

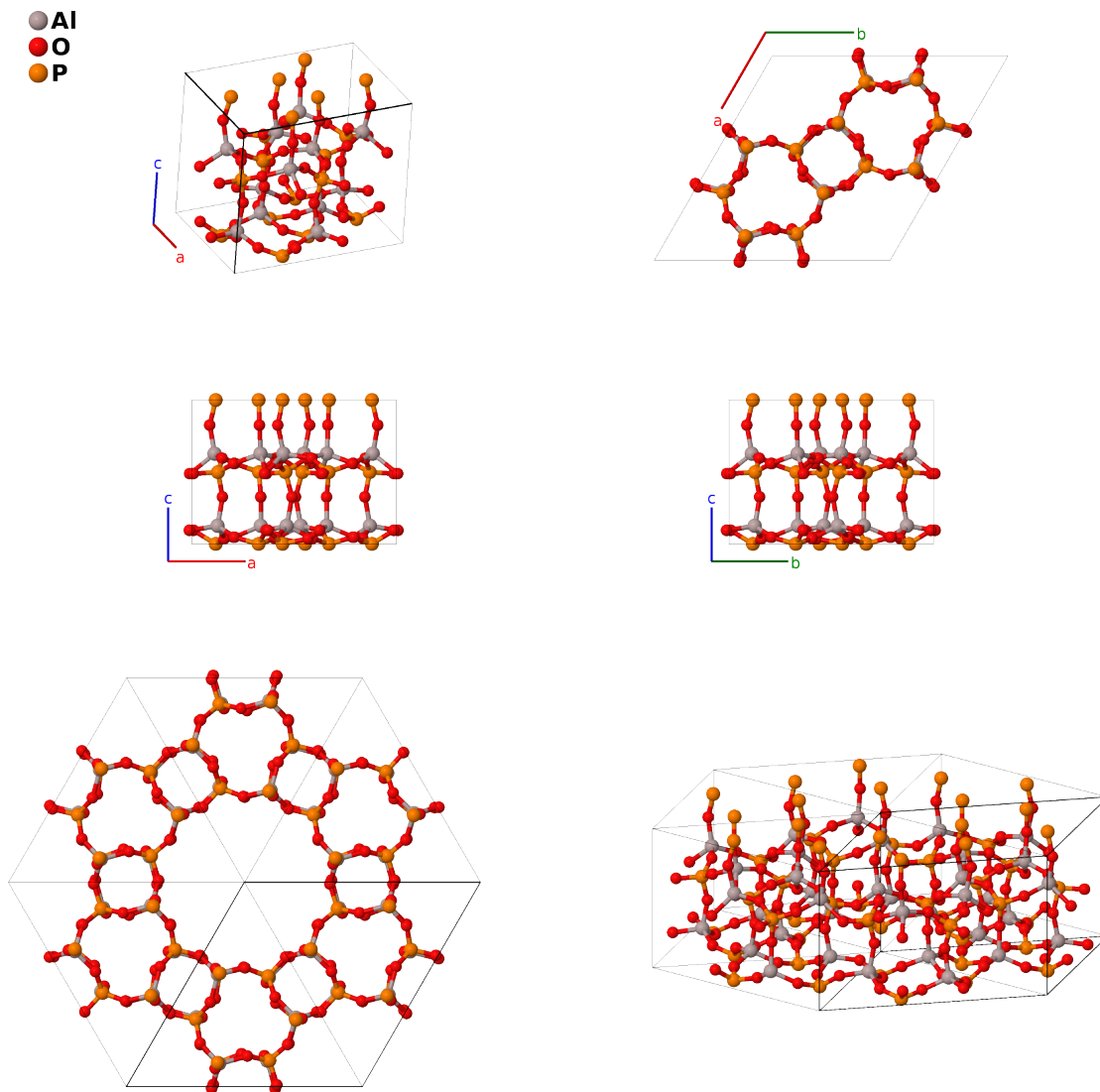
Al[PO₄] Structure: AB4C_hP72_168_2d_8d_2d-001

This structure originally had the label AB4C_hP72_168_2d_8d_2d. Calls to that address will be redirected here.

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<https://aflow.org/p/5X6W>

https://aflow.org/p/AB4C_hP72_168_2d_8d_2d-001



Prototype	AlO ₄ P
AFLOW prototype label	AB4C_hP72_168_2d_8d_2d-001
ICSD	none
Pearson symbol	hP72
Space group number	168

Space group symbol

$P6$

AFLOW prototype command

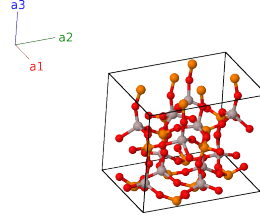
afLOW --proto=AB4C_hP72_168_2d_8d_2d-001

--params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- Polytypes of this compound also appear in space groups $P6cc$ #184 (AB4C_hP72_184_d.4d_d) and $P6/mcc$ #192 (AB2_hP72_192_m.j2kl).

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	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6d)	Al I
\mathbf{B}_2	$= -y_1 \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_1 - 2y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6d)	Al I
\mathbf{B}_3	$= -(x_1 - y_1) \mathbf{a}_1 - x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6d)	Al I
\mathbf{B}_4	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_1 + y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_1 - y_1) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6d)	Al I
\mathbf{B}_5	$= y_1 \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_1 + 2y_1) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6d)	Al I
\mathbf{B}_6	$= (x_1 - y_1) \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_1 - y_1) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(6d)	Al I
\mathbf{B}_7	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6d)	Al II
\mathbf{B}_8	$= -y_2 \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_2 - 2y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6d)	Al II
\mathbf{B}_9	$= -(x_2 - y_2) \mathbf{a}_1 - x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6d)	Al II
\mathbf{B}_{10}	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_2 + y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_2 - y_2) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6d)	Al II
\mathbf{B}_{11}	$= y_2 \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_2 + 2y_2) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6d)	Al II
\mathbf{B}_{12}	$= (x_2 - y_2) \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_2 - y_2) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(6d)	Al II
\mathbf{B}_{13}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6d)	O I
\mathbf{B}_{14}	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6d)	O I
\mathbf{B}_{15}	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6d)	O I
\mathbf{B}_{16}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6d)	O I
\mathbf{B}_{17}	$= y_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_3 + 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6d)	O I
\mathbf{B}_{18}	$= (x_3 - y_3) \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6d)	O I
\mathbf{B}_{19}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{20}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{21}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{22}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O II
\mathbf{B}_{23}	$= y_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(-x_4 + 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6d)	O II

$$\mathbf{B}_{63} = -(x_{11} - y_{11}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = -\frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} \quad (6d) \quad \text{P I}$$

$$\mathbf{B}_{64} = -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = -\frac{1}{2}a(x_{11} + y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{11} - y_{11}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} \quad (6d) \quad \text{P I}$$

$$\mathbf{B}_{65} = y_{11} \mathbf{a}_1 - (x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}a(-x_{11} + 2y_{11}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} \quad (6d) \quad \text{P I}$$

$$\mathbf{B}_{66} = (x_{11} - y_{11}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 = \frac{1}{2}a(2x_{11} - y_{11}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} \quad (6d) \quad \text{P I}$$

$$\mathbf{B}_{67} = x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (6d) \quad \text{P II}$$

$$\mathbf{B}_{68} = -y_{12} \mathbf{a}_1 + (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(x_{12} - 2y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (6d) \quad \text{P II}$$

$$\mathbf{B}_{69} = -(x_{12} - y_{12}) \mathbf{a}_1 - x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = -\frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (6d) \quad \text{P II}$$

$$\mathbf{B}_{70} = -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = -\frac{1}{2}a(x_{12} + y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_{12} - y_{12}) \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (6d) \quad \text{P II}$$

$$\mathbf{B}_{71} = y_{12} \mathbf{a}_1 - (x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(-x_{12} + 2y_{12}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (6d) \quad \text{P II}$$

$$\mathbf{B}_{72} = (x_{12} - y_{12}) \mathbf{a}_1 + x_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 = \frac{1}{2}a(2x_{12} - y_{12}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{12} \hat{\mathbf{y}} + cz_{12} \hat{\mathbf{z}} \quad (6d) \quad \text{P II}$$

References

- [1] A. R. Ruiz-Salvador, G. Sastre, D. W. Lewis, and C. R. A. Catlow, *Space group symmetry and Al—O—P bond angles in $AlPO_4 - 5$* , J. Mater. Chem. **6**, 1837–1842 (1996), doi:10.1039/JM9960601837.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.