β-CuI (Kurdyumova) Structure: AB_hP12_156_3a2bc_3a2bc-001

This structure originally had the label `AB_hP12_156_2ab3c_2ab3c`. Calls to that address will be redirected here.

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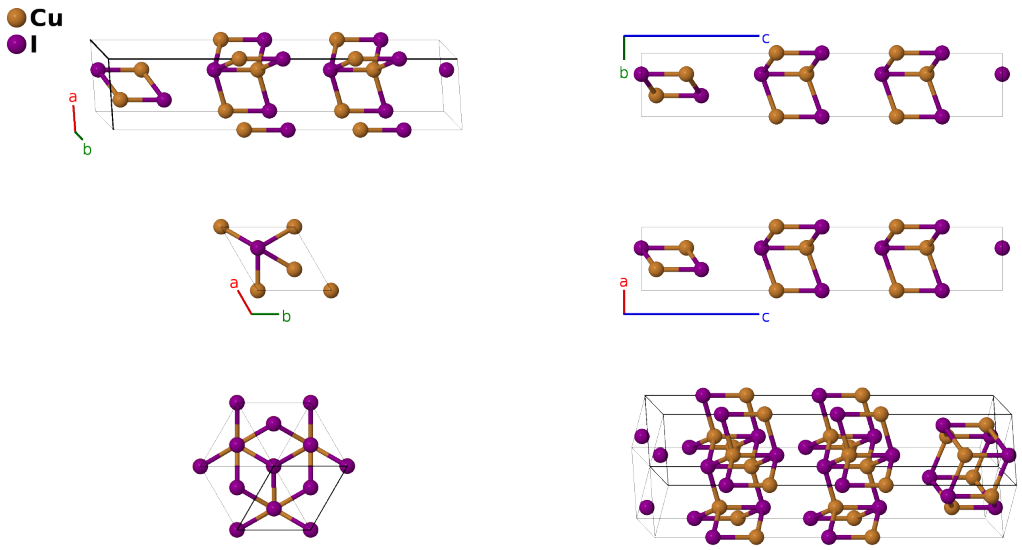
https://aflow.org/p/ZMXD

https://aflow.org/p/AB_hP12_156_3a2bc_3a2bc-001



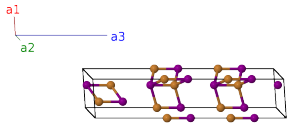
Prototype	CuI
AFLOW prototype label	AB_hP12_156_3a2bc_3a2bc-001
ICSD	30363
Pearson symbol	hP12
Space group number	156
Space group symbol	$P3m1$
AFLOW prototype command	`aflow --proto=AB_hP12_156_3a2bc_3a2bc-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}, z_{11}, z_{12}$

- 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, which is three times larger than the standard cell for this structure and is now considered erroneous, is the one listed on this page. (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 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-III 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)	Cu II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(1a)	Cu III
$\mathbf{B_4}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(1a)	I I
$\mathbf{B_5}$	=	$z_5\,\mathbf{a}_3$	=	$cz_5\,\hat{\mathbf{z}}$	(1a)	I II
$\mathbf{B_6}$	=	$z_6\,\mathbf{a}_3$	=	$cz_6\,\hat{\mathbf{z}}$	(1a)	I III
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(1b)	Cu IV
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(1b)	Cu V
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(1b)	I IV
$\mathbf{B_{10}}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(1b)	I V
$\mathbf{B_{11}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(1c)	Cu VI
$\mathbf{B_{12}}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}}$	(1c)	I VI

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