

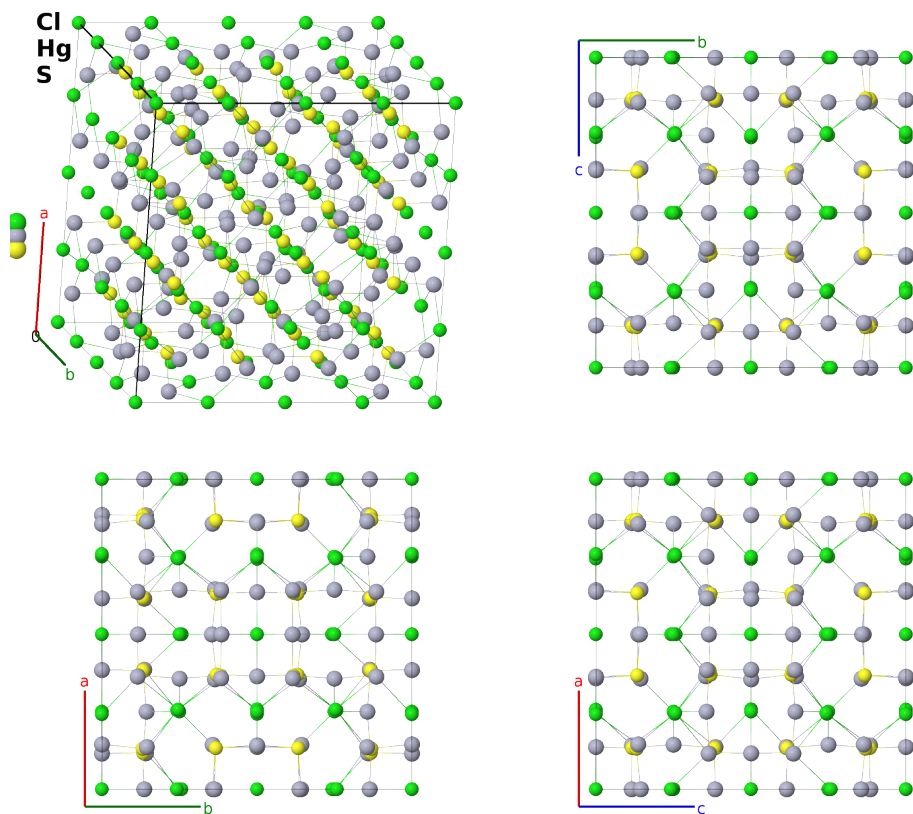
β -Hg₃S₂Cl₂ Structure: A2B3C2_cP224_223_abcdefk_j3k_il-001

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<https://aflow.org/prototype-encyclopedia/UWQ4>

https://aflow.org/prototype-encyclopedia/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
CCDC	1643454
Pearson symbol	cP224
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<pre>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</pre>

- $\text{Hg}_3\text{Cl}_2\text{S}_2$ is found in three forms (Carlson, 1967):

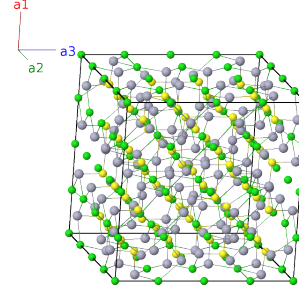
- Corderoite ($\alpha\text{-Hg}_3\text{Cl}_2\text{S}_2$), the cubic ground state.
- $\beta\text{-Hg}_3\text{Cl}_2\text{S}_2$, which appears above 340°C , another cubic phase with a much larger unit cell. (this structure)
- Kenhsuite ($\gamma\text{-Hg}_3\text{Cl}_2\text{S}_2$), which on average has an 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

[illegible]

[illegible]

[illegible]

$$\begin{aligned}
\mathbf{B}_{220} &= -\left(x_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_3 = -a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (48l) & \text{S II} \\
\mathbf{B}_{221} &= -\left(z_{13} - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_3 = -a\left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} & (48l) & \text{S II} \\
\mathbf{B}_{222} &= -\left(z_{13} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_3 = -a\left(z_{13} - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (48l) & \text{S II} \\
\mathbf{B}_{223} &= \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{13} - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_{13} - \frac{1}{2}\right) \mathbf{a}_3 = a\left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_{13} - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_{13} - \frac{1}{2}\right) \hat{\mathbf{z}} & (48l) & \text{S II} \\
\mathbf{B}_{224} &= \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{13} + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_{13} + \frac{1}{2}\right) \mathbf{a}_3 = a\left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_{13} + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} & (48l) & \text{S II}
\end{aligned}$$

References

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