

AlPO₄-5 (Framework type AFI) Structure: AB4C_hP72_184_d_4d_d-001

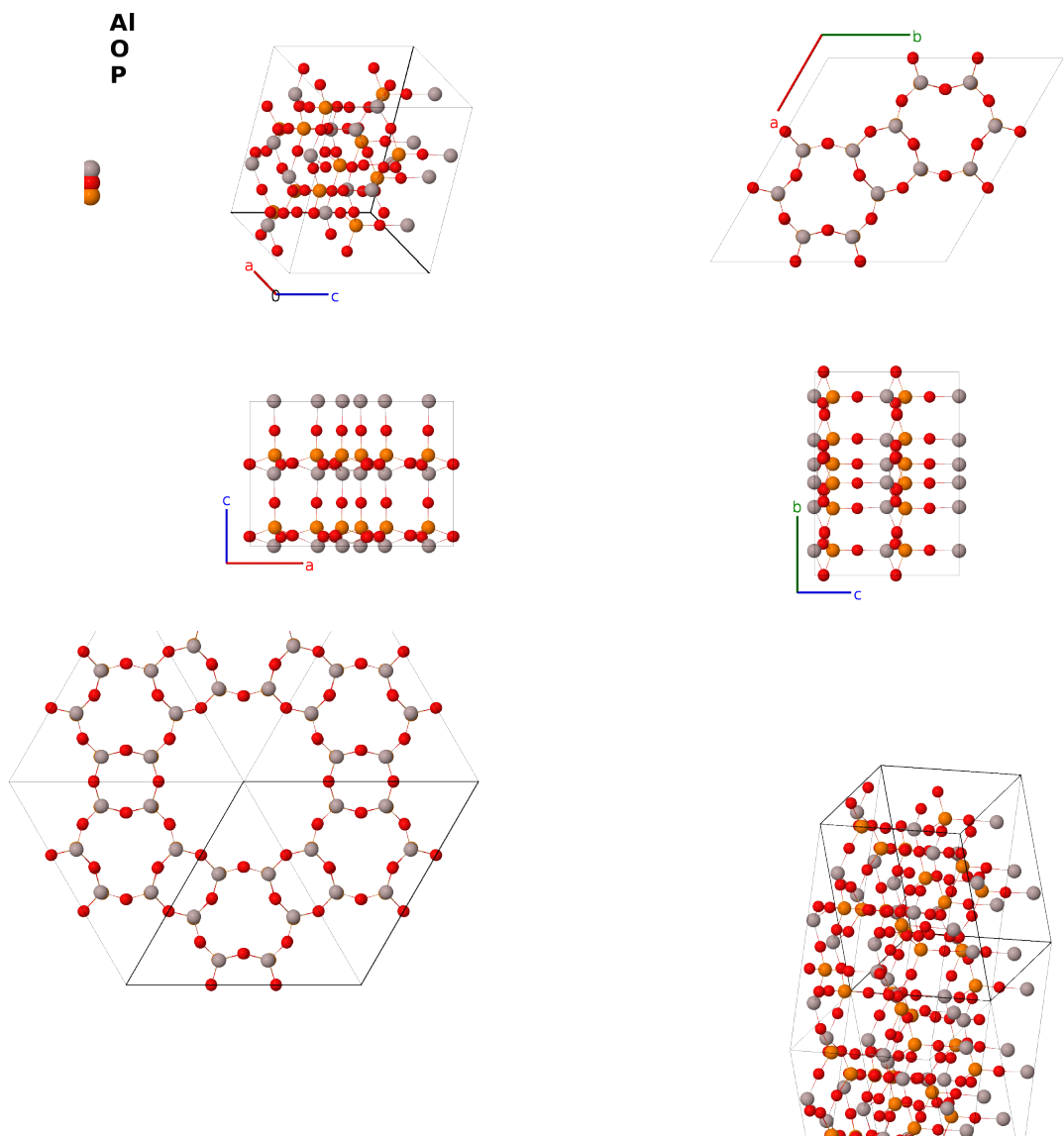
This structure previously used the label(s) **AB4C_hP72_184_d_4d_d**. Calls to these addresses will be redirected here.

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/72JS>

https://aflow.org/prototype-encyclopedia/AB4C_hP72_184_d_4d_d-001



Prototype

AlO₄P

AFLOW prototype label

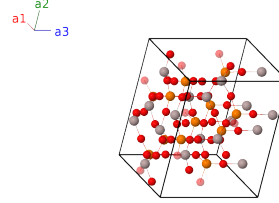
AB4C_hP72_184_d_4d_d-001

ICSD	91671
CCDC	1651197
Pearson symbol	hP72
Space group number	184
Space group symbol	$P6cc$
AFLOW prototype command	<code>aflow --proto=AB4C_hP72_184_d_4d_d-001</code> <code>--params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

- This is one of the large-pore AlPO_4 structures. It is stable up to 34.4 GPa (Lv, 2012).
- The aluminum and phosphorous atoms can be disordered, leading to what we call the (Al,P) O_4 -5 structure.
- The AlPO_4 -5 matrix can contain a wide variety of molecules, leading to structures such as $(\text{AlPO}_4)_6 \cdot \text{NC}_9$.
- Space group $P6cc$ #186 is polar, allowing an arbitrary origin of the z -axis. Here we set $z_1 = 0$ for the Al (12d) site.

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \hat{\mathbf{z}}
\end{aligned}$$



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
$\mathbf{B}_7$	$-y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= -\frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B}_8$	$-(x_1 - y_1) \mathbf{a}_1 + y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= \frac{1}{2}a(-x_1 + 2y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B}_9$	$x_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= \frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B}_{10}$	$y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= \frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B}_{11}$	$(x_1 - y_1) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= \frac{1}{2}a(x_1 - 2y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	Al I
$\mathbf{B}_{12}$	$-x_1 \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= -\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{19} =$	$-y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} +$ $c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{20} =$	$-(x_2 - y_2) \mathbf{a}_1 + y_2 \mathbf{a}_2 +$ $(z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{21} =$	$x_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{22} =$	$y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} +$ $c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{23} =$	$(x_2 - y_2) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{24} =$	$-x_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 +$ $(z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O I
$\mathbf{B}_{25} =$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{26} =$	$-y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{27} =$	$-(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{28} =$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{29} =$	$y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{30} =$	$(x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{31} =$	$-y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} +$ $c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{32} =$	$-(x_3 - y_3) \mathbf{a}_1 + y_3 \mathbf{a}_2 +$ $(z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{33} =$	$x_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{34} =$	$y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} +$ $c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{35} =$	$(x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{36} =$	$-x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 +$ $(z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(12d)	O II
$\mathbf{B}_{37} =$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(12d)	O III

$$\begin{aligned}
\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}} & (12d) & \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}} & (12d) & \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}} & (12d) & \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}} & (12d) & \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}} & (12d) & \text{O IV} \\
\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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{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) & \text{P I}
\end{aligned}$$

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