

*Pnc*2 CuBrSe₃ Structure: ABC3_oP20_30_2a_c_3c-001

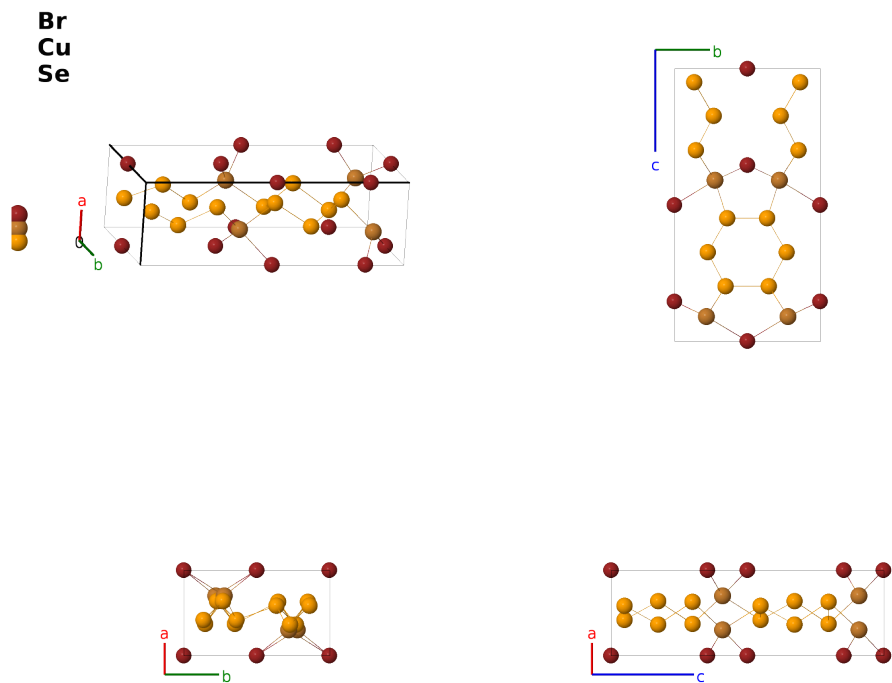
This structure previously used the label(s) **ABC3_oP20_30_2a_c_3c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/2SVA>

https://aflow.org/prototype-encyclopedia/ABC3_oP20_30_2a_c_3c-001



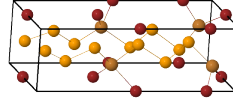
Prototype	BrCuSe ₃
AFLOW prototype label	ABC3_oP20_30_2a_c_3c-001
ICSD	71309
CCDC	1631953
Pearson symbol	oP20
Space group number	30
Space group symbol	<i>Pnc</i> 2
AFLOW prototype command	<code>aflow --proto=ABC3_oP20_30_2a_c_3c-001</code> <code>--params=a, b/a, c/a, z₁, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

- 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

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

a1
a2 a3



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(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
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(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
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - b (y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_8$	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + b (y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_9$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{10}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{11}$	$= x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} - b (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{12}$	$= -x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + b (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se I
$\mathbf{B}_{13}$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{14}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{15}$	$= x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} - b (y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{16}$	$= -x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + b (y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se II
$\mathbf{B}_{17}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{18}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{19}$	$= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} - b (y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se III
$\mathbf{B}_{20}$	$= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_6 \hat{\mathbf{x}} + b (y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Se III

References

- [1] 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.
- [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.

Found in

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

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