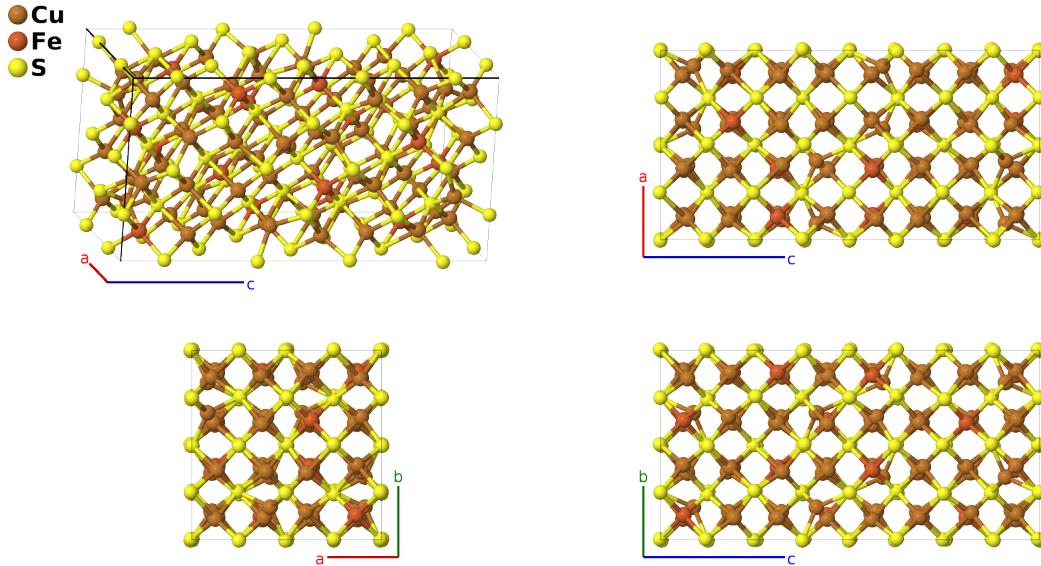


# Room Temperature Bornite ( $\text{Cu}_5\text{FeS}_4$ ) Structure: A5BC4\_oP160\_61\_10c\_2c\_8c-001

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

[https://aflow.org/p/A5BC4\\_oP160\\_61\\_10c\\_2c\\_8c-001](https://aflow.org/p/A5BC4_oP160_61_10c_2c_8c-001)



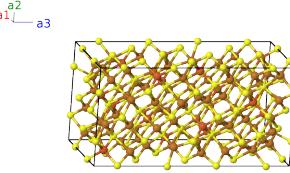
|                                |   |
|--------------------------------|---|
| <b>Prototype</b>               | $\text{Cu}_5\text{FeS}_4$   |
| <b>AFLOW prototype label</b>   | A5BC4_oP160_61_10c_2c_8c-001  |
| <b>Mineral name</b>            | bornite   |
| <b>ICSD</b>                    | 130921  |
| <b>Pearson symbol</b>          | oP160   |
| <b>Space group number</b>      | 61  |
| <b>Space group symbol</b>      | $Pbca$  |
| <b>AFLOW prototype command</b> | <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 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 into 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

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



### Basis vectors

|                   | Lattice coordinates   | Cartesian coordinates   | Wyckoff position | Atom type |
|-------------------|---|---|------------------|-----------|
| $\mathbf{B}_1$    | $x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$                                  | $a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$                                | (8c)             | Cu I      |
| $\mathbf{B}_2$    | $-(x_1 - \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$ | $-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Cu I      |
| $\mathbf{B}_3$    | $-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$ | $-a x_1 \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Cu I      |
| $\mathbf{B}_4$    | $(x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$  | $a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$  | (8c)             | Cu I      |
| $\mathbf{B}_5$    | $-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$                                 | $-a x_1 \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$                               | (8c)             | Cu I      |
| $\mathbf{B}_6$    | $(x_1 + \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$  | $a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Cu I      |
| $\mathbf{B}_7$    | $x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$  | $a x_1 \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Cu I      |
| $\mathbf{B}_8$    | $-(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$ | (8c)             | Cu I      |
| $\mathbf{B}_9$    | $x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$                                  | $a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$                                | (8c)             | Cu II     |
| $\mathbf{B}_{10}$ | $-(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Cu II     |
| $\mathbf{B}_{11}$ | $-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $-a x_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Cu II     |
| $\mathbf{B}_{12}$ | $(x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$  | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$  | (8c)             | Cu II     |
| $\mathbf{B}_{13}$ | $-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$                                 | $-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$                               | (8c)             | Cu II     |
| $\mathbf{B}_{14}$ | $(x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$  | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Cu II     |
| $\mathbf{B}_{15}$ | $x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$  | $a x_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Cu II     |
| $\mathbf{B}_{16}$ | $-(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$ | (8c)             | Cu II     |
| $\mathbf{B}_{17}$ | $x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$                                  | $a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$                                | (8c)             | Cu III    |
| $\mathbf{B}_{18}$ | $-(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Cu III    |
| $\mathbf{B}_{19}$ | $-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $-a x_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c)             | Cu III    |
| $\mathbf{B}_{20}$ | $(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$  | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$  | (8c)             | Cu III    |
| $\mathbf{B}_{21}$ | $-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$                                 | $-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$                               | (8c)             | Cu III    |
| $\mathbf{B}_{22}$ | $(x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$  | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Cu III    |
| $\mathbf{B}_{23}$ | $x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$  | $a x_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c)             | Cu III    |

|                   |     |   |     |   |      |        |
|-------------------|-----|---|-----|---|------|--------|
| $\mathbf{B}_{24}$ | $=$ | $-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$ | (8c) | Cu III |
| $\mathbf{B}_{25}$ | $=$ | $x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$                                  | $=$ | $a x_4 \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$                                | (8c) | Cu IV  |
| $\mathbf{B}_{26}$ | $=$ | $-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu IV  |
| $\mathbf{B}_{27}$ | $=$ | $-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a x_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu IV  |
| $\mathbf{B}_{28}$ | $=$ | $(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$  | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$  | (8c) | Cu IV  |
| $\mathbf{B}_{29}$ | $=$ | $-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$                                 | $=$ | $-a x_4 \hat{\mathbf{x}} - b y_4 \hat{\mathbf{y}} - c z_4 \hat{\mathbf{z}}$                               | (8c) | Cu IV  |
| $\mathbf{B}_{30}$ | $=$ | $(x_4 + \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + b y_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu IV  |
| $\mathbf{B}_{31}$ | $=$ | $x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a x_4 \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu IV  |
| $\mathbf{B}_{32}$ | $=$ | $-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$ | (8c) | Cu IV  |
| $\mathbf{B}_{33}$ | $=$ | $x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$                                  | $=$ | $a x_5 \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$                                | (8c) | Cu V   |
| $\mathbf{B}_{34}$ | $=$ | $-(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu V   |
| $\mathbf{B}_{35}$ | $=$ | $-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a x_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu V   |
| $\mathbf{B}_{36}$ | $=$ | $(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$  | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$  | (8c) | Cu V   |
| $\mathbf{B}_{37}$ | $=$ | $-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$                                 | $=$ | $-a x_5 \hat{\mathbf{x}} - b y_5 \hat{\mathbf{y}} - c z_5 \hat{\mathbf{z}}$                               | (8c) | Cu V   |
| $\mathbf{B}_{38}$ | $=$ | $(x_5 + \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + b y_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu V   |
| $\mathbf{B}_{39}$ | $=$ | $x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a x_5 \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu V   |
| $\mathbf{B}_{40}$ | $=$ | $-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + z_5 \mathbf{a}_3$ | $=$ | $-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$ | (8c) | Cu V   |
| $\mathbf{B}_{41}$ | $=$ | $x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$                                  | $=$ | $a x_6 \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$                                | (8c) | Cu VI  |
| $\mathbf{B}_{42}$ | $=$ | $-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu VI  |
| $\mathbf{B}_{43}$ | $=$ | $-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a x_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu VI  |
| $\mathbf{B}_{44}$ | $=$ | $(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$  | $=$ | $a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c z_6 \hat{\mathbf{z}}$  | (8c) | Cu VI  |
| $\mathbf{B}_{45}$ | $=$ | $-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$                                 | $=$ | $-a x_6 \hat{\mathbf{x}} - b y_6 \hat{\mathbf{y}} - c z_6 \hat{\mathbf{z}}$                               | (8c) | Cu VI  |
| $\mathbf{B}_{46}$ | $=$ | $(x_6 + \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + b y_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu VI  |
| $\mathbf{B}_{47}$ | $=$ | $x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a x_6 \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu VI  |
| $\mathbf{B}_{48}$ | $=$ | $-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$ | $=$ | $-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$ | (8c) | Cu VI  |
| $\mathbf{B}_{49}$ | $=$ | $x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$                                  | $=$ | $a x_7 \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$                                | (8c) | Cu VII |
| $\mathbf{B}_{50}$ | $=$ | $-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu VII |
| $\mathbf{B}_{51}$ | $=$ | $-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a x_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu VII |
| $\mathbf{B}_{52}$ | $=$ | $(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$  | $=$ | $a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - c z_7 \hat{\mathbf{z}}$  | (8c) | Cu VII |
| $\mathbf{B}_{53}$ | $=$ | $-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$                                 | $=$ | $-a x_7 \hat{\mathbf{x}} - b y_7 \hat{\mathbf{y}} - c z_7 \hat{\mathbf{z}}$                               | (8c) | Cu VII |
| $\mathbf{B}_{54}$ | $=$ | $(x_7 + \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + b y_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu VII |
| $\mathbf{B}_{55}$ | $=$ | $x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a x_7 \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu VII |

|                   |     |  |     |   |      |         |
|-------------------|-----|--|-----|---|------|---------|
| $\mathbf{B}_{56}$ | $=$ | $-(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$          | $=$ | $-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$          | (8c) | Cu VII  |
| $\mathbf{B}_{57}$ | $=$ | $x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$   | $=$ | $ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$   | (8c) | Cu VIII |
| $\mathbf{B}_{58}$ | $=$ | $-(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$          | $=$ | $-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$          | (8c) | Cu VIII |
| $\mathbf{B}_{59}$ | $=$ | $-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$          | $=$ | $-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$          | (8c) | Cu VIII |
| $\mathbf{B}_{60}$ | $=$ | $(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$           | $=$ | $a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$           | (8c) | Cu VIII |
| $\mathbf{B}_{61}$ | $=$ | $-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$  | $=$ | $-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$  | (8c) | Cu VIII |
| $\mathbf{B}_{62}$ | $=$ | $(x_8 + \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$           | $=$ | $a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$           | (8c) | Cu VIII |
| $\mathbf{B}_{63}$ | $=$ | $x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$           | $=$ | $ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$           | (8c) | Cu VIII |
| $\mathbf{B}_{64}$ | $=$ | $-(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$          | $=$ | $-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$          | (8c) | Cu VIII |
| $\mathbf{B}_{65}$ | $=$ | $x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$   | $=$ | $ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$   | (8c) | Cu IX   |
| $\mathbf{B}_{66}$ | $=$ | $-(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$          | $=$ | $-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$          | (8c) | Cu IX   |
| $\mathbf{B}_{67}$ | $=$ | $-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$          | $=$ | $-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$          | (8c) | Cu IX   |
| $\mathbf{B}_{68}$ | $=$ | $(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$           | $=$ | $a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$           | (8c) | Cu IX   |
| $\mathbf{B}_{69}$ | $=$ | $-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$  | $=$ | $-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$  | (8c) | Cu IX   |
| $\mathbf{B}_{70}$ | $=$ | $(x_9 + \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$           | $=$ | $a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$           | (8c) | Cu IX   |
| $\mathbf{B}_{71}$ | $=$ | $x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$           | $=$ | $ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$           | (8c) | Cu IX   |
| $\mathbf{B}_{72}$ | $=$ | $-(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$          | $=$ | $-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$          | (8c) | Cu IX   |
| $\mathbf{B}_{73}$ | $=$ | $x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$                                  | $=$ | $ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$                                  | (8c) | Cu X    |
| $\mathbf{B}_{74}$ | $=$ | $-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu X    |
| $\mathbf{B}_{75}$ | $=$ | $-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Cu X    |
| $\mathbf{B}_{76}$ | $=$ | $(x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$  | $=$ | $a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$  | (8c) | Cu X    |
| $\mathbf{B}_{77}$ | $=$ | $-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$                                 | $=$ | $-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$                                 | (8c) | Cu X    |
| $\mathbf{B}_{78}$ | $=$ | $(x_{10} + \frac{1}{2}) \mathbf{a}_1 + y_{10} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu X    |
| $\mathbf{B}_{79}$ | $=$ | $x_{10} \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_{10} \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Cu X    |
| $\mathbf{B}_{80}$ | $=$ | $-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$ | $=$ | $-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$ | (8c) | Cu X    |
| $\mathbf{B}_{81}$ | $=$ | $x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$                                  | $=$ | $ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$                                  | (8c) | Fe I    |
| $\mathbf{B}_{82}$ | $=$ | $-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Fe I    |
| $\mathbf{B}_{83}$ | $=$ | $-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_{11} \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Fe I    |
| $\mathbf{B}_{84}$ | $=$ | $(x_{11} + \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$  | $=$ | $a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$  | (8c) | Fe I    |

|                        |  |   |   |      |       |
|------------------------|--|---|---|------|-------|
| <b>B<sub>85</sub></b>  | $-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$                                 | = | $-ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$                                 | (8c) | Fe I  |
| <b>B<sub>86</sub></b>  | $(x_{11} + \frac{1}{2}) \mathbf{a}_1 + y_{11} \mathbf{a}_2 - (z_{11} - \frac{1}{2}) \mathbf{a}_3$  | = | $a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - c(z_{11} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Fe I  |
| <b>B<sub>87</sub></b>  | $x_{11} \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + (z_{11} + \frac{1}{2}) \mathbf{a}_3$  | = | $ax_{11} \hat{\mathbf{x}} - b(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{11} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Fe I  |
| <b>B<sub>88</sub></b>  | $-(x_{11} - \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$ | = | $-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$ | (8c) | Fe I  |
| <b>B<sub>89</sub></b>  | $x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$                                  | = | $ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$                                  | (8c) | Fe II |
| <b>B<sub>90</sub></b>  | $-(x_{12} - \frac{1}{2}) \mathbf{a}_1 - y_{12} \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$ | = | $-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Fe II |
| <b>B<sub>91</sub></b>  | $-x_{12} \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$ | = | $-ax_{12} \hat{\mathbf{x}} + b(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | Fe II |
| <b>B<sub>92</sub></b>  | $(x_{12} + \frac{1}{2}) \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$  | = | $a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$  | (8c) | Fe II |
| <b>B<sub>93</sub></b>  | $-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$                                 | = | $-ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} - cz_{12} \hat{\mathbf{z}}$                                 | (8c) | Fe II |
| <b>B<sub>94</sub></b>  | $(x_{12} + \frac{1}{2}) \mathbf{a}_1 + y_{12} \mathbf{a}_2 - (z_{12} - \frac{1}{2}) \mathbf{a}_3$  | = | $a(x_{12} + \frac{1}{2}) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - c(z_{12} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Fe II |
| <b>B<sub>95</sub></b>  | $x_{12} \mathbf{a}_1 - (y_{12} - \frac{1}{2}) \mathbf{a}_2 + (z_{12} + \frac{1}{2}) \mathbf{a}_3$  | = | $ax_{12} \hat{\mathbf{x}} - b(y_{12} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{12} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | Fe II |
| <b>B<sub>96</sub></b>  | $-(x_{12} - \frac{1}{2}) \mathbf{a}_1 + (y_{12} + \frac{1}{2}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$ | = | $-a(x_{12} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{12} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$ | (8c) | Fe II |
| <b>B<sub>97</sub></b>  | $x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$                                  | = | $ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$                                  | (8c) | S I   |
| <b>B<sub>98</sub></b>  | $-(x_{13} - \frac{1}{2}) \mathbf{a}_1 - y_{13} \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$ | = | $-a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S I   |
| <b>B<sub>99</sub></b>  | $-x_{13} \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3$ | = | $-ax_{13} \hat{\mathbf{x}} + b(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S I   |
| <b>B<sub>100</sub></b> | $(x_{13} + \frac{1}{2}) \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$  | = | $a(x_{13} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}}$  | (8c) | S I   |
| <b>B<sub>101</sub></b> | $-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$                                 | = | $-ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - cz_{13} \hat{\mathbf{z}}$                                 | (8c) | S I   |
| <b>B<sub>102</sub></b> | $(x_{13} + \frac{1}{2}) \mathbf{a}_1 + y_{13} \mathbf{a}_2 - (z_{13} - \frac{1}{2}) \mathbf{a}_3$  | = | $a(x_{13} + \frac{1}{2}) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - c(z_{13} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S I   |
| <b>B<sub>103</sub></b> | $x_{13} \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 + (z_{13} + \frac{1}{2}) \mathbf{a}_3$  | = | $ax_{13} \hat{\mathbf{x}} - b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S I   |
| <b>B<sub>104</sub></b> | $-(x_{13} - \frac{1}{2}) \mathbf{a}_1 + (y_{13} + \frac{1}{2}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$ | = | $-a(x_{13} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{13} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$ | (8c) | S I   |
| <b>B<sub>105</sub></b> | $x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$                                  | = | $ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$                                  | (8c) | S II  |
| <b>B<sub>106</sub></b> | $-(x_{14} - \frac{1}{2}) \mathbf{a}_1 - y_{14} \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$ | = | $-a(x_{14} - \frac{1}{2}) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S II  |
| <b>B<sub>107</sub></b> | $-x_{14} \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3$ | = | $-ax_{14} \hat{\mathbf{x}} + b(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S II  |
| <b>B<sub>108</sub></b> | $(x_{14} + \frac{1}{2}) \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$  | = | $a(x_{14} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}}$  | (8c) | S II  |
| <b>B<sub>109</sub></b> | $-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$                                 | = | $-ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - cz_{14} \hat{\mathbf{z}}$                                 | (8c) | S II  |
| <b>B<sub>110</sub></b> | $(x_{14} + \frac{1}{2}) \mathbf{a}_1 + y_{14} \mathbf{a}_2 - (z_{14} - \frac{1}{2}) \mathbf{a}_3$  | = | $a(x_{14} + \frac{1}{2}) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S II  |

|                      |  |     |   |      |       |
|----------------------|--|-----|---|------|-------|
| $\mathbf{B}_{111} =$ | $x_{14} \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 + (z_{14} + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_{14} \hat{\mathbf{x}} - b(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S II  |
| $\mathbf{B}_{112} =$ | $-(x_{14} - \frac{1}{2}) \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$ | $=$ | $-a(x_{14} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}}$ | (8c) | S II  |
| $\mathbf{B}_{113} =$ | $x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$                                  | $=$ | $ax_{15} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}}$                                  | (8c) | S III |
| $\mathbf{B}_{114} =$ | $-(x_{15} - \frac{1}{2}) \mathbf{a}_1 - y_{15} \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_{15} - \frac{1}{2}) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S III |
| $\mathbf{B}_{115} =$ | $-x_{15} \mathbf{a}_1 + (y_{15} + \frac{1}{2}) \mathbf{a}_2 - (z_{15} - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_{15} \hat{\mathbf{x}} + b(y_{15} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S III |
| $\mathbf{B}_{116} =$ | $(x_{15} + \frac{1}{2}) \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$  | $=$ | $a(x_{15} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}}$  | (8c) | S III |
| $\mathbf{B}_{117} =$ | $-x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3$                                 | $=$ | $-ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} - cz_{15} \hat{\mathbf{z}}$                                 | (8c) | S III |
| $\mathbf{B}_{118} =$ | $(x_{15} + \frac{1}{2}) \mathbf{a}_1 + y_{15} \mathbf{a}_2 - (z_{15} - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_{15} + \frac{1}{2}) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - c(z_{15} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S III |
| $\mathbf{B}_{119} =$ | $x_{15} \mathbf{a}_1 - (y_{15} - \frac{1}{2}) \mathbf{a}_2 + (z_{15} + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_{15} \hat{\mathbf{x}} - b(y_{15} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{15} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S III |
| $\mathbf{B}_{120} =$ | $-(x_{15} - \frac{1}{2}) \mathbf{a}_1 + (y_{15} + \frac{1}{2}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$ | $=$ | $-a(x_{15} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{15} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}}$ | (8c) | S III |
| $\mathbf{B}_{121} =$ | $x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$                                  | $=$ | $ax_{16} \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$                                  | (8c) | S IV  |
| $\mathbf{B}_{122} =$ | $-(x_{16} - \frac{1}{2}) \mathbf{a}_1 - y_{16} \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_{16} - \frac{1}{2}) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S IV  |
| $\mathbf{B}_{123} =$ | $-x_{16} \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 - (z_{16} - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_{16} \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S IV  |
| $\mathbf{B}_{124} =$ | $(x_{16} + \frac{1}{2}) \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$  | $=$ | $a(x_{16} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}}$  | (8c) | S IV  |
| $\mathbf{B}_{125} =$ | $-x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3$                                 | $=$ | $-ax_{16} \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} - cz_{16} \hat{\mathbf{z}}$                                 | (8c) | S IV  |
| $\mathbf{B}_{126} =$ | $(x_{16} + \frac{1}{2}) \mathbf{a}_1 + y_{16} \mathbf{a}_2 - (z_{16} - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_{16} + \frac{1}{2}) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - c(z_{16} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S IV  |
| $\mathbf{B}_{127} =$ | $x_{16} \mathbf{a}_1 - (y_{16} - \frac{1}{2}) \mathbf{a}_2 + (z_{16} + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_{16} \hat{\mathbf{x}} - b(y_{16} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{16} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S IV  |
| $\mathbf{B}_{128} =$ | $-(x_{16} - \frac{1}{2}) \mathbf{a}_1 + (y_{16} + \frac{1}{2}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$ | $=$ | $-a(x_{16} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{16} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}}$ | (8c) | S IV  |
| $\mathbf{B}_{129} =$ | $x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$                                  | $=$ | $ax_{17} \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$                                  | (8c) | S V   |
| $\mathbf{B}_{130} =$ | $-(x_{17} - \frac{1}{2}) \mathbf{a}_1 - y_{17} \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S V   |
| $\mathbf{B}_{131} =$ | $-x_{17} \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_{17} \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | S V   |
| $\mathbf{B}_{132} =$ | $(x_{17} + \frac{1}{2}) \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$  | $=$ | $a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}}$  | (8c) | S V   |
| $\mathbf{B}_{133} =$ | $-x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3$                                 | $=$ | $-ax_{17} \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}}$                                 | (8c) | S V   |
| $\mathbf{B}_{134} =$ | $(x_{17} + \frac{1}{2}) \mathbf{a}_1 + y_{17} \mathbf{a}_2 - (z_{17} - \frac{1}{2}) \mathbf{a}_3$  | $=$ | $a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S V   |
| $\mathbf{B}_{135} =$ | $x_{17} \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 + (z_{17} + \frac{1}{2}) \mathbf{a}_3$  | $=$ | $ax_{17} \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$  | (8c) | S V   |
| $\mathbf{B}_{136} =$ | $-(x_{17} - \frac{1}{2}) \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$ | $=$ | $-a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$ | (8c) | S V   |

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

## References

- [1] A. Martinelli, G. O. Lepore, F. Bernardini, A. Giaccherini, and F. D. Benedetto, *The puzzling structure of Cu<sub>5</sub>FeS<sub>4</sub> (bornite) at low temperature*, Acta Crystallogr. Sect. B **74**, 405–415 (2018), doi:10.1107/S2052520618009812.