β-CuI (Keen-Hull) Structure: A2B_hP6_164_2d_d-001

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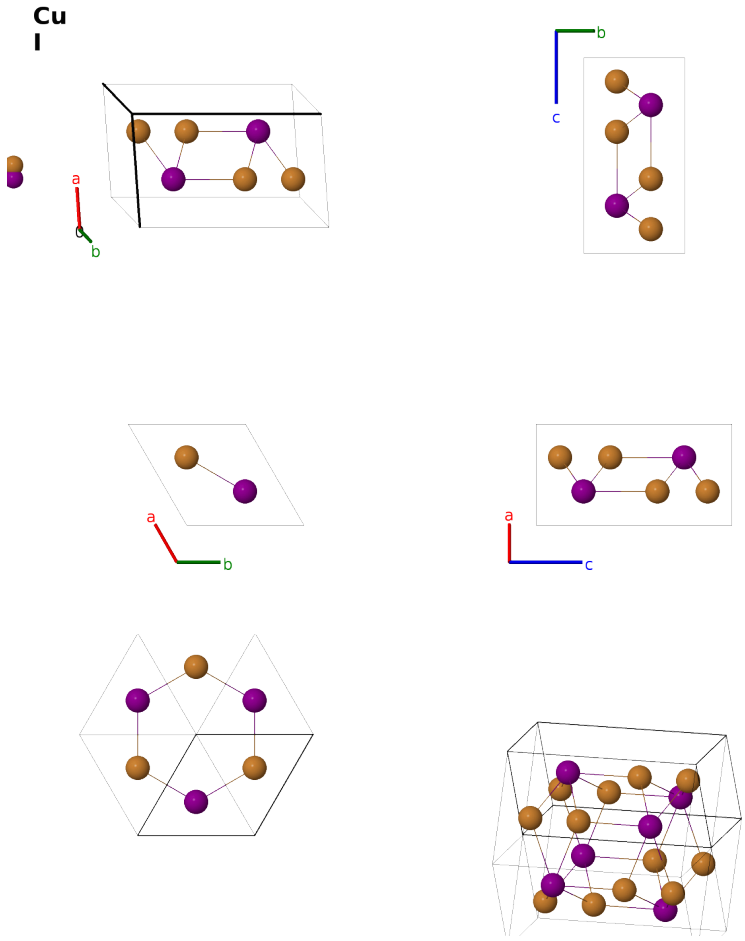
https://aflow.org/prototype-encyclopedia/TVVQ

https://aflow.org/prototype-encyclopedia/A2B_hP6_164_2d_d-001



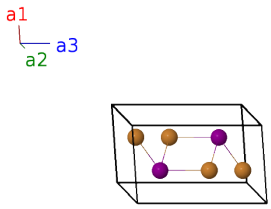
Prototype	CuI
AFLOW prototype label	A2B_hP6_164_2d_d-001
ICSD	78429
CCDC	1638708
Pearson symbol	hP6
Space group number	164
Space group symbol	$P\bar{3}m1$

AFLOW prototype command `aflow --proto=A2B_hP6_164_2d_d-001 --params=`$a, c/a, z_1, z_2, z_3$

- 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 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 (this structure), with a unit cell similar to (Bührer, 1977) and (Sakuma, 1988). Like the former paper, the oxygen positions are disordered.
- The data from (Keen, 1994) was taken at 655K.
- The copper sites are only partially occupied: Cu-I (2d) is 85.1% filled, with the remaining 14.9% of the copper atoms going on the Cu-II (2d) site.

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
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2d)	Cu I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2d)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	Cu II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	Cu II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	I I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	I I

References

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First cited in

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