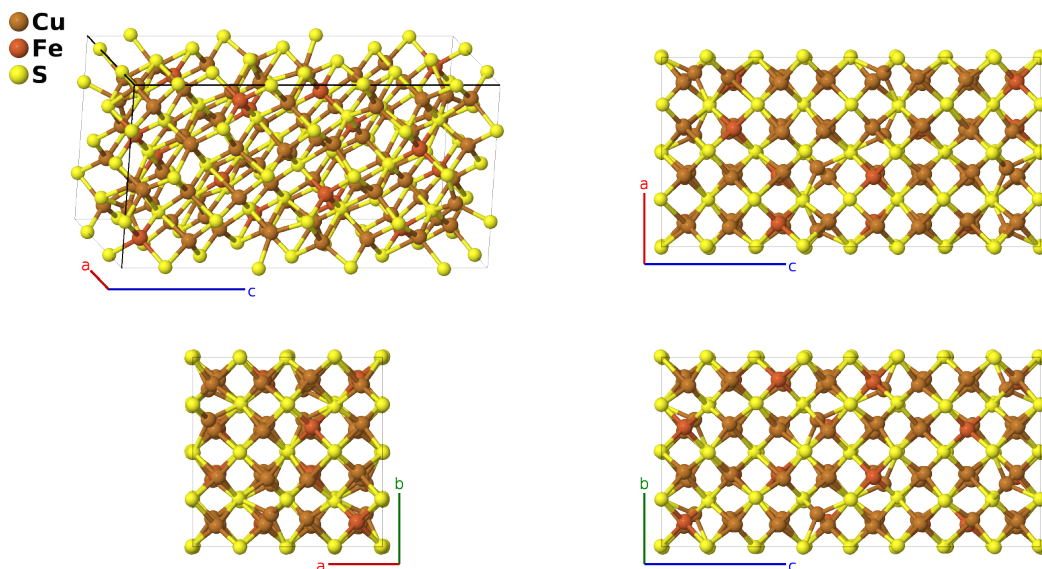


Room Temperature Bornite (Cu_5FeS_4) Structure: A5BC4_oP160_61_10c_2c_8c-001

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<https://aflow.org/p/L8SE>

https://aflow.org/p/A5BC4_oP160_61_10c_2c_8c-001



Prototype	Cu_5FeS_4
AFLOW prototype label	A5BC4_oP160_61_10c_2c_8c-001
Mineral name	bornite
ICSD	130921
Pearson symbol	oP160
Space group number	61
Space group symbol	$Pbca$
AFLOW prototype command	<pre>aflow --proto=A5BC4_oP160_61_10c_2c_8c-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</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 (this structure).
 - 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.

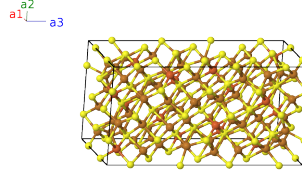
- Data for this room-temperature structure was taken at 275K.

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	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_2	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_5	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_6	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_7	$= x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_8	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	Cu I
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{10}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{11}	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{12}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{13}	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{14}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{15}	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{16}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	Cu II
\mathbf{B}_{17}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Cu III
\mathbf{B}_{18}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu III
\mathbf{B}_{19}	$= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu III
\mathbf{B}_{20}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	Cu III
\mathbf{B}_{21}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8c)	Cu III
\mathbf{B}_{22}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu III
\mathbf{B}_{23}	$= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	Cu III

$$\begin{aligned}
\mathbf{B}_{137} &= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= ax_{18} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (8c) & \text{S VI} \\
\mathbf{B}_{138} &= -\left(x_{18} - \frac{1}{2}\right) \mathbf{a}_1 - y_{18} \mathbf{a}_2 + &= -a\left(x_{18} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c\left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VI} \\
&\quad \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{139} &= -x_{18} \mathbf{a}_1 + \left(y_{18} + \frac{1}{2}\right) \mathbf{a}_2 - &= -ax_{18} \hat{\mathbf{x}} + b\left(y_{18} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{18} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VI} \\
&\quad \left(z_{18} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{140} &= \left(x_{18} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{18} - \frac{1}{2}\right) \mathbf{a}_2 - &= a\left(x_{18} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{18} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}} & (8c) & \text{S VI} \\
&\quad z_{18} \mathbf{a}_3 \\
\mathbf{B}_{141} &= -x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3 &= -ax_{18} \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}} & (8c) & \text{S VI} \\
\mathbf{B}_{142} &= \left(x_{18} + \frac{1}{2}\right) \mathbf{a}_1 + y_{18} \mathbf{a}_2 - &= a\left(x_{18} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - c\left(z_{18} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VI} \\
&\quad \left(z_{18} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{143} &= x_{18} \mathbf{a}_1 - \left(y_{18} - \frac{1}{2}\right) \mathbf{a}_2 + &= ax_{18} \hat{\mathbf{x}} - b\left(y_{18} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{18} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VI} \\
&\quad \left(z_{18} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{144} &= -\left(x_{18} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{18} + \frac{1}{2}\right) \mathbf{a}_2 + &= -a\left(x_{18} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{18} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}} & (8c) & \text{S VI} \\
&\quad z_{18} \mathbf{a}_3 \\
\mathbf{B}_{145} &= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= ax_{19} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8c) & \text{S VII} \\
\mathbf{B}_{146} &= -\left(x_{19} - \frac{1}{2}\right) \mathbf{a}_1 - y_{19} \mathbf{a}_2 + &= -a\left(x_{19} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c\left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VII} \\
&\quad \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{147} &= -x_{19} \mathbf{a}_1 + \left(y_{19} + \frac{1}{2}\right) \mathbf{a}_2 - &= -ax_{19} \hat{\mathbf{x}} + b\left(y_{19} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VII} \\
&\quad \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{148} &= \left(x_{19} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{19} - \frac{1}{2}\right) \mathbf{a}_2 - &= a\left(x_{19} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{19} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8c) & \text{S VII} \\
&\quad z_{19} \mathbf{a}_3 \\
\mathbf{B}_{149} &= -x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= -ax_{19} \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} & (8c) & \text{S VII} \\
\mathbf{B}_{150} &= \left(x_{19} + \frac{1}{2}\right) \mathbf{a}_1 + y_{19} \mathbf{a}_2 - &= a\left(x_{19} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - c\left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VII} \\
&\quad \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{151} &= x_{19} \mathbf{a}_1 - \left(y_{19} - \frac{1}{2}\right) \mathbf{a}_2 + &= ax_{19} \hat{\mathbf{x}} - b\left(y_{19} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VII} \\
&\quad \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{152} &= -\left(x_{19} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{19} + \frac{1}{2}\right) \mathbf{a}_2 + &= -a\left(x_{19} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{19} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} & (8c) & \text{S VII} \\
&\quad z_{19} \mathbf{a}_3 \\
\mathbf{B}_{153} &= x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3 &= ax_{20} \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
\mathbf{B}_{154} &= -\left(x_{20} - \frac{1}{2}\right) \mathbf{a}_1 - y_{20} \mathbf{a}_2 + &= -a\left(x_{20} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c\left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
&\quad \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{155} &= -x_{20} \mathbf{a}_1 + \left(y_{20} + \frac{1}{2}\right) \mathbf{a}_2 - &= -ax_{20} \hat{\mathbf{x}} + b\left(y_{20} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{20} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
&\quad \left(z_{20} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{156} &= \left(x_{20} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{20} - \frac{1}{2}\right) \mathbf{a}_2 - &= a\left(x_{20} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{20} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
&\quad z_{20} \mathbf{a}_3 \\
\mathbf{B}_{157} &= -x_{20} \mathbf{a}_1 - y_{20} \mathbf{a}_2 - z_{20} \mathbf{a}_3 &= -ax_{20} \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
\mathbf{B}_{158} &= \left(x_{20} + \frac{1}{2}\right) \mathbf{a}_1 + y_{20} \mathbf{a}_2 - &= a\left(x_{20} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - c\left(z_{20} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
&\quad \left(z_{20} - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{159} &= x_{20} \mathbf{a}_1 - \left(y_{20} - \frac{1}{2}\right) \mathbf{a}_2 + &= ax_{20} \hat{\mathbf{x}} - b\left(y_{20} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{20} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
&\quad \left(z_{20} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{160} &= -\left(x_{20} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{20} + \frac{1}{2}\right) \mathbf{a}_2 + &= -a\left(x_{20} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{20} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}} & (8c) & \text{S VIII} \\
&\quad z_{20} \mathbf{a}_3
\end{aligned}$$

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.