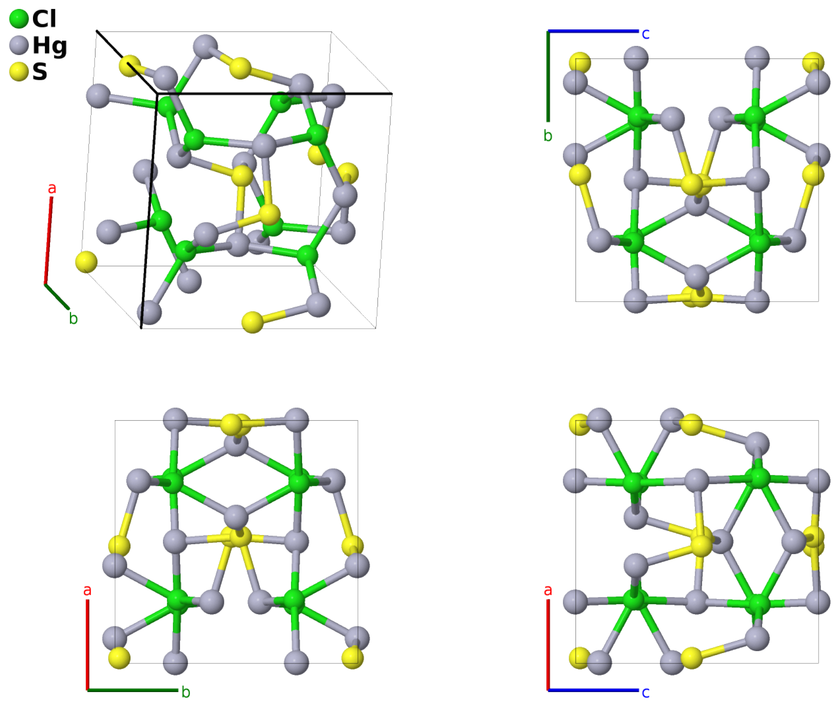
Corderoite (α-$Hg_3S_2Cl_2$) Structure: A2B3C2_cI28_199_a_b_a-002

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/VYHG

https://aflow.org/p/A2B3C2_cI28_199_a_b_a-002



Prototype	$Cl_2Hg_3S_2$
AFLOW prototype label	A2B3C2_cI28_199_a_b_a-002
Mineral name	corderoite
ICSD	27399
Pearson symbol	cI28
Space group number	199
Space group symbol	$I2_13$
AFLOW prototype command	`aflow --proto=A2B3C2_cI28_199_a_b_a-002` `--params=`a, x_1, x_2, x_3

Other compounds with this structure

$Hg_3S_2F_2$, $Hg_3S_2I_2$, $Hg_3Se_2F_2$, $Hg_3Se_2Cl_2$, $Hg_3Te_2Br_2$, $Hg_3Te_2Cl_2$, $K_2Pb_2O_3$, $K_2Sn_2O_3$, $Pd_3S_2Bi_2$

- $Hg_3Cl_2S_2$ is found in three forms (Carlson, 1967):
  - Corderoite (α-$Hg_3Cl_2S_2$), the cubic ground state. (this structure)

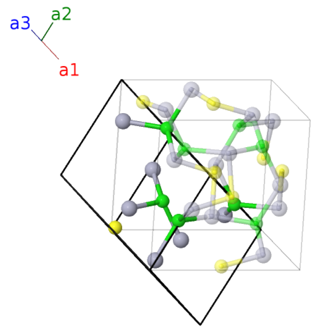
– β-$Hg_3Cl_2S_2$, which appears above 340°C, another cubic phase with a much larger unit cell.

– Kenhsuite (γ-$Hg_3Cl_2S_2$), which on average has an orthorhombic lattice. This state is apparently metastable.

- Corderoite is a cubic variant of the parkerite ($Ni_3Bi_2S_2$) structure.

Body-centered Cubic primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{2}a\,\mathbf{\hat{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\mathbf{\hat{x}} - \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{2}a\,\mathbf{\hat{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}} - \frac{1}{2}a\,\mathbf{\hat{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$2x_1\,\mathbf{a}_1 + 2x_1\,\mathbf{a}_2 + 2x_1\,\mathbf{a}_3$	=	$ax_1\,\mathbf{\hat{x}} + ax_1\,\mathbf{\hat{y}} + ax_1\,\mathbf{\hat{z}}$	(8a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\mathbf{\hat{x}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + ax_1\,\mathbf{\hat{z}}$	(8a)	Cl I
$\mathbf{B_3}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_1\,\mathbf{\hat{y}} - ax_1\,\mathbf{\hat{z}}$	(8a)	Cl I
$\mathbf{B_4}$	=	$-\left(2x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_1\,\mathbf{\hat{x}} - ax_1\,\mathbf{\hat{y}} - a\left(x_1 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8a)	Cl I
$\mathbf{B_5}$	=	$2x_2\,\mathbf{a}_1 + 2x_2\,\mathbf{a}_2 + 2x_2\,\mathbf{a}_3$	=	$ax_2\,\mathbf{\hat{x}} + ax_2\,\mathbf{\hat{y}} + ax_2\,\mathbf{\hat{z}}$	(8a)	S I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\mathbf{\hat{x}} - a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + ax_2\,\mathbf{\hat{z}}$	(8a)	S I
$\mathbf{B_7}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_2\,\mathbf{\hat{y}} - ax_2\,\mathbf{\hat{z}}$	(8a)	S I
$\mathbf{B_8}$	=	$-\left(2x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$ax_2\,\mathbf{\hat{x}} - ax_2\,\mathbf{\hat{y}} - a\left(x_2 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(8a)	S I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{z}}$	(12b)	Hg I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} + \frac{1}{2}a\,\mathbf{\hat{y}} + \frac{1}{4}a\,\mathbf{\hat{z}}$	(12b)	Hg I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}}$	(12b)	Hg I
$\mathbf{B_{12}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}} + \frac{1}{2}a\,\mathbf{\hat{z}}$	(12b)	Hg I
$\mathbf{B_{13}}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\mathbf{\hat{y}} + ax_3\,\mathbf{\hat{z}}$	(12b)	Hg I
$\mathbf{B_{14}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{1}{4}a\,\mathbf{\hat{y}} - ax_3\,\mathbf{\hat{z}}$	(12b)	Hg I

References

[1] H. Puff and J. Küster, *Quecksilberchalkogenid-halogenide*, Naturwissenschaften **49**, 299 (1962), doi:10.1007/BF00622707.

[2] E. H. Carlson, *The growth of HgS and $Hg_3S_2Cl_2$ single crystals by a vapor phase method* **1**, 271–277 (1967), doi:10.1016/0022-0248(67)90033-4.

Found in

[1] E. H. Carlson, *The growth of HgS and $Hg_3S_2Cl_2$ single crystals by a vapor phase method*, J. Cryst. Growth **1**, 271–277 (1967), doi:10.1016/0022-0248(67)90033-4.