

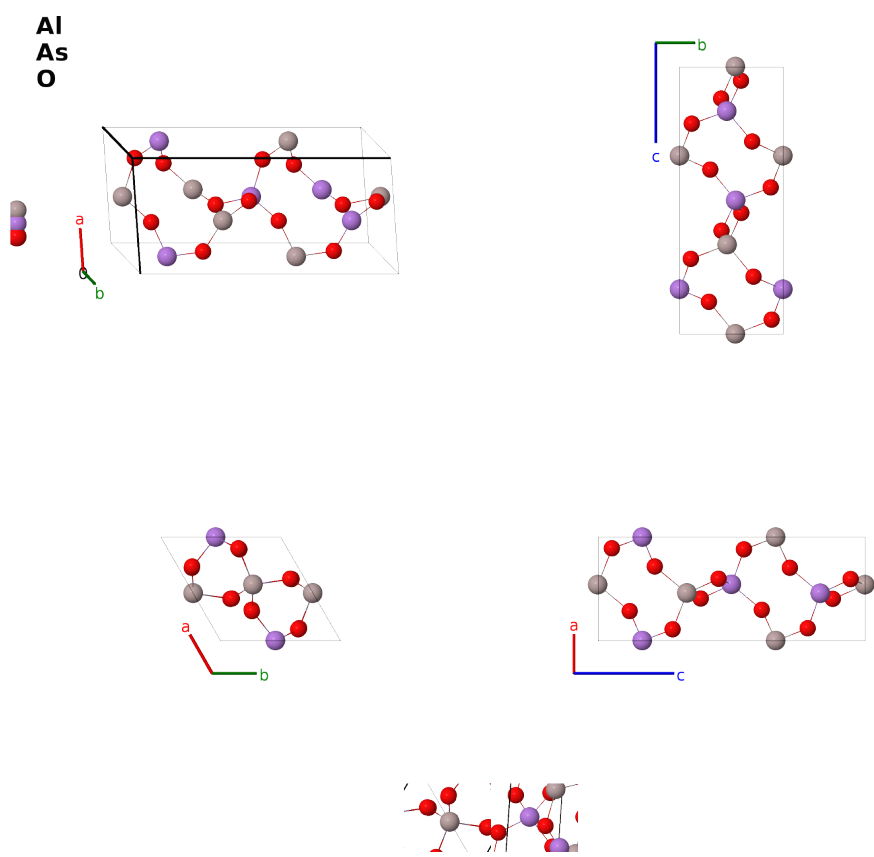
Alarsite (AlAsO₄) Structure: ABC4_hP18_152_a_b_2c-001

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<https://aflow.org/prototype-encyclopedia/P55Q>

https://aflow.org/prototype-encyclopedia/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
CCDC	1606573
Pearson symbol	hP18
Space group number	152
Space group symbol	$P3_121$
AFLOW prototype command	<code>aflow --proto=ABC4_hP18_152_a_b_2c-001</code> <code>--params=a, c/a, x₁, x₂, x₃, y₃, z₃, x₄, y₄, z₄</code>

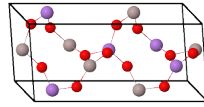
Other compounds with this structure

AlPO₄ (berlinite), AsGaO₄, BLiF₄, BPO₄, FePO₄, GaPO₄

- This structure is chiral, Sohncke Class II, and so may also be found in the enantiomorphic space group $P3_221$ #154.
- The ICSD designates AlPO₄ berlinite as the prototype structure.
- There is a very close relationship between this structure and α -quartz.
- See the silica and aluminum phosphate page for more information on these structures.

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

$$\mathbf{B}_{17} = (x_4 - y_4) \mathbf{a}_1 - y_4 \mathbf{a}_2 - \left(z_4 - \frac{2}{3}\right) \mathbf{a}_3 = \frac{1}{2}a(x_4 - 2y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} - \frac{1}{3}c(3z_4 - 2) \hat{\mathbf{z}} \quad (6c) \quad \text{O II}$$

$$\mathbf{B}_{18} = -x_4 \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - \left(z_4 - \frac{1}{3}\right) \mathbf{a}_3 = -\frac{1}{2}a(2x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{3}\right) \hat{\mathbf{z}} \quad (6c) \quad \text{O II}$$

References

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Found in

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