β (high) Cristobalite $AlPO_4$ Structure: AB12C_cF56_216_a_h_c-001

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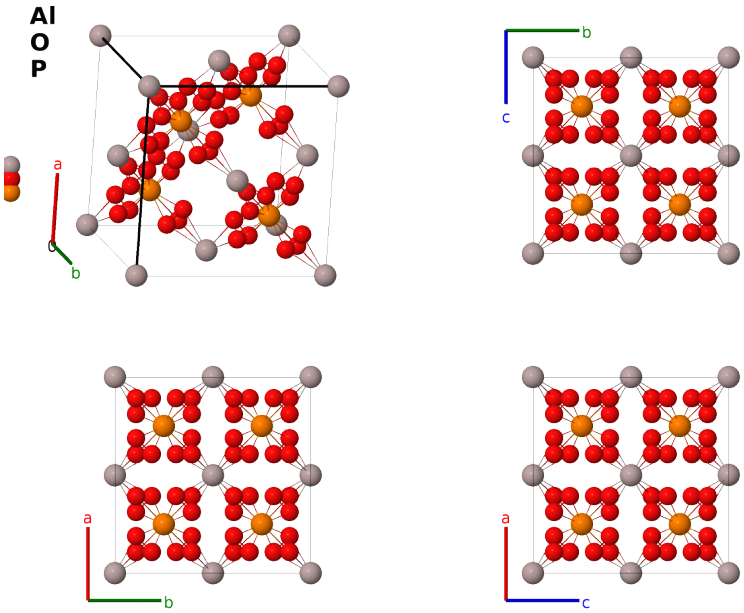
https://aflow.org/prototype-encyclopedia/KWDY

https://aflow.org/prototype-encyclopedia/AB12C_cF56_216_a_h_c-001



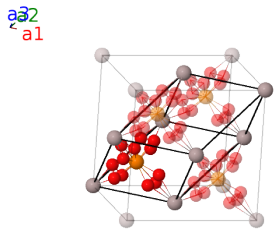
Prototype	AlO_4P
AFLOW prototype label	AB12C_cF56_216_a_h_c-001
ICSD	162669
CCDC	1678996
Pearson symbol	cF56
Space group number	216
Space group symbol	$F\bar{4}3m$
AFLOW prototype command	`aflow --proto=AB12C_cF56_216_a_h_c-001 --params=`a, x_3, z_3

- This is the $AlPO_4$ analog of $C9$ SiO_2 β cristobalite. It transforms to the the orthorhombic α (low) structure at a temperature near 500K (Hatch, 1994).
- The oxygen (48h) sites are only 1/3 filled. If replaced them by an averaged (16e) (x,x,x) site with x $\approx$ 0.136 we would obtain the ideal structure analogous to $C9$ SiO_2, but the Al-O and P-O distances would be slightly too small.

- For more information, see our silica and aluminum phosphate page.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Al I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(4c)	P I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - (2x_3 + z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + az_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_5}$	=	$(2x_3 - z_3)\,\mathbf{a}_1 - (2x_3 + z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_6}$	=	$-(2x_3 + z_3)\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - az_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_7}$	=	$(2x_3 - z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_8}$	=	$-(2x_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_9}$	=	$z_3\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 - (2x_3 + z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_{10}}$	=	$z_3\,\mathbf{a}_1 - (2x_3 + z_3)\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3$	=	$-az_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_{11}}$	=	$z_3\,\mathbf{a}_1 + (2x_3 - z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_{12}}$	=	$z_3\,\mathbf{a}_1 - (2x_3 + z_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_{13}}$	=	$-(2x_3 + z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + (2x_3 - z_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(48h)	O I
$\mathbf{B_{14}}$	=	$(2x_3 - z_3)\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 - (2x_3 + z_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - az_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(48h)	O I

References

[1] B. L. Phillips, J. G. Thompson, Y. Xiao, and R. J. Kirkpatrick, *Constraints on the structure and dynamics of the β-cristobalite polymorphs of SiO_2 and $AlPO_4$ from ^{31}P, ^{27}Al and ^{29}Si NMR spectroscopy to 770 K*, Phys. Chem. Minerals **20**, 341–352 (1993), doi:10.1007/BF00215105.

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