$Al_{22}Mo_5$ Structure: A22B5_oF216_43_11b_a2b-001

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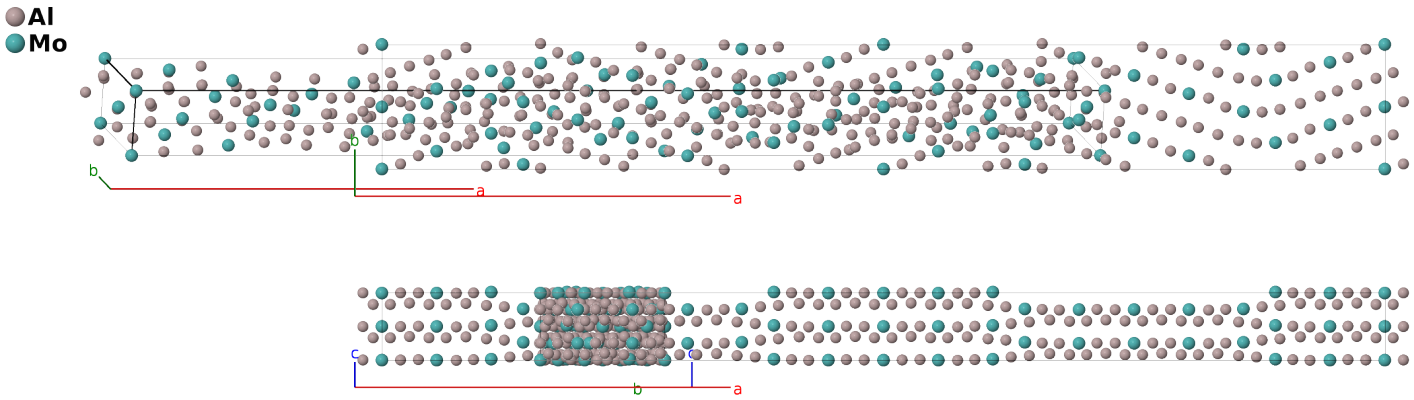
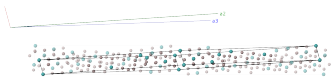


Prototype	$Al_{22}Mo_5$
AFLOW prototype label	A22B5_oF216_43_11b_a2b-001
ICSD	400888
Pearson symbol	oF216
Space group number	43
Space group symbol	$Fdd2$
AFLOW prototype command	`aflow --proto=A22B5_oF216_43_11b_a2b-001 --params=`$a, b/a, c/a, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}$

- Space group $Fdd2$ #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

$$\mathbf{a_1} = \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$



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
$\mathbf{B_3}$	=	$(-x_2+y_2+z_2)\,\mathbf{a}_1+(x_2-y_2+z_2)\,\mathbf{a}_2+(x_2+y_2-z_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}+by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B_4}$	=	$(x_2-y_2+z_2)\,\mathbf{a}_1+(-x_2+y_2+z_2)\,\mathbf{a}_2-(x_2+y_2+z_2)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}-by_2\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B_5}$	=	$-\left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_1+\left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_2+\left(x_2-y_2-z_2+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_2-\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B_6}$	=	$\left(x_2+y_2+z_2+\frac{1}{4}\right)\mathbf{a}_1-\left(x_2+y_2-z_2-\frac{1}{4}\right)\mathbf{a}_2-\left(x_2-y_2+z_2-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_2+\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_2+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al I
$\mathbf{B_7}$	=	$(-x_3+y_3+z_3)\,\mathbf{a}_1+(x_3-y_3+z_3)\,\mathbf{a}_2+(x_3+y_3-z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_8}$	=	$(x_3-y_3+z_3)\,\mathbf{a}_1+(-x_3+y_3+z_3)\,\mathbf{a}_2-(x_3+y_3+z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-by_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_9}$	=	$-\left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_1+\left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_2+\left(x_3-y_3-z_3+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_3-\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_{10}}$	=	$\left(x_3+y_3+z_3+\frac{1}{4}\right)\mathbf{a}_1-\left(x_3+y_3-z_3-\frac{1}{4}\right)\mathbf{a}_2-\left(x_3-y_3+z_3-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_3+\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_3+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al II
$\mathbf{B_{11}}$	=	$(-x_4+y_4+z_4)\,\mathbf{a}_1+(x_4-y_4+z_4)\,\mathbf{a}_2+(x_4+y_4-z_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B_{12}}$	=	$(x_4-y_4+z_4)\,\mathbf{a}_1+(-x_4+y_4+z_4)\,\mathbf{a}_2-(x_4+y_4+z_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B_{13}}$	=	$-\left(x_4+y_4-z_4-\frac{1}{4}\right)\mathbf{a}_1+\left(x_4+y_4+z_4+\frac{1}{4}\right)\mathbf{a}_2+\left(x_4-y_4-z_4+\frac{1}{4}\right)\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_4-\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B_{14}}$	=	$\left(x_4+y_4+z_4+\frac{1}{4}\right)\mathbf{a}_1-\left(x_4+y_4-z_4-\frac{1}{4}\right)\mathbf{a}_2-\left(x_4-y_4+z_4-\frac{1}{4}\right)\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_4+\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(16b)	Al III
$\mathbf{B_{15}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1+(x_5-y_5+z_5)\,\mathbf{a}_2+(x_5+y_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(16b)	Al IV
$\mathbf{B_{16}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1+(-x_5+y_5+z_5)\,\mathbf{a}_2-(x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(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

$$\mathbf{B_{19}} = (-x_6+y_6+z_6)\,\mathbf{a}_1+(x_6-y_6+z_6)\,\mathbf{a}_2+(x_6+y_6-z_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al V}$$

$$\mathbf{B_{20}} = (x_6-y_6+z_6)\,\mathbf{a}_1+(-x_6+y_6+z_6)\,\mathbf{a}_2-(x_6+y_6+z_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al V}$$

$$\mathbf{B_{21}} = -\left(x_6+y_6-z_6-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_6+y_6+z_6+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_6-y_6-z_6+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_6+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_6-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al V}$$

$$\mathbf{B_{22}} = \left(x_6+y_6+z_6+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_6+y_6-z_6-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_6-y_6+z_6-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_6-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_6+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al V}$$

$$\mathbf{B_{23}} = (-x_7+y_7+z_7)\,\mathbf{a}_1+(x_7-y_7+z_7)\,\mathbf{a}_2+(x_7+y_7-z_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al VI}$$

$$\mathbf{B_{24}} = (x_7-y_7+z_7)\,\mathbf{a}_1+(-x_7+y_7+z_7)\,\mathbf{a}_2-(x_7+y_7+z_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al VI}$$

$$\mathbf{B_{25}} = -\left(x_7+y_7-z_7-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_7+y_7+z_7+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_7-y_7-z_7+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_7+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_7-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al VI}$$

$$\mathbf{B_{26}} = \left(x_7+y_7+z_7+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_7+y_7-z_7-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_7-y_7+z_7-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_7-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_7+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al VI}$$

$$\mathbf{B_{27}} = (-x_8+y_8+z_8)\,\mathbf{a}_1+(x_8-y_8+z_8)\,\mathbf{a}_2+(x_8+y_8-z_8)\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al VII}$$

$$\mathbf{B_{28}} = (x_8-y_8+z_8)\,\mathbf{a}_1+(-x_8+y_8+z_8)\,\mathbf{a}_2-(x_8+y_8+z_8)\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al VII}$$

$$\mathbf{B_{29}} = -\left(x_8+y_8-z_8-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_8+y_8+z_8+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_8-y_8-z_8+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_8+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_8-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al VII}$$

$$\mathbf{B_{30}} = \left(x_8+y_8+z_8+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_8+y_8-z_8-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_8-y_8+z_8-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_8-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_8+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al VII}$$

$$\mathbf{B_{31}} = (-x_9+y_9+z_9)\,\mathbf{a}_1+(x_9-y_9+z_9)\,\mathbf{a}_2+(x_9+y_9-z_9)\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al VIII}$$

$$\mathbf{B_{32}} = (x_9-y_9+z_9)\,\mathbf{a}_1+(-x_9+y_9+z_9)\,\mathbf{a}_2-(x_9+y_9+z_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al VIII}$$

$$\mathbf{B_{33}} = -\left(x_9+y_9-z_9-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_9+y_9+z_9+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_9-y_9-z_9+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_9+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_9-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al VIII}$$

$$\mathbf{B_{34}} = \left(x_9+y_9+z_9+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_9+y_9-z_9-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_9-y_9+z_9-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_9-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_9+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al VIII}$$

$$\mathbf{B_{35}} = (-x_{10}+y_{10}+z_{10})\,\mathbf{a}_1+(x_{10}-y_{10}+z_{10})\,\mathbf{a}_2+(x_{10}+y_{10}-z_{10})\,\mathbf{a}_3 = ax_{10}\,\hat{\mathbf{x}}+by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al IX}$$

$$\mathbf{B_{36}} = (x_{10}-y_{10}+z_{10})\,\mathbf{a}_1+(-x_{10}+y_{10}+z_{10})\,\mathbf{a}_2-(x_{10}+y_{10}+z_{10})\,\mathbf{a}_3 = -ax_{10}\,\hat{\mathbf{x}}-by_{10}\,\hat{\mathbf{y}}+cz_{10}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al IX}$$

$$\mathbf{B_{37}} = -\left(x_{10}+y_{10}-z_{10}-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_{10}+y_{10}+z_{10}+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_{10}-y_{10}-z_{10}+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_{10}+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_{10}-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{10}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al IX}$$

$$\mathbf{B_{38}} = \left(x_{10}+y_{10}+z_{10}+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_{10}+y_{10}-z_{10}-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_{10}-y_{10}+z_{10}-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_{10}-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_{10}+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{10}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al IX}$$

$$\mathbf{B_{39}} = (-x_{11}+y_{11}+z_{11})\,\mathbf{a}_1+(x_{11}-y_{11}+z_{11})\,\mathbf{a}_2+(x_{11}+y_{11}-z_{11})\,\mathbf{a}_3 = ax_{11}\,\hat{\mathbf{x}}+by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al X}$$

$$\mathbf{B_{40}} = (x_{11}-y_{11}+z_{11})\,\mathbf{a}_1+(-x_{11}+y_{11}+z_{11})\,\mathbf{a}_2-(x_{11}+y_{11}+z_{11})\,\mathbf{a}_3 = -ax_{11}\,\hat{\mathbf{x}}-by_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al X}$$

$$\mathbf{B_{41}} = -\left(x_{11}+y_{11}-z_{11}-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_{11}+y_{11}+z_{11}+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_{11}-y_{11}-z_{11}+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_{11}+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_{11}-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{11}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al X}$$

$$\mathbf{B_{42}} = \left(x_{11}+y_{11}+z_{11}+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_{11}+y_{11}-z_{11}-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_{11}-y_{11}+z_{11}-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_{11}-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_{11}+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{11}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al X}$$

$$\mathbf{B_{43}} = (-x_{12}+y_{12}+z_{12})\,\mathbf{a}_1+(x_{12}-y_{12}+z_{12})\,\mathbf{a}_2+(x_{12}+y_{12}-z_{12})\,\mathbf{a}_3 = ax_{12}\,\hat{\mathbf{x}}+by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al XI}$$

$$\mathbf{B_{44}} = (x_{12}-y_{12}+z_{12})\,\mathbf{a}_1+(-x_{12}+y_{12}+z_{12})\,\mathbf{a}_2-(x_{12}+y_{12}+z_{12})\,\mathbf{a}_3 = -ax_{12}\,\hat{\mathbf{x}}-by_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Al XI}$$

$$\mathbf{B_{45}} = -\left(x_{12}+y_{12}-z_{12}-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_{12}+y_{12}+z_{12}+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_{12}-y_{12}-z_{12}+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_{12}+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_{12}-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{12}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al XI}$$

$$\mathbf{B_{46}} = \left(x_{12}+y_{12}+z_{12}+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_{12}+y_{12}-z_{12}-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_{12}-y_{12}+z_{12}-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_{12}-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_{12}+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{12}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Al XI}$$

$$\mathbf{B_{47}} = (-x_{13}+y_{13}+z_{13})\,\mathbf{a}_1+(x_{13}-y_{13}+z_{13})\,\mathbf{a}_2+(x_{13}+y_{13}-z_{13})\,\mathbf{a}_3 = ax_{13}\,\hat{\mathbf{x}}+by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Mo II}$$

$$\mathbf{B_{48}} = (x_{13}-y_{13}+z_{13})\,\mathbf{a}_1+(-x_{13}+y_{13}+z_{13})\,\mathbf{a}_2-(x_{13}+y_{13}+z_{13})\,\mathbf{a}_3 = -ax_{13}\,\hat{\mathbf{x}}-by_{13}\,\hat{\mathbf{y}}+cz_{13}\,\hat{\mathbf{z}} \quad (16b) \quad \text{Mo II}$$

$$\mathbf{B_{49}} = -\left(x_{13}+y_{13}-z_{13}-\tfrac{1}{4}\right)\mathbf{a}_1+\left(x_{13}+y_{13}+z_{13}+\tfrac{1}{4}\right)\mathbf{a}_2+\left(x_{13}-y_{13}-z_{13}+\tfrac{1}{4}\right)\mathbf{a}_3 = a\left(x_{13}+\tfrac{1}{4}\right)\hat{\mathbf{x}}-b\left(y_{13}-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{13}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Mo II}$$

$$\mathbf{B_{50}} = \left(x_{13}+y_{13}+z_{13}+\tfrac{1}{4}\right)\mathbf{a}_1-\left(x_{13}+y_{13}-z_{13}-\tfrac{1}{4}\right)\mathbf{a}_2-\left(x_{13}-y_{13}+z_{13}-\tfrac{1}{4}\right)\mathbf{a}_3 = -a\left(x_{13}-\tfrac{1}{4}\right)\hat{\mathbf{x}}+b\left(y_{13}+\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_{13}+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16b) \quad \text{Mo II}$$

$\mathbf{B_{51}}$	$=$	$(-x_{14}+y_{14}+z_{14})\,\mathbf{a}_1+$ $(x_{14}-y_{14}+z_{14})\,\mathbf{a}_2+$ $(x_{14}+y_{14}-z_{14})\,\mathbf{a}_3$	$=$	$ax_{14}\,\hat{\mathbf{x}}+by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(16b)	Mo III
$\mathbf{B_{52}}$	$=$	$(x_{14}-y_{14}+z_{14})\,\mathbf{a}_1+$ $(-x_{14}+y_{14}+z_{14})\,\mathbf{a}_2-$ $(x_{14}+y_{14}+z_{14})\,\mathbf{a}_3$	$=$	$-ax_{14}\,\hat{\mathbf{x}}-by_{14}\,\hat{\mathbf{y}}+cz_{14}\,\hat{\mathbf{z}}$	(16b)	Mo III
$\mathbf{B_{53}}$	$=$	$-\left(x_{14}+y_{14}-z_{14}-\frac{1}{4}\right)\,\mathbf{a}_1+$ $\left(x_{14}+y_{14}+z_{14}+\frac{1}{4}\right)\,\mathbf{a}_2+$ $\left(x_{14}-y_{14}-z_{14}+\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$a\left(x_{14}+\frac{1}{4}\right)\,\hat{\mathbf{x}}-b\left(y_{14}-\frac{1}{4}\right)\,\hat{\mathbf{y}}+$ $c\left(z_{14}+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Mo III
$\mathbf{B_{54}}$	$=$	$\left(x_{14}+y_{14}+z_{14}+\frac{1}{4}\right)\,\mathbf{a}_1-$ $\left(x_{14}+y_{14}-z_{14}-\frac{1}{4}\right)\,\mathbf{a}_2-$ $\left(x_{14}-y_{14}+z_{14}-\frac{1}{4}\right)\,\mathbf{a}_3$	$=$	$-a\left(x_{14}-\frac{1}{4}\right)\,\hat{\mathbf{x}}+b\left(y_{14}+\frac{1}{4}\right)\,\hat{\mathbf{y}}+$ $c\left(z_{14}+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(16b)	Mo III

References

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