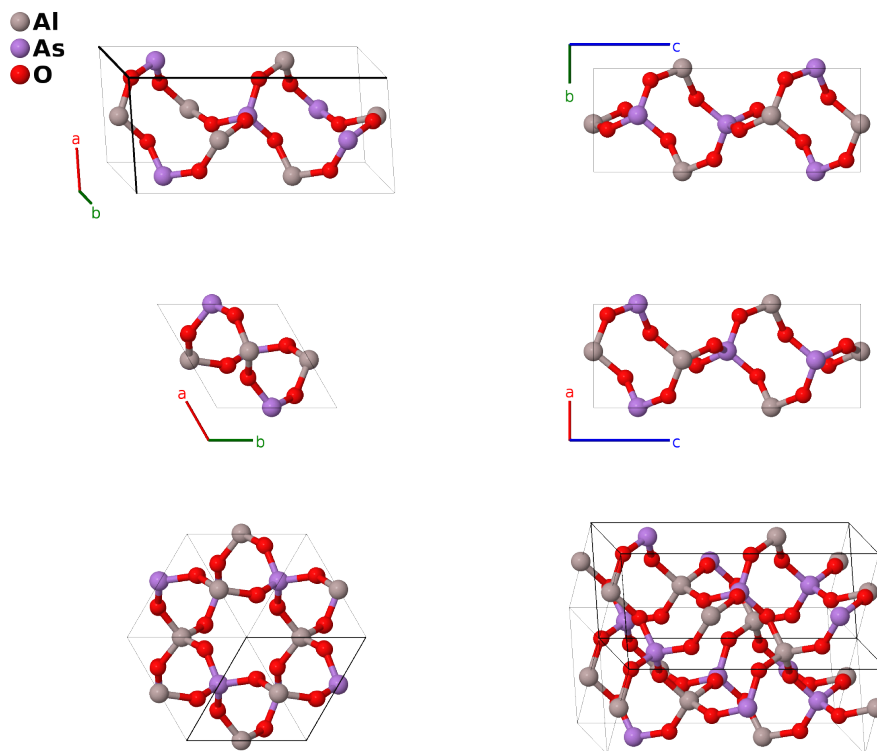


Alarsite (AlAsO₄) Structure: ABC4_hP18_152_a_b_2c-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://afLOW.org/p/P55Q>

https://afLOW.org/p/ABC4_hP18_152_a_b_2c-001



Prototype	AlAsO ₄
AFLOW prototype label	ABC4_hP18_152_a_b_2c-001
Mineral name	alarsite
ICSD	33832
Pearson symbol	hP18
Space group number	152
Space group symbol	<i>P</i> 3 ₁ 21
AFLOW prototype command	<code>afLOW --proto=ABC4_hP18_152_a_b_2c-001 --params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

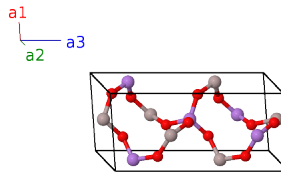
Other compounds with this structure

AlPO₄ (berlinite)

- This structure may also be found in the enantiomorphic space group *P*3₂21 #154.

Trigonal (Hexagonal) primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}$	(3a)	Al I
\mathbf{B}_2	$= x_1 \mathbf{a}_2 + \frac{2}{3} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_1 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1 \hat{\mathbf{y}} + \frac{2}{3}c \hat{\mathbf{z}}$	(3a)	Al I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2$	$=$	$-ax_1 \hat{\mathbf{x}}$	(3a)	Al I
\mathbf{B}_4	$= x_2 \mathbf{a}_1 + \frac{5}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{5}{6}c \hat{\mathbf{z}}$	(3b)	As I
\mathbf{B}_5	$= x_2 \mathbf{a}_2 + \frac{1}{6} \mathbf{a}_3$	$=$	$\frac{1}{2}ax_2 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2 \hat{\mathbf{y}} + \frac{1}{6}c \hat{\mathbf{z}}$	(3b)	As I
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3b)	As I
\mathbf{B}_7	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_8	$= -y_3 \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_9	$= -(x_3 - y_3) \mathbf{a}_1 - x_3 \mathbf{a}_2 + (z_3 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} + \frac{1}{3}c(3z_3 + 2) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{10}	$= y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 + y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_3 - y_3) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{11}	$= (x_3 - y_3) \mathbf{a}_1 - y_3 \mathbf{a}_2 - (z_3 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - 2y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}} - \frac{1}{3}c(3z_3 - 2) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{12}	$= -x_3 \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O I
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{14}	$= -y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{15}	$= -(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2 + (z_4 + \frac{2}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} + \frac{1}{3}c(3z_4 + 2) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{16}	$= y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 + y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a(x_4 - y_4) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{17}	$= (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - (z_4 - \frac{2}{3}) \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}}$	(6c)	O II
\mathbf{B}_{18}	$= -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{3}) \mathbf{a}_3$	$=$	$-\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{3}) \hat{\mathbf{z}}$	(6c)	O II

References

- [1] H. Sowa, *The crystal structure of $AlAsO_4$ at high pressure*, Z. Kristallogr. **304**, 291–304 (1991), doi:10.1524/zkri.1991.194.14.291.

Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).