

Pmna CuBrSe₃ Structure: ABC3_oP20_53_e_g_hi-001

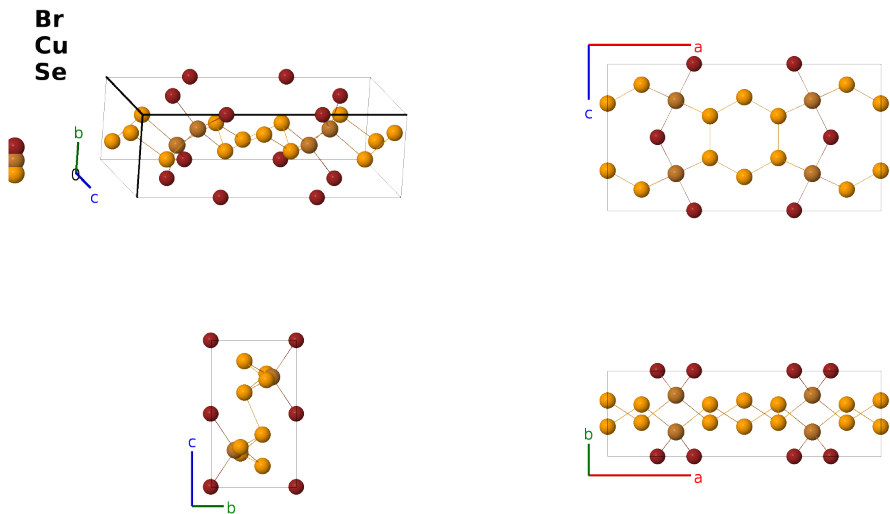
This structure previously used the label(s) **ABC3_oP20_53_e_g_hi**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/SET9>

https://aflow.org/prototype-encyclopedia/ABC3_oP20_53_e_g_hi-001

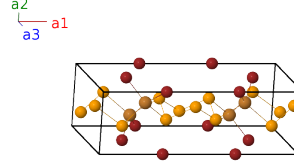


Prototype	BrCuSe ₃
AFLOW prototype label	ABC3_oP20_53_e_g_hi-001
ICSD	10129
CCDC	1595000
Pearson symbol	oP20
Space group number	53
Space group symbol	<i>Pmna</i>
AFLOW prototype command	<code>aflow --proto=ABC3_oP20_53_e_g_hi-001 --params=a, b/a, c/a, x₁, y₂, y₃, z₃, x₄, y₄, z₄</code>

- CuBrSe₃ has also been reported in the *Pnc2* #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

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



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
$\mathbf{B}_2$	$-(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B}_3$	$-x_1 \mathbf{a}_1$	$=$	$-ax_1 \hat{\mathbf{x}}$	(4e)	Br I
$\mathbf{B}_4$	$(x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(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
$\mathbf{B}_{10}$	$\frac{1}{2} \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4h)	Se I
$\mathbf{B}_{11}$	$\frac{1}{2} \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{14}$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B}_{15}$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{18}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8i)	Se II
$\mathbf{B}_{19}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(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, CuBrSe₃*, 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 CuBrSe₃*, 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.

First cited in

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