Provisional δ-Alane (AlH_3) Structure: AB3_tP64_85_2ceg_2cf5g-001

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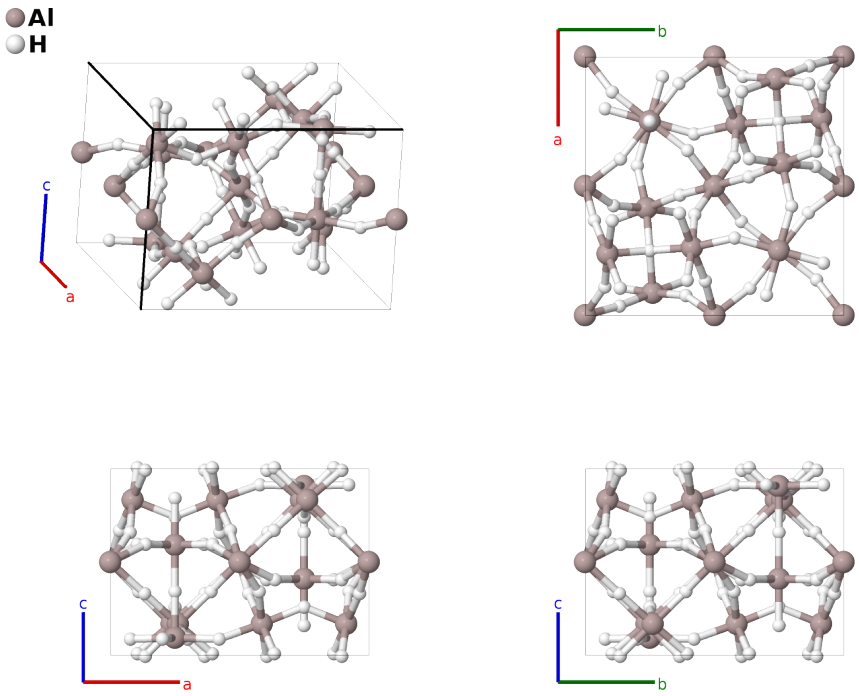
https://aflow.org/p/U4T0

https://aflow.org/p/AB3_tP64_85_2ceg_2cf5g-001



Prototype	AlH_3
AFLOW prototype label	AB3_tP64_85_2ceg_2cf5g-001
Mineral name	δ-alane
ICSD	none
Pearson symbol	tP64
Space group number	85
Space group symbol	$P4/n$
AFLOW prototype command	`aflow --proto=AB3_tP64_85_2ceg_2cf5g-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

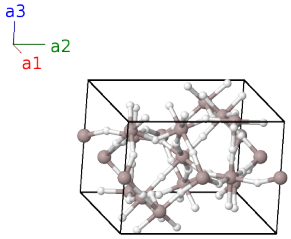
- Alane (AlH_3 or AlD_3) comes a variety of polymorphs (Brower, 1976) which can be accessed by using different preparation methods. We will add to this list as we obtain data on more of the crystal structures. Currently we have
  - α-Alane is the ground state, and has the rhombohedral FeF_3 ($D0_{12}$)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

- α'-Alane, which takes the body-centered orthorhombic β-$AlFe_3$ structure.
- β-Alane is cubic,
- orthorhombic γ-Alane has two hydrogens bridging some of the aluminum atoms, and
- tetragonal δ-Alane (this structure).

- We have not found experimental data for δ-alane, and hence no ICSD entry. (Sun, 2009) used first-principles calculations to find the current structure, stating "that x-ray powder-diffraction patterns [give] simulated main-peak positions for AlH_3 [in] good agreement with experimental (Bower, 1976) δ-AlH_3." Since (Bower, 1976) did not extract a crystal structure from their data and we do not have any other confirmation that this is the correct structure we will list this as a "provisional" structure.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(2c)	Al I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	H I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	H I
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	H II
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2c)	H II
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	Al III
$\mathbf{B_{13}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4f)	H III
$\mathbf{B_{14}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4f)	H III
$\mathbf{B_{15}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4f)	H III
$\mathbf{B_{16}}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(4f)	H III
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B_{18}}$	=	$-\left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B_{19}}$	=	$-\left(y_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-a\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B_{20}}$	=	$y_7\,\mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8g)	Al IV

$$
\begin{array}{lcccccc}
\mathbf{B_{21}} & = & -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 & = & -ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} & (8g) & \text{Al IV} \\
\mathbf{B_{22}} & = & \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 & = & a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} & (8g) & \text{Al IV} \\
\mathbf{B_{23}} & = & \left(y_7+\tfrac{1}{2}\right)\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 & = & a\left(y_7+\tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} & (8g) & \text{Al IV} \\
\mathbf{B_{24}} & = & -y_7\,\mathbf{a}_1 + \left(x_7+\tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 & = & -ay_7\,\hat{\mathbf{x}} + a\left(x_7+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} & (8g) & \text{Al IV} \\
\mathbf{B_{25}} & = & x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{26}} & = & -\left(x_8-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_8-\tfrac{1}{2}\right)\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & -a\left(x_8-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_8-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{27}} & = & -\left(y_8-\tfrac{1}{2}\right)\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & -a\left(y_8-\tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{28}} & = & y_8\,\mathbf{a}_1 - \left(x_8-\tfrac{1}{2}\right)\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & ay_8\,\hat{\mathbf{x}} - a\left(x_8-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{29}} & = & -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 & = & -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{30}} & = & \left(x_8+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8+\tfrac{1}{2}\right)\mathbf{a}_2 - z_8\,\mathbf{a}_3 & = & a\left(x_8+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_8+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{31}} & = & \left(y_8+\tfrac{1}{2}\right)\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 & = & a\left(y_8+\tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{32}} & = & -y_8\,\mathbf{a}_1 + \left(x_8+\tfrac{1}{2}\right)\mathbf{a}_2 - z_8\,\mathbf{a}_3 & = & -ay_8\,\hat{\mathbf{x}} + a\left(x_8+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} & (8g) & \text{H IV} \\
\mathbf{B_{33}} & = & x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{34}} & = & -\left(x_9-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9-\tfrac{1}{2}\right)\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & -a\left(x_9-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_9-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{35}} & = & -\left(y_9-\tfrac{1}{2}\right)\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & -a\left(y_9-\tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{36}} & = & y_9\,\mathbf{a}_1 - \left(x_9-\tfrac{1}{2}\right)\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & ay_9\,\hat{\mathbf{x}} - a\left(x_9-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{37}} & = & -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 & = & -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{38}} & = & \left(x_9+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9+\tfrac{1}{2}\right)\mathbf{a}_2 - z_9\,\mathbf{a}_3 & = & a\left(x_9+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_9+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{39}} & = & \left(y_9+\tfrac{1}{2}\right)\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 & = & a\left(y_9+\tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{40}} & = & -y_9\,\mathbf{a}_1 + \left(x_9+\tfrac{1}{2}\right)\mathbf{a}_2 - z_9\,\mathbf{a}_3 & = & -ay_9\,\hat{\mathbf{x}} + a\left(x_9+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} & (8g) & \text{H V} \\
\mathbf{B_{41}} & = & x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} + ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{42}} & = & -\left(x_{10}-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{10}-\tfrac{1}{2}\right)\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & -a\left(x_{10}-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_{10}-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{43}} & = & -\left(y_{10}-\tfrac{1}{2}\right)\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & -a\left(y_{10}-\tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{44}} & = & y_{10}\,\mathbf{a}_1 - \left(x_{10}-\tfrac{1}{2}\right)\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & ay_{10}\,\hat{\mathbf{x}} - a\left(x_{10}-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{45}} & = & -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} - ay_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{46}} & = & \left(x_{10}+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{10}+\tfrac{1}{2}\right)\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & a\left(x_{10}+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_{10}+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{47}} & = & \left(y_{10}+\tfrac{1}{2}\right)\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & a\left(y_{10}+\tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{48}} & = & -y_{10}\,\mathbf{a}_1 + \left(x_{10}+\tfrac{1}{2}\right)\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & -ay_{10}\,\hat{\mathbf{x}} + a\left(x_{10}+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & (8g) & \text{H VI} \\
\mathbf{B_{49}} & = & x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}} + ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{50}} & = & -\left(x_{11}-\tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_{11}-\tfrac{1}{2}\right)\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & -a\left(x_{11}-\tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_{11}-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{51}} & = & -\left(y_{11}-\tfrac{1}{2}\right)\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & -a\left(y_{11}-\tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{52}} & = & y_{11}\,\mathbf{a}_1 - \left(x_{11}-\tfrac{1}{2}\right)\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & ay_{11}\,\hat{\mathbf{x}} - a\left(x_{11}-\tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{53}} & = & -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}} - ay_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{54}} & = & \left(x_{11}+\tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_{11}+\tfrac{1}{2}\right)\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & a\left(x_{11}+\tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_{11}+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{55}} & = & \left(y_{11}+\tfrac{1}{2}\right)\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & a\left(y_{11}+\tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{56}} & = & -y_{11}\,\mathbf{a}_1 + \left(x_{11}+\tfrac{1}{2}\right)\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & -ay_{11}\,\hat{\mathbf{x}} + a\left(x_{11}+\tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} & (8g) & \text{H VII} \\
\mathbf{B_{57}} & = & x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 & = & ax_{12}\,\hat{\mathbf{x}} + ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} & (8g) & \text{H VIII}
\end{array}
$$

$\mathbf{B_{58}}$	=	$-\left(x_{12}-\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_{12}-\frac{1}{2}\right)\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$-a\left(x_{12}-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(y_{12}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII
$\mathbf{B_{59}}$	=	$-\left(y_{12}-\frac{1}{2}\right)\,\mathbf{a}_1+x_{12}\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$-a\left(y_{12}-\frac{1}{2}\right)\,\hat{\mathbf{x}}+ax_{12}\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII
$\mathbf{B_{60}}$	=	$y_{12}\,\mathbf{a}_1-\left(x_{12}-\frac{1}{2}\right)\,\mathbf{a}_2+z_{12}\,\mathbf{a}_3$	=	$ay_{12}\,\hat{\mathbf{x}}-a\left(x_{12}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII
$\mathbf{B_{61}}$	=	$-x_{12}\,\mathbf{a}_1-y_{12}\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$-ax_{12}\,\hat{\mathbf{x}}-ay_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII
$\mathbf{B_{62}}$	=	$\left(x_{12}+\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_{12}+\frac{1}{2}\right)\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$a\left(x_{12}+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(y_{12}+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII
$\mathbf{B_{63}}$	=	$\left(y_{12}+\frac{1}{2}\right)\,\mathbf{a}_1-x_{12}\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$a\left(y_{12}+\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_{12}\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII
$\mathbf{B_{64}}$	=	$-y_{12}\,\mathbf{a}_1+\left(x_{12}+\frac{1}{2}\right)\,\mathbf{a}_2-z_{12}\,\mathbf{a}_3$	=	$-ay_{12}\,\hat{\mathbf{x}}+a\left(x_{12}+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_{12}\,\hat{\mathbf{z}}$	(8g)	H VIII

References

[1] S. Sun, X. Ke, C. Chen, and I. Tanaka, *First-principles prediction of low-energy structures for AlH_3*, Phys. Rev. B **79**, 024104 (2009), doi:10.1103/PhysRevB.79.024104.

[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.