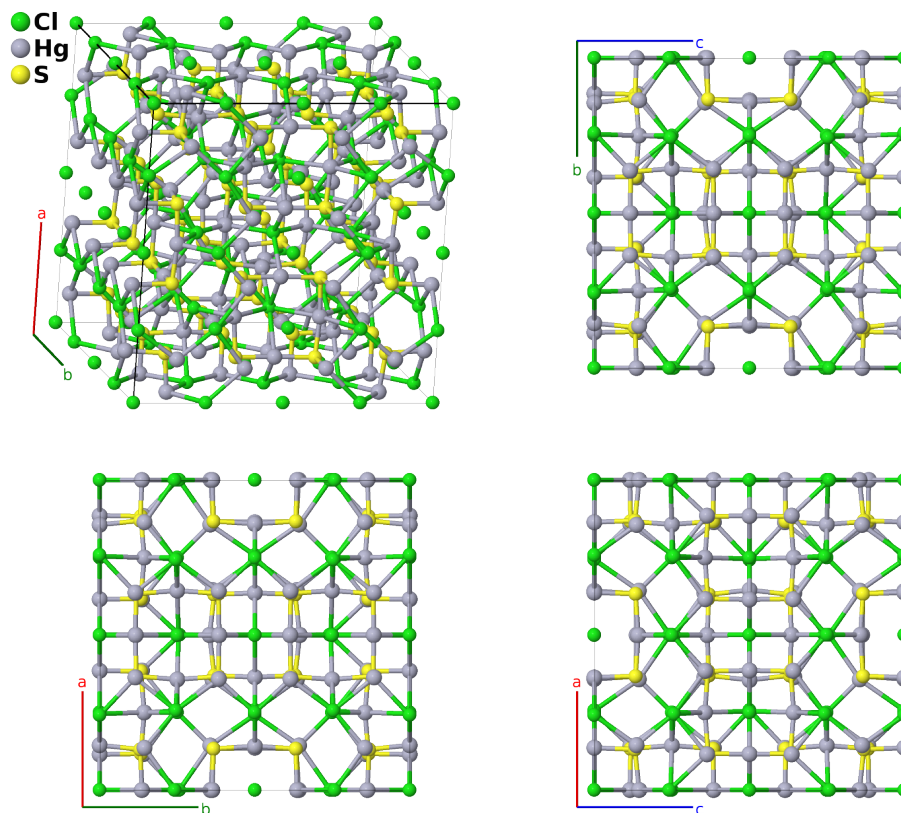


β -Hg₃S₂Cl₂ Structure: A2B3C2_cP224_223_abcdefk_j3k_il-001

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<https://aflow.org/p/UWQ4>

https://aflow.org/p/A2B3C2_cP224_223_abcdefk_j3k_il-001



Prototype	Cl ₂ Hg ₃ S ₂
AFLOW prototype label	A2B3C2_cP224_223_abcdefk_j3k_il-001
ICSD	83407
Pearson symbol	cP224
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A2B3C2_cP224_223_abcdefk_j3k_il-001 --params=a, x₆, x₇, y₈, y₉, z₉, y₁₀, z₁₀, y₁₁, z₁₁, y₁₂, z₁₂, x₁₃, y₁₃, z₁₃</code>

- Hg₃Cl₂S₂ is found in three forms (Carlson, 1967):
 - Corderoite (α -Hg₃Cl₂S₂), the cubic ground state.
 - β -Hg₃Cl₂S₂, which appears above 340°C, another cubic phase with a much larger unit cell. (this structure)

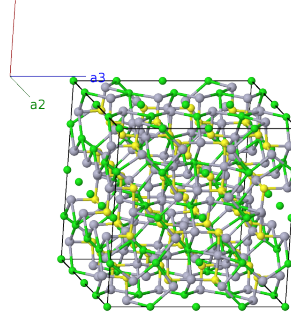
– Kenhsuite (γ -Hg₃Cl₂S₂), which on average has an orthorhombic lattice. This state is apparently metastable.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	Cl I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(2a)	Cl I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6b)	Cl II
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6b)	Cl II
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6b)	Cl II
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(6b)	Cl II
\mathbf{B}_7	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(6b)	Cl II
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(6b)	Cl II
\mathbf{B}_9	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{10}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{11}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(6c)	Cl III
\mathbf{B}_{12}	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(6c)	Cl III
\mathbf{B}_{13}	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{14}	$\frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6c)	Cl III
\mathbf{B}_{15}	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6d)	Cl IV
\mathbf{B}_{16}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(6d)	Cl IV
\mathbf{B}_{17}	$\frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Cl IV
\mathbf{B}_{18}	$\frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(6d)	Cl IV
\mathbf{B}_{19}	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(6d)	Cl IV
\mathbf{B}_{20}	$\frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}}$	(6d)	Cl IV
\mathbf{B}_{21}	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e)	Cl V
\mathbf{B}_{22}	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e)	Cl V
\mathbf{B}_{23}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e)	Cl V
\mathbf{B}_{24}	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e)	Cl V
\mathbf{B}_{25}	$\frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e)	Cl V
\mathbf{B}_{26}	$\frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(8e)	Cl V
\mathbf{B}_{27}	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(8e)	Cl V

$$\mathbf{B}_{221} = \begin{pmatrix} -(z_{13} - \frac{1}{2}) \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a(z_{13} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} + \\ a(x_{13} + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} \quad (481) \quad \text{S II}$$

$$\mathbf{B}_{222} = \begin{pmatrix} -(z_{13} - \frac{1}{2}) \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 - \\ (x_{13} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a(z_{13} - \frac{1}{2}) \hat{\mathbf{x}} + a(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - \\ a(x_{13} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} \quad (481) \quad \text{S II}$$

$$\mathbf{B}_{223} = \begin{pmatrix} (z_{13} + \frac{1}{2}) \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 - \\ (x_{13} - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(z_{13} + \frac{1}{2}) \hat{\mathbf{x}} - a(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} - \\ a(x_{13} - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} \quad (481) \quad \text{S II}$$

$$\mathbf{B}_{224} = \begin{pmatrix} (z_{13} + \frac{1}{2}) \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} a(z_{13} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} + \\ a(x_{13} + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} \quad (481) \quad \text{S II}$$

References

- [1] V. A. Khudolii, V. V. Pan'ko, M. S. Shelemba, L. I. Lopit, A. S. Fedor, and Y. V. Voroshilov, *Phase Equilibria in the Systems HgS-HgSe-HgCl₂(HgBr₂)*, Russ. J. Inorg. Chem. **38**, 1479–1480 (1993).
- [2] E. H. Carlson, *The growth of HgS and Hg₃S₂Cl₂ single crystals by a vapor phase method* **1**, 271–277 (1967), doi:10.1016/0022-0248(67)90033-4.

Found in

- [1] S. A. Magarill, N. V. Pervukhina, S. V. Borisov, and N. A. Pal'chik, *Crystal chemistry and features of the structure formation of mercury oxo- and chalcogenides*, Russ. Chem. Rev. **76**, 101–131 (2007), doi:10.1070/RC2007v076n02ABEH003653.