

CuBi₂O₄ Structure:

A2BC4_tP28_130_f_c-g-001

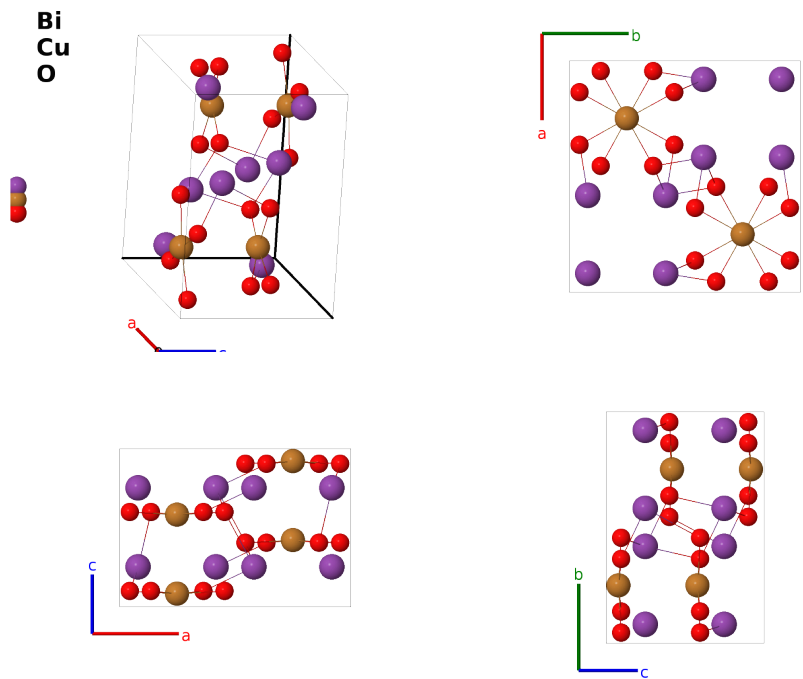
This structure previously used the label(s) **A2BC4_tP28_130_f_c-g**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/N4MV>

https://aflow.org/prototype-encyclopedia/A2BC4_tP28_130_f_c-g-001

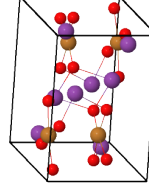


Prototype	Bi ₂ CuO ₄
AFLOW prototype label	A2BC4_tP28_130_f_c-g-001
ICSD	15865
CCDC	1596544
Pearson symbol	tP28
Space group number	130
Space group symbol	<i>P4/ncc</i>
AFLOW prototype command	<code>aflow --proto=A2BC4_tP28_130_f_c-g-001</code> <code>--params=a, c/a, z₁, x₂, x₃, y₃, z₃</code>

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$

a1
a2
a3



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c (z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_3$	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_6$	$= - (x_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_7$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_9$	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_{10}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_{11}$	$= - (x_2 - \frac{1}{2}) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a (x_2 - \frac{1}{2}) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_{12}$	$= x_2 \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a (x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(8f)	Bi I
$\mathbf{B}_{13}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{14}$	$= - (x_3 - \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a (x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{15}$	$= - (y_3 - \frac{1}{2}) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a (y_3 - \frac{1}{2}) \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{16}$	$= y_3 \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a y_3 \hat{\mathbf{x}} - a (x_3 - \frac{1}{2}) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{17}$	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{18}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{19}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{20}$	$= -y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - a y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{22}$	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{23}$	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a (y_3 + \frac{1}{2}) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{24}$	$= -y_3 \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a y_3 \hat{\mathbf{x}} + a (x_3 + \frac{1}{2}) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(16g)	O I
$\mathbf{B}_{25}$	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - a (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(16g)	O I

$$\mathbf{B}_{26} = \begin{matrix} -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 + \\ \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16g) \quad \text{O I}$$

$$\mathbf{B}_{27} = \begin{matrix} -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \\ \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16g) \quad \text{O I}$$

$$\mathbf{B}_{28} = y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 = ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16g) \quad \text{O I}$$

References

- [1] J.-C. Boivin, J. Tréhoux, and D. Thomas, *Étude structurale de CuBi_2O_4* , Bull. Soc. fr. Mineral. Cristallog. **99**, 193–196 (1976), doi:10.3406/bulmi.1976.7065.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

- D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043