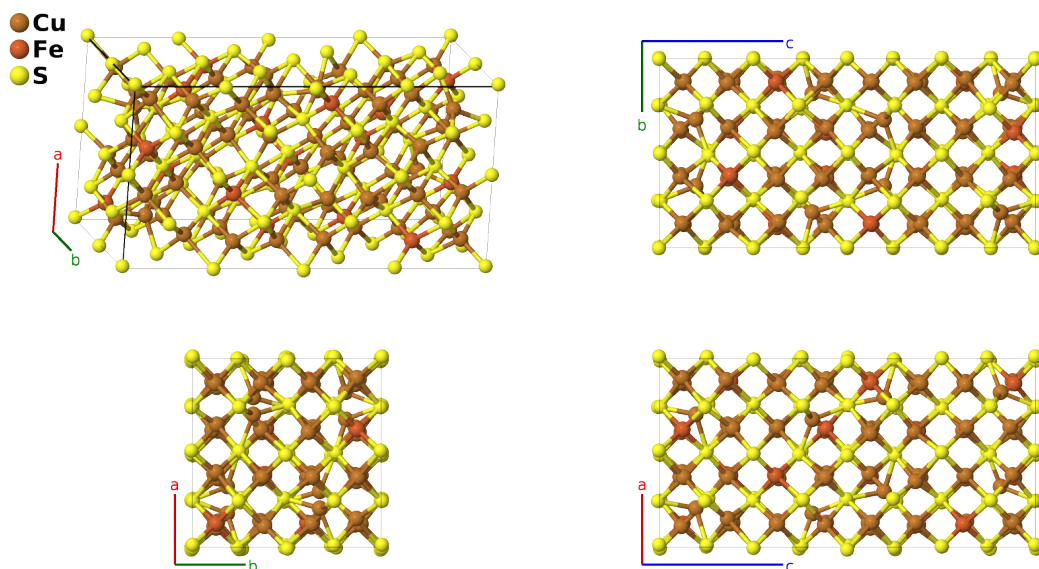


Low Temperature Bornite (Cu_5FeS_4) Structure: A5BC4_oP160_29_20a_4a_16a-001

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<https://afLOW.org/p/H7LS>

https://afLOW.org/p/A5BC4_oP160_29_20a_4a_16a-001



Prototype	Cu_5FeS_4
AFLOW prototype label	A5BC4_oP160_29_20a_4a_16a-001
Mineral name	bornite
ICSD	130920
Pearson symbol	oP160
Space group number	29
Space group symbol	$Pca2_1$
AFLOW prototype command	<pre>afLOW --proto=A5BC4_oP160_29_20a_4a_16a-001 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24, x25, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, z29, x30, y30, z30, x31, y31, z31, x32, y32, z32, x33, y33, z33, x34, y34, z34, x35, y35, z35, x36, y36, z36, x37, y37, z37, x38, y38, z38, x39, y39, z39, x40, y40, z40</pre>

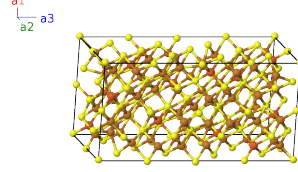
- Bornite can take on several forms at different temperatures (Martinelli, 2018):
 - At temperatures above 508K it is cubic with an “anti”-fluorite ($C1$) structure.
 - From 443K to 508K it becomes a a supercell of an anti-fluorite structure.
 - Below 443K it becomes orthorhombic, in the $Pbca$ #61 space group.

– As temperatures drop into the 50-70K range it transforms into the non-centrosymmetric $Pca2_1$ #29 space group (this structure).

- In all of these cases the sulfur atoms form a face-centered or nearly face-centered cubic lattice.
- Data for this low-temperature structure was taken at 10K.

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	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_3	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_4	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	Cu II
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu II
\mathbf{B}_7	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	Cu II
\mathbf{B}_8	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu II
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	Cu III
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu III
\mathbf{B}_{11}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	Cu III
\mathbf{B}_{12}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu III
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	Cu IV
\mathbf{B}_{14}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu IV
\mathbf{B}_{15}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	Cu IV
\mathbf{B}_{16}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu IV
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	Cu V
\mathbf{B}_{18}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu V
\mathbf{B}_{19}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	Cu V
\mathbf{B}_{20}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu V
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	Cu VI
\mathbf{B}_{22}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu VI
\mathbf{B}_{23}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	Cu VI

$$\mathbf{B}_{160} = \begin{matrix} -\left(x_{40} - \frac{1}{2}\right) \mathbf{a}_1 + y_{40} \mathbf{a}_2 + \\ \left(z_{40} + \frac{1}{2}\right) \mathbf{a}_3 \end{matrix} = -a \left(x_{40} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{40} \hat{\mathbf{y}} + c \left(z_{40} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (4a) \quad \text{S XVI}$$

References

- [1] A. Martinelli, G. O. Lepore, F. Bernardini, A. Giaccherini, and F. D. Benedetto, *The puzzling structure of Cu_5FeS_4 (bornite) at low temperature*, Acta Crystallogr. Sect. B **74**, 405–415 (2018), doi:10.1107/S2052520618009812.