Cuprite (Cu_2O, $C3$) Structure: A2B_cP6_224_b_a-001

This structure originally had the label `A2B_cP6_224_b_a`. Calls to that address will be redirected here.

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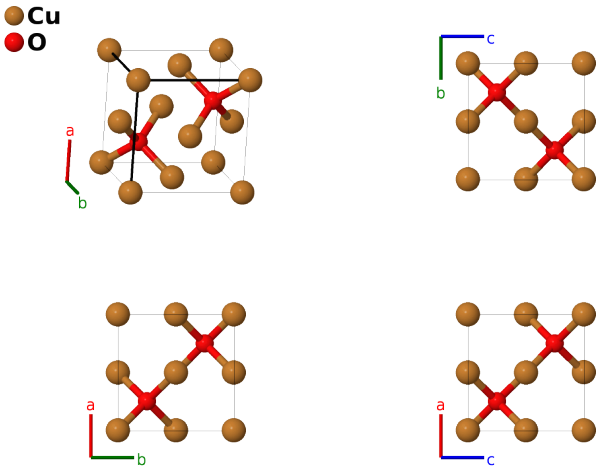
https://aflow.org/p/WUJH

https://aflow.org/p/A2B_cP6_224_b_a-001



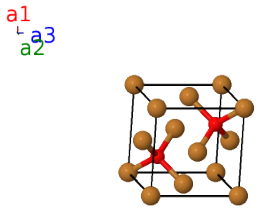
Prototype	Cu_2O
AFLOW prototype label	A2B_cP6_224_b_a-001
***Strukturbericht* designation**	$C3$
Mineral name	cuprite
ICSD	52043
Pearson symbol	cP6
Space group number	224
Space group symbol	$Pn\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B_cP6_224_b_a-001 --params=`a

Other compounds with this structure
Ag_2O, Pb_2O

- (Restori, 1986) gives the equilibrium lattice constant of Cu_2O as a=4.627Å, but gives nearest-neighbor distances which yield a lattice constant of 4.267Å. Since this value agrees with other sources, including those in (Downs, 2003), we use it. The ICSD entry uses 4.2685Å.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_3}$	=	0	=	0	(4b)	Cu I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(4b)	Cu I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(4b)	Cu I

References

[1] R. Restori and D. Schwarzenbach, *Charge Density in Cuprite, Cu_2O*, Acta Crystallogr. Sect. B **42**, 201–208 (1986), doi:10.1107/S0108768186098336.

[2] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

Found in

[1] A. Kirfel and K. Eichhorn, *Accurate structure analysis with synchrotron radiation. The electron density in Al_2O_3 and Cu_2O*, Acta Crystallogr. Sect. A **46**, 271–284 (1990), doi:10.1107/S0108767389012596.