

Disordered (Al,P)O₄-5 Framework Structure: AB2_hP72_192_m_j2kl-001

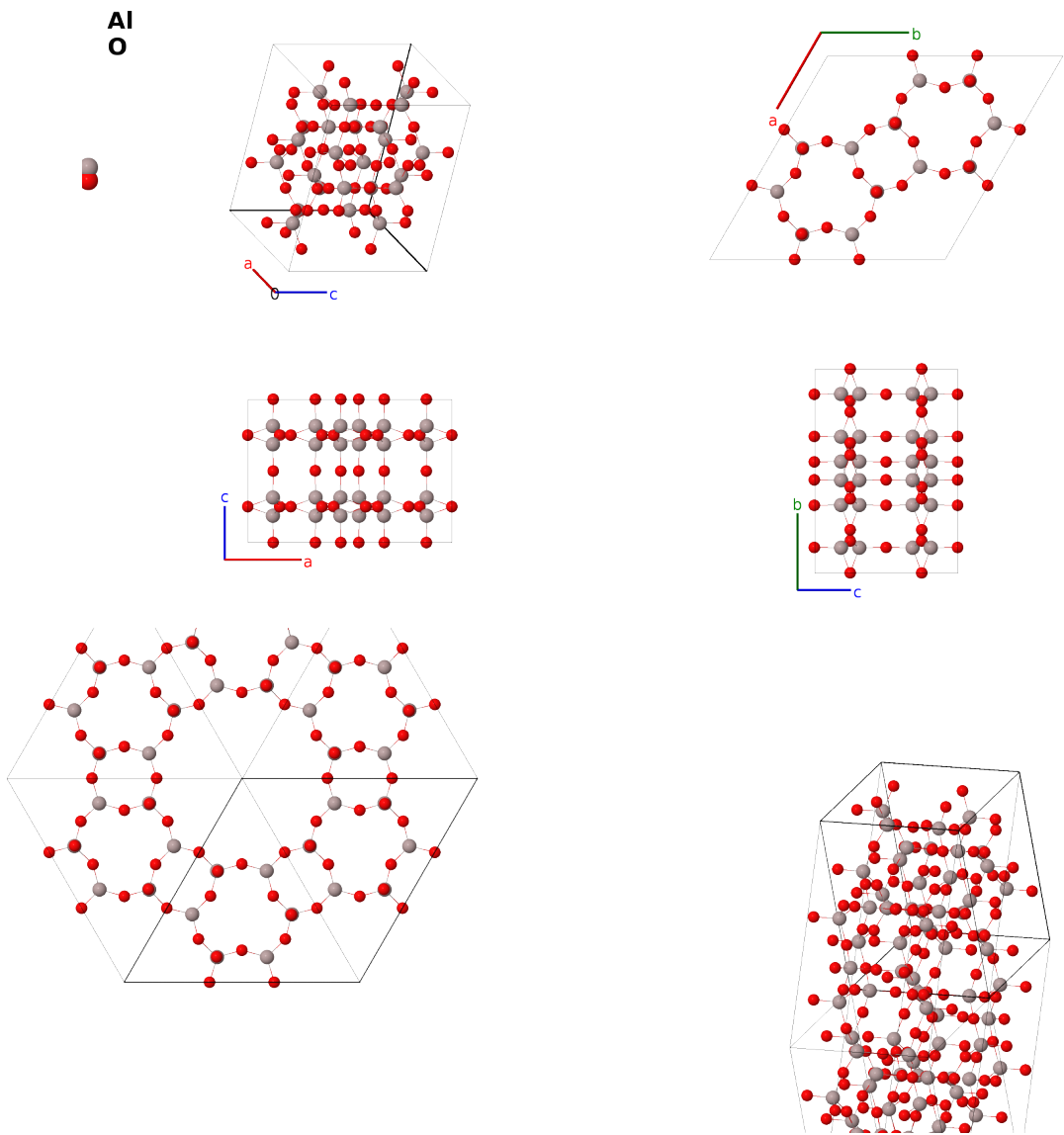
This structure previously used the label(s) **AB2_hP72_192_m_j2kl**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/M1VB>

https://aflow.org/prototype-encyclopedia/AB2_hP72_192_m_j2kl-001



Prototype

AlO₄P

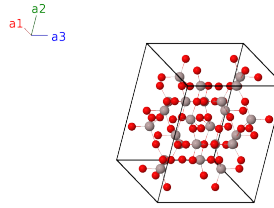
AFLOW prototype label

AB2_hP72_192_m_j2kl-001

ICSD	62772
CCDC	1625975
Pearson symbol	hP72
Space group number	192
Space group symbol	$P6/mcc$
AFLOW prototype command	<code>aflow --proto=AB2_hP72_192_m_j2kl-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄, y₄, x₅, y₅, z₅</code>

- This is a version of AlPO₄-5 with aluminum and phosphorous atoms randomly placed on the metallic sites, changing the space group from polar $P6cc$ #184 to centrosymmetric $P6/mcc$ #192. We arbitrarily label these sites as “Al.”
- For information on similar structures see the SiO₂ and AlPO₄ page.

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

[illegible]

$$\begin{aligned}
\mathbf{B}_{58} &= -y_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \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}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{59} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{60} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\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 + \left(z_5 + \frac{1}{2}\right) \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}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{68} &= -(x_5 - y_5) \mathbf{a}_1 + y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(-x_5 + 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{69} &= x_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{70} &= y_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \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}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{71} &= (x_5 - y_5) \mathbf{a}_1 - y_5 \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= \frac{1}{2}a(x_5 - 2y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I} \\
\mathbf{B}_{72} &= -x_5 \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right) \mathbf{a}_3 &= -\frac{1}{2}a(2x_5 - y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right) \hat{\mathbf{z}} &(24m) &\text{Al I}
\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.

Found in

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

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043