

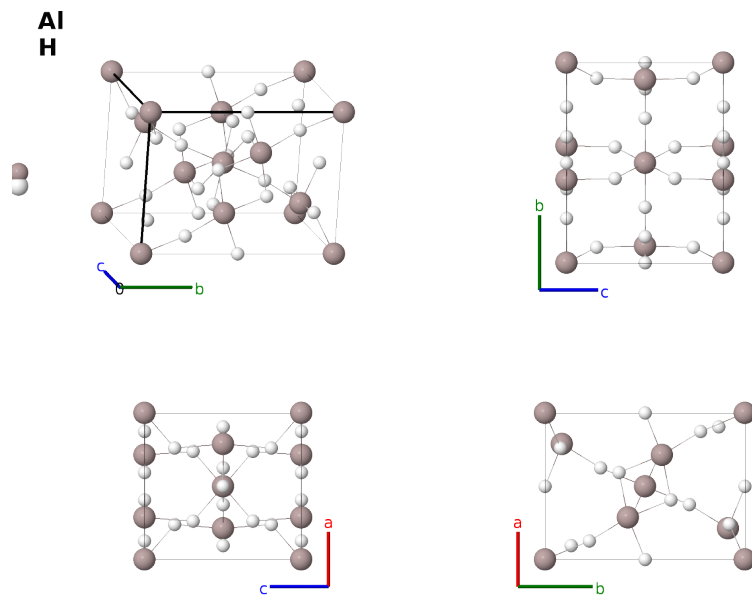
γ -Alane (AlH_3) Structure: AB3_oP24_58_ag_c2gh-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/AB3_oP24_58_ag_c2gh-001



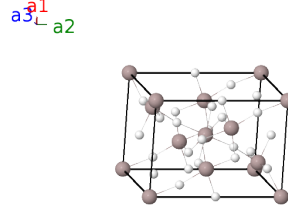
Prototype	AlH_3
AFLOW prototype label	AB3_oP24_58_ag_c2gh-001
Mineral name	γ -alane
ICSD	249407
CCDC	1715636
Pearson symbol	oP24
Space group number	58
Space group symbol	$Pn\bar{m}m$
AFLOW prototype command	<code>aflow --proto=AB3_oP24_58_ag_c2gh-001</code> <code>--params=a,b/a,c/a,x3,y3,x4,y4,x5,y5,x6,y6,z6</code>

- Alane (AlH_3 or AlD_3) comes a variety of polymorphs (Brower, 1976) which can be accessed by using different preparation methods. We will add to this list as we obtain data on more of the crystal structures. Currently we have
 - α -Alane is the ground state, and has the rhombohedral FeF_3 ($D0_{12}$) structure,

- α' -Alane, which takes the body-centered orthorhombic β -AlFe₃ structure.
- β -Alane is cubic,
- orthorhombic γ -Alane (this structure) has two hydrogens bridging some of the aluminum atoms, and
- tetragonal δ -Alane.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Al I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a) Al I
$\mathbf{B}_3$	=	$\frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} b \hat{\mathbf{y}}$	(2c) H I
$\mathbf{B}_4$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2c) H I
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	=	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g) Al II
$\mathbf{B}_6$	=	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g) Al II
$\mathbf{B}_7$	=	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) Al II
$\mathbf{B}_8$	=	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) Al II
$\mathbf{B}_9$	=	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	=	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g) H II
$\mathbf{B}_{10}$	=	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	=	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g) H II
$\mathbf{B}_{11}$	=	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) H II
$\mathbf{B}_{12}$	=	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) H II
$\mathbf{B}_{13}$	=	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	=	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(4g) H III
$\mathbf{B}_{14}$	=	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	=	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(4g) H III
$\mathbf{B}_{15}$	=	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) H III
$\mathbf{B}_{16}$	=	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4g) H III
$\mathbf{B}_{17}$	=	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8h) H IV
$\mathbf{B}_{18}$	=	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(8h) H IV
$\mathbf{B}_{19}$	=	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h) H IV
$\mathbf{B}_{20}$	=	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(8h) H IV
$\mathbf{B}_{21}$	=	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(8h) H IV

$$\mathbf{B}_{22} = x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 = ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}} \quad (8h) \quad \text{H IV}$$

$$\mathbf{B}_{23} = \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_6 + \frac{1}{2} \\ y_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = a \begin{pmatrix} x_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} - b \begin{pmatrix} y_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} x_6 + \frac{1}{2} \\ y_6 - \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} \quad (8h) \quad \text{H IV}$$

$$\mathbf{B}_{24} = - \begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_2 + \begin{pmatrix} x_6 - \frac{1}{2} \\ y_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_3 = -a \begin{pmatrix} x_6 - \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{x}} + b \begin{pmatrix} y_6 + \frac{1}{2} \\ z_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{y}} + c \begin{pmatrix} x_6 - \frac{1}{2} \\ y_6 + \frac{1}{2} \end{pmatrix} \hat{\mathbf{z}} \quad (8h) \quad \text{H IV}$$

References

- [1] V. A. Yartys, R. V. Denys, J. P. Maehlen, C. Frommen, M. Fichtner, B. M. Bulychiev, and H. Emerich, *Double-Bridge Bonding of Aluminium and Hydrogen in the Crystal Structure of γ -AlH₃*, Inorg. Chem. **46**, 1051–1055 (2007), doi:10.1021/ic0617487.
- [2] F. M. Brower, N. E. Matzek, P. F. Reigler, H. W. Rinn, C. B. Roberts, D. L. Schmidt, J. A. Snover, and K. Terada, *Preparation and properties of aluminum hydride*, J. Am. Chem. Soc. **98**, 2450–2453 (1976), doi:10.1021/ja00425a011.

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.