

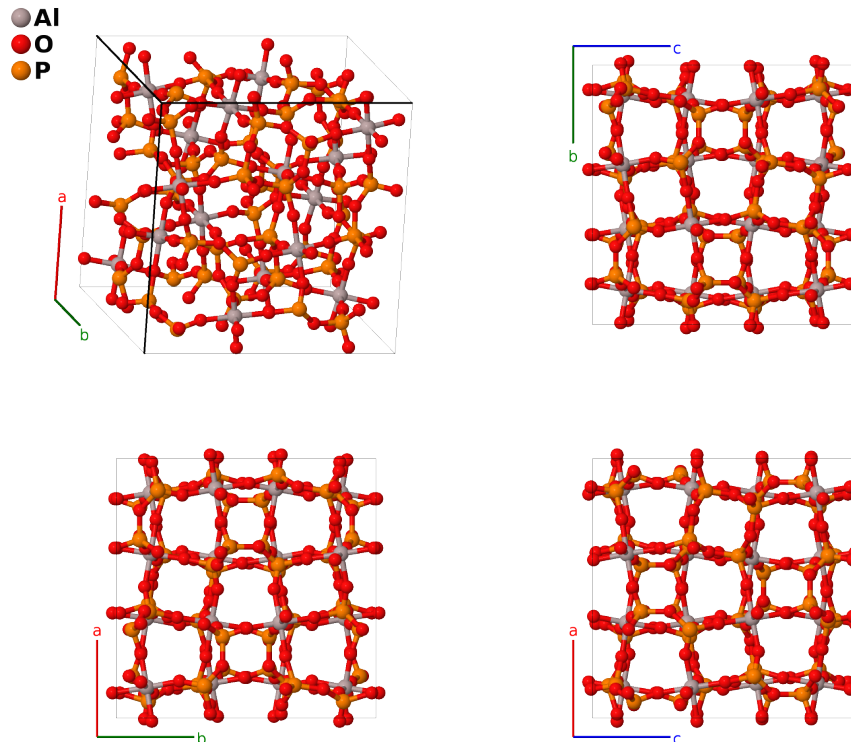
# Al(PO<sub>3</sub>)<sub>3</sub> (*G*5<sub>2</sub>) Structure: AB9C3\_cI208\_220\_c\_3e\_e-001

This structure originally had the label AB9C3\_cI208\_220\_c\_3e\_e. Calls to that address will be redirected here.

Cite this page as: 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/p/2BX1>

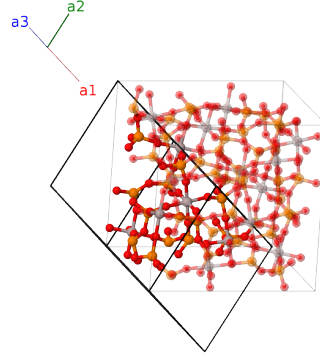
[https://afLOW.org/p/AB9C3\\_cI208\\_220\\_c\\_3e\\_e-001](https://afLOW.org/p/AB9C3_cI208_220_c_3e_e-001)



Prototype	AlO <sub>9</sub> P <sub>3</sub>
AFLOW prototype label	AB9C3_cI208_220_c_3e_e-001
<i>Strukturbericht</i> designation	<i>G</i> 5 <sub>2</sub>
ICSD	26759
Pearson symbol	cI208
Space group number	220
Space group symbol	$\bar{I}43d$
AFLOW prototype command	<code>afLOW --proto=AB9C3_cI208_220_c_3e_e-001</code> <code>--params=<i>a</i>, <i>x</i><sub>1</sub>, <i>x</i><sub>2</sub>, <i>y</i><sub>2</sub>, <i>z</i><sub>2</sub>, <i>x</i><sub>3</sub>, <i>y</i><sub>3</sub>, <i>z</i><sub>3</sub>, <i>x</i><sub>4</sub>, <i>y</i><sub>4</sub>, <i>z</i><sub>4</sub>, <i>x</i><sub>5</sub>, <i>y</i><sub>5</sub>, <i>z</i><sub>5</sub></code>

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
$\mathbf{B}_1$	$= 2x_1 \mathbf{a}_1 + 2x_1 \mathbf{a}_2 + 2x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - (2x_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_3$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_4$	$= -(2x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_5$	$= (2x_1 + \frac{1}{2}) \mathbf{a}_1 + (2x_1 + \frac{1}{2}) \mathbf{a}_2 + (2x_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - 2x_1 \mathbf{a}_3$	$=$	$-a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_7$	$= -2x_1 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$a(x_1 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 - \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_8$	$= -2x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_1 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_1 + \frac{1}{4}) \hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B}_9$	$= (y_2 + z_2) \mathbf{a}_1 + (x_2 + z_2) \mathbf{a}_2 + (x_2 + y_2) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{10}$	$= (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_1 - (x_2 - z_2) \mathbf{a}_2 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{11}$	$= (y_2 - z_2) \mathbf{a}_1 - (x_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{12}$	$= -(y_2 + z_2 - \frac{1}{2}) \mathbf{a}_1 + (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_2 + (x_2 - y_2) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{13}$	$= (x_2 + y_2) \mathbf{a}_1 + (y_2 + z_2) \mathbf{a}_2 + (x_2 + z_2) \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{14}$	$= -(x_2 + y_2 - \frac{1}{2}) \mathbf{a}_1 + (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_2 - (x_2 - z_2) \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{15}$	$= (-x_2 + y_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 - z_2) \mathbf{a}_2 - (x_2 + z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_2 \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{16}$	$= (x_2 - y_2) \mathbf{a}_1 - (y_2 + z_2 - \frac{1}{2}) \mathbf{a}_2 + (x_2 - z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_2 - \frac{1}{2}) \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{17}$	$= (x_2 + z_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + (y_2 + z_2) \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(48e)	O I
$\mathbf{B}_{18}$	$= -(x_2 - z_2) \mathbf{a}_1 - (x_2 + y_2 - \frac{1}{2}) \mathbf{a}_2 + (-y_2 + z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(48e)	O I



$$\begin{aligned}
\mathbf{B}_{41} &= \begin{pmatrix} (x_3 + z_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + \\ (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{42} &= \begin{pmatrix} -(x_3 - z_3) \mathbf{a}_1 - \\ (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_2 + \\ (-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_3 - \frac{1}{2}) \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{43} &= \begin{pmatrix} -(x_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 + \\ (-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{44} &= \begin{pmatrix} (x_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - y_3) \mathbf{a}_2 - (y_3 + z_3 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{45} &= \begin{pmatrix} (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{46} &= \begin{pmatrix} (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3 \end{pmatrix} = -a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{47} &= \begin{pmatrix} -(x_3 + z_3) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 \end{pmatrix} = a(y_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{48} &= \begin{pmatrix} (x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{49} &= \begin{pmatrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{50} &= \begin{pmatrix} -(y_3 - z_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{51} &= \begin{pmatrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - y_3) \mathbf{a}_2 - (x_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{52} &= \begin{pmatrix} -(y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a(x_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{53} &= \begin{pmatrix} (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{54} &= \begin{pmatrix} -(x_3 + y_3) \mathbf{a}_1 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{55} &= \begin{pmatrix} -(x_3 - y_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_3 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{56} &= \begin{pmatrix} (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a(z_3 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O II} \\
\mathbf{B}_{57} &= \begin{pmatrix} (y_4 + z_4) \mathbf{a}_1 + (x_4 + z_4) \mathbf{a}_2 + \\ (x_4 + y_4) \mathbf{a}_3 \end{pmatrix} = ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{58} &= \begin{pmatrix} (-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 \end{pmatrix} = -ax_4 \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + az_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{59} &= \begin{pmatrix} (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{pmatrix} = -a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} - az_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{60} &= \begin{pmatrix} -(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{pmatrix} = ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{61} &= \begin{pmatrix} (x_4 + y_4) \mathbf{a}_1 + (y_4 + z_4) \mathbf{a}_2 + \\ (x_4 + z_4) \mathbf{a}_3 \end{pmatrix} = az_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{62} &= \begin{pmatrix} -(x_4 + y_4 - \frac{1}{2}) \mathbf{a}_1 + \\ (-y_4 + z_4 + \frac{1}{2}) \mathbf{a}_2 - (x_4 - z_4) \mathbf{a}_3 \end{pmatrix} = az_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{O III}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{63} &= \begin{pmatrix} -x_4 + y_4 + \frac{1}{2} \\ y_4 - z_4 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_4 + z_4 - \frac{1}{2} \\ x_4 - z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 &= & -az_4 \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + ay_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{64} &= \begin{pmatrix} x_4 - y_4 \\ x_4 - z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_4 + z_4 - \frac{1}{2} \\ x_4 - z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + &= & -a(z_4 - \frac{1}{2}) \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - ay_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{65} &= \begin{pmatrix} x_4 + z_4 \\ y_4 + z_4 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_4 + y_4 \\ y_4 + z_4 \end{pmatrix} \mathbf{a}_2 + &= & ay_4 \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{66} &= \begin{pmatrix} -(x_4 - z_4) \\ x_4 + y_4 - \frac{1}{2} \\ -y_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= & -a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + az_4 \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{67} &= \begin{pmatrix} -(x_4 + z_4 - \frac{1}{2}) \\ -x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ay_4 \hat{\mathbf{x}} - az_4 \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{68} &= \begin{pmatrix} x_4 - z_4 + \frac{1}{2} \\ x_4 - y_4 \end{pmatrix} \mathbf{a}_1 + &= & -ay_4 \hat{\mathbf{x}} - a(z_4 - \frac{1}{2}) \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{69} &= \begin{pmatrix} x_4 + z_4 + \frac{1}{2} \\ y_4 + z_4 + \frac{1}{2} \\ x_4 + y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{70} &= \begin{pmatrix} -x_4 + z_4 + \frac{1}{2} \\ y_4 - z_4 \end{pmatrix} \mathbf{a}_1 - &= & -a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{71} &= \begin{pmatrix} -(x_4 + z_4) \\ y_4 - z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & a(y_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{72} &= \begin{pmatrix} x_4 - z_4 \\ x_4 - y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_4 + z_4 \\ x_4 - y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + &= & -a(y_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{73} &= \begin{pmatrix} y_4 + z_4 + \frac{1}{2} \\ x_4 + y_4 + \frac{1}{2} \\ x_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{74} &= \begin{pmatrix} -(y_4 - z_4) \\ -x_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_4 + y_4 \\ -x_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + &= & -a(x_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{75} &= \begin{pmatrix} y_4 - z_4 + \frac{1}{2} \\ x_4 - y_4 \end{pmatrix} \mathbf{a}_1 - &= & -a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{76} &= \begin{pmatrix} -(y_4 + z_4) \\ x_4 - y_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & a(x_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{77} &= \begin{pmatrix} x_4 + y_4 + \frac{1}{2} \\ x_4 + z_4 + \frac{1}{2} \\ y_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{78} &= \begin{pmatrix} -(x_4 + y_4) \\ -x_4 + z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{79} &= \begin{pmatrix} -(x_4 - y_4) \\ y_4 - z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_4 + z_4 \\ y_4 - z_4 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + &= & -a(z_4 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{80} &= \begin{pmatrix} x_4 - y_4 + \frac{1}{2} \\ x_4 - z_4 \end{pmatrix} \mathbf{a}_1 + &= & -a(z_4 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{O III} \\
\mathbf{B}_{81} &= \begin{pmatrix} y_5 + z_5 \\ x_5 + y_5 \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} x_5 + z_5 \\ x_5 + y_5 \end{pmatrix} \mathbf{a}_2 + &= & ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{82} &= \begin{pmatrix} -y_5 + z_5 + \frac{1}{2} \\ x_5 - z_5 \end{pmatrix} \mathbf{a}_1 - &= & -ax_5 \hat{\mathbf{x}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{83} &= \begin{pmatrix} y_5 - z_5 \\ -x_5 + y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} x_5 + z_5 - \frac{1}{2} \\ -x_5 + y_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + &= & -a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{84} &= \begin{pmatrix} -(y_5 + z_5 - \frac{1}{2}) \\ x_5 - z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= & ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{P I}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{85} &= \begin{pmatrix} (x_5 + y_5) \mathbf{a}_1 + (y_5 + z_5) \mathbf{a}_2 + \\ (x_5 + z_5) \mathbf{a}_3 \end{pmatrix} = az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{86} &= \begin{pmatrix} -(x_5 + y_5 - \frac{1}{2}) \mathbf{a}_1 + \\ (-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - (x_5 - z_5) \mathbf{a}_3 \end{pmatrix} = az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - a(y_5 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{87} &= \begin{pmatrix} (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_5 - z_5) \mathbf{a}_2 - (x_5 + z_5 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -az_5 \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{88} &= \begin{pmatrix} (x_5 - y_5) \mathbf{a}_1 - (y_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_5 - z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_5 - \frac{1}{2}) \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{89} &= \begin{pmatrix} (x_5 + z_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + \\ (y_5 + z_5) \mathbf{a}_3 \end{pmatrix} = ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{90} &= \begin{pmatrix} -(x_5 - z_5) \mathbf{a}_1 - \\ (x_5 + y_5 - \frac{1}{2}) \mathbf{a}_2 + \\ (-y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{91} &= \begin{pmatrix} -(x_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 + \\ (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_2 + (y_5 - z_5) \mathbf{a}_3 \end{pmatrix} = ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{92} &= \begin{pmatrix} (x_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 - y_5) \mathbf{a}_2 - (y_5 + z_5 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{93} &= \begin{pmatrix} (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{pmatrix} = a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{94} &= \begin{pmatrix} (-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{pmatrix} = -a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{95} &= \begin{pmatrix} -(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{pmatrix} = a(y_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_5 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{96} &= \begin{pmatrix} (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{pmatrix} = -a(y_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{y}} - a(z_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{97} &= \begin{pmatrix} (y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{98} &= \begin{pmatrix} -(y_5 - z_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 + \\ (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(x_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{99} &= \begin{pmatrix} (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_5 - y_5) \mathbf{a}_2 - (x_5 + z_5) \mathbf{a}_3 \end{pmatrix} = -a(x_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_5 - \frac{1}{4}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{100} &= \begin{pmatrix} -(y_5 + z_5) \mathbf{a}_1 + \\ (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - z_5) \mathbf{a}_3 \end{pmatrix} = a(x_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(z_5 + \frac{1}{4}) \hat{\mathbf{y}} - a(y_5 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{101} &= \begin{pmatrix} (x_5 + y_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(z_5 + \frac{1}{4}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{102} &= \begin{pmatrix} -(x_5 + y_5) \mathbf{a}_1 + \\ (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - (y_5 - z_5) \mathbf{a}_3 \end{pmatrix} = a(z_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_5 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_5 - \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{103} &= \begin{pmatrix} -(x_5 - y_5) \mathbf{a}_1 - (x_5 + z_5) \mathbf{a}_2 + \\ (y_5 - z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(z_5 - \frac{1}{4}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{4}) \hat{\mathbf{y}} - a(x_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I} \\
\mathbf{B}_{104} &= \begin{pmatrix} (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 - z_5) \mathbf{a}_2 - (y_5 + z_5) \mathbf{a}_3 \end{pmatrix} = -a(z_5 + \frac{1}{4}) \hat{\mathbf{x}} - a(y_5 - \frac{1}{4}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{4}) \hat{\mathbf{z}} & (48e) & \text{P I}
\end{aligned}$$

## References

- [1] L. Pauling and J. Sherman, *The Crystal Structure of Aluminum Metaphosphate,  $Al(PO_3)_3$* , Z. Krystallogr. **96**, 481–487 (1937).

## Found in

- [1] H. van der Meer, *The crystal structure of a monoclinic form of aluminium metaphosphate,  $Al(PO_3)_3$* , Acta Crystallogr. Sect. B **32**, 2423–2426 (1976), doi:10.1107/S0567740876007899.