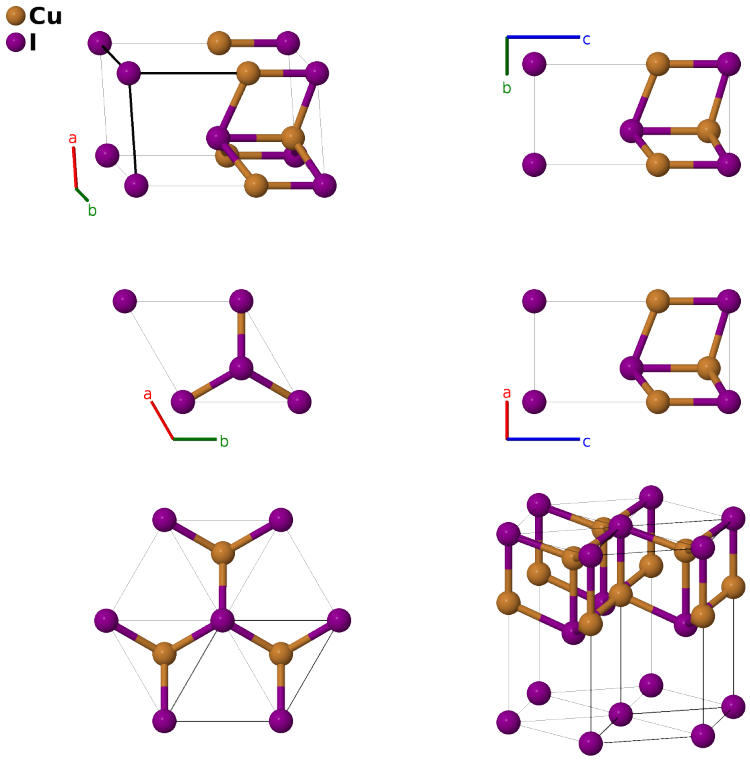
β-CuI (Sakuma) Structure: AB_hP4_156_ab_ab-001

This structure originally had the label `AB_hP4_156_ab_ab`. 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/1M22

https://aflow.org/p/AB_hP4_156_ab_ab-001



Prototype	CuI
AFLOW prototype label	AB_hP4_156_ab_ab-001
ICSD	84217
Pearson symbol	hP4
Space group number	156
Space group symbol	$P3m1$
AFLOW prototype command	`aflow --proto=AB_hP4_156_ab_ab-001 --params=`$a, c/a, z_1, z_2, z_3, z_4$

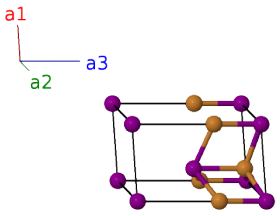
- Copper(I) iodide can be found in three forms (Keen, 1995):
  - α-CuI is stable above 673 ± 8K, and is in the δ-Bi_2O_3 structure, with the iodine atoms on the (2a) Wyckoff positions and the copper atoms occupying 1/8 of the (32f) positions.

- γ-CuI (marshite) is the ground state, stable below 643 ± 2K, and is also in the δ-Bi_2O_3 structure.
- In the intermediate temperature range β-CuI is generally agreed to be trigonal or hexagonal, but the exact structure is under dispute:
  * (Kurdyumova, 1961) placed it in trigonal space group $P3m1$ #156. Their unit cell is three times larger than the standard cell for this structure, and is now considered erroneous. (Abrahams, 2008).
  * (Bührer, 1977) placed it in hexagonal space group $P\bar{6}m2$ #187, with the copper atoms partially occupying two sites.
  * (Sakuma, 1988) placed it in trigonal space group $P3m1$ #156 (this structure) with a smaller unit cell than (Kurdyumova, 1961) and no disorder on the copper sites.
  * (Keen, 1994) placed it in trigonal space group $P\bar{3}m1$ #164, with a unit cell similar to (Bührer, 1977) and (Sakuma, 1988). Like the former paper, the oxygen positions are disordered.

- Space group $P3m1$ #156 allows an arbitary choice of origin for the z-axis. Used this freedom to place the I-I atom at the origin.
- This structure originally appeared in (Hicks, 2019). This page has been rewritten, but the structure itself has not changed.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(1a)	Cu I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(1a)	I I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(1b)	Cu II
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(1b)	I II

References

[1] T. Sakuma, *Crystal Structure of β-CuI*, J. Phys. Soc. Jpn. **57**, 565–569 (1988), doi:10.1143/JPSJ.57.565.

[2] R. N. Kurdyumova and R. V. Baranova, *An electron diffraction study of thin films of cuprous iodide*, Sov. Phys. Cryst. **6**, 318–321 (1961).

[3] W. Bührer and W. Hälg, *Crystal structure of high-temperature cuprous iodide and cuprous bromide*, Electrochimica Acta **22**, 701–704 (1977), doi:10.1016/0013-4686(77)80021-2.

[4] D. A. Keen and S. Hull, *Determination of the structure of β-CuI by high-resolution neutron powder diffraction*, J. Phys.: Condens. Matter **6**, 1637–1644 (1994), doi:10.1088/0953-8984/6/9/006.

[5] D. A. Keen and S. Hull, *The high-temperature structural behaviour of copper(I) iodide*, J. Phys.: Condens. Matter **7**, 5793–5804 (1995), doi:10.1088/0953-8984/7/29/007.

[6] 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–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

[1] S. C. Abrahams, *Inorganic structures in space group $P3m1$; coordinate analysis and systematic prediction of new ferroelectrics*, Acta Crystallogr. Sect. B **64**, 426–437 (2008), doi:10.1107/S0108768108018144.