

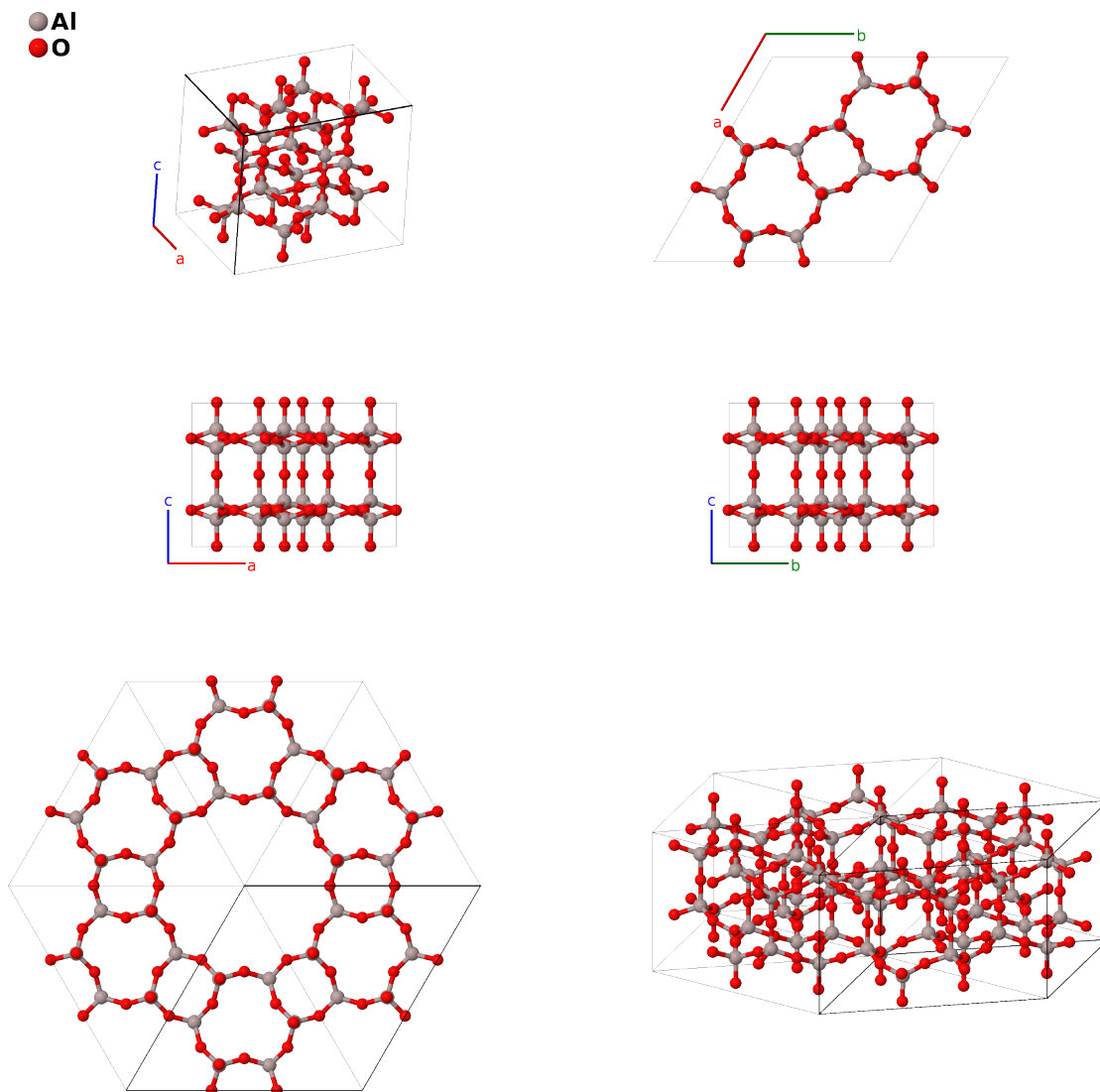
AlPO₄ Structure: AB2_hP72_192_m_j2kl-001

This structure originally had the label AB2_hP72_192_m_j2kl. Calls to that address will be redirected here.

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<https://aflow.org/p/M1VB>

https://aflow.org/p/AB2_hP72_192_m_j2kl-001



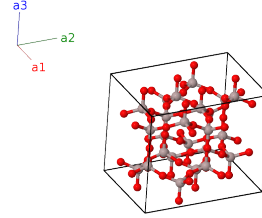
Prototype	AlO ₄ P
AFLOW prototype label	AB2_hP72_192_m_j2kl-001
ICSD	62772
Pearson symbol	hP72

Space group number 192
Space group symbol $P6/mcc$
AFLOW prototype command `aflow --proto=AB2_hP72_192_m_j2k1-001`
`--params=a, c/a, x1, x2, x3, x4, y4, x5, y5, z5`

- Here, the metallic (“M”) sites are alloyed, $Al_{0.5}P_{0.5}$. The Jmol image represents the M sites with aluminum atoms. Polytypes of this compound also appear in space groups $P6$ #168 (AB4C_hP72_168_2d_8d_2d) and $P6_3mc$ #184 (AB4C_hP72_184_d_4d_d).

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	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_2	$= x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_4	$= -x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_5	$= -x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_6	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_7	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_8	$= -x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_9	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_{10}	$= x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_{11}	$= x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_{12}	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12j)	O I
\mathbf{B}_{13}	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{14}	$= -2x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{15}	$= x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{16}	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{17}	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{18}	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{19}	$= -x_2 \mathbf{a}_1 - 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{20}	$= 2x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{21}	$= -x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\sqrt{3}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12k)	O II
\mathbf{B}_{22}	$= x_2 \mathbf{a}_1 + 2x_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(12k)	O II

$$\begin{aligned}
\mathbf{B}_{61} &= -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}} &(24m) & \text{Al I} \\
\mathbf{B}_{62} &= 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}} &(24m) & \text{Al I} \\
\mathbf{B}_{63} &= (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}} &(24m) & \text{Al I} \\
\mathbf{B}_{64} &= 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}} &(24m) & \text{Al I} \\
\mathbf{B}_{65} &= -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}} &(24m) & \text{Al I} \\
\mathbf{B}_{66} &= -(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}} &(24m) & \text{Al I} \\
\mathbf{B}_{67} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \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}} + &(24m) & \text{Al I} \\
&&& c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} \\
\mathbf{B}_{68} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} &(24m) & \text{Al I} \\
&& (z_5 + \frac{1}{2}) \mathbf{a}_3 \\
\mathbf{B}_{69} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} &(24m) & \text{Al I} \\
\mathbf{B}_{70} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \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}} + &(24m) & \text{Al I} \\
&&& c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} \\
\mathbf{B}_{71} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3 &= \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} &(24m) & \text{Al I} \\
\mathbf{B}_{72} &= -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + &= -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}} &(24m) & \text{Al I} \\
&& (z_5 + \frac{1}{2}) \mathbf{a}_3
\end{aligned}$$

References

- [1] J. W. R. Jr., J. J. Pluth, and J. V. Smith, *Aluminophosphate number 5: time-of-flight neutron powder diffraction study of calcined powder at 295 K*, Acta Crystallogr. Sect. C **43**, 1469–1472 (1987), doi:10.1107/S0108270187091418.

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