

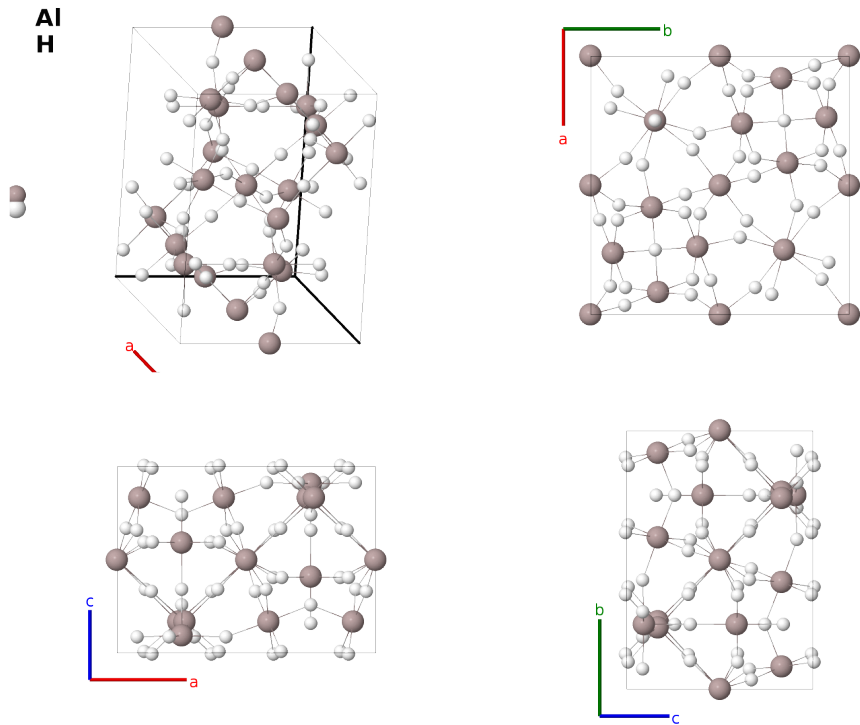
Provisional δ -Alane (AlH_3) Structure: AB3_tP64_85_2ceg_2cf5g-001

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- 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/U4T0>

https://aflow.org/prototype-encyclopedia/AB3_tP64_85_2ceg_2cf5g-001



Prototype	AlH_3
AFLOW prototype label	AB3_tP64_85_2ceg_2cf5g-001
Mineral name	δ -alane
Pearson symbol	tP64
Space group number	85
Space group symbol	$P4/n$
AFLOW prototype command	<pre>aflow --proto=AB3_tP64_85_2ceg_2cf5g-001 --params=a, c/a, z1, z2, z3, z4, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12</pre>

- 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

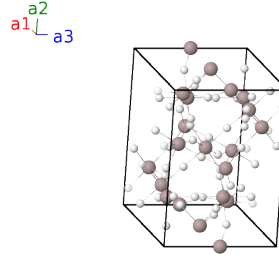
- α -Alane is the ground state, and has the rhombohedral FeF_3 ($D0_{12}$) structure,
 - α' -Alane, which takes the body-centered orthorhombic $\beta\text{-AlFe}_3$ structure.
 - β -Alane is cubic,
 - orthorhombic γ -Alane has two hydrogens bridging some of the aluminum atoms, and
 - tetragonal δ -Alane (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) $\delta\text{-AlH}_3$.” 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

$\mathbf{B}_{19} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B}_{20} =$	$y_7 \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B}_{21} =$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B}_{22} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B}_{23} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	Al IV
$\mathbf{B}_{24} =$	$-y_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(8g)	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)	H IV
$\mathbf{B}_{26} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	H IV
$\mathbf{B}_{27} =$	$-(y_8 - \frac{1}{2}) \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	H IV
$\mathbf{B}_{28} =$	$y_8 \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8g)	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)	H IV
$\mathbf{B}_{30} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	H IV
$\mathbf{B}_{31} =$	$(y_8 + \frac{1}{2}) \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	H IV
$\mathbf{B}_{32} =$	$-y_8 \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8g)	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)	H V
$\mathbf{B}_{34} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	H V
$\mathbf{B}_{35} =$	$-(y_9 - \frac{1}{2}) \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} + ax_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	H V
$\mathbf{B}_{36} =$	$y_9 \mathbf{a}_1 - (x_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} - a(x_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8g)	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)	H V
$\mathbf{B}_{38} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	H V
$\mathbf{B}_{39} =$	$(y_9 + \frac{1}{2}) \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(y_9 + \frac{1}{2}) \hat{\mathbf{x}} - ax_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	H V
$\mathbf{B}_{40} =$	$-y_9 \mathbf{a}_1 + (x_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + a(x_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8g)	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)	H VI
$\mathbf{B}_{42} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	H VI
$\mathbf{B}_{43} =$	$-(y_{10} - \frac{1}{2}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(y_{10} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	H VI
$\mathbf{B}_{44} =$	$y_{10} \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ay_{10} \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8g)	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)	H VI
$\mathbf{B}_{46} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	H VI
$\mathbf{B}_{47} =$	$(y_{10} + \frac{1}{2}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(y_{10} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	H VI
$\mathbf{B}_{48} =$	$-y_{10} \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ay_{10} \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8g)	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)	H VII
$\mathbf{B}_{50} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	H VII
$\mathbf{B}_{51} =$	$-(y_{11} - \frac{1}{2}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-a(y_{11} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	H VII
$\mathbf{B}_{52} =$	$y_{11} \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ay_{11} \hat{\mathbf{x}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(8g)	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)	H VII
$\mathbf{B}_{54} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8g)	H VII
$\mathbf{B}_{55} =$	$(y_{11} + \frac{1}{2}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(y_{11} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(8g)	H VII

$$\begin{aligned}
\mathbf{B}_{56} &= -y_{11} \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= -ay_{11} \hat{\mathbf{x}} + a \left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(8g) &\quad \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) &\quad \text{H VIII} \\
\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) &\quad \text{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) &\quad \text{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) &\quad \text{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) &\quad \text{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) &\quad \text{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) &\quad \text{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) &\quad \text{H VIII}
\end{aligned}$$

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