

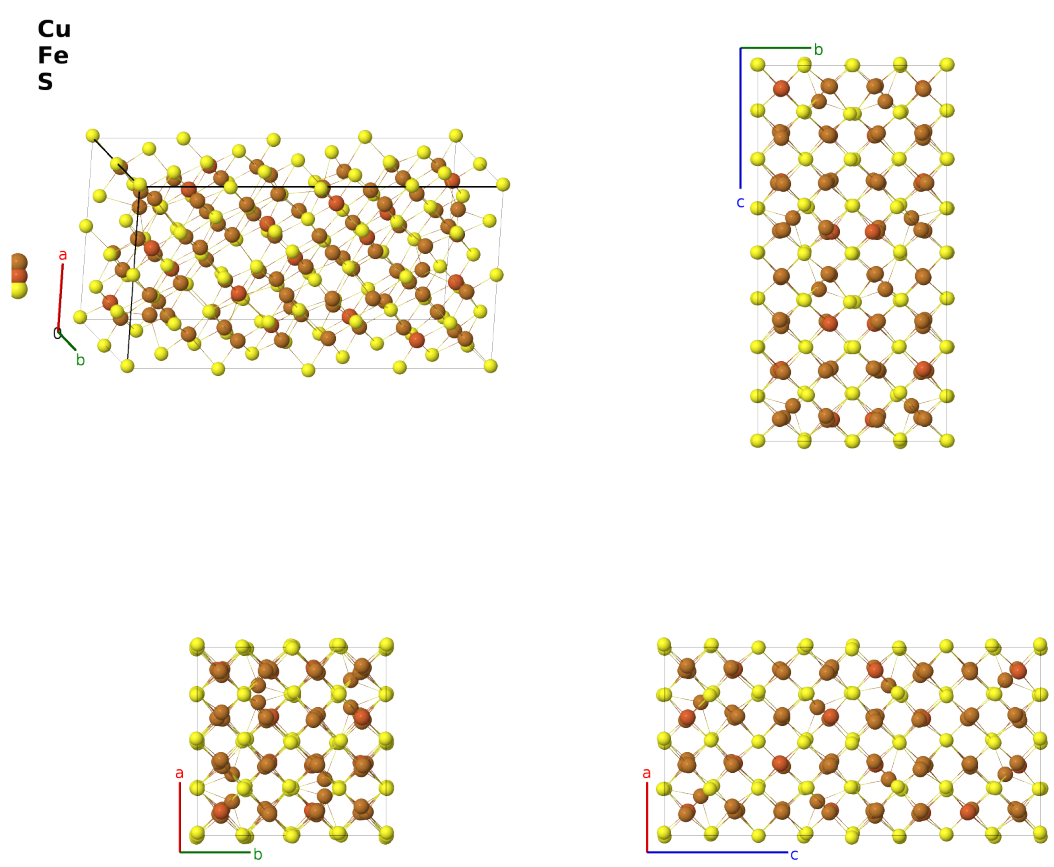
Low Temperature Bornite (Cu₅FeS₄) Structure: A5BC4_oP160_29_20a_4a_16a-001

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- 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.

<https://aflow.org/prototype-encyclopedia/H7LS>

https://aflow.org/prototype-encyclopedia/A5BC4_oP160_29_20a_4a_16a-001



Prototype	Cu ₅ FeS ₄
AFLOW prototype label	A5BC4_oP160_29_20a_4a_16a-001
Mineral name	bornite
ICSD	130920
CCDC	2147010
Pearson symbol	oP160
Space group number	29

Space group symbol

$Pca2_1$

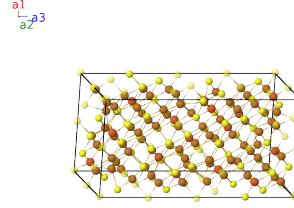
AFLOW prototype command

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y15,z15,x16,y16,z16,x17,y17,z17,x18,y18,z18,x19,y19,z19,x20,y20,z20,x21,y21,z21,x22,y22,
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y37,z37,x38,y38,z38,x39,y39,z39,x40,y40,z40
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- 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 in to 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
$\mathbf{B}_{24} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 +$ $(z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu VI
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4a)	Cu VII
$\mathbf{B}_{26} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu VII
$\mathbf{B}_{27} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4a)	Cu VII
$\mathbf{B}_{28} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 +$ $(z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu VII
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4a)	Cu VIII
$\mathbf{B}_{30} =$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu VIII
$\mathbf{B}_{31} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4a)	Cu VIII
$\mathbf{B}_{32} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 +$ $(z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu VIII
$\mathbf{B}_{33} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4a)	Cu IX
$\mathbf{B}_{34} =$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu IX
$\mathbf{B}_{35} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4a)	Cu IX
$\mathbf{B}_{36} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 +$ $(z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu IX
$\mathbf{B}_{37} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4a)	Cu X
$\mathbf{B}_{38} =$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu X
$\mathbf{B}_{39} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4a)	Cu X
$\mathbf{B}_{40} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 +$ $(z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu X
$\mathbf{B}_{41} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4a)	Cu XI
$\mathbf{B}_{42} =$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu XI
$\mathbf{B}_{43} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(4a)	Cu XI
$\mathbf{B}_{44} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + y_{11} \mathbf{a}_2 +$ $(z_{11} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Cu XI

$$\begin{aligned}
\mathbf{B}_{148} &= -\left(x_{37} - \frac{1}{2}\right) \mathbf{a}_1 + y_{37} \mathbf{a}_2 + \left(z_{37} + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_{37} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{37} \hat{\mathbf{y}} + c \left(z_{37} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\quad \text{S XIII} \\
\mathbf{B}_{149} &= x_{38} \mathbf{a}_1 + y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 &= ax_{38} \hat{\mathbf{x}} + by_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} &(4a) &\quad \text{S XIV} \\
\mathbf{B}_{150} &= -x_{38} \mathbf{a}_1 - y_{38} \mathbf{a}_2 + \left(z_{38} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{38} \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + c \left(z_{38} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\quad \text{S XIV} \\
\mathbf{B}_{151} &= \left(x_{38} + \frac{1}{2}\right) \mathbf{a}_1 - y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 &= a \left(x_{38} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} + cz_{38} \hat{\mathbf{z}} &(4a) &\quad \text{S XIV} \\
\mathbf{B}_{152} &= -\left(x_{38} - \frac{1}{2}\right) \mathbf{a}_1 + y_{38} \mathbf{a}_2 + \left(z_{38} + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_{38} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{38} \hat{\mathbf{y}} + c \left(z_{38} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\quad \text{S XIV} \\
\mathbf{B}_{153} &= x_{39} \mathbf{a}_1 + y_{39} \mathbf{a}_2 + z_{39} \mathbf{a}_3 &= ax_{39} \hat{\mathbf{x}} + by_{39} \hat{\mathbf{y}} + cz_{39} \hat{\mathbf{z}} &(4a) &\quad \text{S XV} \\
\mathbf{B}_{154} &= -x_{39} \mathbf{a}_1 - y_{39} \mathbf{a}_2 + \left(z_{39} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{39} \hat{\mathbf{x}} - by_{39} \hat{\mathbf{y}} + c \left(z_{39} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\quad \text{S XV} \\
\mathbf{B}_{155} &= \left(x_{39} + \frac{1}{2}\right) \mathbf{a}_1 - y_{39} \mathbf{a}_2 + z_{39} \mathbf{a}_3 &= a \left(x_{39} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{39} \hat{\mathbf{y}} + cz_{39} \hat{\mathbf{z}} &(4a) &\quad \text{S XV} \\
\mathbf{B}_{156} &= -\left(x_{39} - \frac{1}{2}\right) \mathbf{a}_1 + y_{39} \mathbf{a}_2 + \left(z_{39} + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_{39} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{39} \hat{\mathbf{y}} + c \left(z_{39} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\quad \text{S XV} \\
\mathbf{B}_{157} &= x_{40} \mathbf{a}_1 + y_{40} \mathbf{a}_2 + z_{40} \mathbf{a}_3 &= ax_{40} \hat{\mathbf{x}} + by_{40} \hat{\mathbf{y}} + cz_{40} \hat{\mathbf{z}} &(4a) &\quad \text{S XVI} \\
\mathbf{B}_{158} &= -x_{40} \mathbf{a}_1 - y_{40} \mathbf{a}_2 + \left(z_{40} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{40} \hat{\mathbf{x}} - by_{40} \hat{\mathbf{y}} + c \left(z_{40} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4a) &\quad \text{S XVI} \\
\mathbf{B}_{159} &= \left(x_{40} + \frac{1}{2}\right) \mathbf{a}_1 - y_{40} \mathbf{a}_2 + z_{40} \mathbf{a}_3 &= a \left(x_{40} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{40} \hat{\mathbf{y}} + cz_{40} \hat{\mathbf{z}} &(4a) &\quad \text{S XVI} \\
\mathbf{B}_{160} &= -\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 &= -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}} &(4a) &\quad \text{S XVI}
\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.

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