β-CuI (Bührer-Hälg) Structure: A2B_hP6_187_gi_ad-001

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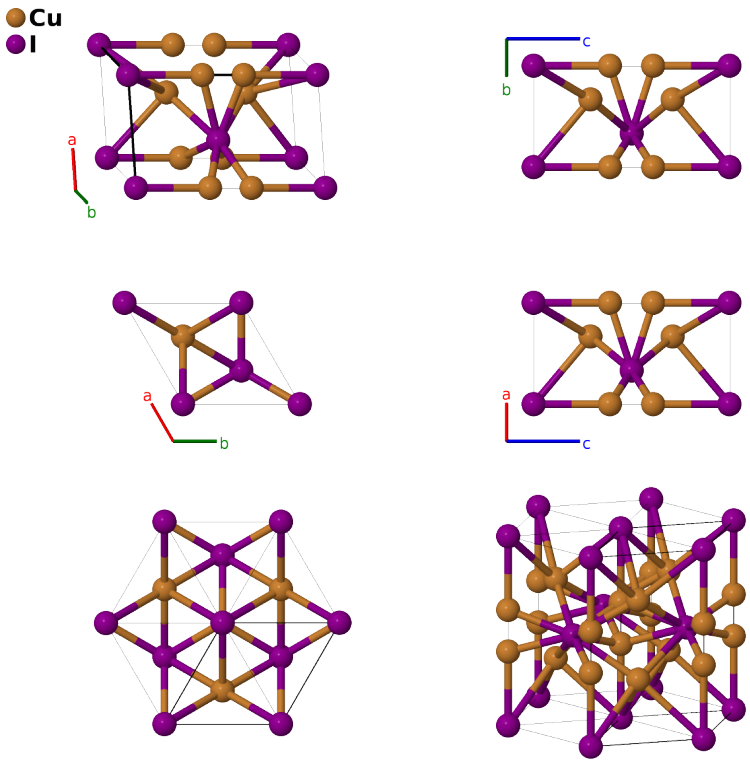
https://aflow.org/p/P31P

https://aflow.org/p/A2B_hP6_187_gi_ad-001



Prototype	CuI
AFLOW prototype label	A2B_hP6_187_gi_ad-001
ICSD	30088
Pearson symbol	hP6
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=A2B_hP6_187_gi_ad-001 --params=`$a, c/a, z_3, z_4$

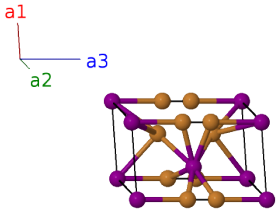
- Copper(I) iodide can be found in three forms (Keen, 1995):
  - α-CuI is stable above 673 ± 8K, and is in the δ-Bi_2O_3 structure, with the iodine atoms on the (2a) Wyckoff positions and the copper atoms occupying 1/8 of the (32f) positions.
  - γ-CuI (marshite) is the ground state, stable below 643 ± 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 (this structure), 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.

- The data from (Bührer, 1977) was taken at 653K.
- The copper sites are only partially occupied: Cu-I (2g) is 70% filled, with the remaining 30% of the copper atoms going on the Cu-II (2i) site.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	I I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	I II
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2g)	Cu I
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2g)	Cu I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2i)	Cu II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2i)	Cu II

References

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