

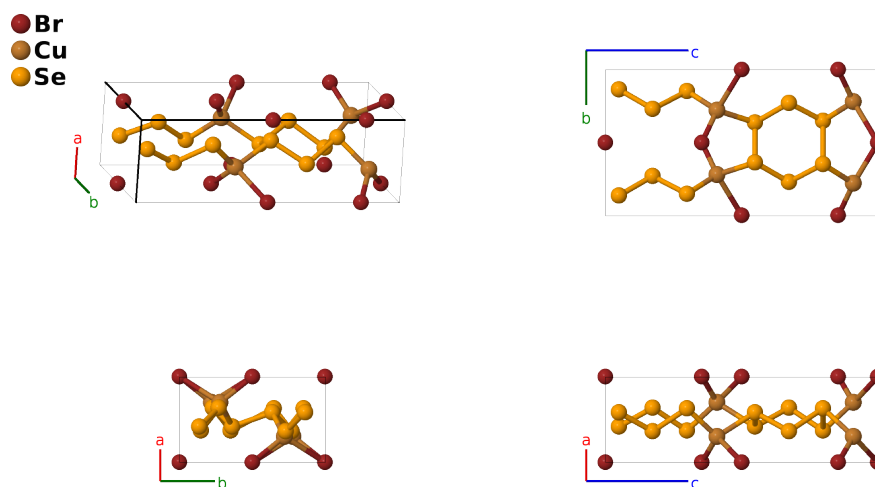
Pnc2 CuBrSe₃ Structure: ABC3_oP20_30_2a_c_3c-001

This structure originally had the label ABC3_oP20_30_2a_c_3c. Calls to that address will be redirected here.

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<https://aflow.org/p/2SVA>

https://aflow.org/p/ABC3_oP20_30_2a_c_3c-001



Prototype	BrCuSe ₃
AFLOW prototype label	ABC3_oP20_30_2a_c_3c-001
ICSD	71309
Pearson symbol	oP20
Space group number	30
Space group symbol	<i>Pnc2</i>
AFLOW prototype command	aflow --proto=ABC3_oP20_30_2a_c_3c-001 --params=a, b/a, c/a, z ₁ , z ₂ , x ₃ , y ₃ , z ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅ , x ₆ , y ₆ , z ₆

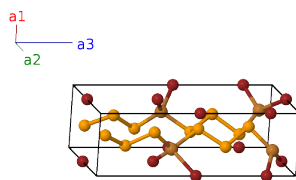
- CuBrSe₃ has also been reported in the *Pmna* #53 orthorhombic space group. It is not clear that (Sakuma, 1991) knew of the work of (Haendler, 1979). The two structures are very similar.

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	$= z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	Br I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Br I
\mathbf{B}_3	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(2a)	Br II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Br II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Cu I
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4c)	Cu I
\mathbf{B}_7	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cu I
\mathbf{B}_8	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cu I
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Se I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4c)	Se I
\mathbf{B}_{11}	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se I
\mathbf{B}_{12}	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + b (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se I
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Se II
\mathbf{B}_{14}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4c)	Se II
\mathbf{B}_{15}	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} - b (y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se II
\mathbf{B}_{16}	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + b (y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se II
\mathbf{B}_{17}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Se III
\mathbf{B}_{18}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4c)	Se III
\mathbf{B}_{19}	$= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - b (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se III
\mathbf{B}_{20}	$= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + b (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se III

References

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- [2] 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.

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