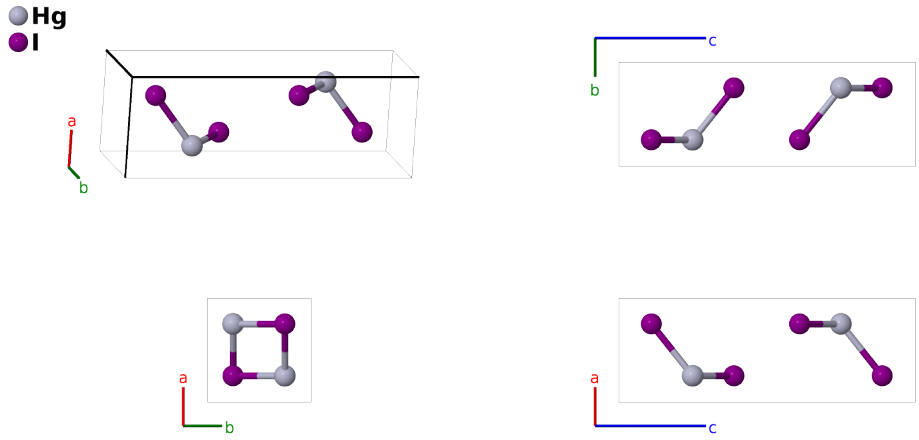
Coccinite (Red HgI_2, $C13$) Structure: AB2_tP6_137_a_d-001

This structure originally had the label `AB2_tP6_137_a_d`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/2F93

https://aflow.org/p/AB2_tP6_137_a_d-001



Prototype	HgI_2
AFLOW prototype label	AB2_tP6_137_a_d-001
***Strukturbericht* designation**	$C13$
Mineral name	coccinite
ICSD	241175
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=`$a, c/a, z_2$

- HgI_2 can be found in a variety of forms (Gumiński, 1997):
  - The ground state, coccinite (this structure), also known as red or α-HgI_2 and given the *Strukturbericht* designation $C13$. It is stable up to 135°C.
  - At higher temperatures this transforms into yellow or β-HgI_2 in the $HgBr_2$ ($C24$) structure. This is stable up to the melting point at 258°C.
  - (Schwarzenbach, 1969) studied the metastable orange HgI_2 body-centered tetragonal ($I4_1/amd$ #141) phase. This structure was refined by (Hostettler, 2002).
  - (Hostettler, 2002) also found a second orange HgI_2 phase in a simple tetragonal ($P4_2/nmc$ #137) cell.

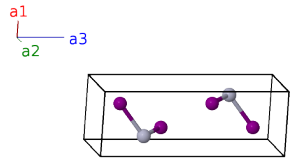
  - The last two structures differ by stacking order. (Hostettler, 2002) used them to produce an averaged orange HgI_2 structure, space group $P\bar{4}m2$ #115.

- 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. ZrO_2 (A2B_tP6_137_d_a) and HgI_2 (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

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4d)	I I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	I I
$\mathbf{B_5}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4d)	I I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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 HgI_2*, Acta Crystallogr. Sect. B **63**, 826–835 (2007), doi:10.1107/S0108768107043327.

[2] M. Hostettler, H. Birkedal, and D. Schwarzenbach, *The structure of orange HgI_2. 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 HgI_2*, 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).