$Al[PO_4]$ (Framework type AFI) Structure: AB4C_hP72_184_d_4d_d-001

This structure originally had the label `AB4C_hP72_184_d_4d_d`. Calls to that address will be redirected here.

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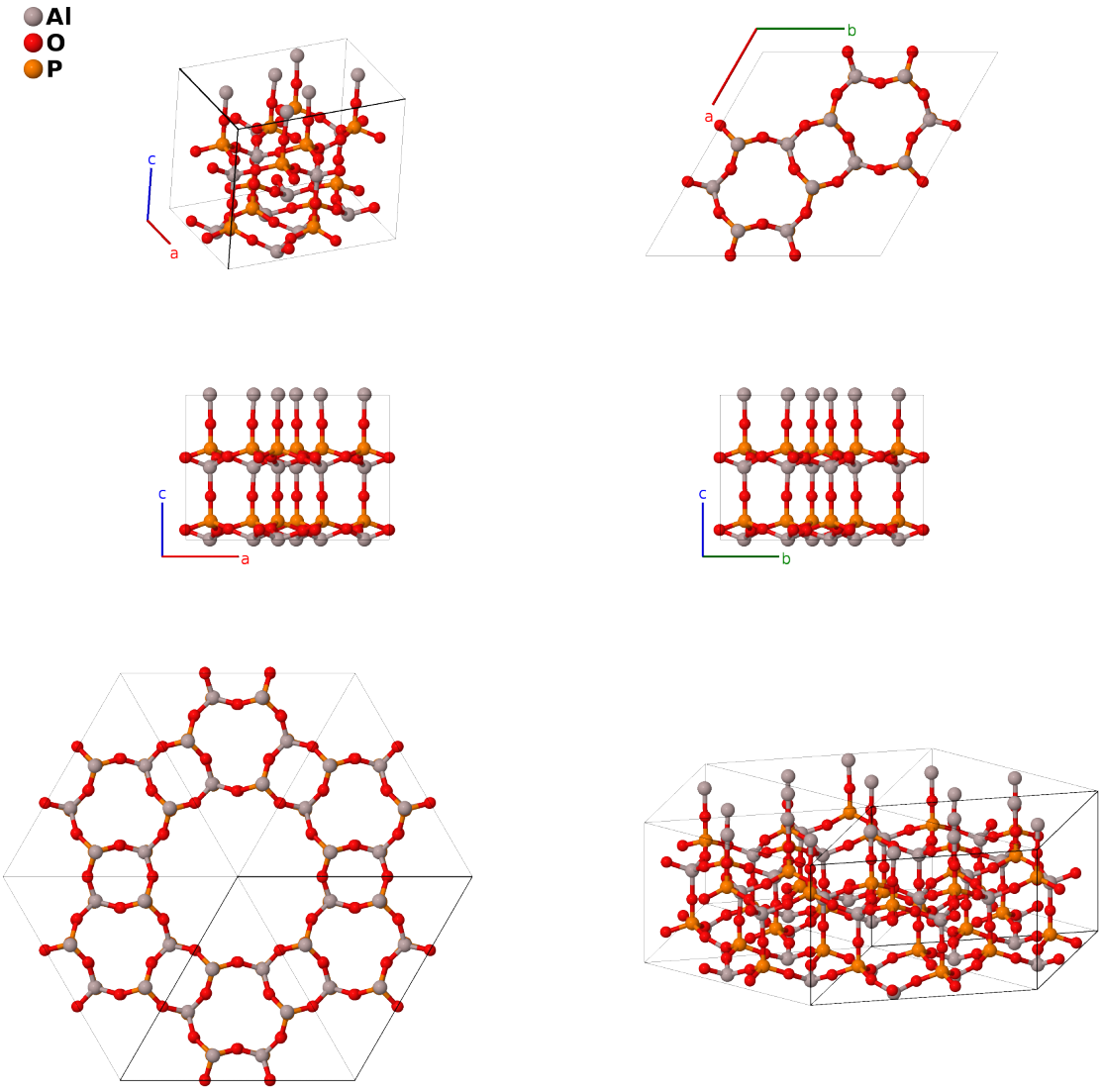
https://aflow.org/p/72JS

https://aflow.org/p/AB4C_hP72_184_d_4d_d-001



Prototype	AlO_4P
AFLOW prototype label	AB4C_hP72_184_d_4d_d-001
ICSD	91671
Pearson symbol	hP72
Space group number	184

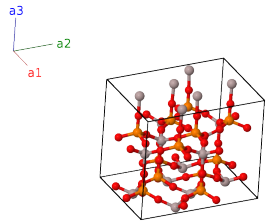
Space group symbol $P6cc$

AFLOW prototype command `aflow --proto=AB4C_hP72_184_d_4d_d-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- Klap refers calls this $AlPO_4$-5.
- Space group $P6cc$ #186 allows an arbitary origin of the z-axis. Here we set $z_1 = 0$ for the Al (12d) site.
- Polytypes of this compound also appear in space groups $P6$ #168 (AB4C_hP72_168_2d_8d_2d) and $P6/mcc$ #192 (AB2_hP72_192_m_j2kl).

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 + y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_1 - y_1)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - 2y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_3}$	=	$-(x_1 - y_1)\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 + y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_1 - y_1)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_5}$	=	$y_1\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_1 + 2y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_6}$	=	$(x_1 - y_1)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_1 - y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_7}$	=	$-y_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_1 + y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_1 - y_1)\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_8}$	=	$-(x_1 - y_1)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_1 + 2y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_9}$	=	$x_1\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_1 - y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_{10}}$	=	$y_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 + y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_1 - y_1)\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_{11}}$	=	$(x_1 - y_1)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_1 - 2y_1)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_{12}}$	=	$-x_1\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_1 - y_1)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B_{13}}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{14}}$	=	$-y_2\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_2 - 2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{15}}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{16}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_2 + y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_2 - y_2)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{17}}$	=	$y_2\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_2 + 2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B_{18}}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_2 - y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(12d)	O I

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\begin{array}{lcccccc}
\mathbf{B_{19}} & = & -y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O I} \\
\mathbf{B_{20}} & = & -(x_2-y_2)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_2+2y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O I} \\
\mathbf{B_{21}} & = & x_2\,\mathbf{a}_1 + (x_2-y_2)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O I} \\
\mathbf{B_{22}} & = & y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_2+y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_2-y_2)\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O I} \\
\mathbf{B_{23}} & = & (x_2-y_2)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_2-2y_2)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O I} \\
\mathbf{B_{24}} & = & -x_2\,\mathbf{a}_1 - (x_2-y_2)\,\mathbf{a}_2 + \left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_2-y_2)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + c\left(z_2+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O I} \\
\mathbf{B_{25}} & = & x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{26}} & = & -y_3\,\mathbf{a}_1 + (x_3-y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{27}} & = & -(x_3-y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{28}} & = & -x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{29}} & = & y_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{30}} & = & (x_3-y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{31}} & = & -y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{32}} & = & -(x_3-y_3)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{33}} & = & x_3\,\mathbf{a}_1 + (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{34}} & = & y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{35}} & = & (x_3-y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{36}} & = & -x_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O II} \\
\mathbf{B_{37}} & = & x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{38}} & = & -y_4\,\mathbf{a}_1 + (x_4-y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{39}} & = & -(x_4-y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{40}} & = & -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{41}} & = & y_4\,\mathbf{a}_1 - (x_4-y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{42}} & = & (x_4-y_4)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{43}} & = & -y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{44}} & = & -(x_4-y_4)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(-x_4+2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{45}} & = & x_4\,\mathbf{a}_1 + (x_4-y_4)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{46}} & = & y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4+y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_4-y_4)\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{47}} & = & (x_4-y_4)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_4-2y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{48}} & = & -x_4\,\mathbf{a}_1 - (x_4-y_4)\,\mathbf{a}_2 + \left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_4-y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4+\frac{1}{2}\right)\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O III} \\
\mathbf{B_{49}} & = & x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O IV} \\
\mathbf{B_{50}} & = & -y_5\,\mathbf{a}_1 + (x_5-y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & \frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O IV} \\
\mathbf{B_{51}} & = & -(x_5-y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 & = & -\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} & (12\mathrm{d}) & \text{O IV}
\end{array}
$$

$\mathbf{B_{52}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{53}}$	=	$y_5\,\mathbf{a}_1 - (x_5-y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{54}}$	=	$(x_5-y_5)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{55}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{56}}$	=	$-(x_5-y_5)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_5+2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{57}}$	=	$x_5\,\mathbf{a}_1 + (x_5-y_5)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{58}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5+y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_5-y_5)\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{59}}$	=	$(x_5-y_5)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5-2y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{60}}$	=	$-x_5\,\mathbf{a}_1 - (x_5-y_5)\,\mathbf{a}_2 + \left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_5-y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}} + c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	O IV
$\mathbf{B_{61}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{62}}$	=	$-y_6\,\mathbf{a}_1 + (x_6-y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{63}}$	=	$-(x_6-y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{64}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{65}}$	=	$y_6\,\mathbf{a}_1 - (x_6-y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6+2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{66}}$	=	$(x_6-y_6)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{67}}$	=	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{68}}$	=	$-(x_6-y_6)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6+2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{69}}$	=	$x_6\,\mathbf{a}_1 + (x_6-y_6)\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{70}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6+y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6-y_6)\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{71}}$	=	$(x_6-y_6)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6-2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	P I
$\mathbf{B_{72}}$	=	$-x_6\,\mathbf{a}_1 - (x_6-y_6)\,\mathbf{a}_2 + \left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6-y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12d)	P I

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