$AlPO_4$ "low cristobalite type" Structure: AB4C_oC24_20_a_2c_b-001

This structure originally had the label `AB4C_oC24_20_b_2c_a`. Calls to that address will be redirected here.

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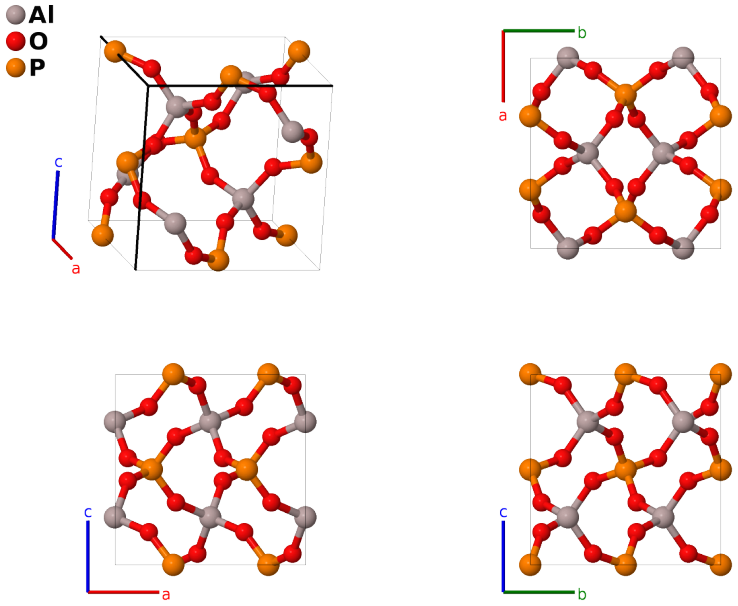
https://aflow.org/p/HRBV

https://aflow.org/p/AB4C_oC24_20_a_2c_b-001



Prototype	AlO_4P
AFLOW prototype label	AB4C_oC24_20_a_2c_b-001
Mineral name	low cristobalite type
ICSD	16651
Pearson symbol	oC24
Space group number	20
Space group symbol	$C222_1$
AFLOW prototype command	`aflow --proto=AB4C_oC24_20_a_2c_b-001 --params=`$a, b/a, c/a, x_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4$

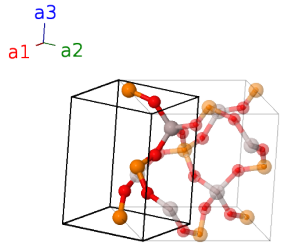
Other compounds with this structure
$GaPO_4$

- Aluminum and Gallium Phosphate are closely related to the low cristobalite structure of SiO_2.
- The change in symmetry from $Fd\bar{3}m$ #227 in SiO_2 to $C222_1$ #20 in $AlPO_4$ is caused by the replacement of the silicon atoms by two types of atoms.

- The structure is "pseudo-tetragonal," with $a = b$, but the presence of ordered aluminum and phosphorous atoms reduces the symmetry to orthogonal.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(4a)	Al I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4b)	P I
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_6}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_7}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_8}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{10}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{11}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8c)	O II

References

[1] R. C. L. Mooney, *The crystal structure of aluminium phosphate and gallium phosphate, low-cristobalite type*, Acta Cryst. **9** (1956), doi:10.1107/S0365110X56001996.

Found in

[1] D. M. Hatch, S. Ghose, and J. L. Bjorkstam, *The $\alpha-$ phase transition in $AlPO_4$ cristobalite: Symmetry analysis, domain structure and transition dynamics*, Phys. Chem. Minerals **21**, 67–77 (1994), doi:10.1007/BF00205217.