

Calcined AlPO₄-34 Structure: AB4C_hR36_148_f_4f_f-001

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<https://aflow.org/prototype-encyclopedia/GX1Z>

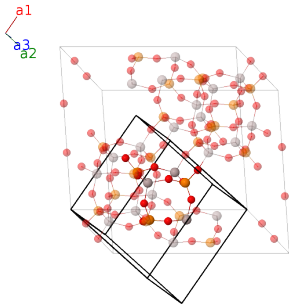
https://aflow.org/prototype-encyclopedia/AB4C_hR36_148_f_4f_f-001

Prototype	AlO ₄ P
AFLOW prototype label	AB4C_hR36_148_f_4f_f-001
ICSD	38957
CCDC	1817054
Pearson symbol	hR36
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=AB4C_hR36_148_f_4f_f-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 yet another of the many possible crystal structures in the silica/aluminum phosphate system. (Szostak, 1989) relates it to chabazite. Like all such crystals, it consists of connected AlO₄ and PO₄ tetrahedra.
- This sample was calcined, *e.g.* heated below the melting temperature to remove any organic and water molecules. The rehydrated samples have *P*1 symmetry, and neither (Tuel, 2000) nor (Poulet, 2002) give the positions of the hydrogen atoms, so we pass on showing that structure for now.

Rhombohedral primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
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$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 - z_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_1 - 2y_1 + z_1) \hat{\mathbf{y}} + \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_2$	$=$	$z_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_1 - z_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_1 - y_1 - z_1) \hat{\mathbf{y}} + \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_3$	$=$	$y_1 \mathbf{a}_1 + z_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_1 + y_1 - 2z_1) \hat{\mathbf{y}} + \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_4$	$=$	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_1 - z_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_1 - 2y_1 + z_1) \hat{\mathbf{y}} - \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_5$	$=$	$-z_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_1 - z_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_1 - y_1 - z_1) \hat{\mathbf{y}} - \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_6$	$=$	$-y_1 \mathbf{a}_1 - z_1 \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 - y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_1 + y_1 - 2z_1) \hat{\mathbf{y}} - \frac{1}{3}c(x_1 + y_1 + z_1) \hat{\mathbf{z}}$	(6f)	Al I
$\mathbf{B}_7$	$=$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_8$	$=$	$z_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + y_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_9$	$=$	$y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} + \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{10}$	$=$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 - z_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_2 - 2y_2 + z_2) \hat{\mathbf{y}} - \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{11}$	$=$	$-z_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - y_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_2 - z_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_2 - y_2 - z_2) \hat{\mathbf{y}} - \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{12}$	$=$	$-y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_2 + y_2 - 2z_2) \hat{\mathbf{y}} - \frac{1}{3}c(x_2 + y_2 + z_2) \hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B}_{13}$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B}_{14}$	$=$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B}_{15}$	$=$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B}_{16}$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B}_{17}$	$=$	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B}_{18}$	$=$	$-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f)	O II
$\mathbf{B}_{19}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{20}$	$=$	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{21}$	$=$	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{22}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{23}$	$=$	$-z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O III
$\mathbf{B}_{24}$	$=$	$-y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f)	O III

$$\begin{aligned}
\mathbf{B}_{25} &= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O IV} \\
\mathbf{B}_{26} &= z_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + y_5 \mathbf{a}_3 &= -\frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O IV} \\
\mathbf{B}_{27} &= y_5 \mathbf{a}_1 + z_5 \mathbf{a}_2 + x_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} + \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O IV} \\
\mathbf{B}_{28} &= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3 &= -\frac{1}{2}a(x_5 - z_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 - 2y_5 + z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O IV} \\
\mathbf{B}_{29} &= -z_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - y_5 \mathbf{a}_3 &= \frac{1}{2}a(y_5 - z_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_5 - y_5 - z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O IV} \\
\mathbf{B}_{30} &= -y_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 - x_5 \mathbf{a}_3 &= \frac{1}{2}a(x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_5 + y_5 - 2z_5) \hat{\mathbf{y}} - \frac{1}{3}c(x_5 + y_5 + z_5) \hat{\mathbf{z}} &(6f) &\quad \text{O IV} \\
\mathbf{B}_{31} &= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{P I} \\
\mathbf{B}_{32} &= z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3 &= -\frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{P I} \\
\mathbf{B}_{33} &= y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} + \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{P I} \\
\mathbf{B}_{34} &= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -\frac{1}{2}a(x_6 - z_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 - 2y_6 + z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{P I} \\
\mathbf{B}_{35} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= \frac{1}{2}a(y_6 - z_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_6 - y_6 - z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{P I} \\
\mathbf{B}_{36} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= \frac{1}{2}a(x_6 - y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_6 + y_6 - 2z_6) \hat{\mathbf{y}} - \frac{1}{3}c(x_6 + y_6 + z_6) \hat{\mathbf{z}} &(6f) &\quad \text{P I}
\end{aligned}$$

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First cited in

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