

Al₂₂Mo₅ Structure:

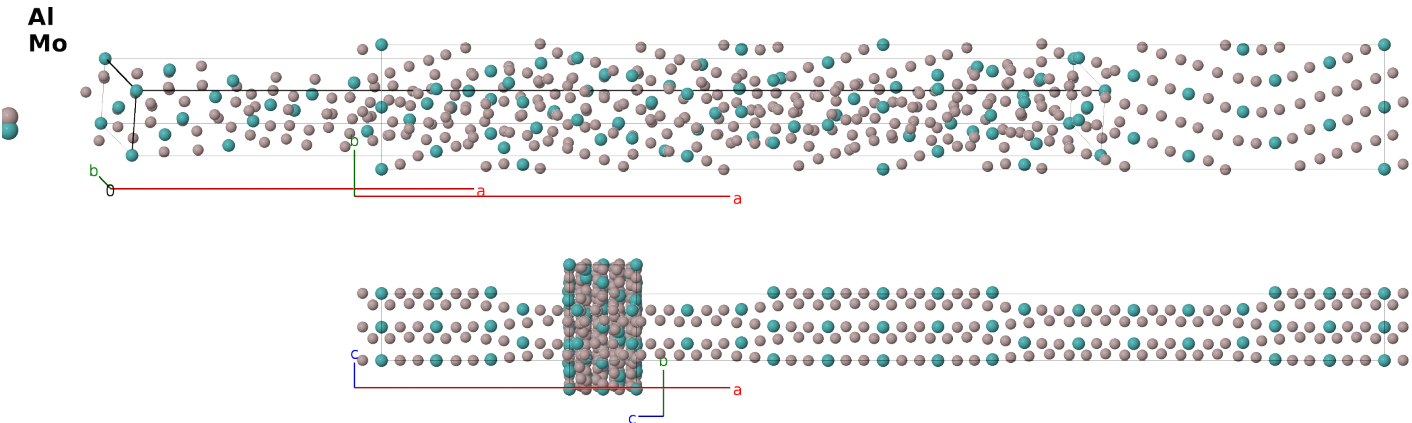
A22B5_oF216_43_11b_a2b-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/15LF>

https://aflow.org/prototype-encyclopedia/A22B5_oF216_43_11b_a2b-001

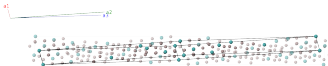


Prototype	Al ₂₂ Mo ₅
AFLOW prototype label	A22B5_oF216_43_11b_a2b-001
ICSD	400888
CCDC	1724610
Pearson symbol	oF216
Space group number	43
Space group symbol	<i>Fdd</i> 2
AFLOW prototype command	<pre>aflow --proto=A22B5_oF216_43_11b_a2b-001 --params=a,b/a,c/a,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈, y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄</pre>

- Space group *Fdd*2 #43 allows an arbitrary choice of the origin of the *z*-axis. Here we follow (Grin, 1995) and set *z*₁ = 0 for the Mo-I atom.

Face-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(8a)	Mo I
$\mathbf{B}_2$	$= \left(z_1 + \frac{1}{4}\right) \mathbf{a}_1 + \left(z_1 + \frac{1}{4}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8a)	Mo I
$\mathbf{B}_3$	$= \begin{aligned} &(-x_2 + y_2 + z_2) \mathbf{a}_1 + \\ &(x_2 - y_2 + z_2) \mathbf{a}_2 + \\ &(x_2 + y_2 - z_2) \mathbf{a}_3 \end{aligned}$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B}_4$	$= \begin{aligned} &(x_2 - y_2 + z_2) \mathbf{a}_1 + \\ &(-x_2 + y_2 + z_2) \mathbf{a}_2 - \\ &(x_2 + y_2 + z_2) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B}_5$	$= \begin{aligned} &-(x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_1 + \\ &(x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_2 - y_2 - z_2 + \frac{1}{4}) \mathbf{a}_3 \end{aligned}$	$=$	$a \left(x_2 + \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B}_6$	$= \begin{aligned} &(x_2 + y_2 + z_2 + \frac{1}{4}) \mathbf{a}_1 - \\ &(x_2 + y_2 - z_2 - \frac{1}{4}) \mathbf{a}_2 - \\ &(x_2 - y_2 + z_2 - \frac{1}{4}) \mathbf{a}_3 \end{aligned}$	$=$	$-a \left(x_2 - \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B}_7$	$= \begin{aligned} &(-x_3 + y_3 + z_3) \mathbf{a}_1 + \\ &(x_3 - y_3 + z_3) \mathbf{a}_2 + \\ &(x_3 + y_3 - z_3) \mathbf{a}_3 \end{aligned}$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B}_8$	$= \begin{aligned} &(x_3 - y_3 + z_3) \mathbf{a}_1 + \\ &(-x_3 + y_3 + z_3) \mathbf{a}_2 - \\ &(x_3 + y_3 + z_3) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B}_9$	$= \begin{aligned} &-(x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_1 + \\ &(x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_3 - y_3 - z_3 + \frac{1}{4}) \mathbf{a}_3 \end{aligned}$	$=$	$a \left(x_3 + \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B}_{10}$	$= \begin{aligned} &(x_3 + y_3 + z_3 + \frac{1}{4}) \mathbf{a}_1 - \\ &(x_3 + y_3 - z_3 - \frac{1}{4}) \mathbf{a}_2 - \\ &(x_3 - y_3 + z_3 - \frac{1}{4}) \mathbf{a}_3 \end{aligned}$	$=$	$-a \left(x_3 - \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B}_{11}$	$= \begin{aligned} &(-x_4 + y_4 + z_4) \mathbf{a}_1 + \\ &(x_4 - y_4 + z_4) \mathbf{a}_2 + \\ &(x_4 + y_4 - z_4) \mathbf{a}_3 \end{aligned}$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B}_{12}$	$= \begin{aligned} &(x_4 - y_4 + z_4) \mathbf{a}_1 + \\ &(-x_4 + y_4 + z_4) \mathbf{a}_2 - \\ &(x_4 + y_4 + z_4) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B}_{13}$	$= \begin{aligned} &-(x_4 + y_4 - z_4 - \frac{1}{4}) \mathbf{a}_1 + \\ &(x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_2 + \\ &(x_4 - y_4 - z_4 + \frac{1}{4}) \mathbf{a}_3 \end{aligned}$	$=$	$a \left(x_4 + \frac{1}{4}\right) \hat{\mathbf{x}} - b \left(y_4 - \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B}_{14}$	$= \begin{aligned} &(x_4 + y_4 + z_4 + \frac{1}{4}) \mathbf{a}_1 - \\ &(x_4 + y_4 - z_4 - \frac{1}{4}) \mathbf{a}_2 - \\ &(x_4 - y_4 + z_4 - \frac{1}{4}) \mathbf{a}_3 \end{aligned}$	$=$	$-a \left(x_4 - \frac{1}{4}\right) \hat{\mathbf{x}} + b \left(y_4 + \frac{1}{4}\right) \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B}_{15}$	$= \begin{aligned} &(-x_5 + y_5 + z_5) \mathbf{a}_1 + \\ &(x_5 - y_5 + z_5) \mathbf{a}_2 + \\ &(x_5 + y_5 - z_5) \mathbf{a}_3 \end{aligned}$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16b)	Al IV
$\mathbf{B}_{16}$	$= \begin{aligned} &(x_5 - y_5 + z_5) \mathbf{a}_1 + \\ &(-x_5 + y_5 + z_5) \mathbf{a}_2 - \\ &(x_5 + y_5 + z_5) \mathbf{a}_3 \end{aligned}$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(16b)	Al IV

$\mathbf{B}_{17} =$	$-\left(x_5 + y_5 - z_5 - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_5 + y_5 + z_5 + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_5 - y_5 - z_5 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_5 - \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al IV
$\mathbf{B}_{18} =$	$\left(x_5 + y_5 + z_5 + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_5 + y_5 - z_5 - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_5 - y_5 + z_5 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_5 + \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al IV
$\mathbf{B}_{19} =$	$\left(-x_6 + y_6 + z_6\right) \mathbf{a}_1 +$ $\left(x_6 - y_6 + z_6\right) \mathbf{a}_2 +$ $\left(x_6 + y_6 - z_6\right) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16b)	Al V
$\mathbf{B}_{20} =$	$\left(x_6 - y_6 + z_6\right) \mathbf{a}_1 +$ $\left(-x_6 + y_6 + z_6\right) \mathbf{a}_2 -$ $\left(x_6 + y_6 + z_6\right) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(16b)	Al V
$\mathbf{B}_{21} =$	$-\left(x_6 + y_6 - z_6 - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_6 + y_6 + z_6 + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_6 - y_6 - z_6 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_6 + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_6 - \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al V
$\mathbf{B}_{22} =$	$\left(x_6 + y_6 + z_6 + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_6 + y_6 - z_6 - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_6 - y_6 + z_6 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_6 - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_6 + \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_6 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al V
$\mathbf{B}_{23} =$	$\left(-x_7 + y_7 + z_7\right) \mathbf{a}_1 +$ $\left(x_7 - y_7 + z_7\right) \mathbf{a}_2 +$ $\left(x_7 + y_7 - z_7\right) \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(16b)	Al VI
$\mathbf{B}_{24} =$	$\left(x_7 - y_7 + z_7\right) \mathbf{a}_1 +$ $\left(-x_7 + y_7 + z_7\right) \mathbf{a}_2 -$ $\left(x_7 + y_7 + z_7\right) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(16b)	Al VI
$\mathbf{B}_{25} =$	$-\left(x_7 + y_7 - z_7 - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_7 + y_7 + z_7 + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_7 - y_7 - z_7 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_7 + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_7 - \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al VI
$\mathbf{B}_{26} =$	$\left(x_7 + y_7 + z_7 + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_7 + y_7 - z_7 - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_7 - y_7 + z_7 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_7 - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_7 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al VI
$\mathbf{B}_{27} =$	$\left(-x_8 + y_8 + z_8\right) \mathbf{a}_1 +$ $\left(x_8 - y_8 + z_8\right) \mathbf{a}_2 +$ $\left(x_8 + y_8 - z_8\right) \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(16b)	Al VII
$\mathbf{B}_{28} =$	$\left(x_8 - y_8 + z_8\right) \mathbf{a}_1 +$ $\left(-x_8 + y_8 + z_8\right) \mathbf{a}_2 -$ $\left(x_8 + y_8 + z_8\right) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(16b)	Al VII
$\mathbf{B}_{29} =$	$-\left(x_8 + y_8 - z_8 - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_8 + y_8 + z_8 + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_8 - y_8 - z_8 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_8 + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al VII
$\mathbf{B}_{30} =$	$\left(x_8 + y_8 + z_8 + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_8 + y_8 - z_8 - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_8 - y_8 + z_8 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_8 - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al VII
$\mathbf{B}_{31} =$	$\left(-x_9 + y_9 + z_9\right) \mathbf{a}_1 +$ $\left(x_9 - y_9 + z_9\right) \mathbf{a}_2 +$ $\left(x_9 + y_9 - z_9\right) \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(16b)	Al VIII
$\mathbf{B}_{32} =$	$\left(x_9 - y_9 + z_9\right) \mathbf{a}_1 +$ $\left(-x_9 + y_9 + z_9\right) \mathbf{a}_2 -$ $\left(x_9 + y_9 + z_9\right) \mathbf{a}_3$	$=$	$-ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(16b)	Al VIII

$\mathbf{B}_{33} =$	$-\left(x_9 + y_9 - z_9 - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_9 + y_9 + z_9 + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_9 - y_9 - z_9 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_9 + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al VIII
$\mathbf{B}_{34} =$	$\left(x_9 + y_9 + z_9 + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_9 + y_9 - z_9 - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_9 - y_9 + z_9 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_9 - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{4}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al VIII
$\mathbf{B}_{35} =$	$\left(-x_{10} + y_{10} + z_{10}\right) \mathbf{a}_1 +$ $\left(x_{10} - y_{10} + z_{10}\right) \mathbf{a}_2 +$ $\left(x_{10} + y_{10} - z_{10}\right) \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(16b)	Al IX
$\mathbf{B}_{36} =$	$\left(x_{10} - y_{10} + z_{10}\right) \mathbf{a}_1 +$ $\left(-x_{10} + y_{10} + z_{10}\right) \mathbf{a}_2 -$ $\left(x_{10} + y_{10} + z_{10}\right) \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(16b)	Al IX
$\mathbf{B}_{37} =$	$-\left(x_{10} + y_{10} - z_{10} - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_{10} + y_{10} + z_{10} + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_{10} - y_{10} - z_{10} + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_{10} + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{4}\right) \hat{\mathbf{y}} +$ $c\left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al IX
$\mathbf{B}_{38} =$	$\left(x_{10} + y_{10} + z_{10} + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_{10} + y_{10} - z_{10} - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_{10} - y_{10} + z_{10} - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_{10} - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{4}\right) \hat{\mathbf{y}} +$ $c\left(z_{10} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al IX
$\mathbf{B}_{39} =$	$\left(-x_{11} + y_{11} + z_{11}\right) \mathbf{a}_1 +$ $\left(x_{11} - y_{11} + z_{11}\right) \mathbf{a}_2 +$ $\left(x_{11} + y_{11} - z_{11}\right) \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(16b)	Al X
$\mathbf{B}_{40} =$	$\left(x_{11} - y_{11} + z_{11}\right) \mathbf{a}_1 +$ $\left(-x_{11} + y_{11} + z_{11}\right) \mathbf{a}_2 -$ $\left(x_{11} + y_{11} + z_{11}\right) \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(16b)	Al X
$\mathbf{B}_{41} =$	$-\left(x_{11} + y_{11} - z_{11} - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_{11} + y_{11} + z_{11} + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_{11} - y_{11} - z_{11} + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_{11} + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_{11} - \frac{1}{4}\right) \hat{\mathbf{y}} +$ $c\left(z_{11} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al X
$\mathbf{B}_{42} =$	$\left(x_{11} + y_{11} + z_{11} + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_{11} + y_{11} - z_{11} - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_{11} - y_{11} + z_{11} - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_{11} - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_{11} + \frac{1}{4}\right) \hat{\mathbf{y}} +$ $c\left(z_{11} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al X
$\mathbf{B}_{43} =$	$\left(-x_{12} + y_{12} + z_{12}\right) \mathbf{a}_1 +$ $\left(x_{12} - y_{12} + z_{12}\right) \mathbf{a}_2 +$ $\left(x_{12} + y_{12} - z_{12}\right) \mathbf{a}_3$	$=$	$ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(16b)	Al XI
$\mathbf{B}_{44} =$	$\left(x_{12} - y_{12} + z_{12}\right) \mathbf{a}_1 +$ $\left(-x_{12} + y_{12} + z_{12}\right) \mathbf{a}_2 -$ $\left(x_{12} + y_{12} + z_{12}\right) \mathbf{a}_3$	$=$	$-ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}}$	(16b)	Al XI
$\mathbf{B}_{45} =$	$-\left(x_{12} + y_{12} - z_{12} - \frac{1}{4}\right) \mathbf{a}_1 +$ $\left(x_{12} + y_{12} + z_{12} + \frac{1}{4}\right) \mathbf{a}_2 +$ $\left(x_{12} - y_{12} - z_{12} + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_{12} + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_{12} - \frac{1}{4}\right) \hat{\mathbf{y}} +$ $c\left(z_{12} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al XI
$\mathbf{B}_{46} =$	$\left(x_{12} + y_{12} + z_{12} + \frac{1}{4}\right) \mathbf{a}_1 -$ $\left(x_{12} + y_{12} - z_{12} - \frac{1}{4}\right) \mathbf{a}_2 -$ $\left(x_{12} - y_{12} + z_{12} - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_{12} - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_{12} + \frac{1}{4}\right) \hat{\mathbf{y}} +$ $c\left(z_{12} + \frac{1}{4}\right) \hat{\mathbf{z}}$	(16b)	Al XI
$\mathbf{B}_{47} =$	$\left(-x_{13} + y_{13} + z_{13}\right) \mathbf{a}_1 +$ $\left(x_{13} - y_{13} + z_{13}\right) \mathbf{a}_2 +$ $\left(x_{13} + y_{13} - z_{13}\right) \mathbf{a}_3$	$=$	$ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(16b)	Mo II
$\mathbf{B}_{48} =$	$\left(x_{13} - y_{13} + z_{13}\right) \mathbf{a}_1 +$ $\left(-x_{13} + y_{13} + z_{13}\right) \mathbf{a}_2 -$ $\left(x_{13} + y_{13} + z_{13}\right) \mathbf{a}_3$	$=$	$-ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}}$	(16b)	Mo II

$$\begin{aligned}
\mathbf{B}_{49} &= -\left(x_{13} + y_{13} - z_{13} - \frac{1}{4}\right) \mathbf{a}_1 + &= a\left(x_{13} + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_{13} - \frac{1}{4}\right) \hat{\mathbf{y}} + & (16b) & \text{Mo II} \\
&\quad \left(x_{13} + y_{13} + z_{13} + \frac{1}{4}\right) \mathbf{a}_2 + && c\left(z_{13} + \frac{1}{4}\right) \hat{\mathbf{z}} \\
&\quad \left(x_{13} - y_{13} - z_{13} + \frac{1}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{50} &= \left(x_{13} + y_{13} + z_{13} + \frac{1}{4}\right) \mathbf{a}_1 - &= -a\left(x_{13} - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_{13} + \frac{1}{4}\right) \hat{\mathbf{y}} + & (16b) & \text{Mo II} \\
&\quad \left(x_{13} + y_{13} - z_{13} - \frac{1}{4}\right) \mathbf{a}_2 - && c\left(z_{13} + \frac{1}{4}\right) \hat{\mathbf{z}} \\
&\quad \left(x_{13} - y_{13} + z_{13} - \frac{1}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{51} &= \left(-x_{14} + y_{14} + z_{14}\right) \mathbf{a}_1 + &= ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16b) & \text{Mo III} \\
&\quad \left(x_{14} - y_{14} + z_{14}\right) \mathbf{a}_2 + \\
&\quad \left(x_{14} + y_{14} - z_{14}\right) \mathbf{a}_3 \\
\mathbf{B}_{52} &= \left(x_{14} - y_{14} + z_{14}\right) \mathbf{a}_1 + &= -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (16b) & \text{Mo III} \\
&\quad \left(-x_{14} + y_{14} + z_{14}\right) \mathbf{a}_2 - \\
&\quad \left(x_{14} + y_{14} + z_{14}\right) \mathbf{a}_3 \\
\mathbf{B}_{53} &= -\left(x_{14} + y_{14} - z_{14} - \frac{1}{4}\right) \mathbf{a}_1 + &= a\left(x_{14} + \frac{1}{4}\right) \hat{\mathbf{x}} - b\left(y_{14} - \frac{1}{4}\right) \hat{\mathbf{y}} + & (16b) & \text{Mo III} \\
&\quad \left(x_{14} + y_{14} + z_{14} + \frac{1}{4}\right) \mathbf{a}_2 + && c\left(z_{14} + \frac{1}{4}\right) \hat{\mathbf{z}} \\
&\quad \left(x_{14} - y_{14} - z_{14} + \frac{1}{4}\right) \mathbf{a}_3 \\
\mathbf{B}_{54} &= \left(x_{14} + y_{14} + z_{14} + \frac{1}{4}\right) \mathbf{a}_1 - &= -a\left(x_{14} - \frac{1}{4}\right) \hat{\mathbf{x}} + b\left(y_{14} + \frac{1}{4}\right) \hat{\mathbf{y}} + & (16b) & \text{Mo III} \\
&\quad \left(x_{14} + y_{14} - z_{14} - \frac{1}{4}\right) \mathbf{a}_2 - && c\left(z_{14} + \frac{1}{4}\right) \hat{\mathbf{z}} \\
&\quad \left(x_{14} - y_{14} + z_{14} - \frac{1}{4}\right) \mathbf{a}_3
\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.

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