High-Temperature $AlPO_4$-25 Structure: AB2_oC72_67_mo_cgilno-001

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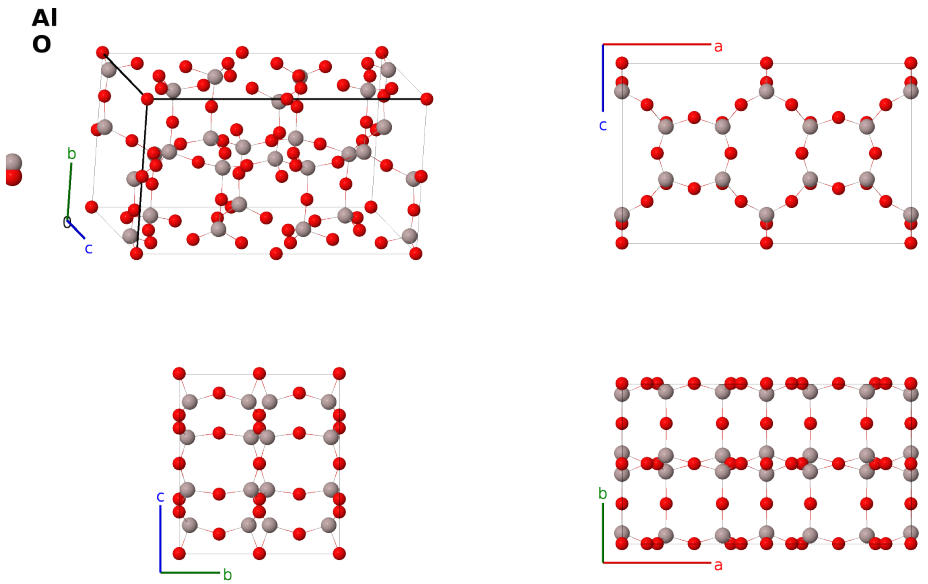
https://aflow.org/prototype-encyclopedia/E8FK

https://aflow.org/prototype-encyclopedia/AB2_oC72_67_mo_cgilno-001



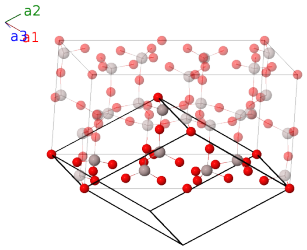
Prototype	AlO_4P
AFLOW prototype label	AB2_oC72_67_mo_cgilno-001
ICSD	108832
CCDC	1666476
Pearson symbol	oC72
Space group number	67
Space group symbol	*Cmme*
AFLOW prototype command	`aflow --proto=AB2_oC72_67_mo_cgilno-001 --params=`$a, b/a, c/a, z_2, x_3, z_4, y_5, z_5, x_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- Calcinated (heated below the melting temperature) $AlPO_4$-21 loses its water molecules and accompaning embedded materials and transforms into the $AlPO_4$-25 phase, with a structure in space group *Ibam* #72 that (Richardson, 1990) were unable to resolve.
- Above 530K the structure transforms into this high-temperature structure, with a conventional unit cell half the size of the low-temperature cell.

- (Richardson, 1990) give the structure in the *Acmm* setting of space group #67. AFLOW transforms this to the standard *Cmme* setting. Enforcing the AFLOW label convention then shifts the first oxygen atom from the (4e) to the (4c) Wyckoff position, with corrsponding shifts in other Wyckoff positions.
- The metallic (8n) and (16o) sites randomly occupied by aluminum and phosphorous atoms. We arbitrarily chose aluminum to represent these sites.
- More information about $AlPO_4$ and related structures can be found on the silica and aluminum phosphate page.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4c)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	O I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4g)	O II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	O III
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	O III
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	O III
$\mathbf{B_8}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8i)	O III
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8l)	O IV
$\mathbf{B_{10}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(8l)	O IV
$\mathbf{B_{11}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(8l)	O IV
$\mathbf{B_{12}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(8l)	O IV
$\mathbf{B_{13}}$	=	$-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Al I
$\mathbf{B_{14}}$	=	$\left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Al I
$\mathbf{B_{15}}$	=	$-\left(y_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Al I
$\mathbf{B_{16}}$	=	$y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Al I
$\mathbf{B_{17}}$	=	$\left(x_6 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{1}{4}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8n)	O V
$\mathbf{B_{18}}$	=	$-\left(x_6 - \frac{3}{4}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{1}{4}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - \frac{1}{4}b\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8n)	O V
$\mathbf{B_{19}}$	=	$-\left(x_6 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_6 - \frac{3}{4}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8n)	O V
$\mathbf{B_{20}}$	=	$\left(x_6 + \frac{1}{4}\right)\,\mathbf{a}_1 + \left(x_6 + \frac{3}{4}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8n)	O V

$$\mathbf{B_{21}} = (x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{22}} = \left(-x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(x_7 + y_7 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{23}} = -\left(x_7 + y_7 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{24}} = (x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{25}} = -(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{26}} = \left(x_7 - y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{27}} = \left(x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{28}} = -(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16o) \quad \text{Al II}$$

$$\mathbf{B_{29}} = (x_8 - y_8)\,\mathbf{a}_1 + (x_8 + y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{30}} = \left(-x_8 + y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - \left(x_8 + y_8 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -a\left(x_8 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{31}} = -\left(x_8 + y_8 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_8 + y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -a\left(x_8 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{32}} = (x_8 + y_8)\,\mathbf{a}_1 + (x_8 - y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{33}} = -(x_8 - y_8)\,\mathbf{a}_1 - (x_8 + y_8)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{34}} = \left(x_8 - y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 + y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = a\left(x_8 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{35}} = \left(x_8 + y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 - y_8 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = a\left(x_8 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

$$\mathbf{B_{36}} = -(x_8 + y_8)\,\mathbf{a}_1 - (x_8 - y_8)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (16o) \quad \text{O VI}$$

References

[1] J. W. Richardson, J. V. Smith, and J. J. Pluth, *$AlPO_4$-25: framework topology, topotactic transformation from $AlPO_4$-21, and high-low displacive transition*, J. Phys. Chem. **94**, 3365–3367 (1990), doi:10.1021/j100372a002.

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