$PPrS_4$ Structure: ABC4_tI96_142_e_ab_2g-001

This structure previously used the label(s) `ABC4_tI96_142_e_ab_2g`. Calls to these addresses will be redirected here.

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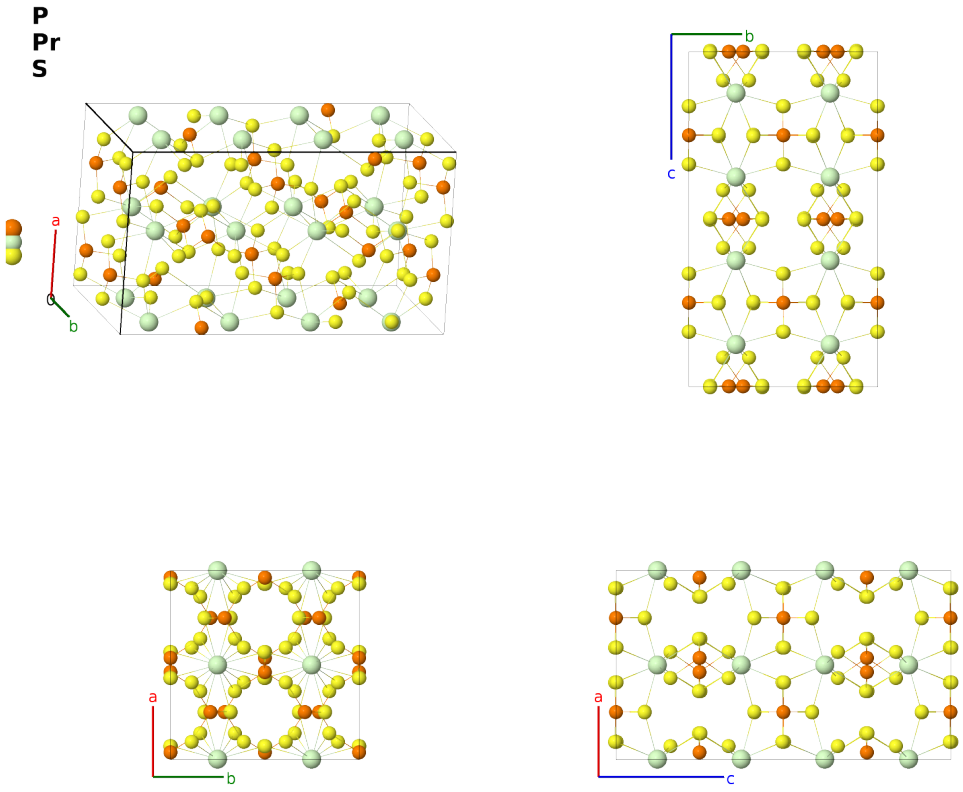
https://aflow.org/prototype-encyclopedia/B2Y6

https://aflow.org/prototype-encyclopedia/ABC4_tI96_142_e_ab_2g-001

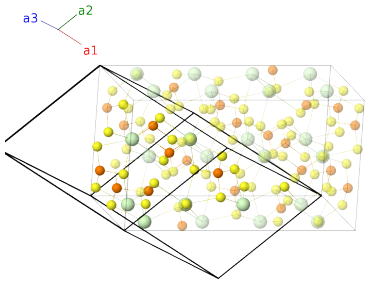


Prototype	$PPrS_4$
AFLOW prototype label	ABC4_tI96_142_e_ab_2g-001
ICSD	201897
CCDC	1706525
Pearson symbol	tI96
Space group number	142
Space group symbol	$I4_1/acd$

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

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



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
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	P I
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	P I
$\mathbf{B_{11}}$	=	$\left(x_3 + \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	P I
$\mathbf{B_{12}}$	=	$-\left(x_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}}$	(16e)	P I
$\mathbf{B_{13}}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(16e)	P I
$\mathbf{B_{14}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16e)	P I
$\mathbf{B_{15}}$	=	$-\left(x_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(16e)	P I
$\mathbf{B_{16}}$	=	$\left(x_3 + \frac{3}{4}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	=	$\left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - \left(x_4 + y_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{19}}$	=	$(x_4 + z_4)\,\mathbf{a}_1 + \left(-y_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{20}}$	=	$-(x_4 - z_4)\,\mathbf{a}_1 + (y_4 + z_4)\,\mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_4 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{21}}$	=	$(y_4 - z_4)\,\mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_4 + y_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(32g)	S I

$\mathbf{B_{22}}$	$=$	$-\left(y_4+z_4-\frac{1}{2}\right)\mathbf{a}_1+\left(x_4-z_4+\frac{1}{2}\right)\mathbf{a}_2+(x_4-y_4)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{23}}$	$=$	$\left(x_4-z_4+\frac{1}{2}\right)\mathbf{a}_1+(y_4-z_4)\mathbf{a}_2+(x_4+y_4)\mathbf{a}_3$	$=$	$a\left(y_4-\frac{1}{4}\right)\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{24}}$	$=$	$-\left(x_4+z_4-\frac{1}{2}\right)\mathbf{a}_1-\left(y_4+z_4-\frac{1}{2}\right)\mathbf{a}_2-\left(x_4+y_4-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{4}\right)\hat{\mathbf{x}}-a\left(x_4-\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(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
$\mathbf{B_{26}}$	$=$	$\left(y_4-z_4+\frac{1}{2}\right)\mathbf{a}_1+(x_4-z_4)\,\mathbf{a}_2+\left(x_4+y_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_4\,\hat{\mathbf{x}}+a\left(y_4+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{27}}$	$=$	$-(x_4+z_4)\,\mathbf{a}_1+\left(y_4-z_4+\frac{1}{2}\right)\mathbf{a}_2-(x_4-y_4)\,\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{4}\right)\hat{\mathbf{x}}-a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_4-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{28}}$	$=$	$(x_4-z_4)\,\mathbf{a}_1-(y_4+z_4)\,\mathbf{a}_2+\left(x_4-y_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_4-\frac{1}{4}\right)\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{29}}$	$=$	$-(y_4-z_4)\,\mathbf{a}_1+\left(x_4+z_4+\frac{1}{2}\right)\mathbf{a}_2+\left(x_4-y_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(x_4+\frac{1}{2}\right)\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{30}}$	$=$	$\left(y_4+z_4+\frac{1}{2}\right)\mathbf{a}_1+\left(-x_4+z_4+\frac{1}{2}\right)\mathbf{a}_2-(x_4-y_4)\,\mathbf{a}_3$	$=$	$-ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{31}}$	$=$	$\left(-x_4+z_4+\frac{1}{2}\right)\mathbf{a}_1-(y_4-z_4)\,\mathbf{a}_2-(x_4+y_4)\,\mathbf{a}_3$	$=$	$-a\left(y_4+\frac{1}{4}\right)\hat{\mathbf{x}}-a\left(x_4-\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{32}}$	$=$	$\left(x_4+z_4+\frac{1}{2}\right)\mathbf{a}_1+\left(y_4+z_4+\frac{1}{2}\right)\mathbf{a}_2+\left(x_4+y_4+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_4+\frac{1}{4}\right)\hat{\mathbf{x}}+a\left(x_4+\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_4+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S I
$\mathbf{B_{33}}$	$=$	$(y_5+z_5)\,\mathbf{a}_1+(x_5+z_5)\,\mathbf{a}_2+(x_5+y_5)\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{34}}$	$=$	$\left(-y_5+z_5+\frac{1}{2}\right)\mathbf{a}_1-(x_5-z_5)\,\mathbf{a}_2-\left(x_5+y_5-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}}-a\left(y_5-\frac{1}{2}\right)\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{35}}$	$=$	$(x_5+z_5)\,\mathbf{a}_1+\left(-y_5+z_5+\frac{1}{2}\right)\mathbf{a}_2+(x_5-y_5)\,\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{4}\right)\hat{\mathbf{x}}+a\left(x_5-\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_5+\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{36}}$	$=$	$-(x_5-z_5)\,\mathbf{a}_1+(y_5+z_5)\,\mathbf{a}_2+\left(-x_5+y_5+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$a\left(y_5+\frac{1}{4}\right)\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_5-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{37}}$	$=$	$(y_5-z_5)\,\mathbf{a}_1-\left(x_5+z_5-\frac{1}{2}\right)\mathbf{a}_2+\left(-x_5+y_5+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(x_5-\frac{1}{2}\right)\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{38}}$	$=$	$-\left(y_5+z_5-\frac{1}{2}\right)\mathbf{a}_1+\left(x_5-z_5+\frac{1}{2}\right)\mathbf{a}_2+(x_5-y_5)\,\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{39}}$	$=$	$\left(x_5-z_5+\frac{1}{2}\right)\mathbf{a}_1+(y_5-z_5)\,\mathbf{a}_2+(x_5+y_5)\,\mathbf{a}_3$	$=$	$a\left(y_5-\frac{1}{4}\right)\hat{\mathbf{x}}+a\left(x_5+\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{40}}$	$=$	$-\left(x_5+z_5-\frac{1}{2}\right)\mathbf{a}_1-\left(y_5+z_5-\frac{1}{2}\right)\mathbf{a}_2-\left(x_5+y_5-\frac{1}{2}\right)\mathbf{a}_3$	$=$	$-a\left(y_5-\frac{1}{4}\right)\hat{\mathbf{x}}-a\left(x_5-\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{41}}$	$=$	$-(y_5+z_5)\,\mathbf{a}_1-(x_5+z_5)\,\mathbf{a}_2-(x_5+y_5)\,\mathbf{a}_3$	$=$	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{42}}$	$=$	$\left(y_5-z_5+\frac{1}{2}\right)\mathbf{a}_1+(x_5-z_5)\,\mathbf{a}_2+\left(x_5+y_5+\frac{1}{2}\right)\mathbf{a}_3$	$=$	$ax_5\,\hat{\mathbf{x}}+a\left(y_5+\frac{1}{2}\right)\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{43}}$	$=$	$-(x_5+z_5)\,\mathbf{a}_1+\left(y_5-z_5+\frac{1}{2}\right)\mathbf{a}_2-(x_5-y_5)\,\mathbf{a}_3$	$=$	$a\left(y_5+\frac{1}{4}\right)\hat{\mathbf{x}}-a\left(x_5+\frac{1}{4}\right)\hat{\mathbf{y}}-c\left(z_5-\frac{1}{4}\right)\hat{\mathbf{z}}$	(32g)	S II

$\mathbf{B_{44}}$	=	$(x_5 - z_5)\,\mathbf{a}_1 - (y_5 + z_5)\,\mathbf{a}_2 + \left(x_5 - y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - c\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{45}}$	=	$-\left(y_5 - z_5\right)\,\mathbf{a}_1 + \left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 - y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a y_5\,\hat{\mathbf{y}} + c z_5\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{46}}$	=	$\left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3$	=	$-a x_5\,\hat{\mathbf{x}} + a y_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{47}}$	=	$\left(-x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (y_5 - z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3$	=	$-a\left(y_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	S II
$\mathbf{B_{48}}$	=	$\left(x_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 + y_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5 + \frac{1}{4}\right)\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(32g)	S II

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Found in

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M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017