Orange (averaged) HgI_2 Structure: AB2_tP12_115_j_egi-001

This structure previously used the label(s) `AB2_tP12_115_j_egi`. Calls to these addresses will be redirected here.

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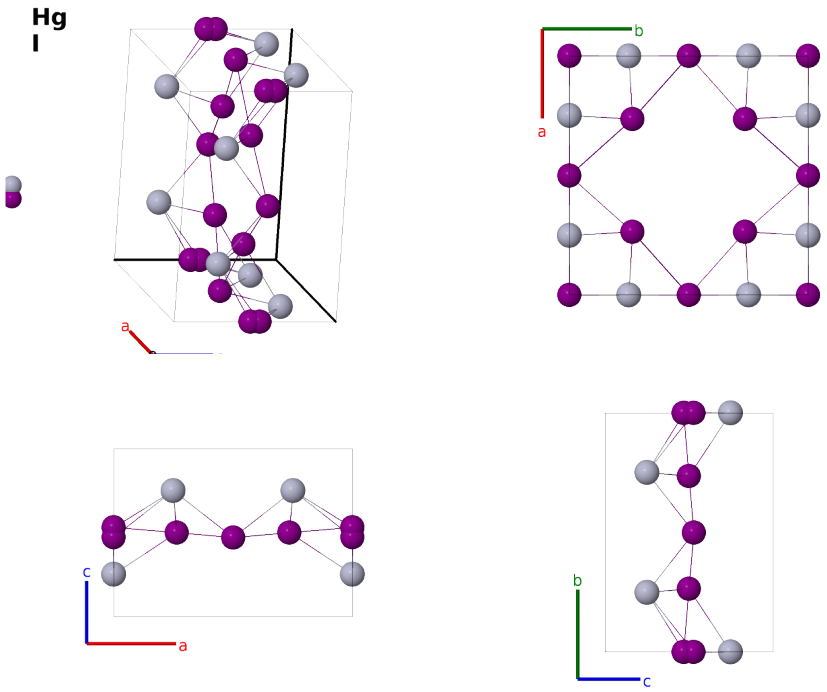
https://aflow.org/prototype-encyclopedia/RJ86

https://aflow.org/prototype-encyclopedia/AB2_tP12_115_j_egi-001



Prototype	HgI_2
AFLOW prototype label	AB2_tP12_115_j_egi-001
ICSD	95272
CCDC	1654679
Pearson symbol	tP12
Space group number	115
Space group symbol	$P\bar{4}m2$
AFLOW prototype command	`aflow --proto=AB2_tP12_115_j_egi-001 --params=`$a, c/a, z_1, z_2, x_3, x_4, z_4$

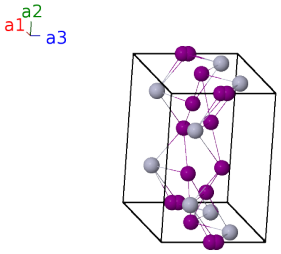
- HgI_2 can be found in a variety of forms (Gumiński, 1997):

  - The ground state, coccinite, 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 (this structure), space group $P\bar{4}m2$ #115.

- This structure is an "average" of the Orange I and Orange II structures. The averaging procedure places the iodine I atoms only 0.36Å apart, so this is not a physical structure. We retain it as an example of a structure in space group $P\bar{4}m2$ #115.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2e)	I I
$\mathbf{B_2}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(2e)	I I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2g)	I II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$	(2g)	I II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4i)	I III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4i)	I III
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4i)	I III
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4i)	I III
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4j)	Hg I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(4j)	Hg I
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4j)	Hg I
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(4j)	Hg I

References

[1] 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.

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[3] 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.

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First cited in

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