Hexagonal high-temperature tridymite $AlPO_4$: AB4C_hP12_186_b_bc_b-001

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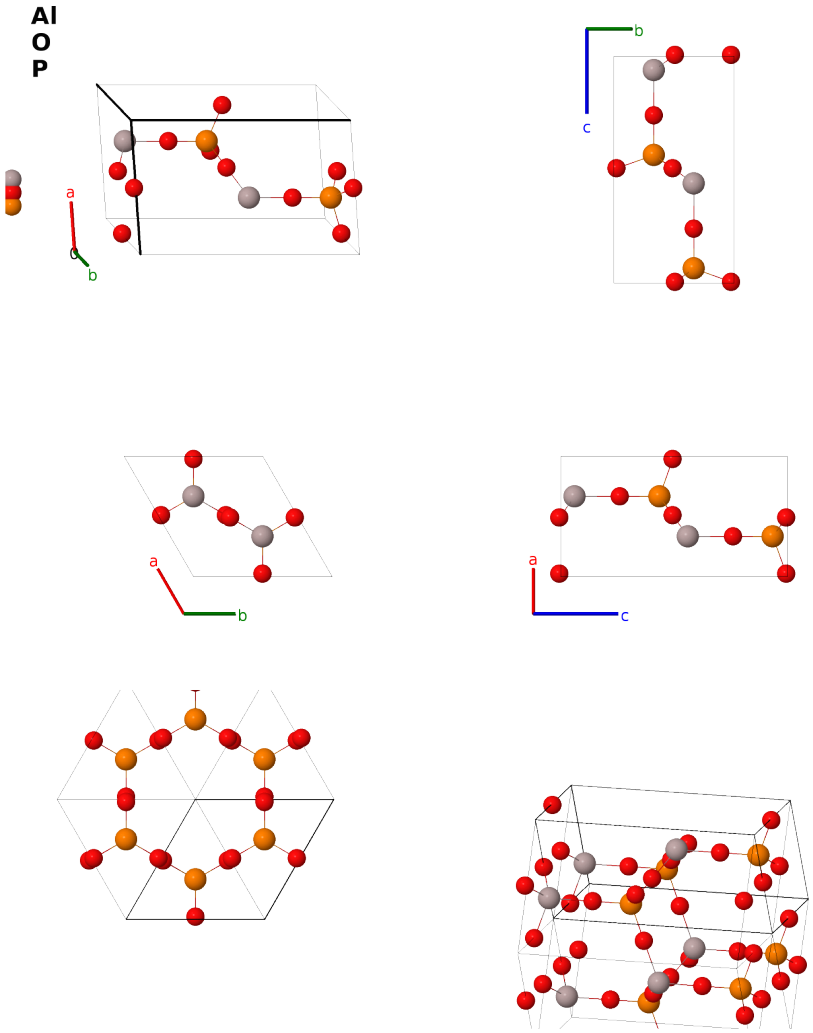
https://aflow.org/prototype-encyclopedia/CVY6

https://aflow.org/prototype-encyclopedia/AB4C_hP12_186_b_bc_b-001



Prototype	AlO_4P
AFLOW prototype label	AB4C_hP12_186_b_bc_b-001
ICSD	279582
CCDC	1720706
Pearson symbol	hP12
Space group number	186

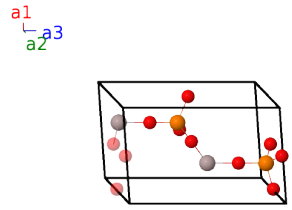
Space group symbol $P6_3mc$

AFLOW prototype command `aflow --proto=AB4C_hP12_186_b_bc_b-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4$

- 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 (this structure)
  - The first intermediate form is monoclinic, space group $P2_1$ #4 at temperatures above $\approx$ 460K
  - The second intermediate form, $P2_1(\alpha\beta0)$ (ICSD 279583), 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.
- (Graetsch, 2001) gives two forms for this structure: one with the O II atoms on the (6c) site, and the second with those atoms partially occupying four (12d) sites near that (6c) site. Since the distance of those atoms is less that 0.5Å from the "averaged" (6c) site we use the first form.
- The ICSD lists $LiBH_4$ as the structure type, but even though both this structure and $LiBH_4$ share the same AFLOW prototype label, AB4C_hP12_186_b_bc_b, the structures are very different and we define them as two independent prototypes.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	P I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	P I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\sqrt{3}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II

$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 + 2x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_9}$	=	$-2x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\sqrt{3}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{11}}$	=	$-x_4\,\mathbf{a}_1 - 2x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II
$\mathbf{B_{12}}$	=	$2x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{3}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(6c)	O II

References

[1] H. A. Graetsch, *Hexagonal high-temperature form of aluminium phosphate tridymite from X-ray powder data*, Acta Crystallogr. Sect. C **57**, 665–667 (2001), doi:10.1107/S0108270101005133.

[2] 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.

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