

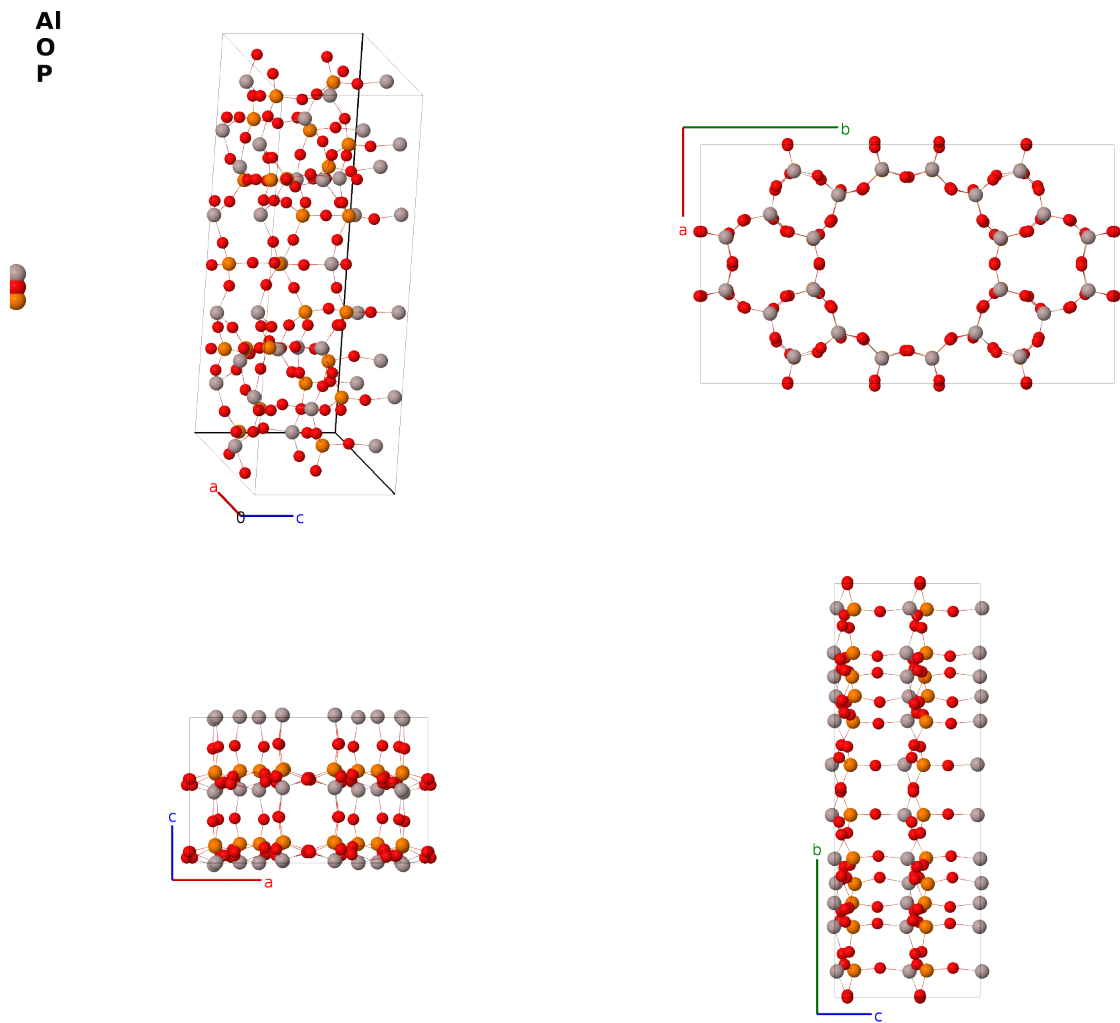
Orthorhombic AlPO_4 -5 Structure: AB4C_oP144_27_6e_24e_6e-001

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<https://aflow.org/prototype-encyclopedia/Y4G8>

https://aflow.org/prototype-encyclopedia/AB4C_oP144_27_6e_24e_6e-001



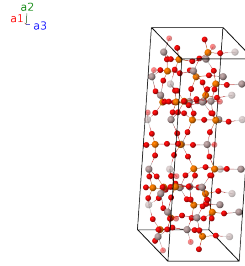
Prototype	AlO_4P
AFLOW prototype label	AB4C_oP144_27_6e_24e_6e-001
ICSD	82863
CCDC	1642920
Pearson symbol	oP144

Space group number	27
Space group symbol	<i>Pcc2</i>
AFLOW prototype command	aflow --proto=AB4C_oP144_27_6e_24e_6e-001 --params= <i>a, b/a, c/a, 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, x₃₁, y₃₁, z₃₁, x₃₂, y₃₂, z₃₂, x₃₃, y₃₃, z₃₃, x₃₄, y₃₄, z₃₄, x₃₅, y₃₅, z₃₅, x₃₆, y₃₆, z₃₆</i>

- AlPO₄ can be found in a wide variety of structures (Wilson, 1982). The variants included in the Encyclopedia can be found on the silica/AlPO₄ page.
- Ordered AlPO₄-5 can have the metallic atoms ordered, space group *P6cc* #186 (Klapp, 184), although (Ruiz-Salvador, 1996) find it in space group *P6* #168, and (Mora, 1996) find it in space group *Pcc2* #27 (this structure).
- It may also have disordered aluminum/phosphorous sites, space group *P6/mcc* #192 (Richardson, 1987).

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_3$	$= x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_4$	$= -x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Al I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4e)	Al II
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4e)	Al II
$\mathbf{B}_7$	$= x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Al II
$\mathbf{B}_8$	$= -x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Al II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B}_{11}$	$= x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B}_{12}$	$= -x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	Al IV
$\mathbf{B}_{14}$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	Al IV

$$\begin{aligned}
\mathbf{B}_{138} &= -x_{35} \mathbf{a}_1 - y_{35} \mathbf{a}_2 + z_{35} \mathbf{a}_3 &= -ax_{35} \hat{\mathbf{x}} - by_{35} \hat{\mathbf{y}} + cz_{35} \hat{\mathbf{z}} &(4e) &\text{P V} \\
\mathbf{B}_{139} &= x_{35} \mathbf{a}_1 - y_{35} \mathbf{a}_2 + \left(z_{35} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{35} \hat{\mathbf{x}} - by_{35} \hat{\mathbf{y}} + c \left(z_{35} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4e) &\text{P V} \\
\mathbf{B}_{140} &= -x_{35} \mathbf{a}_1 + y_{35} \mathbf{a}_2 + \left(z_{35} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{35} \hat{\mathbf{x}} + by_{35} \hat{\mathbf{y}} + c \left(z_{35} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4e) &\text{P V} \\
\mathbf{B}_{141} &= x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3 &= ax_{36} \hat{\mathbf{x}} + by_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}} &(4e) &\text{P VI} \\
\mathbf{B}_{142} &= -x_{36} \mathbf{a}_1 - y_{36} \mathbf{a}_2 + z_{36} \mathbf{a}_3 &= -ax_{36} \hat{\mathbf{x}} - by_{36} \hat{\mathbf{y}} + cz_{36} \hat{\mathbf{z}} &(4e) &\text{P VI} \\
\mathbf{B}_{143} &= x_{36} \mathbf{a}_1 - y_{36} \mathbf{a}_2 + \left(z_{36} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{36} \hat{\mathbf{x}} - by_{36} \hat{\mathbf{y}} + c \left(z_{36} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4e) &\text{P VI} \\
\mathbf{B}_{144} &= -x_{36} \mathbf{a}_1 + y_{36} \mathbf{a}_2 + \left(z_{36} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{36} \hat{\mathbf{x}} + by_{36} \hat{\mathbf{y}} + c \left(z_{36} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4e) &\text{P VI}
\end{aligned}$$

References

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First cited in

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