

Mg₂₃Al₃₀ Structure:

A30B23_hR53_148_5f_a2c3f-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/DB0A>

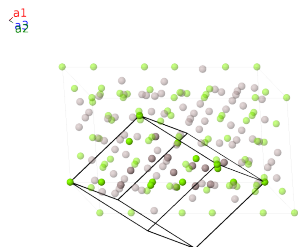
https://aflow.org/prototype-encyclopedia/A30B23_hR53_148_5f_a2c3f-001

Prototype	Al ₃₀ Mg ₂₃
AFLOW prototype label	A30B23_hR53_148_5f_a2c3f-001
ICSD	57965
CCDC	1622003
Pearson symbol	hR53
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<pre>aflow --proto=A30B23_hR53_148_5f_a2c3f-001 --params=a, c/a, x₂, x₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀, x₁₁, y₁₁, z₁₁</pre>

- (Samson, 1968) finds that the stoichiometry of this system is closer to Mg₂₂Al₃₁ than Mg₂₃Al₃₀, so there must be some substitutional disorder in this structure.
- We have shifted the origin so that the first magnesium atom is at (1a) (0 0 0) instead of (1b) (0 0 1/2).
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
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$\mathbf{B}_1$	$=$	0	$=$	0	(1a)	Mg I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c)	Mg II
$\mathbf{B}_3$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c)	Mg II
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$cx_3 \hat{\mathbf{z}}$	(2c)	Mg III
$\mathbf{B}_5$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-cx_3 \hat{\mathbf{z}}$	(2c)	Mg III
$\mathbf{B}_6$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_7$	$=$	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_8$	$=$	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_9$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_{10}$	$=$	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_{11}$	$=$	$-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_{12}$	$=$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B}_{13}$	$=$	$z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B}_{14}$	$=$	$y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B}_{15}$	$=$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B}_{16}$	$=$	$-z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B}_{17}$	$=$	$-y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}}$	(6f)	Al II
$\mathbf{B}_{18}$	$=$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B}_{19}$	$=$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B}_{20}$	$=$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B}_{21}$	$=$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B}_{22}$	$=$	$-z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B}_{23}$	$=$	$-y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}}$	(6f)	Al III
$\mathbf{B}_{24}$	$=$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al IV
$\mathbf{B}_{25}$	$=$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al IV
$\mathbf{B}_{26}$	$=$	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} + \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}}$	(6f)	Al IV

$$\begin{aligned}
\mathbf{B}_{27} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= -\frac{1}{2}a(x_7 - z_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 - 2y_7 + z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Al IV} \\
\mathbf{B}_{28} &= -z_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - y_7 \mathbf{a}_3 &= \frac{1}{2}a(y_7 - z_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_7 - y_7 - z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Al IV} \\
\mathbf{B}_{29} &= -y_7 \mathbf{a}_1 - z_7 \mathbf{a}_2 - x_7 \mathbf{a}_3 &= \frac{1}{2}a(x_7 - y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_7 + y_7 - 2z_7) \hat{\mathbf{y}} - \frac{1}{3}c(x_7 + y_7 + z_7) \hat{\mathbf{z}} &(6f) &\text{Al IV} \\
\mathbf{B}_{30} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= \frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} &(6f) &\text{Al V} \\
\mathbf{B}_{31} &= z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + y_8 \mathbf{a}_3 &= -\frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} &(6f) &\text{Al V} \\
\mathbf{B}_{32} &= y_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3 &= -\frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} + \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} &(6f) &\text{Al V} \\
\mathbf{B}_{33} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= -\frac{1}{2}a(x_8 - z_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 - 2y_8 + z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} &(6f) &\text{Al V} \\
\mathbf{B}_{34} &= -z_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - y_8 \mathbf{a}_3 &= \frac{1}{2}a(y_8 - z_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_8 - y_8 - z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} &(6f) &\text{Al V} \\
\mathbf{B}_{35} &= -y_8 \mathbf{a}_1 - z_8 \mathbf{a}_2 - x_8 \mathbf{a}_3 &= \frac{1}{2}a(x_8 - y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_8 + y_8 - 2z_8) \hat{\mathbf{y}} - \frac{1}{3}c(x_8 + y_8 + z_8) \hat{\mathbf{z}} &(6f) &\text{Al V} \\
\mathbf{B}_{36} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= \frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}} &(6f) &\text{Mg IV} \\
\mathbf{B}_{37} &= z_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + y_9 \mathbf{a}_3 &= -\frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}} &(6f) &\text{Mg IV} \\
\mathbf{B}_{38} &= y_9 \mathbf{a}_1 + z_9 \mathbf{a}_2 + x_9 \mathbf{a}_3 &= -\frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} + \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}} &(6f) &\text{Mg IV} \\
\mathbf{B}_{39} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= -\frac{1}{2}a(x_9 - z_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_9 - 2y_9 + z_9) \hat{\mathbf{y}} - \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}} &(6f) &\text{Mg IV} \\
\mathbf{B}_{40} &= -z_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - y_9 \mathbf{a}_3 &= \frac{1}{2}a(y_9 - z_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_9 - y_9 - z_9) \hat{\mathbf{y}} - \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}} &(6f) &\text{Mg IV} \\
\mathbf{B}_{41} &= -y_9 \mathbf{a}_1 - z_9 \mathbf{a}_2 - x_9 \mathbf{a}_3 &= \frac{1}{2}a(x_9 - y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_9 + y_9 - 2z_9) \hat{\mathbf{y}} - \frac{1}{3}c(x_9 + y_9 + z_9) \hat{\mathbf{z}} &(6f) &\text{Mg IV} \\
\mathbf{B}_{42} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= \frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} &(6f) &\text{Mg V} \\
\mathbf{B}_{43} &= z_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + y_{10} \mathbf{a}_3 &= -\frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} &(6f) &\text{Mg V} \\
\mathbf{B}_{44} &= y_{10} \mathbf{a}_1 + z_{10} \mathbf{a}_2 + x_{10} \mathbf{a}_3 &= -\frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} + \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} &(6f) &\text{Mg V} \\
\mathbf{B}_{45} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= -\frac{1}{2}a(x_{10} - z_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{10} - 2y_{10} + z_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} &(6f) &\text{Mg V} \\
\mathbf{B}_{46} &= -z_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - y_{10} \mathbf{a}_3 &= \frac{1}{2}a(y_{10} - z_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_{10} - y_{10} - z_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} &(6f) &\text{Mg V} \\
\mathbf{B}_{47} &= -y_{10} \mathbf{a}_1 - z_{10} \mathbf{a}_2 - x_{10} \mathbf{a}_3 &= \frac{1}{2}a(x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_{10} + y_{10} - 2z_{10}) \hat{\mathbf{y}} - \frac{1}{3}c(x_{10} + y_{10} + z_{10}) \hat{\mathbf{z}} &(6f) &\text{Mg V}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{48} &= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= & \frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} - & (6f) & \text{Mg VI} \\
& & & \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} + \\
& & & \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} \\
\mathbf{B}_{49} &= z_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + y_{11} \mathbf{a}_3 &= & -\frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} + & (6f) & \text{Mg VI} \\
& & & \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} + \\
& & & \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} \\
\mathbf{B}_{50} &= y_{11} \mathbf{a}_1 + z_{11} \mathbf{a}_2 + x_{11} \mathbf{a}_3 &= & -\frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} - & (6f) & \text{Mg VI} \\
& & & \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} + \\
& & & \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} \\
\mathbf{B}_{51} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & -\frac{1}{2}a(x_{11} - z_{11}) \hat{\mathbf{x}} + & (6f) & \text{Mg VI} \\
& & & \frac{\sqrt{3}}{6}a(x_{11} - 2y_{11} + z_{11}) \hat{\mathbf{y}} - \\
& & & \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} \\
\mathbf{B}_{52} &= -z_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - y_{11} \mathbf{a}_3 &= & \frac{1}{2}a(y_{11} - z_{11}) \hat{\mathbf{x}} - & (6f) & \text{Mg VI} \\
& & & \frac{\sqrt{3}}{6}a(2x_{11} - y_{11} - z_{11}) \hat{\mathbf{y}} - \\
& & & \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}} \\
\mathbf{B}_{53} &= -y_{11} \mathbf{a}_1 - z_{11} \mathbf{a}_2 - x_{11} \mathbf{a}_3 &= & \frac{1}{2}a(x_{11} - y_{11}) \hat{\mathbf{x}} + & (6f) & \text{Mg VI} \\
& & & \frac{\sqrt{3}}{6}a(x_{11} + y_{11} - 2z_{11}) \hat{\mathbf{y}} - \\
& & & \frac{1}{3}c(x_{11} + y_{11} + z_{11}) \hat{\mathbf{z}}
\end{aligned}$$

References

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Al
Mg

