# $\beta$-CuI (Keen-Hull) Structure: A2B_hP6_164_2d_d-001

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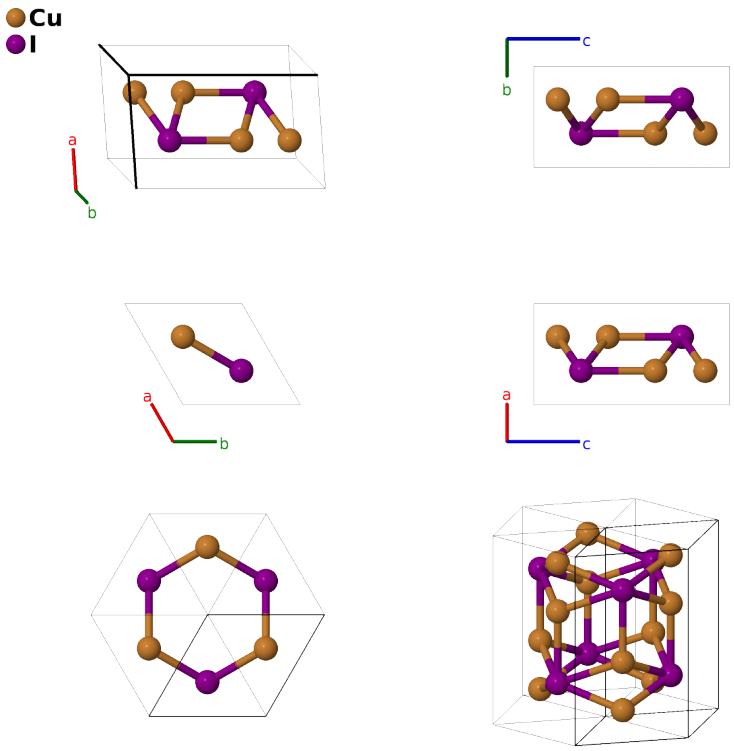
https://aflow.org/p/TVVQ

https://aflow.org/p/A2B_hP6_164_2d_d-001




| | |
|---|---|
| **Prototype** | CuI |
| **AFLOW prototype label** | A2B_hP6_164_2d_d-001 |
| **ICSD** | 78429 |
| **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):
  - $\alpha$-CuI is stable above $673 \pm 8$K, and is in the $\delta$-$Bi_2O_3$ structure, with the iodine atoms on the (2a) Wyckoff positions and the copper atoms occupying 1/8 of the (32f) positions.
  - $\gamma$-CuI (marshite) is the ground state, stable below $643 \pm 2$K, and is also in the $\delta$-$Bi_2O_3$ structure.

– In the intermediate temperature range $\beta$-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.

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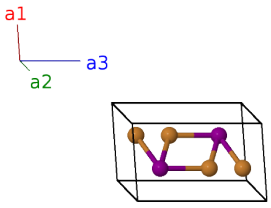
**Trigonal (Hexagonal) primitive vectors**

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

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**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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[4] 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.

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**Found in**

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