$CuTeO_4$ Structure: AB4C_mP24_14_ac_4e_e-001

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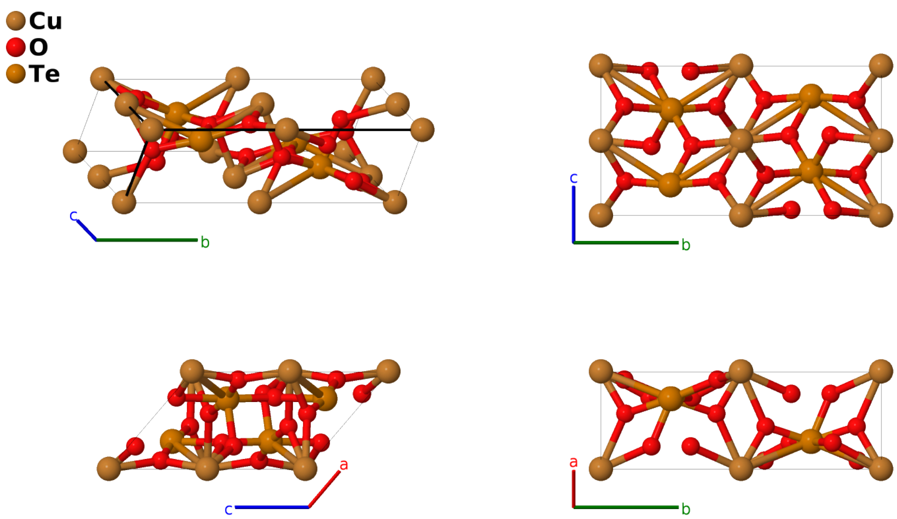
https://aflow.org/p/LRGD

https://aflow.org/p/AB4C_mP24_14_ac_4e_e-001

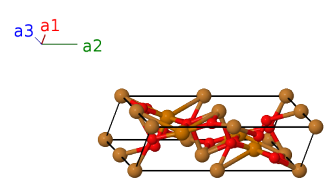


Prototype	CuO_4Te
AFLOW prototype label	AB4C_mP24_14_ac_4e_e-001
ICSD	1671
Pearson symbol	mP24
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=AB4C_mP24_14_ac_4e_e-001` `--params=`$a, b/a, c/a, \beta, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

- (Falck, 1978) give this structure in the $P2_1/n$ setting of space group #14. We used FINDSYM to transform this to our standard $P2_1/c$ structure.

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a_1} &= a\,\hat{\mathbf{x}} \\ \mathbf{a_2} &= b\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}} \end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(2c)	Cu II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{12}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{15}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{16}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{19}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{20}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	Te I
$\mathbf{B_{22}}$	=	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Te I
$\mathbf{B_{23}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	Te I
$\mathbf{B_{24}}$	=	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Te I

References

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