Intermediate Temperature Bornite $(Cu_{5/6}Fe_{1/6})_3S_2$ Structure: A7B_cF256_225_f2k_ce-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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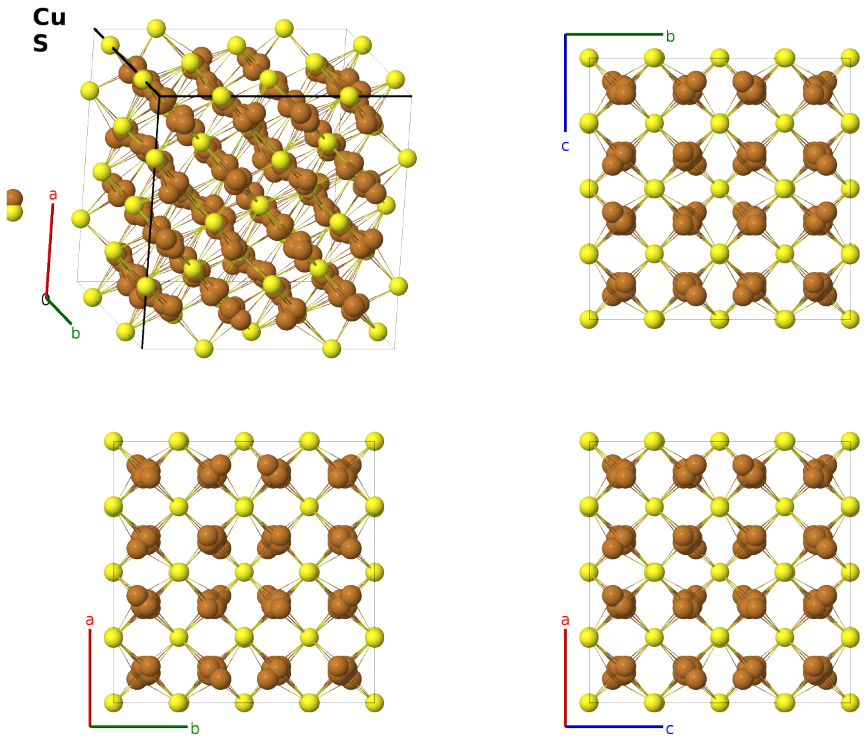
https://aflow.org/prototype-encyclopedia/EMLR

https://aflow.org/prototype-encyclopedia/A7B_cF256_225_f2k_ce-001

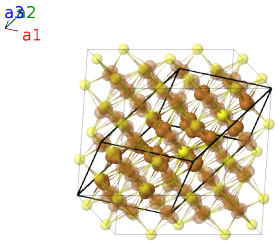


Prototype	Cu_5FeS_4
AFLOW prototype label	A7B_cF256_225_f2k_ce-001
Mineral name	bornite
ICSD	200424
CCDC	1705359
Pearson symbol	cF256
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A7B_cF256_225_f2k_ce-001 --params=`$a, x_2, x_3, x_4, z_4, x_5, z_5$

- Bornite can take on several forms at different temperatures (Martinelli, 2018).
  - At temperatures above 508K it is cubic with an "anti"-fluorite ($C1$) structure.
  - From 443K to 508K it becomes a a supercell of an anti-fluorite structure (this structure).
  - Below 443K it becomes orthorhombic, in the $Pbca$ #61 space group.
  - As temperatures drop into the 50-70K range it transforms in to the non-centrosymmetric $Pca2_1$ #29 space group.
- In all of these cases the sulfur atoms form a face-centered or nearly face-centered cubic lattice.
- Data for this structure was taken at 458K. There is considerable disorder here. The site we labeled Cu-II is occupied 33% of the time with a mixture of copper and iron atoms. The Cu-I and Cu-III sites are occupied 31% and 7% of the time, respectively, and are purely copper. The sulfur atoms form a nearly cubic fcc lattice, with one of the tetrahedral sites is occupied by a copper or iron atom, and the other site is either filled by a copper atom or remains vacant. (Kanazawa, 1978)

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	S I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	S I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(24e)	S II
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(24e)	S II
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{y}}$	(24e)	S II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{y}}$	(24e)	S II
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{z}}$	(24e)	S II
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{z}}$	(24e)	S II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{12}}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + 3x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 + 3x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{16}}$	=	$3x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32f)	Cu I
$\mathbf{B_{17}}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + (2x_4 - z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}}$	(96k)	Cu II

$$\mathbf{B_{18}} = z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - (2x_4 + z_4)\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{19}} = (2x_4 - z_4)\,\mathbf{a}_1 - (2x_4 + z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{20}} = -(2x_4 + z_4)\,\mathbf{a}_1 + (2x_4 - z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{21}} = (2x_4 - z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{22}} = -(2x_4 + z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{23}} = z_4\,\mathbf{a}_1 + (2x_4 - z_4)\,\mathbf{a}_2 - (2x_4 + z_4)\,\mathbf{a}_3 = -az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{24}} = z_4\,\mathbf{a}_1 - (2x_4 + z_4)\,\mathbf{a}_2 + (2x_4 - z_4)\,\mathbf{a}_3 = -az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{25}} = z_4\,\mathbf{a}_1 + (2x_4 - z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{26}} = z_4\,\mathbf{a}_1 - (2x_4 + z_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{27}} = -(2x_4 + z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + (2x_4 - z_4)\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{28}} = (2x_4 - z_4)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 - (2x_4 + z_4)\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{29}} = -z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + (2x_4 + z_4)\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{30}} = -z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - (2x_4 - z_4)\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{31}} = -(2x_4 - z_4)\,\mathbf{a}_1 + (2x_4 + z_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{32}} = (2x_4 + z_4)\,\mathbf{a}_1 - (2x_4 - z_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + az_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{33}} = -(2x_4 - z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + (2x_4 + z_4)\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{34}} = (2x_4 + z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - (2x_4 - z_4)\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} + az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{35}} = -z_4\,\mathbf{a}_1 - (2x_4 - z_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{36}} = -z_4\,\mathbf{a}_1 + (2x_4 + z_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = ax_4\,\hat{\mathbf{x}} - az_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{37}} = -z_4\,\mathbf{a}_1 - (2x_4 - z_4)\,\mathbf{a}_2 + (2x_4 + z_4)\,\mathbf{a}_3 = az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{38}} = -z_4\,\mathbf{a}_1 + (2x_4 + z_4)\,\mathbf{a}_2 - (2x_4 - z_4)\,\mathbf{a}_3 = az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{39}} = (2x_4 + z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -az_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{40}} = -(2x_4 - z_4)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -az_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu II}$$

$$\mathbf{B_{41}} = z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$$\mathbf{B_{42}} = z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - (2x_5 + z_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$$\mathbf{B_{43}} = (2x_5 - z_5)\,\mathbf{a}_1 - (2x_5 + z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$$\mathbf{B_{44}} = -(2x_5 + z_5)\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$$\mathbf{B_{45}} = (2x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$$\mathbf{B_{46}} = -(2x_5 + z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$$\mathbf{B_{47}} = z_5\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 - (2x_5 + z_5)\,\mathbf{a}_3 = -az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}} \quad \text{(96k)} \quad \text{Cu III}$$

$\mathbf{B_{48}}$	=	$z_5\,\mathbf{a}_1 - (2x_5 + z_5)\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{49}}$	=	$z_5\,\mathbf{a}_1 + (2x_5 - z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{50}}$	=	$z_5\,\mathbf{a}_1 - (2x_5 + z_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{51}}$	=	$-(2x_5 + z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + (2x_5 - z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{52}}$	=	$(2x_5 - z_5)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 - (2x_5 + z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{53}}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + (2x_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{54}}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - az_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{55}}$	=	$-(2x_5 - z_5)\,\mathbf{a}_1 + (2x_5 + z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{56}}$	=	$(2x_5 + z_5)\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + az_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{57}}$	=	$-(2x_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + (2x_5 + z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{58}}$	=	$(2x_5 + z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{59}}$	=	$-z_5\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{60}}$	=	$-z_5\,\mathbf{a}_1 + (2x_5 + z_5)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - az_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{61}}$	=	$-z_5\,\mathbf{a}_1 - (2x_5 - z_5)\,\mathbf{a}_2 + (2x_5 + z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{62}}$	=	$-z_5\,\mathbf{a}_1 + (2x_5 + z_5)\,\mathbf{a}_2 - (2x_5 - z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{63}}$	=	$(2x_5 + z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III
$\mathbf{B_{64}}$	=	$-(2x_5 - z_5)\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - ax_5\,\hat{\mathbf{z}}$	(96k)	Cu III

References

[1] Y. Kanazawa, K. Koto, and N. Morimoto, *Bornite (Cu_5FeS_4); stability and crystal structure of the intermediate form*, Can. Mineral. **16**, 397–404 (1978).

Found in

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First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.