

AlPO₄-41 Structure:

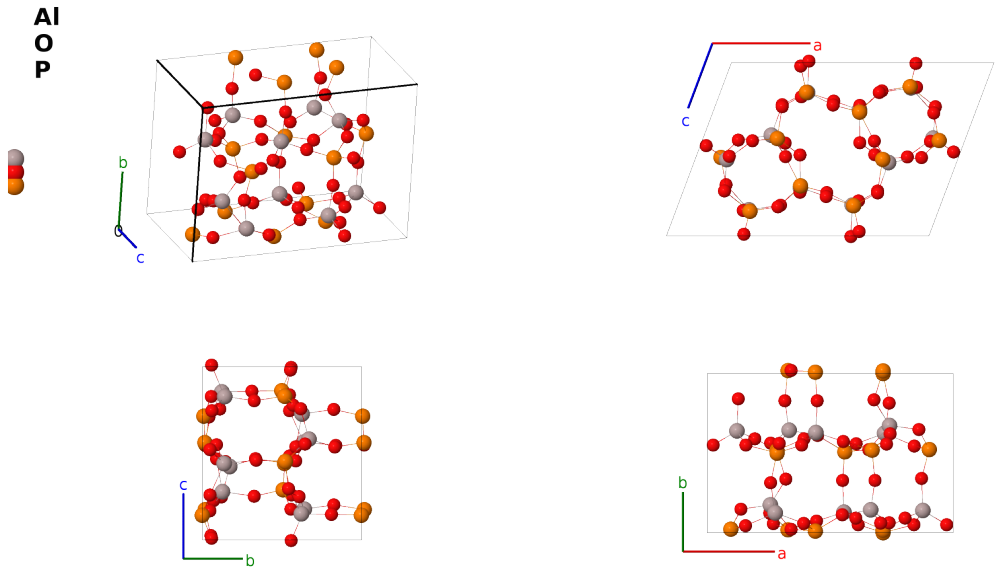
AB4C_mP60_4_5a_20a_5a-001

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<https://aflow.org/prototype-encyclopedia/5V2E>

https://aflow.org/prototype-encyclopedia/AB4C_mP60_4_5a_20a_5a-001



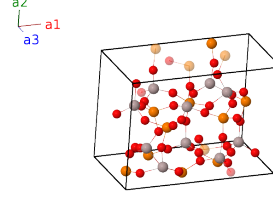
Prototype	AlO ₄ P
AFLOW prototype label	AB4C_mP60_4_5a_20a_5a-001
ICSD	75906
CCDC	1636548
Pearson symbol	mP60
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	<pre>aflow --proto=AB4C_mP60_4_5a_20a_5a-001 --params=a,b/a,c/a,β,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, 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,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉,x₂₀,y₂₀,z₂₀,x₂₁,y₂₁,z₂₁,x₂₂,y₂₂, z₂₂,x₂₃,y₂₃,z₂₃,x₂₄,y₂₄,z₂₄,x₂₅,y₂₅,z₂₅,x₂₆,y₂₆,z₂₆,x₂₇,y₂₇,z₂₇,x₂₈,y₂₈,z₂₈,x₂₉,y₂₉,z₂₉, x₃₀,y₃₀,z₃₀</pre>

- This is yet another of the many possible crystal structures in the silica/aluminum phosphate system. Like all such crystals, it consists of connected AlO₄ and PO₄ tetrahedra. In some cases silicon can replace the aluminum and phosphorous atoms (Ma, 2011).

- While the view of this structure along the unique axis suggests that this is a layered compound, the distance between the aluminum and phosphorous atoms in different layers (roughly 3Å) is approximately the same it is in an Al-O-P chain in other parts of the structure. This allows us to define an effective microporous ring with a minimum distance of 7.06Å.
- (Kirchner, 1994) give the structure in the unique axis c setting of space group $P2_1$ #4. We rotated the axes so that $c \rightarrow b \rightarrow a \rightarrow c$ to change this to the standard unique axis b setting.

Simple Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Al IV
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	Al IV
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	Al V
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	Al V
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_{12}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_{14}$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{16}$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{18}$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	=	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{19}$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	O V

$$\begin{aligned}
\mathbf{B}_{50} &= -x_{25} \mathbf{a}_1 + \left(y_{25} + \frac{1}{2}\right) \mathbf{a}_2 - z_{25} \mathbf{a}_3 = -\left(ax_{25} + cz_{25} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{25} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{25} \sin \beta \hat{\mathbf{z}} & (2a) & \text{O XX} \\
\mathbf{B}_{51} &= x_{26} \mathbf{a}_1 + y_{26} \mathbf{a}_2 + z_{26} \mathbf{a}_3 = \left(ax_{26} + cz_{26} \cos \beta\right) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P I} \\
\mathbf{B}_{52} &= -x_{26} \mathbf{a}_1 + \left(y_{26} + \frac{1}{2}\right) \mathbf{a}_2 - z_{26} \mathbf{a}_3 = -\left(ax_{26} + cz_{26} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{26} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{26} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P I} \\
\mathbf{B}_{53} &= x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3 = \left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P II} \\
\mathbf{B}_{54} &= -x_{27} \mathbf{a}_1 + \left(y_{27} + \frac{1}{2}\right) \mathbf{a}_2 - z_{27} \mathbf{a}_3 = -\left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{27} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P II} \\
\mathbf{B}_{55} &= x_{28} \mathbf{a}_1 + y_{28} \mathbf{a}_2 + z_{28} \mathbf{a}_3 = \left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P III} \\
\mathbf{B}_{56} &= -x_{28} \mathbf{a}_1 + \left(y_{28} + \frac{1}{2}\right) \mathbf{a}_2 - z_{28} \mathbf{a}_3 = -\left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{28} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{28} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P III} \\
\mathbf{B}_{57} &= x_{29} \mathbf{a}_1 + y_{29} \mathbf{a}_2 + z_{29} \mathbf{a}_3 = \left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P IV} \\
\mathbf{B}_{58} &= -x_{29} \mathbf{a}_1 + \left(y_{29} + \frac{1}{2}\right) \mathbf{a}_2 - z_{29} \mathbf{a}_3 = -\left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{29} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{29} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P IV} \\
\mathbf{B}_{59} &= x_{30} \mathbf{a}_1 + y_{30} \mathbf{a}_2 + z_{30} \mathbf{a}_3 = \left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P V} \\
\mathbf{B}_{60} &= -x_{30} \mathbf{a}_1 + \left(y_{30} + \frac{1}{2}\right) \mathbf{a}_2 - z_{30} \mathbf{a}_3 = -\left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + b\left(y_{30} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{30} \sin \beta \hat{\mathbf{z}} & (2a) & \text{P V}
\end{aligned}$$

References

- [1] R. M. Kirchner and J. M. Bennett, *The structure of calcined $\text{AlPO}_4\text{-41}$: A new framework topology containing one-dimensional 10-ring pores*, *Zeolites* **14**, 523–528 (1994), doi:10.1016/0144-2449(94)90185-6.
- [2] Y. Ma, N. Li, N. Guan, and S. Xiang, *Crystals morphology of AFO-type structure $\text{AlPO}_4\text{-41}$ and SAPO-41 molecular sieves*, *Microporous and Mesoporous Materials* **142**, 680–687 (2011), doi:10.1016/j.micromeso.2011.01.017.

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