$CuCr_2O_4$ Structure: A2BC4_tI28_141_c_b_h-001

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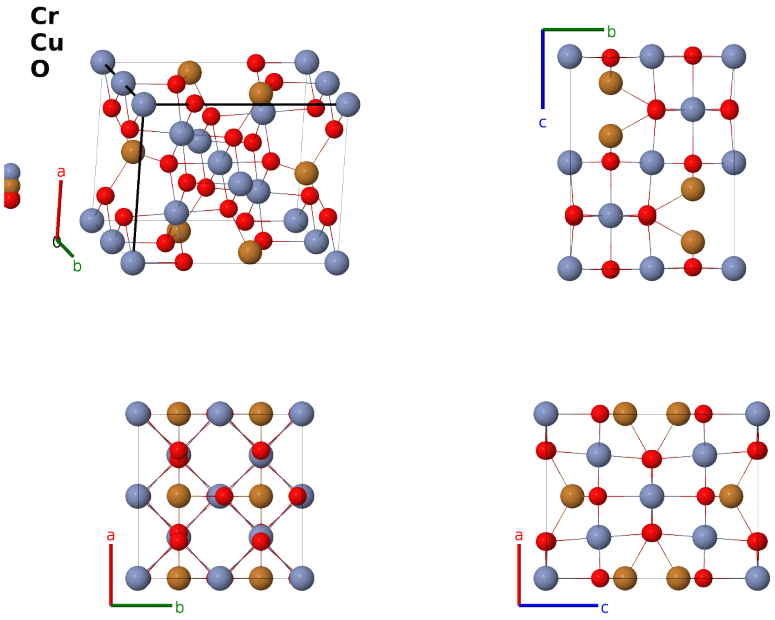
https://aflow.org/prototype-encyclopedia/763J

https://aflow.org/prototype-encyclopedia/A2BC4_tI28_141_c_b_h-001



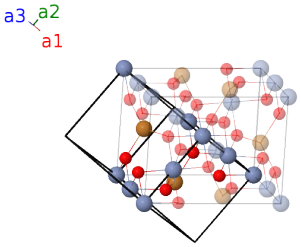
Prototype	Cr_2CuO_4
AFLOW prototype label	A2BC4_tI28_141_c_b_h-001
ICSD	84378
CCDC	1644382
Pearson symbol	tI28
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A2BC4_tI28_141_c_b_h-001 --params=`$a, c/a, y_3, z_3$

Other compounds with this structure
$CdMn_2O_4$, $CoMn_2O_4$, $CuMn_2O_4$, $FeCr_2S_4$, $GeCo_2O_4$, $MgMn_2O_4$, $NiCr_2O_4$, $ZnMn_2O_4$

- This is a tetragonal distortion of the spinel ($H1_1$) structure.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B_2}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(4b)	Cu I
$\mathbf{B_3}$	=	0	=	0	(8c)	Cr I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(8c)	Cr 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)	Cr 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)	Cr I
$\mathbf{B_7}$	=	$(y_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_8}$	=	$\left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_9}$	=	$z_3\,\mathbf{a}_1 + \left(-y_3 + z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{10}}$	=	$z_3\,\mathbf{a}_1 + (y_3 + z_3)\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{11}}$	=	$\left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{12}}$	=	$-\left(y_3 + z_3\right)\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{13}}$	=	$-z_3\,\mathbf{a}_1 + \left(y_3 - z_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$a\left(y_3 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I
$\mathbf{B_{14}}$	=	$-z_3\,\mathbf{a}_1 - (y_3 + z_3)\,\mathbf{a}_2 - \left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_3 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16h)	O I

References

[1] O. Crottaz, F. Kubel, and H. Schmid, *Jumping crystals of the spinels $NiCr_2O_4$ and $CuCr_2O_4$*, J. Mater. Chem. **7**, 143–146 (1997), doi:10.1039/A604758K.

Found in

[1] I. Naik, S. Mohanta, and S. D. Kaushik, *Structural and magnetic properties of tetragonal distorted spinel $CuMn_2O_4$ prepared by single step method*, AIP Conf. Proc. **1832**, 130013 (2017), doi:10.1063/1.4980733.

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