Tenorite (CuO, $B26$) Structure: AB_mC8_15_a_e-001

This structure previously used the label(s) `AB_mC8_15_c_e`. Calls to these addresses will be redirected here.

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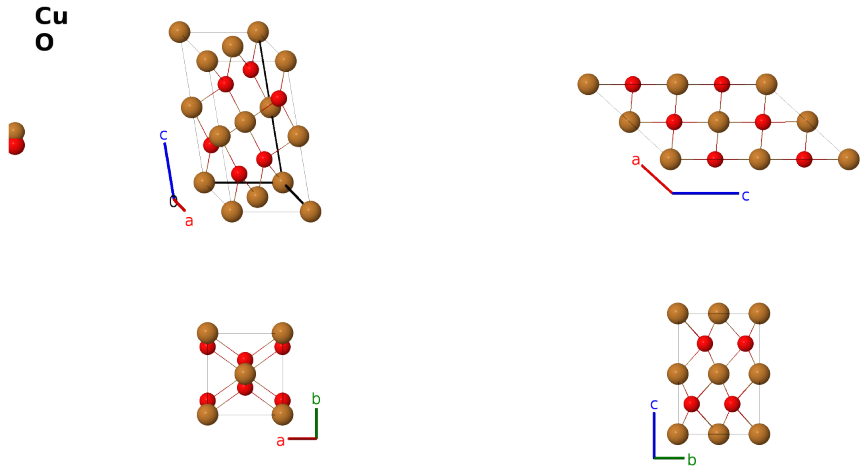
https://aflow.org/prototype-encyclopedia/HRJX

https://aflow.org/prototype-encyclopedia/AB_mC8_15_a_e-001



Prototype	CuO
AFLOW prototype label	AB_mC8_15_a_e-001
***Strukturbericht* designation**	$B26$
Mineral name	tenorite
ICSD	16025
CCDC	752807
Pearson symbol	mC8
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=AB_mC8_15_a_e-001 --params=`$a, b/a, c/a, \beta, y_2$

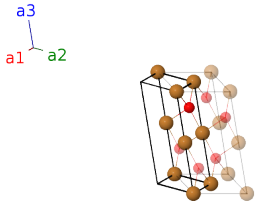
Other compounds with this structure
AgO

- In (Mehl, 2017) we inadvertently used $\beta = 120.34°$ rather than the correct value of 99.54°. We apologize for the error, and correct it here.

- In any case, the AFLOW prototype label protocol rearranges the lattice vectors and shifts the origin, moving the copper atom from the (4c) to the (4a) Wyckoff position.
- Tenorite (CuO) and low-temperature CrS have the same AFLOW prototype label, AB_mC8_15_a_e. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I

References

[1] S. Åsbrink and N.-J. Norrby, *A refinement of the crystal structure of copper(II) oxide with a discussion of some exceptional e.s.d.'s*, Acta Crystallogr. Sect. B **26**, 8–15 (1970), doi:10.1107/S0567740870001838.

[2] M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW library of crystallographic prototypes: part 1*, Comput. Mater. Sci. **136**, S1–S828 (2017), doi:10.1016/j.commatsci.2017.01.017.

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