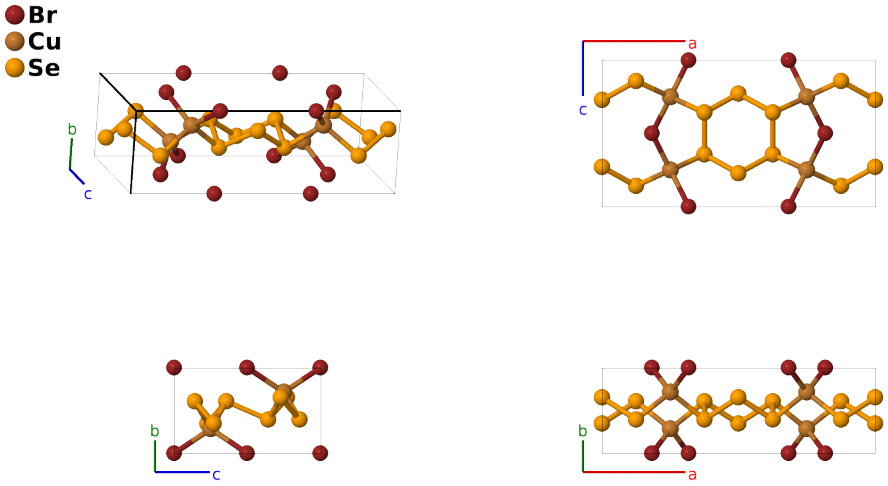
Pmna $CuBrSe_3$ Structure: ABC3_oP20_53_e_g_hi-001

This structure originally had the label `ABC3_oP20_53_e_g_hi`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/SET9

https://aflow.org/p/ABC3_oP20_53_e_g_hi-001

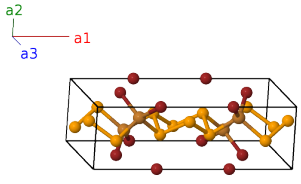


Prototype	$BrCuSe_3$
AFLOW prototype label	ABC3_oP20_53_e_g_hi-001
ICSD	10129
Pearson symbol	oP20
Space group number	53
Space group symbol	*Pmna*
AFLOW prototype command	`aflow --proto=ABC3_oP20_53_e_g_hi-001 --params=`$a, b/a, c/a, x_1, y_2, y_3, z_3, x_4, y_4, z_4$

- $CuBrSe_3$ has also been reported in the *Pnc*2 #30 orthorhombic space group. It is not clear that (Sakuma, 1991) knew of the work of (Haendler, 1979). The two structures are very similar.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1$	=	$ax_1\,\hat{\mathbf{x}}$	(4e)	Br I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1$	=	$-ax_1\,\hat{\mathbf{x}}$	(4e)	Br I
$\mathbf{B_4}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1+y_2\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B_6}$	=	$\frac{1}{4}\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1-y_2\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1+y_2\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(4g)	Cu I
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1-y_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1+y_3\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B_{12}}$	=	$-y_3\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{14}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{15}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{16}}$	=	$x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{18}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{19}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8i)	Se II

References

[1] H. M. Haendler and P. M. Carkner, *The crystal structure of copper bromide triselenide, $CuBrSe_3$*, J. Solid State Chem. **29**, 35–39 (1979), doi:10.1016/0022-4596(79)90206-8.

[2] T. Sakuma, T. Kaneko, T. Kurita, and H. Takahashi, *Crystal Structure of $CuBrSe_3$*, J. Phys. Soc. Jpn. **60**, 1608–1611 (1991), doi:10.1143/JPSJ.60.1608.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.