Monoclinic tridymite (473K) $AlPO_4$ Structure: AB4C_mP12_4_a_4a_a-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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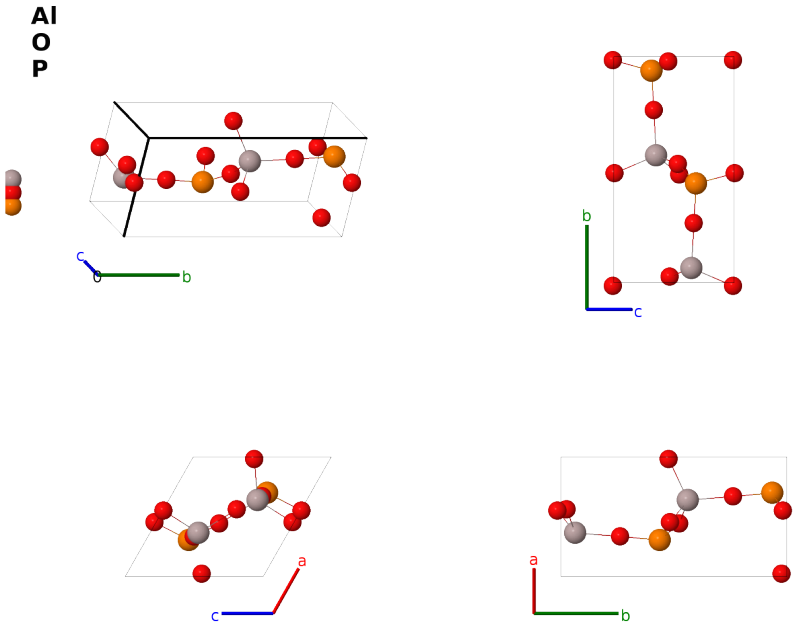
https://aflow.org/prototype-encyclopedia/H7X6

https://aflow.org/prototype-encyclopedia/AB4C_mP12_4_a_4a_a-001

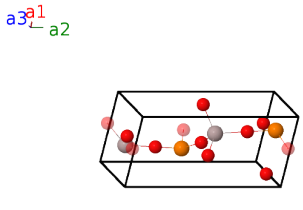


Prototype	AlO_4P
AFLOW prototype label	AB4C_mP12_4_a_4a_a-001
ICSD	280772
CCDC	1721418
Pearson symbol	mP12
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	`aflow --proto=AB4C_mP12_4_a_4a_a-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- The tridymite form of $AlPO_4$ is related to the tridymite forms of SiO_2. Like SiO_2 it undergoes a series of temperature driven phase transitions (Graetsch, 2002):
  - The high temperature form is hexagonal, space group $P6_3mc$ #186 at temperatures above $\approx$ 590K

  - The first intermediate form is monoclinic, space group $P2_1$ #4 at temperatures above $\approx$ 460K (this structure)
  - The second intermediate form, $P2_1(\alpha\beta0)$, is incommensurate but averages to a structure similar to the previous one
  - This is followed by an orthorhombic form, space group $P2_12_12_1$ #19, for which we have no data.
  - Near room temperature we find another monoclinic structure, space group Pc #7
  - The low temperature structure is triclinic, space group $P1$ #1, also measured at room temperature.
- The astute reader will recognize that we are very vague about these phase transitions, as we have found no definitive phase diagram.
- For more information on realted structures see our silica and aluminum phosphate page.
- Data for this structure was taken at 473K, with the associated incommensurate structure measured at 463K.
- (Graetsch, 2002) gave the data in the unique-axis c representation of space group $P2_1$ #4. AFLOW automatically converted this to the standard unique-axis b representation.

Simple Monoclinic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$

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
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\left(ax_1 + cz_1\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(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)	O I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\left(ax_3 + cz_3\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	P I
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	P I

References

[1] H. A. Graetsch, *Monoclinic $AlPO_4$ tridymite at 473 and 463K from X-ray powder data*, Acta Crystallographica C **58**, i18–i20 (2002), doi:10.1107/S0108270101015773.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).