

Computational AlPO_4 -5 Structure: AB4C_hP72_168_2d_8d_2d-001

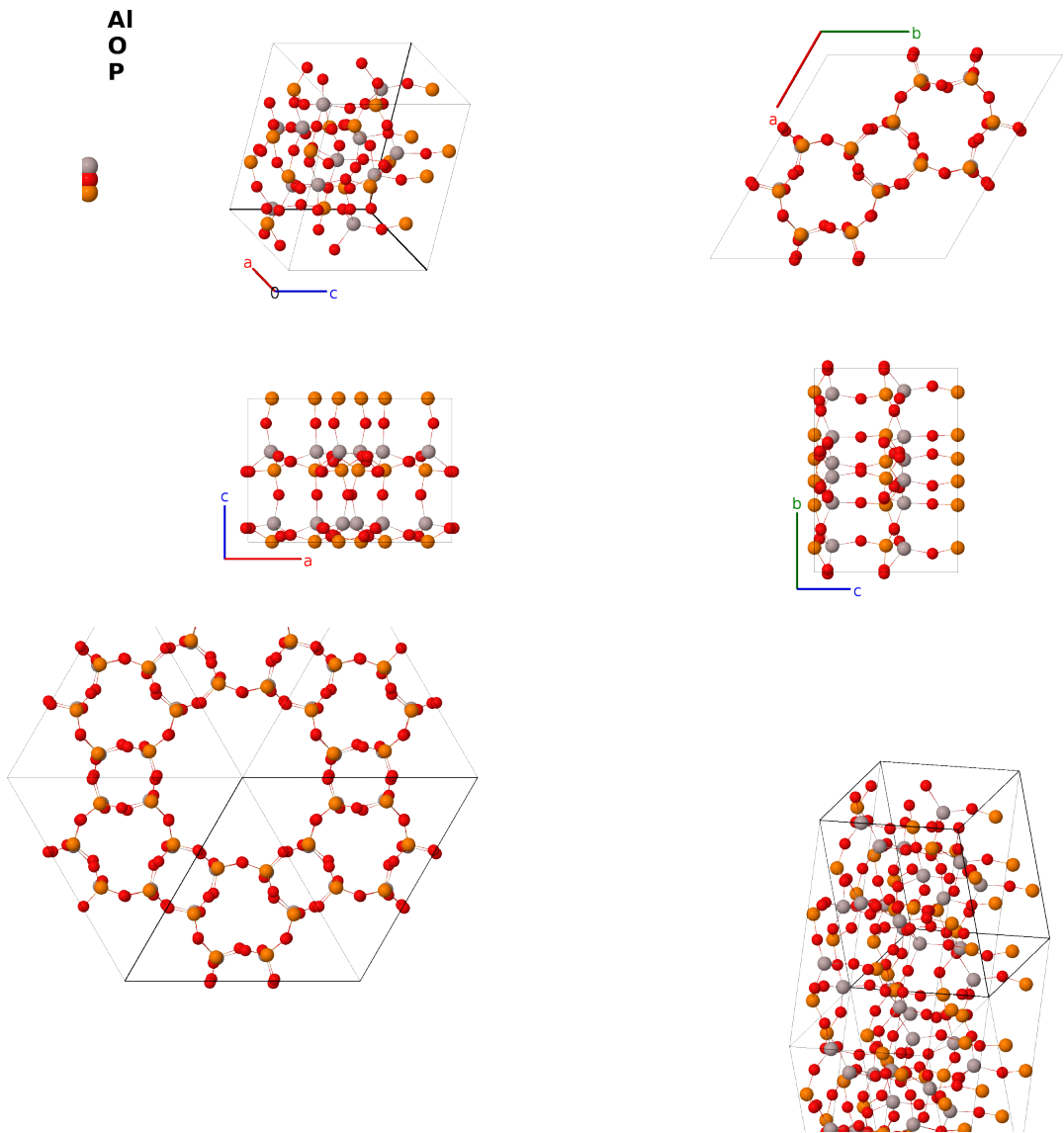
This structure previously used the label(s) **AB4C_hP72_168_2d_8d_2d**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/5X6W>

https://aflow.org/prototype-encyclopedia/AB4C_hP72_168_2d_8d_2d-001



Prototype

AlO_4P

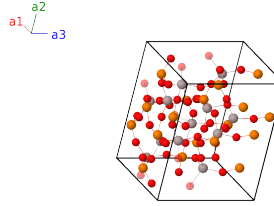
AFLOW prototype label

AB4C_hP72_168_2d_8d_2d-001

Pearson symbol	hP72
Space group number	168
Space group symbol	$P6$
AFLOW prototype command	aflow --proto=AB4C_hP72_168_2d_8d_2d-001 --params= $a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- This is a computational prediction of the structure of microporous AlPO_4 -5. It is somewhat different than the experimental AlPO_4 -5 framework.
- A list of AlPO_4 polymorphs in the Encyclopedia can be found on our SiO_2 and AlPO_4 page.
- We have updated the bibliographic information for this page (2025).

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

$$\begin{aligned}
\mathbf{B}_{59} &= y_{10} \mathbf{a}_1 - (x_{10} - y_{10}) \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(-x_{10} + 2y_{10}) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{60} &= (x_{10} - y_{10}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 = \frac{1}{2}a(2x_{10} - y_{10}) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (6d) & \text{O VIII} \\
\mathbf{B}_{61} &= 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}} & (6d) & \text{P I} \\
\mathbf{B}_{62} &= -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}} & (6d) & \text{P I} \\
\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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \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}} & (6d) & \text{P II}
\end{aligned}$$

References

- [1] N. J. Henson, A. K. Cheetham, and J. D. Gale, *Computational Studies of Aluminum Phosphate Polymorphs*, Chem. Mater. **8**, 664–670 (1996), doi:10.1021/cm9503238.

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- [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 AlPO₄ - 5*, J. Mater. Chem. **6**, 1837–1842 (1996), doi:10.1039/JM9960601837.
- [2] P. Villars and K. Cenzual, eds., *Structure Types. Part 5: Space Groups (173) P6₃ - (166) R-3m* (Springer-Verlag, 2007), chap. Al[PO₄], doi:10.1007/978-3-540-46933-9_164.

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