$SrMg_4$ Structure: A4B_hP90_194_e2fgh4k_hk-001

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https://aflow.org/prototype-encyclopedia/DU5B

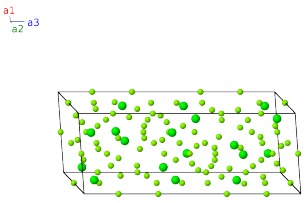
https://aflow.org/prototype-encyclopedia/A4B_hP90_194_e2fgh4k_hk-001

Prototype	Mg_4Sr
AFLOW prototype label	A4B_hP90_194_e2fgh4k_hk-001
ICSD	104874
CCDC	1662775
Pearson symbol	hP90
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A4B_hP90_194_e2fgh4k_hk-001 --params=`$a, c/a, z_1, z_2, z_3, x_5, x_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}$

- If we use the (Wang, 1965) coordinate $x_6 = 0.0478$ the Sr-I (6h) atom we get distances that do not agree with their listed interatomic distances, and some distances are too short and physically unreasonable. (Villars, 2016) solved this by assuming the "0" in front of the "478" in Table 3 was extraneous, and that the number should actually be "-0.478." This makes the distances much more reasonable, although still not exactly in agreement with (Wang, 1965). It is also in agreement with the ICSD entry and in near agreement with first-principles relaxed structure found by the Materials Project (Jain, 2103). Accordingly we use "0.522" (1 - 0.478) for x_6.
- Although (Villars, 2016) imply that the actually stoichiometry of this system is Sr_9Mg_{38}, the stoichiometry in their description is $SrMg_4$.

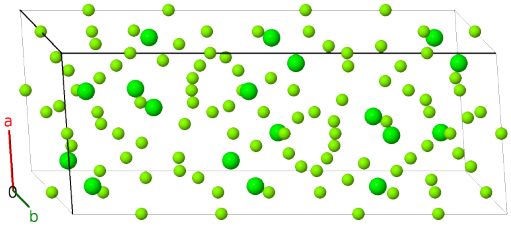
Hexagonal primitive vectors

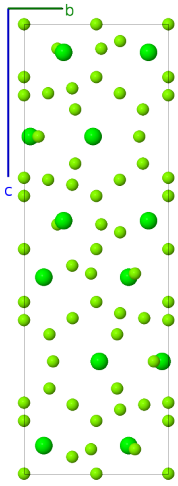
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

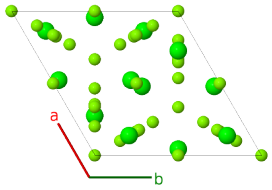


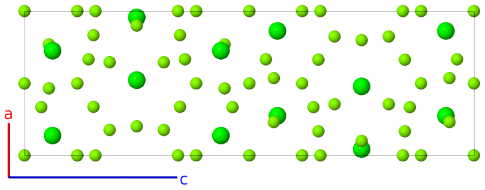
Basis vectors

Mg
Sr









		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_4}$	=	$-\left(z_1-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_1-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Mg I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_7}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-cz_2\,\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_8}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_2-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_2-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mg II
$\mathbf{B_9}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4f)	Mg III
$\mathbf{B_{10}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mg III
$\mathbf{B_{11}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(4f)	Mg III
$\mathbf{B_{12}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Mg III
$\mathbf{B_{13}}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Mg IV
$\mathbf{B_{14}}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(6g)	Mg IV
$\mathbf{B_{15}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(6g)	Mg IV
$\mathbf{B_{16}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Mg IV
$\mathbf{B_{17}}$	=	$\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Mg IV
$\mathbf{B_{18}}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(6g)	Mg IV
$\mathbf{B_{19}}$	=	$x_5\,\mathbf{a}_1+2x_5\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Mg V
$\mathbf{B_{20}}$	=	$-2x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Mg V
$\mathbf{B_{21}}$	=	$x_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_5\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Mg V
$\mathbf{B_{22}}$	=	$-x_5\,\mathbf{a}_1-2x_5\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Mg V
$\mathbf{B_{23}}$	=	$2x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_5\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Mg V
$\mathbf{B_{24}}$	=	$-x_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_5\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Mg V
$\mathbf{B_{25}}$	=	$x_6\,\mathbf{a}_1+2x_6\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sr I
$\mathbf{B_{26}}$	=	$-2x_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sr I
$\mathbf{B_{27}}$	=	$x_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\frac{1}{4}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_6\,\hat{\mathbf{y}}+\frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	Sr I
$\mathbf{B_{28}}$	=	$-x_6\,\mathbf{a}_1-2x_6\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sr I
$\mathbf{B_{29}}$	=	$2x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_6\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sr I
$\mathbf{B_{30}}$	=	$-x_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\frac{3}{4}\,\mathbf{a}_3$	=	$\sqrt{3}ax_6\,\hat{\mathbf{y}}+\frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	Sr I
$\mathbf{B_{31}}$	=	$x_7\,\mathbf{a}_1+2x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{32}}$	=	$-2x_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{33}}$	=	$x_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-\sqrt{3}ax_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{34}}$	=	$-x_7\,\mathbf{a}_1-2x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{35}}$	=	$2x_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{36}}$	=	$-x_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{37}}$	=	$2x_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$\frac{3}{2}ax_7\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{38}}$	=	$-x_7\,\mathbf{a}_1-2x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_7\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(12k)	Mg VI
$\mathbf{B_{39}}$	=	$-x_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2-z_7\,\mathbf{a}_3$	=	$\sqrt{3}ax_7\,\hat{\mathbf{y}}-cz_7\,\hat{\mathbf{z}}$	(12k)	Mg VI

$$\mathbf{B_{40}} = -2x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_7\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VI}$$

$$\mathbf{B_{41}} = x_7\,\mathbf{a}_1 + 2x_7\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_7\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VI}$$

$$\mathbf{B_{42}} = x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\sqrt{3}ax_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VI}$$

$$\mathbf{B_{43}} = x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \tfrac{3}{2}ax_8\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{44}} = -2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -\tfrac{3}{2}ax_8\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{45}} = x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -\sqrt{3}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{46}} = -x_8\,\mathbf{a}_1 - 2x_8\,\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_8\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{47}} = 2x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_8\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{48}} = -x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \sqrt{3}ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{49}} = 2x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = \tfrac{3}{2}ax_8\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{50}} = -x_8\,\mathbf{a}_1 - 2x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -\tfrac{3}{2}ax_8\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{51}} = -x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = \sqrt{3}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{52}} = -2x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_8\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{53}} = x_8\,\mathbf{a}_1 + 2x_8\,\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_8\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{54}} = x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - \left(z_8 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\sqrt{3}ax_8\,\hat{\mathbf{y}} - c\left(z_8 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VII}$$

$$\mathbf{B_{55}} = x_9\,\mathbf{a}_1 + 2x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = \tfrac{3}{2}ax_9\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{56}} = -2x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = -\tfrac{3}{2}ax_9\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{57}} = x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = -\sqrt{3}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{58}} = -x_9\,\mathbf{a}_1 - 2x_9\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_9\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{59}} = 2x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_9\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{60}} = -x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \sqrt{3}ax_9\,\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{61}} = 2x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = \tfrac{3}{2}ax_9\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{62}} = -x_9\,\mathbf{a}_1 - 2x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -\tfrac{3}{2}ax_9\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{63}} = -x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = \sqrt{3}ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{64}} = -2x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_9\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{65}} = x_9\,\mathbf{a}_1 + 2x_9\,\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_9\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{66}} = x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - \left(z_9 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\sqrt{3}ax_9\,\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg VIII}$$

$$\mathbf{B_{67}} = x_{10}\,\mathbf{a}_1 + 2x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = \tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{68}} = -2x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -\tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{69}} = x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 = -\sqrt{3}ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{70}} = -x_{10}\,\mathbf{a}_1 - 2x_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{71}} = 2x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{72}} = -x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10} + \tfrac{1}{2}\right)\,\mathbf{a}_3 = \sqrt{3}ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10} + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{73}} = 2x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = \tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{74}} = -x_{10}\,\mathbf{a}_1 - 2x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -\tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{75}} = -x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = \sqrt{3}ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{76}} = -2x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{77}} = x_{10}\,\mathbf{a}_1 + 2x_{10}\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = \tfrac{3}{2}ax_{10}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{78}} = x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - \left(z_{10} - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -\sqrt{3}ax_{10}\,\hat{\mathbf{y}} - c\left(z_{10} - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Mg IX}$$

$$\mathbf{B_{79}} = x_{11}\,\mathbf{a}_1 + 2x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \tfrac{3}{2}ax_{11}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Sr II}$$

$$\mathbf{B_{80}} = -2x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = -\tfrac{3}{2}ax_{11}\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} \quad \text{(12k)} \quad \text{Sr II}$$

$\mathbf{B_{81}}$	=	$x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$-\sqrt{3}ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{82}}$	=	$-x_{11}\,\mathbf{a}_1 - 2x_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_{11}\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{83}}$	=	$2x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_{11}\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{84}}$	=	$-x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11} + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11} + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{85}}$	=	$2x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$\frac{3}{2}ax_{11}\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{86}}$	=	$-x_{11}\,\mathbf{a}_1 - 2x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_{11}\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{87}}$	=	$-x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$	=	$\sqrt{3}ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{88}}$	=	$-2x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_{11}\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{89}}$	=	$x_{11}\,\mathbf{a}_1 + 2x_{11}\,\mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_{11}\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{11}\,\hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Sr II
$\mathbf{B_{90}}$	=	$x_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - \left(z_{11} - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\sqrt{3}ax_{11}\,\hat{\mathbf{y}} - c\left(z_{11} - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12k)	Sr II

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