

# Al<sub>17</sub>Mo<sub>4</sub> Structure:

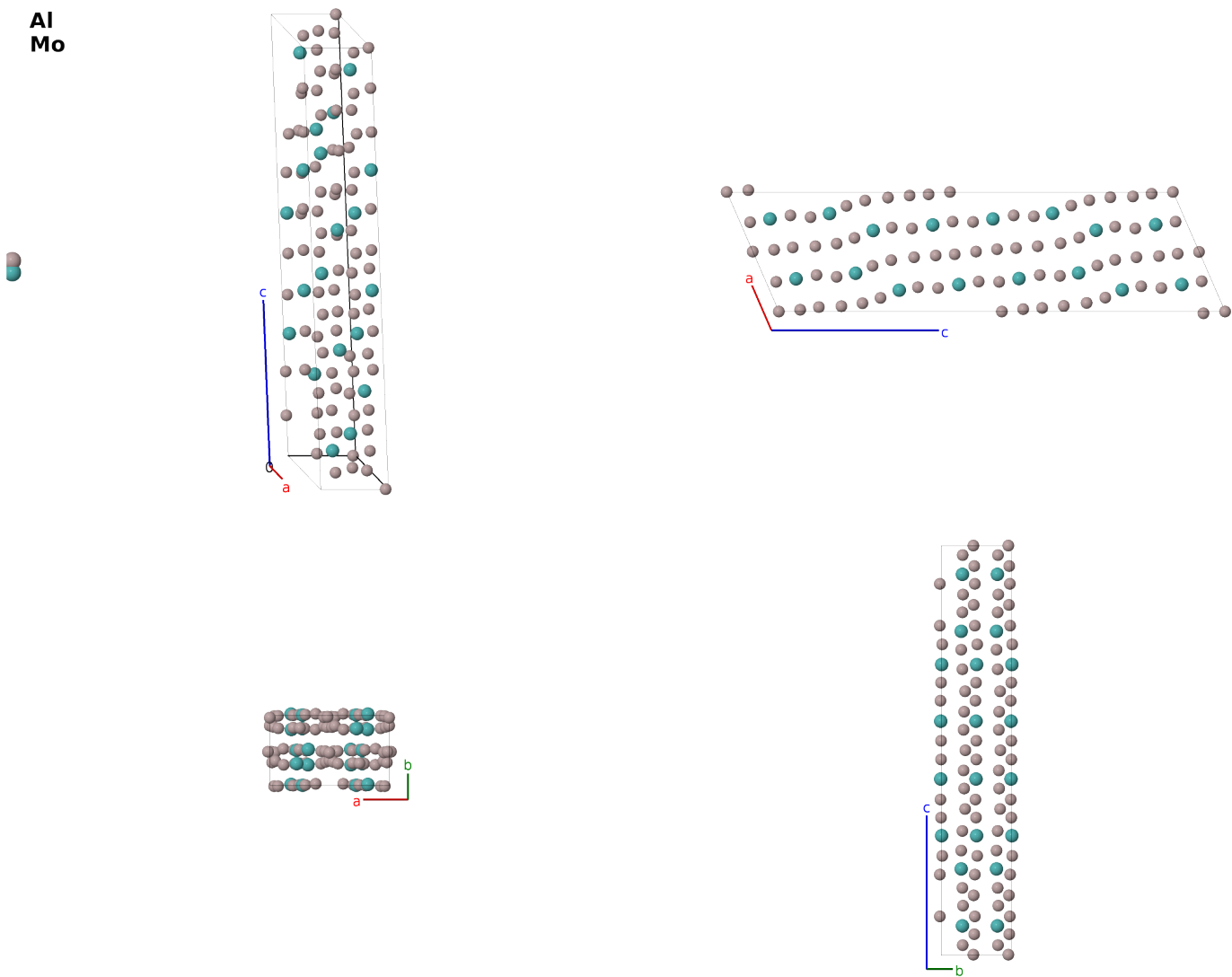
## A17B4\_mC84\_5\_ab16c\_4c-001

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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/QL9A>

[https://aflow.org/prototype-encyclopedia/A17B4\\_mC84\\_5\\_ab16c\\_4c-001](https://aflow.org/prototype-encyclopedia/A17B4_mC84_5_ab16c_4c-001)



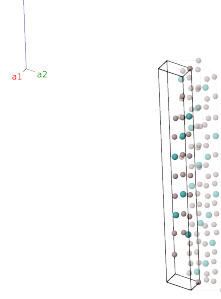
|                       |                                  |
|-----------------------|----------------------------------|
| Prototype             | Al <sub>17</sub> Mo <sub>4</sub> |
| AFLOW prototype label | A17B4_mC84_5_ab16c_4c-001        |
| ICSD                  | 400887                           |
| CCDC                  | 1724609                          |

|                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|-------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Pearson symbol          | mC84                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Space group number      | 5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Space group symbol      | $C2$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| AFLOW prototype command | aflow --proto=A17B4_mC84_5_ab16c_4c-001<br>--params= $a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}$ |

- Space group  $C2$  #5 allows an arbitrary choice of the origin of the  $y$ -axis. Here we follow (Grin, 1995) and set  $y_{19} = 0$  for the Mo-I atom.

### Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$



### Basis vectors

|                   | Lattice coordinates                                                         |     | Cartesian coordinates                                                                                         | Wyckoff position | Atom type |
|-------------------|-----------------------------------------------------------------------------|-----|---------------------------------------------------------------------------------------------------------------|------------------|-----------|
| $\mathbf{B}_1$    | $= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$                                    | $=$ | $by_1 \hat{\mathbf{y}}$                                                                                       | (2a)             | Al I      |
| $\mathbf{B}_2$    | $= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$         | $=$ | $\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$ | (2b)             | Al II     |
| $\mathbf{B}_3$    | $= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$  | $=$ | $(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$        | (4c)             | Al III    |
| $\mathbf{B}_4$    | $= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$       | (4c)             | Al III    |
| $\mathbf{B}_5$    | $= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$  | $=$ | $(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$        | (4c)             | Al IV     |
| $\mathbf{B}_6$    | $= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$ | $=$ | $-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$       | (4c)             | Al IV     |
| $\mathbf{B}_7$    | $= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$  | $=$ | $(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$        | (4c)             | Al V      |
| $\mathbf{B}_8$    | $= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$ | $=$ | $-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$       | (4c)             | Al V      |
| $\mathbf{B}_9$    | $= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$  | $=$ | $(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$        | (4c)             | Al VI     |
| $\mathbf{B}_{10}$ | $= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$ | $=$ | $-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$       | (4c)             | Al VI     |
| $\mathbf{B}_{11}$ | $= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$  | $=$ | $(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$        | (4c)             | Al VII    |

|                     |                                                                                          |     |                                                                                                                     |      |          |
|---------------------|------------------------------------------------------------------------------------------|-----|---------------------------------------------------------------------------------------------------------------------|------|----------|
| $\mathbf{B}_{12} =$ | $-(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$                | $=$ | $-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$             | (4c) | Al VII   |
| $\mathbf{B}_{13} =$ | $(x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$                 | $=$ | $(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$              | (4c) | Al VIII  |
| $\mathbf{B}_{14} =$ | $-(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$                | $=$ | $-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$             | (4c) | Al VIII  |
| $\mathbf{B}_{15} =$ | $(x_9 - y_9) \mathbf{a}_1 + (x_9 + y_9) \mathbf{a}_2 + z_9 \mathbf{a}_3$                 | $=$ | $(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$              | (4c) | Al IX    |
| $\mathbf{B}_{16} =$ | $-(x_9 + y_9) \mathbf{a}_1 - (x_9 - y_9) \mathbf{a}_2 - z_9 \mathbf{a}_3$                | $=$ | $-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$             | (4c) | Al IX    |
| $\mathbf{B}_{17} =$ | $(x_{10} - y_{10}) \mathbf{a}_1 + (x_{10} + y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$  | $=$ | $(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al X     |
| $\mathbf{B}_{18} =$ | $-(x_{10} + y_{10}) \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$ | $=$ | $-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al X     |
| $\mathbf{B}_{19} =$ | $(x_{11} - y_{11}) \mathbf{a}_1 + (x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$  | $=$ | $(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XI    |
| $\mathbf{B}_{20} =$ | $-(x_{11} + y_{11}) \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$ | $=$ | $-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} - cz_{11} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XI    |
| $\mathbf{B}_{21} =$ | $(x_{12} - y_{12}) \mathbf{a}_1 + (x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$  | $=$ | $(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XII   |
| $\mathbf{B}_{22} =$ | $-(x_{12} + y_{12}) \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$ | $=$ | $-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} - cz_{12} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XII   |
| $\mathbf{B}_{23} =$ | $(x_{13} - y_{13}) \mathbf{a}_1 + (x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$  | $=$ | $(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XIII  |
| $\mathbf{B}_{24} =$ | $-(x_{13} + y_{13}) \mathbf{a}_1 - (x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$ | $=$ | $-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} - cz_{13} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XIII  |
| $\mathbf{B}_{25} =$ | $(x_{14} - y_{14}) \mathbf{a}_1 + (x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$  | $=$ | $(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XIV   |
| $\mathbf{B}_{26} =$ | $-(x_{14} + y_{14}) \mathbf{a}_1 - (x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$ | $=$ | $-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} - cz_{14} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XIV   |
| $\mathbf{B}_{27} =$ | $(x_{15} - y_{15}) \mathbf{a}_1 + (x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$  | $=$ | $(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XV    |
| $\mathbf{B}_{28} =$ | $-(x_{15} + y_{15}) \mathbf{a}_1 - (x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$ | $=$ | $-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} - cz_{15} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XV    |
| $\mathbf{B}_{29} =$ | $(x_{16} - y_{16}) \mathbf{a}_1 + (x_{16} + y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$  | $=$ | $(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XVI   |
| $\mathbf{B}_{30} =$ | $-(x_{16} + y_{16}) \mathbf{a}_1 - (x_{16} - y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$ | $=$ | $-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} - cz_{16} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XVI   |
| $\mathbf{B}_{31} =$ | $(x_{17} - y_{17}) \mathbf{a}_1 + (x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$  | $=$ | $(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XVII  |
| $\mathbf{B}_{32} =$ | $-(x_{17} + y_{17}) \mathbf{a}_1 - (x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$ | $=$ | $-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} - cz_{17} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XVII  |
| $\mathbf{B}_{33} =$ | $(x_{18} - y_{18}) \mathbf{a}_1 + (x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$  | $=$ | $(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$  | (4c) | Al XVIII |
| $\mathbf{B}_{34} =$ | $-(x_{18} + y_{18}) \mathbf{a}_1 - (x_{18} - y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$ | $=$ | $-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} - cz_{18} \sin \beta \hat{\mathbf{z}}$ | (4c) | Al XVIII |
| $\mathbf{B}_{35} =$ | $(x_{19} - y_{19}) \mathbf{a}_1 + (x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3$  | $=$ | $(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}}$  | (4c) | Mo I     |

$$\begin{aligned}
\mathbf{B}_{36} &= \begin{matrix} -(x_{19} + y_{19}) \mathbf{a}_1 - \\ (x_{19} - y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - \\ cz_{19} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo I} \\
\mathbf{B}_{37} &= \begin{matrix} (x_{20} - y_{20}) \mathbf{a}_1 + \\ (x_{20} + y_{20}) \mathbf{a}_2 + z_{20} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo II} \\
\mathbf{B}_{38} &= \begin{matrix} -(x_{20} + y_{20}) \mathbf{a}_1 - \\ (x_{20} - y_{20}) \mathbf{a}_2 - z_{20} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{20} + cz_{20} \cos \beta) \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} - \\ cz_{20} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo II} \\
\mathbf{B}_{39} &= \begin{matrix} (x_{21} - y_{21}) \mathbf{a}_1 + \\ (x_{21} + y_{21}) \mathbf{a}_2 + z_{21} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo III} \\
\mathbf{B}_{40} &= \begin{matrix} -(x_{21} + y_{21}) \mathbf{a}_1 - \\ (x_{21} - y_{21}) \mathbf{a}_2 - z_{21} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{21} + cz_{21} \cos \beta) \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} - \\ cz_{21} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo III} \\
\mathbf{B}_{41} &= \begin{matrix} (x_{22} - y_{22}) \mathbf{a}_1 + \\ (x_{22} + y_{22}) \mathbf{a}_2 + z_{22} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} (ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo IV} \\
\mathbf{B}_{42} &= \begin{matrix} -(x_{22} + y_{22}) \mathbf{a}_1 - \\ (x_{22} - y_{22}) \mathbf{a}_2 - z_{22} \mathbf{a}_3 \end{matrix} &= & \begin{matrix} -(ax_{22} + cz_{22} \cos \beta) \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} - \\ cz_{22} \sin \beta \hat{\mathbf{z}} \end{matrix} &(4c) & \text{Mo IV}
\end{aligned}$$

## References

- [1] Y. N. Grin, M. Ellner, K. Peters, and J. C. Schuster, *The crystal structures of  $\text{Mo}_4\text{Al}_{17}$  and  $\text{Mo}_5\text{Al}_{22}$* , Z. Kristallogr. **210**, 96–99 (1995), doi:10.1524/zkri.1995.210.2.96.

## First cited in

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