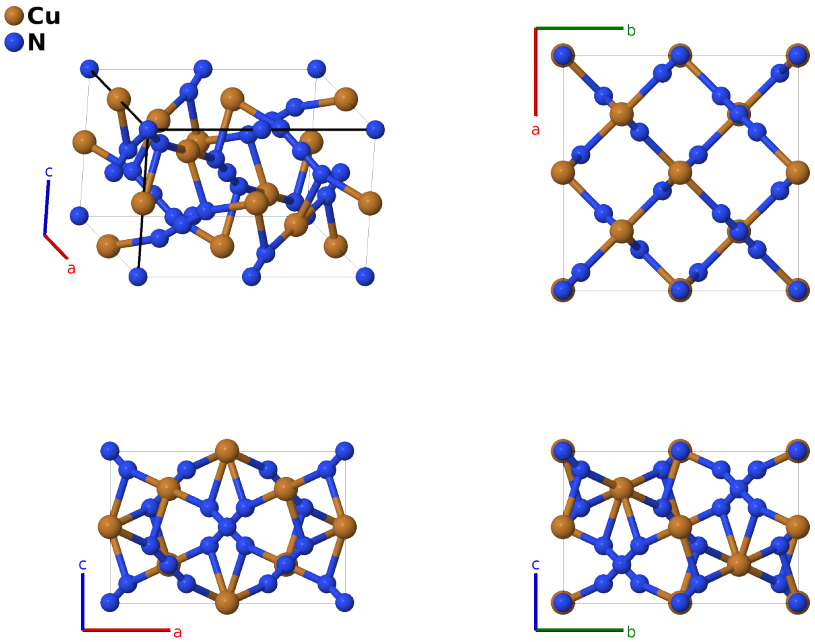
Copper (I) Azide (CuN_3) Structure: AB3_tI32_88_c_df-001

This structure originally had the label `AB3_tI32_88_d_cf`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/L0WX

https://aflow.org/p/AB3_tI32_88_c_df-001



Prototype	CuN_3
AFLOW prototype label	AB3_tI32_88_c_df-001
Mineral name	copper (I) azide
ICSD	30633
Pearson symbol	tI32
Space group number	88
Space group symbol	$I4_1/a$
AFLOW prototype command	`aflow --proto=AB3_tI32_88_c_df-001 --params=`$a, c/a, x_3, y_3, z_3$

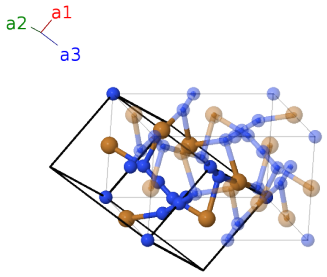
Other compounds with this structure
AgN_3, TiN_3

- Not to be confused with Copper (II) Azide, $Cu(N_3)_2$, an explosive.

- (Wilsdorf, 1948) gave the Wyckoff positions in setting 1 of space group $P4_1/a$ #88. We used findsym to translate this to the standard setting 2.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(8c)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(8c)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	Cu I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	N I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(8d)	N I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8d)	N I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(8d)	N I
$\mathbf{B_9}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + (x_3 + y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{10}}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - \left(x_3 + y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{11}}$	=	$\left(x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - (y_3 - z_3)\,\mathbf{a}_2 + (x_3 - y_3)\,\mathbf{a}_3$	=	$-a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{12}}$	=	$\left(-x_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{13}}$	=	$-(y_3 + z_3)\,\mathbf{a}_1 - (x_3 + z_3)\,\mathbf{a}_2 - (x_3 + y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{14}}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_3 - z_3)\,\mathbf{a}_2 + \left(x_3 + y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{15}}$	=	$-\left(x_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + (y_3 - z_3)\,\mathbf{a}_2 - (x_3 - y_3)\,\mathbf{a}_3$	=	$a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16f)	N II
$\mathbf{B_{16}}$	=	$\left(x_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3 + z_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3 - y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16f)	N II

References

[1] H. Wilsdorf, *Die Kristallstruktur des einwertigen Kupferazids,* CuN_3, Acta Cryst. **1**, 115–118 (1948), doi:10.1107/S0365110X48000314.

Found in

[1] W. Zhu and H. Xiao, *Ab initio study of electronic structure and optical properties of heavy-metal azides:* TlN_3, AgN_3, *and* CuN_3, J. Comput. Chem. **29**, 176–184 (2008), doi:10.1002/jcc.20682.