

Paramelaconite (Cu₄O₃) Structure:

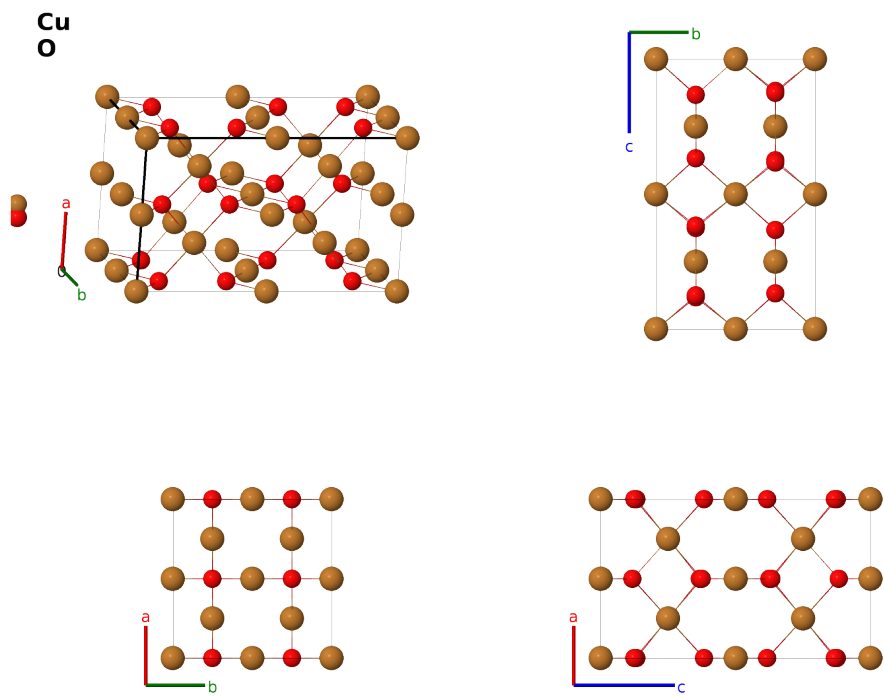
A4B3_tI28_141_cd_ae-002

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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/P57T>

https://aflow.org/prototype-encyclopedia/A4B3_tI28_141_cd_ae-002

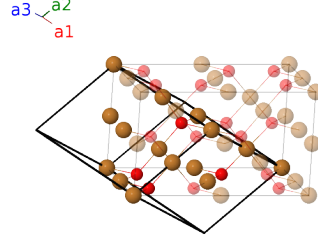


Prototype	Cu ₄ O ₃
AFLOW prototype label	A4B3_tI28_141_cd_ae-002
Mineral name	paramelaconite
ICSD	100566
CCDC	1659698
Pearson symbol	tI28
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	<code>aflow --proto=A4B3_tI28_141_cd_ae-002</code> <code>--params=a, c/a, z₄</code>

- (O’Keeffe, 1968) indicate that the atom they call O(2) (our O-I) is located at the (4a) Wyckoff position, but give the coordinates of the (4b) Wyckoff position. The coordinates are correct, however we shift the origin so that the O-I atom is on the (4a) site. This maps their atom Cu(1) to our Cu-II, and Cu(2) to Cu-I.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates		Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{y}} + \frac{1}{8}c \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_2$	$= \frac{1}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} + \frac{3}{8}c \hat{\mathbf{z}}$		(4a)	O I
$\mathbf{B}_3$	$= 0$	$=$	0		(8c)	Cu I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}}$		(8c)	Cu I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$		(8c)	Cu I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - \frac{1}{4}c \hat{\mathbf{z}}$		(8c)	Cu I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}c \hat{\mathbf{z}}$		(8d)	Cu II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$		(8d)	Cu II
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$		(8d)	Cu II
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$		(8d)	Cu II
$\mathbf{B}_{11}$	$= \left(z_4 + \frac{1}{4}\right) \mathbf{a}_1 + z_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$		(8e)	O II
$\mathbf{B}_{12}$	$= z_4 \mathbf{a}_1 + \left(z_4 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}}$		(8e)	O II
$\mathbf{B}_{13}$	$= -\left(z_4 - \frac{3}{4}\right) \mathbf{a}_1 - z_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$		(8e)	O II
$\mathbf{B}_{14}$	$= -z_4 \mathbf{a}_1 - \left(z_4 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}}$		(8e)	O II

References

- [1] M. O’Keeffe and J.-O. Brovin, *The crystal structure of paramelaconite, Cu_4O_3* , Am. Mineral. **63**, 180–185 (1978).

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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.