β-Berlinite ($AlPO_4$) Structure: AB4C_hP18_181_c_k_d-001

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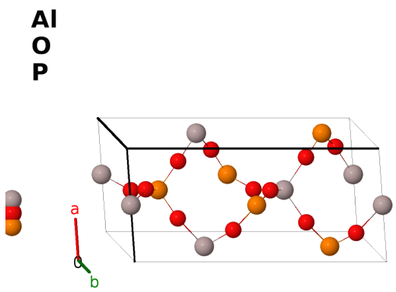
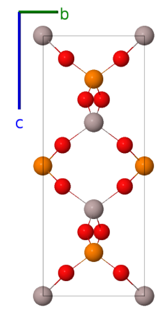
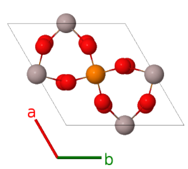
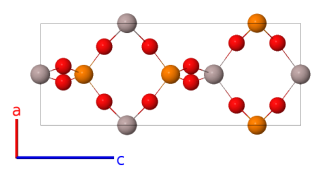
https://aflow.org/prototype-encyclopedia/U1X5

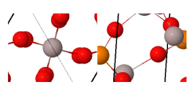
https://aflow.org/prototype-encyclopedia/AB4C_hP18_181_c_k_d-001









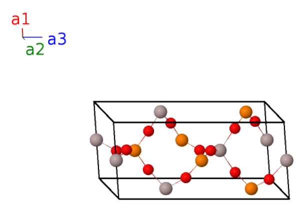


Prototype	AlO_4P
AFLOW prototype label	AB4C_hP18_181_c_k_d-001
Mineral name	berlinite
ICSD	9643
CCDC	1594615
Pearson symbol	hP18
Space group number	181
Space group symbol	$P6_422$
AFLOW prototype command	`aflow --proto=AB4C_hP18_181_c_k_d-001` `--params=`$a, c/a, x_3, y_3, z_3$

- This is the high-temperature form of berlinite, the analog of β-quartz ($C8$).
- Below 853K (Ng, 1976) it transforms into α-berlinite in the alarsite ($AlAsO_4$) structure.
- Our silica and aluminum phosphate page has much more about the relationship between these structures.
- We originally found this structure described in (Muraoka, 1997), but their aluminum and phosphorous coordinates are inconsistent with the Al-O and P-O distances and bond angles, so we use this earlier work.
- Like β-quartz, this structure is chiral, Sohncke Class II, and so may also be found in the enantiomorphic space group $P6_222$ #180.
- (Ng, 1976) put the phosphorous atoms on the (3c) Wyckoff postion, but the AFLOW Wyckoff ordering protocol shifts the origin of the z-axis by c/2, moving the aluminum atoms to the (3c) site.

Hexagonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3c)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3c)	Al I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{2}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(3c)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3d)	P I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(3d)	P I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{6}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3d)	P I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_8}$	=	$-y_3\,\mathbf{a}_1 + (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_9}$	=	$-(x_3-y_3)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{11}}$	=	$y_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 + \left(z_3+\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_3+2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + c\left(z_3+\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{12}}$	=	$(x_3-y_3)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3+\frac{2}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{3}c\,(3z_3+2)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{13}}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - \left(z_3-\frac{1}{3}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3+y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_3-y_3)\,\hat{\mathbf{y}} - c\left(z_3-\frac{1}{3}\right)\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{14}}$	=	$(x_3-y_3)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3-2y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(12k)	O I
$\mathbf{B_{15}}$	=	$-x_3\,\mathbf{a}_1 - (x_3-y_3)\,\mathbf{a}_2 - \left(z_3-\frac{2}{3}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_3-y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - \frac{1}{3}c\,(3z_3-2)\,\hat{\mathbf{z}}$	(12k)	O I

$$\mathbf{B_{16}} = -y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(z_3 - \tfrac{1}{3}\right)\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(x_3 + y_3)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,(x_3 - y_3)\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{3}\right)\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{O I}$$

$$\mathbf{B_{17}} = -\,(x_3 - y_3)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3 = \tfrac{1}{2}a\,(-x_3 + 2y_3)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{O I}$$

$$\mathbf{B_{18}} = x_3\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \tfrac{2}{3}\right)\,\mathbf{a}_3 = \tfrac{1}{2}a\,(2x_3 - y_3)\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} - \tfrac{1}{3}c\,(3z_3 - 2)\,\hat{\mathbf{z}} \qquad \text{(12k)} \qquad \text{O I}$$

References

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