

PPrS₄ Structure:

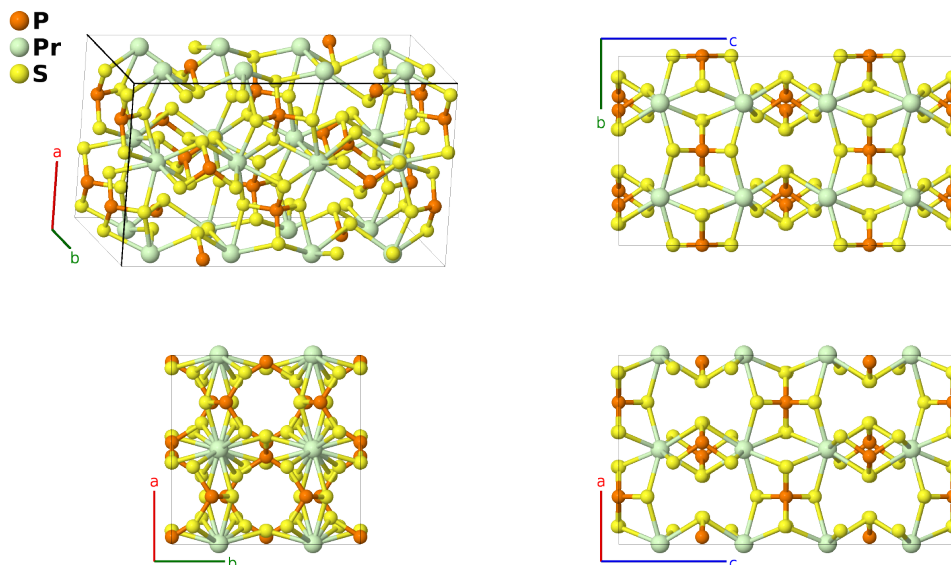
ABC4_tI96_142_e_ab_2g-001

This structure originally had the label ABC4_tI96_142_e_ab_2g. Calls to that address will be redirected here.

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<https://aflow.org/p/B2Y6>

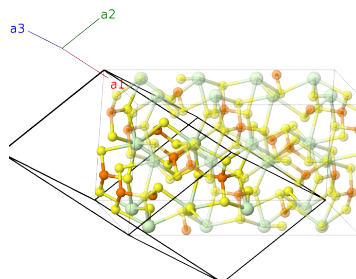
https://aflow.org/p/ABC4_tI96_142_e_ab_2g-001



Prototype	PPrS ₄
AFLOW prototype label	ABC4.tI96_142_e_ab_2g-001
ICSD	201897
Pearson symbol	tI96
Space group number	142
Space group symbol	$I4_1/acd$
AFLOW prototype command	aflow --proto=ABC4_tI96_142_e_ab_2g-001 --params=a, c/a, x ₃ , x ₄ , y ₄ , z ₄ , x ₅ , y ₅ , z ₅

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{5}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(8a)	Pr I
\mathbf{B}_2	$= \frac{3}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(8a)	Pr I
\mathbf{B}_3	$= \frac{7}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(8a)	Pr I
\mathbf{B}_4	$= \frac{1}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(8a)	Pr I
\mathbf{B}_5	$= \frac{3}{8} \mathbf{a}_1 + \frac{1}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{8} c \hat{\mathbf{z}}$	(8b)	Pr II
\mathbf{B}_6	$= \frac{1}{8} \mathbf{a}_1 + \frac{3}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - \frac{1}{8} c \hat{\mathbf{z}}$	(8b)	Pr II
\mathbf{B}_7	$= \frac{5}{8} \mathbf{a}_1 + \frac{7}{8} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{8} c \hat{\mathbf{z}}$	(8b)	Pr II
\mathbf{B}_8	$= \frac{7}{8} \mathbf{a}_1 + \frac{5}{8} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{5}{8} c \hat{\mathbf{z}}$	(8b)	Pr II
\mathbf{B}_9	$= \frac{1}{4} \mathbf{a}_1 + (x_3 + \frac{1}{4}) \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{10}	$= \frac{3}{4} \mathbf{a}_1 - (x_3 - \frac{1}{4}) \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{11}	$= (x_3 + \frac{1}{4}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a (x_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{12}	$= -(x_3 - \frac{1}{4}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 -$ $(x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (x_3 - \frac{1}{4}) \hat{\mathbf{y}}$	(16e)	P I
\mathbf{B}_{13}	$= \frac{3}{4} \mathbf{a}_1 - (x_3 - \frac{3}{4}) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{3}{4} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{14}	$= \frac{1}{4} \mathbf{a}_1 + (x_3 + \frac{3}{4}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (x_3 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{15}	$= -(x_3 - \frac{3}{4}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$-\frac{1}{4} a \hat{\mathbf{x}} - a (x_3 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{16}	$= (x_3 + \frac{3}{4}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + a (x_3 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(16e)	P I
\mathbf{B}_{17}	$= (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 +$ $(x_4 + y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{18}	$= (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 -$ $(x_4 - z_4) \mathbf{a}_2 - (x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{19}	$= (x_4 + z_4) \mathbf{a}_1 +$ $(-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$-a (y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a (x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c (z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{20}	$= -(x_4 - z_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 +$ $(-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c (z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{21}	$= (y_4 - z_4) \mathbf{a}_1 - (x_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 +$ $(-x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{22}	$= -(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 +$ $(x_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 - y_4) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - c (z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{23}	$= (x_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 +$ $(y_4 - z_4) \mathbf{a}_2 + (x_4 + y_4) \mathbf{a}_3$	$=$	$a (y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{24}	$= -(x_4 + z_4 - \frac{1}{2}) \mathbf{a}_1 -$ $(y_4 + z_4 - \frac{1}{2}) \mathbf{a}_2 -$ $(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_4 - \frac{1}{4}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{4}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{25}	$= -(y_4 + z_4) \mathbf{a}_1 - (x_4 + z_4) \mathbf{a}_2 -$ $(x_4 + y_4) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{26}	$= (y_4 - z_4 + \frac{1}{2}) \mathbf{a}_1 +$ $(x_4 - z_4) \mathbf{a}_2 + (x_4 + y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{27}	$= -(x_4 + z_4) \mathbf{a}_1 +$ $(y_4 - z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3$	$=$	$a (y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a (x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c (z_4 - \frac{1}{4}) \hat{\mathbf{z}}$	(32g)	S I
\mathbf{B}_{28}	$= (x_4 - z_4) \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 +$ $(x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a (x_4 + \frac{1}{4}) \hat{\mathbf{y}} - c (z_4 + \frac{1}{4}) \hat{\mathbf{z}}$	(32g)	S I

$$\begin{aligned}
\mathbf{B}_{29} &= \begin{aligned} &-(y_4 - z_4) \mathbf{a}_1 + \\ &(x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_4 - y_4 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} &(32g) & \text{S I} \\
\mathbf{B}_{30} &= \begin{aligned} &(y_4 + z_4 + \frac{1}{2}) \mathbf{a}_1 + \\ &(-x_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - y_4) \mathbf{a}_3 \end{aligned} &= -ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}} &(32g) & \text{S I} \\
\mathbf{B}_{31} &= \begin{aligned} &(-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{aligned} &= -a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S I} \\
\mathbf{B}_{32} &= \begin{aligned} &(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{aligned} &= a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S I} \\
\mathbf{B}_{33} &= \begin{aligned} &(y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + \\ &(x_5 + y_5) \mathbf{a}_3 \end{aligned} &= ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{34} &= \begin{aligned} &(-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ &(x_5 - z_5) \mathbf{a}_2 - (x_5 + y_5 - \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= -ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{35} &= \begin{aligned} &(x_5 + z_5) \mathbf{a}_1 + \\ &(-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3 \end{aligned} &= -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{36} &= \begin{aligned} &-(x_5 - z_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + \\ &(-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{37} &= \begin{aligned} &(y_5 - z_5) \mathbf{a}_1 - (x_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + \\ &(-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= -a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{38} &= \begin{aligned} &-(y_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 + \\ &(x_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5) \mathbf{a}_3 \end{aligned} &= ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{39} &= \begin{aligned} &(x_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ &(y_5 - z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3 \end{aligned} &= a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{40} &= \begin{aligned} &-(x_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 - \\ &(y_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 - \\ &(x_5 + y_5 - \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{41} &= \begin{aligned} &-(y_5 + z_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2 - \\ &(x_5 + y_5) \mathbf{a}_3 \end{aligned} &= -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{42} &= \begin{aligned} &(y_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ &(x_5 - z_5) \mathbf{a}_2 + (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= ax_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{43} &= \begin{aligned} &-(x_5 + z_5) \mathbf{a}_1 + \\ &(y_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 - (x_5 - y_5) \mathbf{a}_3 \end{aligned} &= a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{44} &= \begin{aligned} &(x_5 - z_5) \mathbf{a}_1 - (y_5 + z_5) \mathbf{a}_2 + \\ &(x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{45} &= \begin{aligned} &-(y_5 - z_5) \mathbf{a}_1 + \\ &(x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{46} &= \begin{aligned} &(y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ &(-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - (x_5 - y_5) \mathbf{a}_3 \end{aligned} &= -ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{47} &= \begin{aligned} &(-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ &(y_5 - z_5) \mathbf{a}_2 - (x_5 + y_5) \mathbf{a}_3 \end{aligned} &= -a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II} \\
\mathbf{B}_{48} &= \begin{aligned} &(x_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ &(y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ &(x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3 \end{aligned} &= a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{4}) \hat{\mathbf{z}} &(32g) & \text{S II}
\end{aligned}$$

References

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Found in

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