

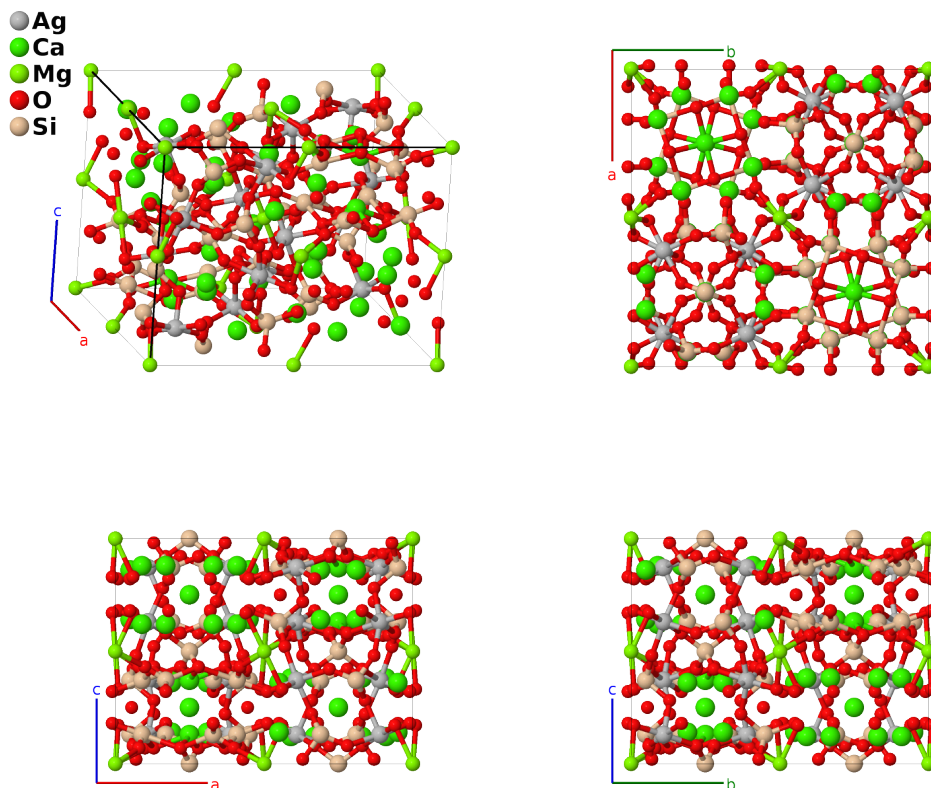
Vesuvianite ($\text{Ca}_{10}\text{Al}_4(\text{Mg},\text{Fe})_2\text{Si}_9\text{O}_{34}(\text{OH})_4$, $S2_3$) Structure: A4B10C2D34E4F9_tP252_126_k_ce2k_f_h8k_k_d2k-001

This structure originally had the label A4B10C2D34E4F9_tP252_126_k_ce2k_f_h8k_k_d2k. Calls to that address will be redirected here.

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<https://afLOW.org/p/QSJ3>

https://afLOW.org/p/A4B10C2D34E4F9_tP252_126_k_ce2k_f_h8k_k_d2k-001



Prototype	$\text{Ag}_4\text{Ca}_{10}\text{Mg}_2\text{O}_{34}(\text{OH})_4\text{Si}_9$
AFLOW prototype label	A4B10C2D34E4F9_tP252_126_k_ce2k_f_h8k_k_d2k-001
Strukturbericht designation	$S2_3$
Mineral name	vesuvianite
ICSD	36198
Pearson symbol	tP252
Space group number	126
Space group symbol	$P4/nnc$
AFLOW prototype command	afLOW --proto=A4B10C2D34E4F9_tP252_126_k_ce2k_f_h8k_k_d2k-001 --params= $a, c/a, z_3, x_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}$

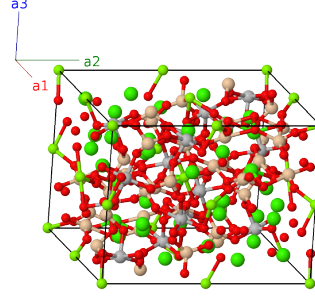
- Vesuvianite, also known as idocrase, comes in a variety of compositions and structures, see *e.g.*, (Allen, 1992) and (Rucklidge, 1975) and references therein. For our example we use the original structure of (Warren, 1931), where the magnesium (8f) site is filled by a random (Mg,Fe) alloy.
- The positions of the hydrogen atoms in the OH ions were not determined, so we only give the positions of the oxygen atoms (labeled as OH).

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
\mathbf{B}_2	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
\mathbf{B}_3	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
\mathbf{B}_4	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4c)	Ca I
\mathbf{B}_5	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}}$	(4d)	Si I
\mathbf{B}_6	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(4d)	Si I
\mathbf{B}_7	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Si I
\mathbf{B}_8	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4d)	Si I
\mathbf{B}_9	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + z_3 c \hat{\mathbf{z}}$	(4e)	Ca II
\mathbf{B}_{10}	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - c (z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ca II
\mathbf{B}_{11}	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(4e)	Ca II
\mathbf{B}_{12}	$= \frac{3}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Ca II
\mathbf{B}_{13}	$= 0$	$=$	0	(8f)	Mg I
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(8f)	Mg I
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(8f)	Mg I
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(8f)	Mg I
\mathbf{B}_{17}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8f)	Mg I
\mathbf{B}_{18}	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8f)	Mg I
\mathbf{B}_{19}	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(8f)	Mg I
\mathbf{B}_{20}	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8f)	Mg I
\mathbf{B}_{21}	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8h)	O I
\mathbf{B}_{22}	$= - (x_5 - \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (x_5 - \frac{1}{2}) \hat{\mathbf{x}} - a (x_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(8h)	O I

$$\begin{aligned}
\mathbf{B}_{23} &= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= & -a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8h) & \text{O I} \\
\mathbf{B}_{24} &= x_5 \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= & ax_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}} & (8h) & \text{O I} \\
\mathbf{B}_{25} &= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= & -ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8h) & \text{O I} \\
\mathbf{B}_{26} &= (x_5 + \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= & a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8h) & \text{O I} \\
\mathbf{B}_{27} &= (x_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= & a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8h) & \text{O I} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= & -ax_5 \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}} & (8h) & \text{O I} \\
\mathbf{B}_{29} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= & ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{30} &= -(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + &= & -a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
& \quad z_6 \mathbf{a}_3 \\
\mathbf{B}_{31} &= -(y_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= & -a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{32} &= y_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3 &= & ay_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{33} &= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - &= & -a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
& \quad (z_6 - \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{34} &= x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 &= & ax_6 \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{35} &= y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3 &= & ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{36} &= -(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - &= & -a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
& \quad (z_6 - \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{37} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & -ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{38} &= (x_6 + \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{39} &= (y_6 + \frac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{40} &= -y_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= & -ay_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{41} &= (x_6 + \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= & a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{42} &= -x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 + &= & -ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
& \quad (z_6 + \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{43} &= -y_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3 &= & -ay_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
\mathbf{B}_{44} &= (y_6 + \frac{1}{2}) \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 + &= & a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ag I} \\
& \quad (z_6 + \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{45} &= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{46} &= -(x_7 - \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 + &= & -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
& \quad z_7 \mathbf{a}_3 \\
\mathbf{B}_{47} &= -(y_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{48} &= y_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & ay_7 \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{49} &= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + y_7 \mathbf{a}_2 - &= & -a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
& \quad (z_7 - \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{50} &= x_7 \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 &= & ax_7 \hat{\mathbf{x}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{51} &= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3 &= & ay_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{52} &= -(y_7 - \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - &= & -a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
& \quad (z_7 - \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{53} &= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & -ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{54} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{55} &= (y_7 + \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{56} &= -y_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3 &= & -ay_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{57} &= (x_7 + \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 &= & a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{58} &= -x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = -ax_7 \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{59} &= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = -ay_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{60} &= (y_7 + \frac{1}{2}) \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3 = a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca III} \\
\mathbf{B}_{61} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{62} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3 = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{63} &= -(y_8 - \frac{1}{2}) \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 = -a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{64} &= y_8 \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3 = ay_8 \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{65} &= -(x_8 - \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{66} &= x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{67} &= y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = ay_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{68} &= -(y_8 - \frac{1}{2}) \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = -a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{69} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{70} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{71} &= (y_8 + \frac{1}{2}) \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 = a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{72} &= -y_8 \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3 = -ay_8 \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{73} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{74} &= -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -ax_8 \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{75} &= -y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = -ay_8 \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{76} &= (y_8 + \frac{1}{2}) \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{Ca IV} \\
\mathbf{B}_{77} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{78} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3 = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{79} &= -(y_9 - \frac{1}{2}) \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = -a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{80} &= y_9 \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3 = ay_9 \hat{\mathbf{x}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{81} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{82} &= x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{83} &= y_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = ay_9 \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{84} &= -(y_9 - \frac{1}{2}) \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = -a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{85} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{86} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{87} &= (y_9 + \frac{1}{2}) \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 = a(y_9 + \frac{1}{2}) \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{88} &= -y_9 \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3 = -ay_9 \hat{\mathbf{x}} + a(x_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{89} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{O II} \\
\mathbf{B}_{90} &= -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} + a(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (16k) & \text{O II}
\end{aligned}$$

$$\mathbf{B}_{240} = y_{19} \mathbf{a}_1 - \left(x_{19} - \frac{1}{2}\right) \mathbf{a}_2 + z_{19} \mathbf{a}_3 = ay_{19} \hat{\mathbf{x}} - a \left(x_{19} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{241} = -\left(x_{19} - \frac{1}{2}\right) \mathbf{a}_1 + y_{19} \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 = -a \left(x_{19} - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_{19} \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{242} = x_{19} \mathbf{a}_1 - \left(y_{19} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 = ax_{19} \hat{\mathbf{x}} - a \left(y_{19} - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{243} = y_{19} \mathbf{a}_1 + x_{19} \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 = ay_{19} \hat{\mathbf{x}} + ax_{19} \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{244} = -\left(y_{19} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{19} - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{19} - \frac{1}{2}\right) \mathbf{a}_3 = -a \left(y_{19} - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_{19} - \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{19} - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{245} = -x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 = -ax_{19} \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{246} = \left(x_{19} + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{19} + \frac{1}{2}\right) \mathbf{a}_2 - z_{19} \mathbf{a}_3 = a \left(x_{19} + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_{19} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{247} = \left(y_{19} + \frac{1}{2}\right) \mathbf{a}_1 - x_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 = a \left(y_{19} + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{248} = -y_{19} \mathbf{a}_1 + \left(x_{19} + \frac{1}{2}\right) \mathbf{a}_2 - z_{19} \mathbf{a}_3 = -ay_{19} \hat{\mathbf{x}} + a \left(x_{19} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{249} = \left(x_{19} + \frac{1}{2}\right) \mathbf{a}_1 - y_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 = a \left(x_{19} + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{250} = -x_{19} \mathbf{a}_1 + \left(y_{19} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 = -ax_{19} \hat{\mathbf{x}} + a \left(y_{19} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{251} = -y_{19} \mathbf{a}_1 - x_{19} \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 = -ay_{19} \hat{\mathbf{x}} - ax_{19} \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

$$\mathbf{B}_{252} = \left(y_{19} + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_{19} + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{19} + \frac{1}{2}\right) \mathbf{a}_3 = a \left(y_{19} + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_{19} + \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{19} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (16k) \quad \text{Si III}$$

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