

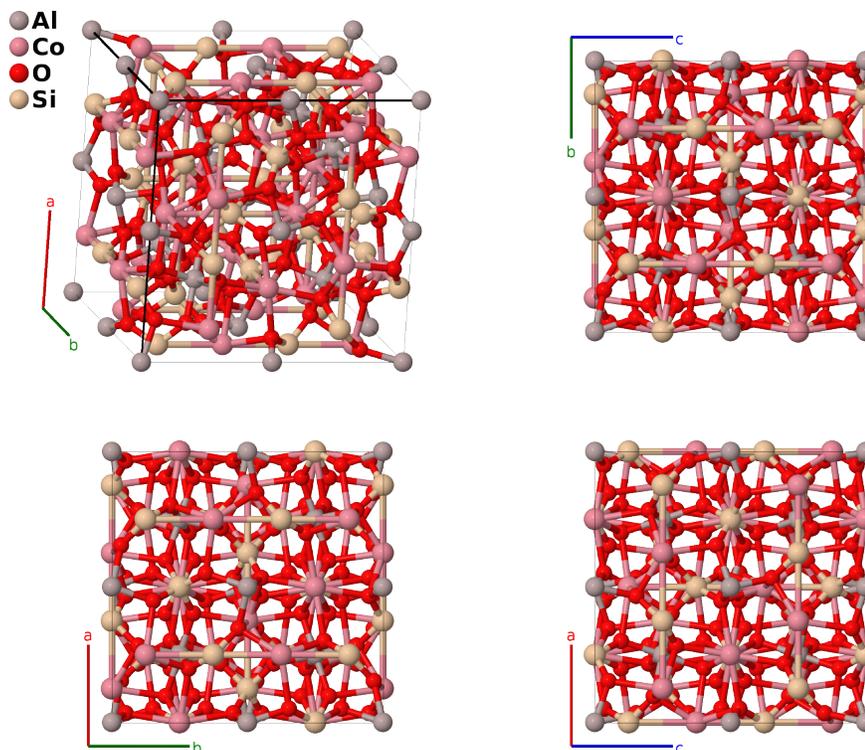
Garnet [$S1_4$, $\text{Co}_3\text{Al}_2(\text{SiO}_4)_3$] Structure: A2B3C12D3_cI160_230_a_c_h_d-001

This structure originally had the label A2B3C12D3_cI160_230_a_c_h_d. Calls to that address will be redirected here.

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<https://aflow.org/p/YMRU>

https://aflow.org/p/A2B3C12D3_cI160_230_a_c_h_d-001



Prototype	$\text{Al}_2\text{Co}_3\text{O}_{12}\text{Si}_3$
AFLOW prototype label	A2B3C12D3_cI160_230_a_c_h_d-001
<i>Strukturbericht</i> designation	$S1_4$
Mineral name	garnet
ICSD	81358
Pearson symbol	cI160
Space group number	230
Space group symbol	$Ia\bar{3}d$
AFLOW prototype command	<code>aflow --proto=A2B3C12D3_cI160_230_a_c_h_d-001 --params=a, x₄, y₄, z₄</code>

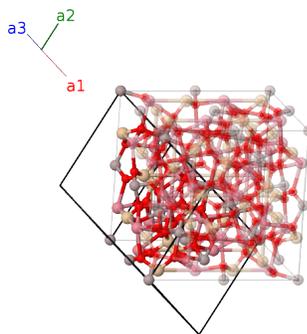
Other compounds with this structure

(Al, Fe)₂Ca₃(SiO₄)₃ (hibschite), Al₂(Ca, Fe)₃(SiO₄)₃ (almandine), Al₂(Mg, Fe)₃(SiO₄)₃ (pyrope), Al₂(Mg, Ni)₃(SiO₄)₃, Al₂Ca₃(SiO₄)₃ (grossular), Al₂Fe₃(SiO₄)₃, Al₂Mg₃(SiO₄)₃, Al₂Mn₃(SiO₄)₃ (spessartite), Ca₂V₃(SiO₄)₃ (goldmanite), Cr₂Ca₃(SiO₄)₃ (uvarovite), Fe₂Ca₃(SiO₄)₃ (topazolite), Fe₂Mn₃(GeO₄)₃, Fe₂Mn₃(SiO₄)₃ (calderite), Al₃Fe₅O₁₂, Al_xLi_{7-3x}Zr₂O₁₂, Mn₅(SiO₄)₃, Sc₂Ca₃(SiO₄)₃, Si₂(Li₂Mg)(SiO₄)₃, Zr₂Ca₃(Fe₂Si)O₁₂ (kerimasite), Al₅(GdO₄)₃, Al₅(LuO₄)₃, Al₅(YO₄)₃, Al₅(YbO₄)₃, Ga₅(GdO₄)₃, Ga₅(LuO₄)₃, Ga₅(YO₄)₃, Ga₅(YbO₄)₃, Fe₅(LuO₄)₃, Fe₅(PyO₄)₃, Fe₅(SmO₄)₃, Fe₅(YO₄)₃, Fe₅(YbO₄)₃, Ga₅(ErO₄)₃, Gd₃Fe₅O₁₂, Y₃Fe₅O₁₂

- (Ross, 1996) does not explicitly give the positions of the Al and Si atoms, which we take from (Downs, 2003).
- (Ewald, 1937) originally gave Ca₃Al₂(SiO₄)₃ garnet the *Strukturbericht* designation *H31* or *H31*. It was reclassified as a silicate and given the designation *S14* by (Gottfried, 1937).
- Although the original prototype was Ca₃Al₂(SiO₄)₃, we have better data for the isostructural Co₃Al₂(SiO₄)₃ and so use it as our example.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(16a)	Al I
\mathbf{B}_2	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}}$	(16a)	Al I
\mathbf{B}_3	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(16a)	Al I
\mathbf{B}_4	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{z}}$	(16a)	Al I
\mathbf{B}_5	$\frac{1}{2} \mathbf{a}_1$	$=$	$-\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(16a)	Al I
\mathbf{B}_6	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(16a)	Al I
\mathbf{B}_7	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - \frac{1}{4}a \hat{\mathbf{z}}$	(16a)	Al I
\mathbf{B}_8	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(16a)	Al I
\mathbf{B}_9	$\frac{1}{4} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{10}	$\frac{3}{4} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$-\frac{1}{8}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{11}	$\frac{1}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{8}a \hat{\mathbf{y}}$	(24c)	Co I
\mathbf{B}_{12}	$\frac{3}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - \frac{1}{8}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{13}	$\frac{3}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{14}	$\frac{1}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - \frac{1}{8}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{15}	$\frac{3}{4} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3$	$=$	$\frac{3}{8}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{16}	$\frac{1}{4} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$\frac{5}{8}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{z}}$	(24c)	Co I
\mathbf{B}_{17}	$\frac{7}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}}$	(24c)	Co I

$$\begin{aligned}
\mathbf{B}_{18} &= \frac{5}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{5}{8} a \hat{\mathbf{y}} & (24c) & \text{Co I} \\
\mathbf{B}_{19} &= \frac{5}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (24c) & \text{Co I} \\
\mathbf{B}_{20} &= \frac{7}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{y}} + \frac{5}{8} a \hat{\mathbf{z}} & (24c) & \text{Co I} \\
\mathbf{B}_{21} &= \frac{1}{4} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{22} &= \frac{3}{4} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{23} &= \frac{3}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} & (24d) & \text{Si I} \\
\mathbf{B}_{24} &= \frac{1}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} & (24d) & \text{Si I} \\
\mathbf{B}_{25} &= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{26} &= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{27} &= \frac{5}{8} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{3}{8} \mathbf{a}_3 &= \frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{8} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{28} &= \frac{7}{8} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{8} \mathbf{a}_3 &= -\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{8} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{29} &= \frac{3}{4} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{5}{8} \mathbf{a}_3 &= \frac{1}{8} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{30} &= \frac{1}{4} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{7}{8} \mathbf{a}_3 &= \frac{3}{8} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - \frac{1}{4} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{31} &= \frac{1}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{32} &= \frac{3}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3 &= \frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} a \hat{\mathbf{z}} & (24d) & \text{Si I} \\
\mathbf{B}_{33} &= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + &= ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (x_4 + y_4) \mathbf{a}_3 \\
\mathbf{B}_{34} &= \left(-y_4 + z_4 + \frac{1}{2}\right) \mathbf{a}_1 - &= -ax_4 \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (x_4 - z_4) \mathbf{a}_2 - \left(x_4 + y_4 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{35} &= (y_4 - z_4) \mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(-x_4 + y_4 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{36} &= -\left(y_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_1 + &= ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(x_4 - z_4 + \frac{1}{2}\right) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3 \\
\mathbf{B}_{37} &= (x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + &= az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (x_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{38} &= -\left(x_4 + y_4 - \frac{1}{2}\right) \mathbf{a}_1 + &= az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(-y_4 + z_4 + \frac{1}{2}\right) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{39} &= \left(-x_4 + y_4 + \frac{1}{2}\right) \mathbf{a}_1 + &= -az_4 \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (y_4 - z_4) \mathbf{a}_2 - \left(x_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{40} &= (x_4 - y_4) \mathbf{a}_1 - \left(y_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(x_4 - z_4 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{41} &= (x_4 + z_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + &= ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (y_4 + z_4) \mathbf{a}_3 \\
\mathbf{B}_{42} &= -\left(x_4 - z_4\right) \mathbf{a}_1 - &= -a \left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(x_4 + y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \\
&\quad \left(-y_4 + z_4 + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{43} &= -\left(x_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_1 + &= ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(-x_4 + y_4 + \frac{1}{2}\right) \mathbf{a}_2 + (y_4 - z_4) \mathbf{a}_3 \\
\mathbf{B}_{44} &= \left(x_4 - z_4 + \frac{1}{2}\right) \mathbf{a}_1 + &= -ay_4 \hat{\mathbf{x}} - a \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (x_4 - y_4) \mathbf{a}_2 - \left(y_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{45} &= \left(x_4 - z_4 + \frac{1}{2}\right) \mathbf{a}_1 + &= a \left(y_4 - \frac{1}{4}\right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad (y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3 \\
\mathbf{B}_{46} &= -\left(x_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_1 - &= -a \left(y_4 - \frac{1}{4}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{4}\right) \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{4}\right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
&\quad \left(y_4 + z_4 - \frac{1}{2}\right) \mathbf{a}_2 - \\
&\quad \left(x_4 + y_4 - \frac{1}{2}\right) \mathbf{a}_3
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{69} &= \begin{pmatrix} (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_4 - z_4) \mathbf{a}_2 - (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = -a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{70} &= \begin{pmatrix} (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{71} &= \begin{pmatrix} (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(y_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{72} &= \begin{pmatrix} -(x_4 + z_4) \mathbf{a}_1 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{pmatrix} = a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(z_4 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{73} &= \begin{pmatrix} (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_4 - y_4) \mathbf{a}_2 - (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(z_4 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{74} &= \begin{pmatrix} -(y_4 + z_4) \mathbf{a}_1 + \\ (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(y_4 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{75} &= \begin{pmatrix} (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{76} &= \begin{pmatrix} -(y_4 - z_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{77} &= \begin{pmatrix} (x_4 - y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 - z_4) \mathbf{a}_2 - (y_4 + z_4) \mathbf{a}_3 \end{pmatrix} = -a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(y_4 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{78} &= \begin{pmatrix} -(x_4 - y_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 + \\ (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(z_4 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{79} &= \begin{pmatrix} -(x_4 + y_4) \mathbf{a}_1 + \\ (-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3 \end{pmatrix} = a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{80} &= \begin{pmatrix} (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 + z_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(z_4 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_4 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I}
\end{aligned}$$

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