β-Alane (AlD_3) Structure: AB3_cF64_227_c_f-001

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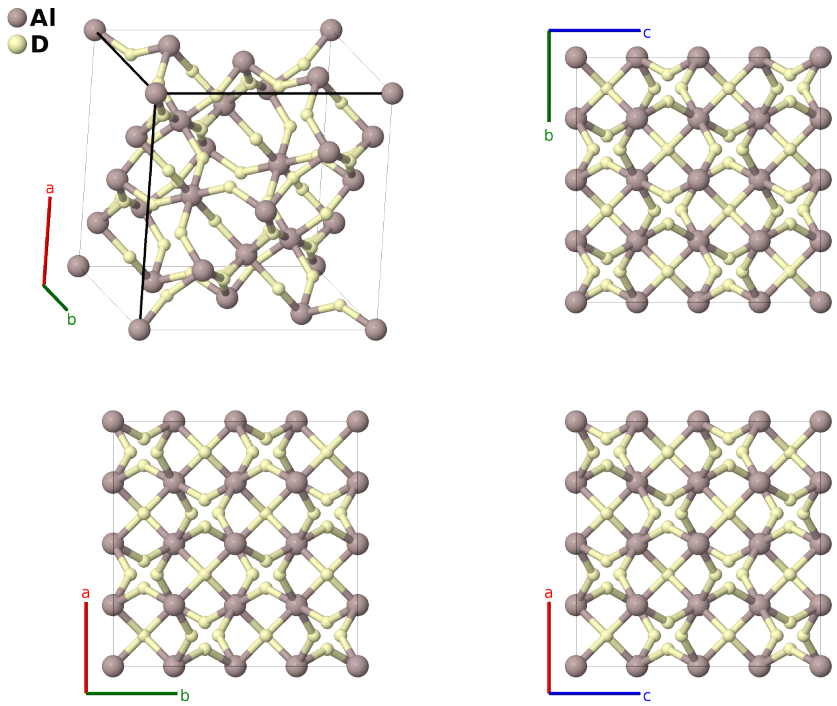
https://aflow.org/p/9LSQ

https://aflow.org/p/AB3_cF64_227_c_f-001



Prototype	AlH_3
AFLOW prototype label	AB3_cF64_227_c_f-001
Mineral name	β-alane
ICSD	156310
Pearson symbol	cF64
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3_cF64_227_c_f-001 --params=`a, x_2

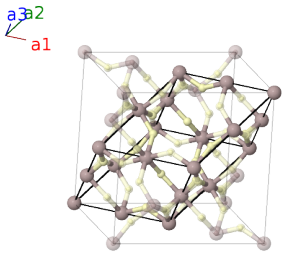
Other compounds with this structure
β-AlH_3, η-AlF_3

- 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-$AlFe_3$ structure.
– β-Alane (this structure) is cubic,
– orthorhombic γ-Alane has two hydrogens bridging some of the aluminum atoms, and
– tetragonal δ-Alane.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(16c)	Al I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(16c)	Al I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(16c)	Al I
$\mathbf{B_5}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_6}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_7}$	=	$x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_8}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{11}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{12}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{15}}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(48f)	D I
$\mathbf{B_{16}}$	=	$\left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(48f)	D I

References

[1] H. W. Brinks, W. Langley, C. M. Jensen, J. Graetz, J. J. Reilly, and B. C. Hauback, *Synthesis and crystal structure of β-AlD_3*, J. Alloys Compd. **433**, 180–183 (2007), doi:10.1016/j.jallcom.2006.06.072.

[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.