

Coccinite (Red HgI_2 , $C13$) Structure: AB2_tP6_137_a_d-001

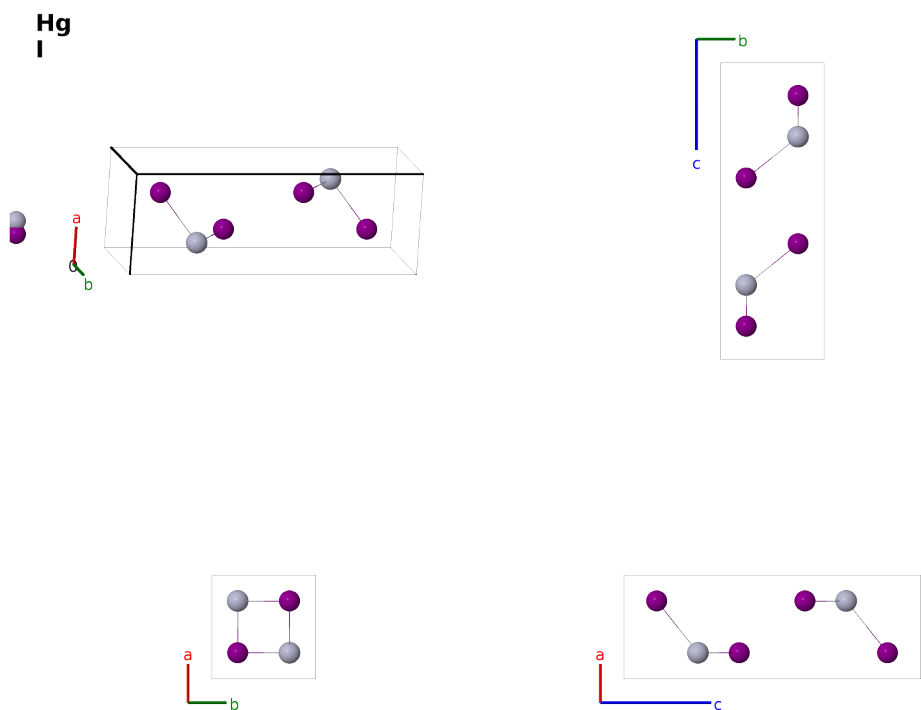
This structure previously used the label(s) **AB2_tP6_137_a_d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/2F93>

https://aflow.org/prototype-encyclopedia/AB2_tP6_137_a_d-001



Prototype	HgI_2
AFLOW prototype label	AB2_tP6_137_a_d-001
<i>Strukturbericht</i> designation	$C13$
Mineral name	coccinite
ICSD	241175
CCDC	1711650
Pearson symbol	tP6
Space group number	137

Space group symbol $P4_2/nmc$

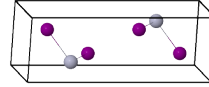
AFLOW prototype command `aflow --proto=AB2_tP6_137_a_d-001
--params=a,c/a,z2`

- HgI₂ can be found in a variety of forms (Gumiński, 1997):
 - The ground state, coccinite (this structure), also known as red or α -HgI₂ and given the *Strukturbericht* designation C13. It is stable up to 135°C.
 - At higher temperatures this transforms into yellow or β -HgI₂ in the HgBr₂ (C24) structure. This is stable up to the melting point at 258°C.
 - (Schwarzenbach, 1969) studied the metastable orange HgI₂ body-centered tetragonal ($I4_1/amd$ #141) phase. This structure was refined by (Hostettler, 2002).
 - (Hostettler, 2002) also found a second orange HgI₂ phase in a simple tetragonal ($P4_2/nmc$ #137) cell.
 - The last two structures differ by stacking order. (Hostettler, 2002) used them to produce an averaged orange HgI₂ structure, space group $P4m2$ #115.
- We use the data for coccinite taken by (Schwarzenbach, 2007) at 293 K.
- The CIF and POSCAR files contain the data at room temperature, 293 K. ZrO₂ (A2B_tP6_137_d_a) and HgI₂ (AB2_tP6_137_a_d) have similar AFLOW prototype labels (i.e., same symmetry and set of Wyckoff positions with different stoichiometry labels due to alphabetic ordering of atomic species). They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files

Simple Tetragonal primitive vectors

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

$\mathbf{a}_1$
 $\mathbf{a}_2$ $\mathbf{a}_3$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(2a)	Hg I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(2a)	Hg I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(4d)	I I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	I I
$\mathbf{B}_5$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(4d)	I I
$\mathbf{B}_6$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4d)	I I

References

- [1] D. Schwarzenbach, H. Birkedal, M. Hostettler, and P. Fischer, *Neutron diffraction investigation of the temperature dependence of crystal structure and thermal motions of red HgI₂*, Acta Crystallogr. Sect. B **63**, 826–835 (2007), doi:10.1107/S0108768107043327.

- [2] M. Hostettler, H. Birkedal, and D. Schwarzenbach, *The structure of orange HgI₂. I. Polytypic layer structure*, Acta Crystallogr. Sect. B **58**, 903–913 (2002), doi:10.1107/S010876810201618X.
- [3] D. Schwarzenbach, *The crystal structure and one-dimensional disorder of the orange modification of HgI₂*, Z. Kristallogr. **128**, 97–114 (1969), doi:10.1524/zkri.1969.128.1-2.97.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

First cited in

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