

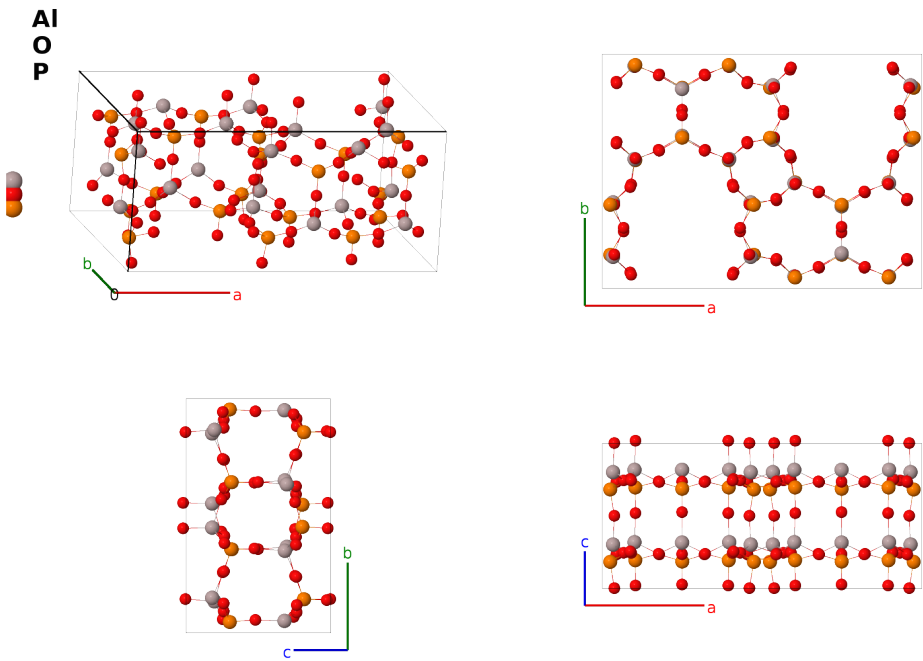
Ordered Calcined AlPO₄-11 Structure: AB4C_oI120_46_b2c_2b9c_b2c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/R2HW>

https://aflow.org/prototype-encyclopedia/AB4C_oI120_46_b2c_2b9c_b2c-001



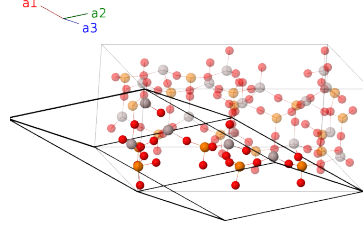
Prototype	AlO ₄ P
AFLOW prototype label	AB4C_oI120_46_b2c_2b9c_b2c-001
ICSD	63664
CCDC	1626745
Pearson symbol	oI120
Space group number	46
Space group symbol	<i>Ima</i> 2
AFLOW prototype command	<pre>aflow --proto=AB4C_oI120_46_b2c_2b9c_b2c-001 --params=a,b/a,c/a,y1,z1,y2,z2,y3,z3,y4,z4,x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8, x9,y9,z9,x10,y10,z10,x11,y11,z11,x12,y12,z12,x13,y13,z13,x14,y14,z14,x15,y15,z15,x16,y16, z16,x17,y17,z17</pre>

- Samples of large-pore AlPO₄-11 were calcined at 873K to remove impurities and then dehydrated at 573K. Data was collected at 295K.

- (Richardson, 1988) found the ordered structure shown here, but also found a good fit to the data by assuming a disordered phase where the aluminum and phosphorous atoms are randomly distributed.
- Unlike the 12-member nearly circular ring in $\text{AlPO}_4\text{-5}$, here the ring onl has aluminum and phosphorous atoms and is elliptical.
- More information about AlPO_4 structures can be found on the SiO_2 and AlPO_4 page.
- (Richardson, 1988) give the data for this structure in the $Icm2$ setting of space group #46. Fortunately the ICSD entry is given in the standard $Ima2$ setting.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$(y_1 + z_1) \mathbf{a}_1 + (z_1 + \frac{1}{4}) \mathbf{a}_2 + (y_1 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Al I
$\mathbf{B}_2$	$-(y_1 - z_1) \mathbf{a}_1 + (z_1 + \frac{3}{4}) \mathbf{a}_2 - (y_1 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4b)	Al I
$\mathbf{B}_3$	$(y_2 + z_2) \mathbf{a}_1 + (z_2 + \frac{1}{4}) \mathbf{a}_2 + (y_2 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_4$	$-(y_2 - z_2) \mathbf{a}_1 + (z_2 + \frac{3}{4}) \mathbf{a}_2 - (y_2 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4b)	O I
$\mathbf{B}_5$	$(y_3 + z_3) \mathbf{a}_1 + (z_3 + \frac{1}{4}) \mathbf{a}_2 + (y_3 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_6$	$-(y_3 - z_3) \mathbf{a}_1 + (z_3 + \frac{3}{4}) \mathbf{a}_2 - (y_3 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4b)	O II
$\mathbf{B}_7$	$(y_4 + z_4) \mathbf{a}_1 + (z_4 + \frac{1}{4}) \mathbf{a}_2 + (y_4 + \frac{1}{4}) \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B}_8$	$-(y_4 - z_4) \mathbf{a}_1 + (z_4 + \frac{3}{4}) \mathbf{a}_2 - (y_4 - \frac{3}{4}) \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B}_9$	$(y_5 + z_5) \mathbf{a}_1 + (x_5 + z_5) \mathbf{a}_2 + (x_5 + y_5) \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Al II
$\mathbf{B}_{10}$	$-(y_5 - z_5) \mathbf{a}_1 - (x_5 - z_5) \mathbf{a}_2 - (x_5 + y_5) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Al II
$\mathbf{B}_{11}$	$-(y_5 - z_5) \mathbf{a}_1 + (x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 - y_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Al II
$\mathbf{B}_{12}$	$(y_5 + z_5) \mathbf{a}_1 + (-x_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + (-x_5 + y_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(8c)	Al II

$$\begin{aligned}
\mathbf{B}_{13} &= \begin{pmatrix} (y_6 + z_6) \mathbf{a}_1 + (x_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6) \mathbf{a}_3 \end{pmatrix} = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8c) & \text{Al III} \\
\mathbf{B}_{14} &= \begin{pmatrix} -(y_6 - z_6) \mathbf{a}_1 - (x_6 - z_6) \mathbf{a}_2 - \\ (x_6 + y_6) \mathbf{a}_3 \end{pmatrix} = -ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8c) & \text{Al III} \\
\mathbf{B}_{15} &= \begin{pmatrix} -(y_6 - z_6) \mathbf{a}_1 + \\ (x_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_6 - y_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8c) & \text{Al III} \\
\mathbf{B}_{16} &= \begin{pmatrix} (y_6 + z_6) \mathbf{a}_1 + \\ (-x_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_6 + y_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}} & (8c) & \text{Al III} \\
\mathbf{B}_{17} &= \begin{pmatrix} (y_7 + z_7) \mathbf{a}_1 + (x_7 + z_7) \mathbf{a}_2 + \\ (x_7 + y_7) \mathbf{a}_3 \end{pmatrix} = ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O III} \\
\mathbf{B}_{18} &= \begin{pmatrix} -(y_7 - z_7) \mathbf{a}_1 - (x_7 - z_7) \mathbf{a}_2 - \\ (x_7 + y_7) \mathbf{a}_3 \end{pmatrix} = -ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O III} \\
\mathbf{B}_{19} &= \begin{pmatrix} -(y_7 - z_7) \mathbf{a}_1 + \\ (x_7 + z_7 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_7 - y_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O III} \\
\mathbf{B}_{20} &= \begin{pmatrix} (y_7 + z_7) \mathbf{a}_1 + \\ (-x_7 + z_7 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_7 + y_7 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{O III} \\
\mathbf{B}_{21} &= \begin{pmatrix} (y_8 + z_8) \mathbf{a}_1 + (x_8 + z_8) \mathbf{a}_2 + \\ (x_8 + y_8) \mathbf{a}_3 \end{pmatrix} = ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{22} &= \begin{pmatrix} -(y_8 - z_8) \mathbf{a}_1 - (x_8 - z_8) \mathbf{a}_2 - \\ (x_8 + y_8) \mathbf{a}_3 \end{pmatrix} = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{23} &= \begin{pmatrix} -(y_8 - z_8) \mathbf{a}_1 + \\ (x_8 + z_8 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_8 - y_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{24} &= \begin{pmatrix} (y_8 + z_8) \mathbf{a}_1 + \\ (-x_8 + z_8 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_8 + y_8 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O IV} \\
\mathbf{B}_{25} &= \begin{pmatrix} (y_9 + z_9) \mathbf{a}_1 + (x_9 + z_9) \mathbf{a}_2 + \\ (x_9 + y_9) \mathbf{a}_3 \end{pmatrix} = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{26} &= \begin{pmatrix} -(y_9 - z_9) \mathbf{a}_1 - (x_9 - z_9) \mathbf{a}_2 - \\ (x_9 + y_9) \mathbf{a}_3 \end{pmatrix} = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{27} &= \begin{pmatrix} -(y_9 - z_9) \mathbf{a}_1 + \\ (x_9 + z_9 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_9 - y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{28} &= \begin{pmatrix} (y_9 + z_9) \mathbf{a}_1 + \\ (-x_9 + z_9 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_9 + y_9 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O V} \\
\mathbf{B}_{29} &= \begin{pmatrix} (y_{10} + z_{10}) \mathbf{a}_1 + (x_{10} + z_{10}) \mathbf{a}_2 + \\ (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{30} &= \begin{pmatrix} -(y_{10} - z_{10}) \mathbf{a}_1 - \\ (x_{10} - z_{10}) \mathbf{a}_2 - (x_{10} + y_{10}) \mathbf{a}_3 \end{pmatrix} = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{31} &= \begin{pmatrix} -(y_{10} - z_{10}) \mathbf{a}_1 + \\ (x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{10} - y_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VI}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{32} &= \begin{pmatrix} (y_{10} + z_{10}) \mathbf{a}_1 + \\ (-x_{10} + z_{10} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{10} + y_{10} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{10} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{O VI} \\
\mathbf{B}_{33} &= \begin{pmatrix} (y_{11} + z_{11}) \mathbf{a}_1 + (x_{11} + z_{11}) \mathbf{a}_2 + \\ (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = ax_{11} \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{34} &= \begin{pmatrix} -(y_{11} - z_{11}) \mathbf{a}_1 - \\ (x_{11} - z_{11}) \mathbf{a}_2 - (x_{11} + y_{11}) \mathbf{a}_3 \end{pmatrix} = -ax_{11} \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{35} &= \begin{pmatrix} -(y_{11} - z_{11}) \mathbf{a}_1 + \\ (x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{11} - y_{11} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{11} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{36} &= \begin{pmatrix} (y_{11} + z_{11}) \mathbf{a}_1 + \\ (-x_{11} + z_{11} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{11} + y_{11} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{11} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} & (8c) & \text{O VII} \\
\mathbf{B}_{37} &= \begin{pmatrix} (y_{12} + z_{12}) \mathbf{a}_1 + (x_{12} + z_{12}) \mathbf{a}_2 + \\ (x_{12} + y_{12}) \mathbf{a}_3 \end{pmatrix} = ax_{12} \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{38} &= \begin{pmatrix} -(y_{12} - z_{12}) \mathbf{a}_1 - \\ (x_{12} - z_{12}) \mathbf{a}_2 - (x_{12} + y_{12}) \mathbf{a}_3 \end{pmatrix} = -ax_{12} \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{39} &= \begin{pmatrix} -(y_{12} - z_{12}) \mathbf{a}_1 + \\ (x_{12} + z_{12} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{12} - y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{12} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{40} &= \begin{pmatrix} (y_{12} + z_{12}) \mathbf{a}_1 + \\ (-x_{12} + z_{12} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{12} + y_{12} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{12} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} & (8c) & \text{O VIII} \\
\mathbf{B}_{41} &= \begin{pmatrix} (y_{13} + z_{13}) \mathbf{a}_1 + (x_{13} + z_{13}) \mathbf{a}_2 + \\ (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = ax_{13} \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{42} &= \begin{pmatrix} -(y_{13} - z_{13}) \mathbf{a}_1 - \\ (x_{13} - z_{13}) \mathbf{a}_2 - (x_{13} + y_{13}) \mathbf{a}_3 \end{pmatrix} = -ax_{13} \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{43} &= \begin{pmatrix} -(y_{13} - z_{13}) \mathbf{a}_1 + \\ (x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{13} - y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{13} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{44} &= \begin{pmatrix} (y_{13} + z_{13}) \mathbf{a}_1 + \\ (-x_{13} + z_{13} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{13} + y_{13} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{13} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \hat{\mathbf{z}} & (8c) & \text{O IX} \\
\mathbf{B}_{45} &= \begin{pmatrix} (y_{14} + z_{14}) \mathbf{a}_1 + (x_{14} + z_{14}) \mathbf{a}_2 + \\ (x_{14} + y_{14}) \mathbf{a}_3 \end{pmatrix} = ax_{14} \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O X} \\
\mathbf{B}_{46} &= \begin{pmatrix} -(y_{14} - z_{14}) \mathbf{a}_1 - \\ (x_{14} - z_{14}) \mathbf{a}_2 - (x_{14} + y_{14}) \mathbf{a}_3 \end{pmatrix} = -ax_{14} \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O X} \\
\mathbf{B}_{47} &= \begin{pmatrix} -(y_{14} - z_{14}) \mathbf{a}_1 + \\ (x_{14} + z_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{14} - y_{14} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{14} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O X} \\
\mathbf{B}_{48} &= \begin{pmatrix} (y_{14} + z_{14}) \mathbf{a}_1 + \\ (-x_{14} + z_{14} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{14} + y_{14} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{14} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \hat{\mathbf{z}} & (8c) & \text{O X} \\
\mathbf{B}_{49} &= \begin{pmatrix} (y_{15} + z_{15}) \mathbf{a}_1 + (x_{15} + z_{15}) \mathbf{a}_2 + \\ (x_{15} + y_{15}) \mathbf{a}_3 \end{pmatrix} = ax_{15} \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O XI} \\
\mathbf{B}_{50} &= \begin{pmatrix} -(y_{15} - z_{15}) \mathbf{a}_1 - \\ (x_{15} - z_{15}) \mathbf{a}_2 - (x_{15} + y_{15}) \mathbf{a}_3 \end{pmatrix} = -ax_{15} \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O XI}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{51} &= \begin{pmatrix} -(y_{15} - z_{15}) \mathbf{a}_1 + \\ (x_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{15} - y_{15} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{15} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O XI} \\
\mathbf{B}_{52} &= \begin{pmatrix} (y_{15} + z_{15}) \mathbf{a}_1 + \\ (-x_{15} + z_{15} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{15} + y_{15} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{15} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \hat{\mathbf{z}} & (8c) & \text{O XI} \\
\mathbf{B}_{53} &= \begin{pmatrix} (y_{16} + z_{16}) \mathbf{a}_1 + (x_{16} + z_{16}) \mathbf{a}_2 + \\ (x_{16} + y_{16}) \mathbf{a}_3 \end{pmatrix} = ax_{16} \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8c) & \text{P II} \\
\mathbf{B}_{54} &= \begin{pmatrix} -(y_{16} - z_{16}) \mathbf{a}_1 - \\ (x_{16} - z_{16}) \mathbf{a}_2 - (x_{16} + y_{16}) \mathbf{a}_3 \end{pmatrix} = -ax_{16} \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8c) & \text{P II} \\
\mathbf{B}_{55} &= \begin{pmatrix} -(y_{16} - z_{16}) \mathbf{a}_1 + \\ (x_{16} + z_{16} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{16} - y_{16} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{16} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8c) & \text{P II} \\
\mathbf{B}_{56} &= \begin{pmatrix} (y_{16} + z_{16}) \mathbf{a}_1 + \\ (-x_{16} + z_{16} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{16} + y_{16} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{16} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \hat{\mathbf{z}} & (8c) & \text{P II} \\
\mathbf{B}_{57} &= \begin{pmatrix} (y_{17} + z_{17}) \mathbf{a}_1 + (x_{17} + z_{17}) \mathbf{a}_2 + \\ (x_{17} + y_{17}) \mathbf{a}_3 \end{pmatrix} = ax_{17} \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (8c) & \text{P III} \\
\mathbf{B}_{58} &= \begin{pmatrix} -(y_{17} - z_{17}) \mathbf{a}_1 - \\ (x_{17} - z_{17}) \mathbf{a}_2 - (x_{17} + y_{17}) \mathbf{a}_3 \end{pmatrix} = -ax_{17} \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (8c) & \text{P III} \\
\mathbf{B}_{59} &= \begin{pmatrix} -(y_{17} - z_{17}) \mathbf{a}_1 + \\ (x_{17} + z_{17} + \frac{1}{2}) \mathbf{a}_2 + \\ (x_{17} - y_{17} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_{17} + \frac{1}{2} \right) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (8c) & \text{P III} \\
\mathbf{B}_{60} &= \begin{pmatrix} (y_{17} + z_{17}) \mathbf{a}_1 + \\ (-x_{17} + z_{17} + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_{17} + y_{17} + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_{17} - \frac{1}{2} \right) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}} & (8c) & \text{P III}
\end{aligned}$$

References

- [1] J. R. Richardson, Jr., J. J. Pluth, and J. V. Smith, *Rietveld profile analysis of calcined $\text{AlPO}_4\text{-11}$ using pulsed neutron powder diffraction*, Acta Crystallographica B **44**, 367–373 (1988), doi:10.1107/S0108768188003076.

Found in

- [1] M. Fischer, *Revisiting the Structure of Calcined and Hydrated $\text{AlPO}_4\text{-11}$ with DFT-Based Molecular Dynamics Simulations*, ChemPhysChem **22**, 2063–2077 (2021), doi:10.1002/cphc.202100486.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).