# $CuN_8$ Structure: AB8_oI36_46_b_a3b2c-001

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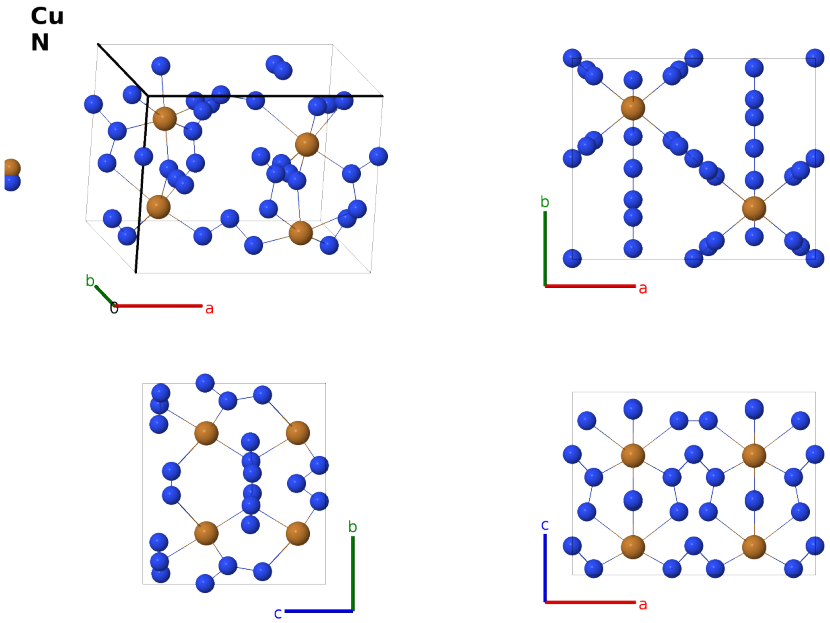
https://aflow.org/prototype-encyclopedia/159P

https://aflow.org/prototype-encyclopedia/AB8_oI36_46_b_a3b2c-001




| | |
|---|---|
| **Prototype** | $CuN_8$ |
| **AFLOW prototype label** | AB8_oI36_46_b_a3b2c-001 |
| **ICSD** | 9713 |
| **CCDC** | 2134216 |
| **Pearson symbol** | oI36 |
| **Space group number** | 46 |
| **Space group symbol** | $Ima2$ |
| **AFLOW prototype command** | `aflow --proto=AB8_oI36_46_b_a3b2c-001 --params=`$a, b/a, c/a, z_1, y_2, z_2, y_3, z_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$ |

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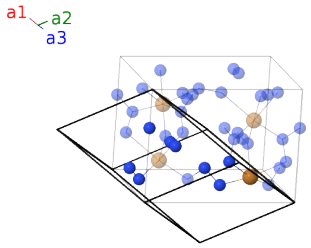
- The ICSD puts this into the TiFeSi structure type, but the only thing the two structures share is the space group and the Wyckoff positions occupied.
- (Xu, 2018) only give interatomic distances, not the coordinates. Fortunately the ICSD entry has atomic coordinates, and we use these. We have checked these to verify that the structure presented here is in reasonable agreement with these distances.

## Body-centered Orthorhombic primitive vectors

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




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$ | = | $cz_1\,\hat{\mathbf{z}}$ | (4a) | N I |
| $\mathbf{B_2}$ | = | $z_1\,\mathbf{a}_1 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_1\,\hat{\mathbf{z}}$ | (4a) | N I |
| $\mathbf{B_3}$ | = | $(y_2 + z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_2 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4b) | Cu I |
| $\mathbf{B_4}$ | = | $-(y_2 - z_2)\,\mathbf{a}_1 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_2 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (4b) | Cu I |
| $\mathbf{B_5}$ | = | $(y_3 + z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (4b) | N II |
| $\mathbf{B_6}$ | = | $-(y_3 - z_3)\,\mathbf{a}_1 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (4b) | N II |
| $\mathbf{B_7}$ | = | $(y_4 + z_4)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4b) | N III |
| $\mathbf{B_8}$ | = | $-(y_4 - z_4)\,\mathbf{a}_1 + \left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_4 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4b) | N III |
| $\mathbf{B_9}$ | = | $(y_5 + z_5)\,\mathbf{a}_1 + \left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_2 + \left(y_5 + \frac{1}{4}\right)\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4b) | N IV |
| $\mathbf{B_{10}}$ | = | $-(y_5 - z_5)\,\mathbf{a}_1 + \left(z_5 + \frac{3}{4}\right)\,\mathbf{a}_2 - \left(y_5 - \frac{3}{4}\right)\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4b) | N IV |
| $\mathbf{B_{11}}$ | = | $(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | N V |
| $\mathbf{B_{12}}$ | = | $-(y_6 - z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | N V |
| $\mathbf{B_{13}}$ | = | $-(y_6 - z_6)\,\mathbf{a}_1 + \left(x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 - y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | N V |
| $\mathbf{B_{14}}$ | = | $(y_6 + z_6)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8c) | N V |
| $\mathbf{B_{15}}$ | = | $(y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3$ | = | $ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | N VI |
| $\mathbf{B_{16}}$ | = | $-(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3$ | = | $-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | N VI |

| | | | | | | |
|---|---|---|---|---|---|---|
| $\mathbf{B_{17}}$ | = | $-\left(y_7 - z_7\right)\,\mathbf{a}_1 + \left(x_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_7 - y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $a\left(x_7 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | N VI |
| $\mathbf{B_{18}}$ | = | $\left(y_7 + z_7\right)\,\mathbf{a}_1 + \left(-x_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_7 + y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8c) | N VI |

## References


[1] Y. Xu, Q. Lin, P. Wang, and M. Lu, *Syntheses, Crystal Structures and Properties of a Series of 3D Metal–Inorganic Frameworks Containing Pentazolate Anion*, Chem. Asian J. **13**, 1669–1673 (2018), doi:10.1002/asia.201800476.


## Found in


[1] ICSD, *Inorganic Crystal Structure Database [CuN8]*. ID 9713.


## First cited in


N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).