

θ -AlF₃ Structure:

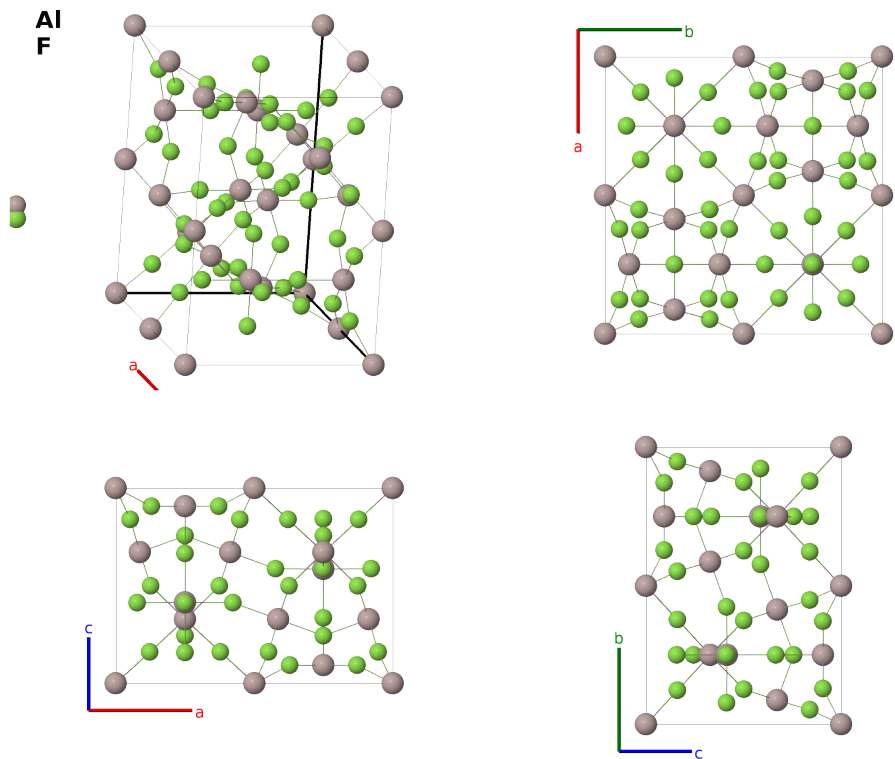
AB3_tP64_129_2cdi_2cfhijk-001

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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/HQ3Z>

https://aflow.org/prototype-encyclopedia/AB3_tP64_129_2cdi_2cfhijk-001



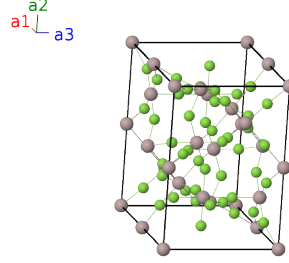
Prototype	AlF ₃
AFLOW prototype label	AB3_tP64_129_2cdi_2cfhijk-001
ICSD	79814
CCDC	1640049
Pearson symbol	tP64
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	<pre>aflow --proto=AB3_tP64_129_2cdi_2cfhijk-001 --params=a, c/a, z₁, z₂, z₃, z₄, z₆, x₇, y₈, z₈, y₉, z₉, x₁₀, z₁₀, x₁₁, y₁₁, z₁₁</pre>

- AlF₃ has a variety of polymorphs (Le Bail, 2006) including:

- α -AlF₃, which takes the rhombohedral FeF₃ ($D0_{12}$) structure.
- β -AlF₃ has a body-centered orthorhombic structure.
- η -AlF₃ has the β -AlH₃ structure.
- κ -AlF₃ is tetragonal structure.
- θ -AlF₃ (this structure), also known as τ -AlF₃, is a larger tetragonal structure.
- Above 713K AlF₃ transforms into the cubic ReO₃ ($D0_9$) structure (Morelock, 2014).

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(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)	F 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)	F 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)	F 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)	F II
$\mathbf{B}_9$	$= 0$	$=$	0	(4d)	Al III
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}$	(4d)	Al III
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2}a \hat{\mathbf{x}}$	(4d)	Al III
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{y}}$	(4d)	Al III
$\mathbf{B}_{13}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	F III
$\mathbf{B}_{14}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	F III
$\mathbf{B}_{15}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	F III
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	F III
$\mathbf{B}_{17}$	$= x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{18}$	$= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_7 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{19}$	$= \left(x_7 + \frac{1}{2}\right) \mathbf{a}_1 + x_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a\left(x_7 + \frac{1}{2}\right) \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{20}$	$= -x_7 \mathbf{a}_1 - \left(x_7 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} - a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{21}$	$= -x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	F IV

$\mathbf{B}_{22} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{23} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{24} =$	$x_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B}_{25} =$	$\frac{1}{4} \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{26} =$	$\frac{1}{4} \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{27} =$	$-(y_8 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{28} =$	$y_8 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ay_8 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{29} =$	$\frac{3}{4} \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{30} =$	$\frac{3}{4} \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{31} =$	$(y_8 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{32} =$	$-y_8 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-ay_8 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(8i)	Al IV
$\mathbf{B}_{33} =$	$\frac{1}{4} \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{34} =$	$\frac{1}{4} \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{35} =$	$-(y_9 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$-a(y_9 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{36} =$	$y_9 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ay_9 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{37} =$	$\frac{3}{4} \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{38} =$	$\frac{3}{4} \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{39} =$	$(y_9 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(y_9 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{40} =$	$-y_9 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-ay_9 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(8i)	F V
$\mathbf{B}_{41} =$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{42} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{43} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{44} =$	$x_{10} \mathbf{a}_1 - (x_{10} - \frac{1}{2}) \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} - a(x_{10} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{45} =$	$-x_{10} \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{46} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{47} =$	$(x_{10} + \frac{1}{2}) \mathbf{a}_1 + (x_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} + a(x_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{48} =$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-ax_{10} \hat{\mathbf{x}} - ax_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(8j)	F VI
$\mathbf{B}_{49} =$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ax_{11} \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{50} =$	$-(x_{11} - \frac{1}{2}) \mathbf{a}_1 - (y_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-a(x_{11} - \frac{1}{2}) \hat{\mathbf{x}} - a(y_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{51} =$	$-(y_{11} - \frac{1}{2}) \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$-a(y_{11} - \frac{1}{2}) \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{52} =$	$y_{11} \mathbf{a}_1 - (x_{11} - \frac{1}{2}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$ay_{11} \hat{\mathbf{x}} - a(x_{11} - \frac{1}{2}) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{53} =$	$-x_{11} \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} + a(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{54} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{55} =$	$(y_{11} + \frac{1}{2}) \mathbf{a}_1 + (x_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(y_{11} + \frac{1}{2}) \hat{\mathbf{x}} + a(x_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{56} =$	$-y_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ay_{11} \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{57} =$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-ax_{11} \hat{\mathbf{x}} - ay_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{58} =$	$(x_{11} + \frac{1}{2}) \mathbf{a}_1 + (y_{11} + \frac{1}{2}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(x_{11} + \frac{1}{2}) \hat{\mathbf{x}} + a(y_{11} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B}_{59} =$	$(y_{11} + \frac{1}{2}) \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$a(y_{11} + \frac{1}{2}) \hat{\mathbf{x}} - ax_{11} \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}}$	(16k)	F VII

$$\begin{aligned}
\mathbf{B}_{60} &= -y_{11} \mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right) \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= -ay_{11} \hat{\mathbf{x}} + a \left(x_{11} + \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{11} \hat{\mathbf{z}} &(16k) &\text{F VII} \\
\mathbf{B}_{61} &= x_{11} \mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right) \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= ax_{11} \hat{\mathbf{x}} - a \left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(16k) &\text{F VII} \\
\mathbf{B}_{62} &= -\left(x_{11} - \frac{1}{2}\right) \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= -a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} + ay_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(16k) &\text{F VII} \\
\mathbf{B}_{63} &= -\left(y_{11} - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_{11} - \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(y_{11} - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_{11} - \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(16k) &\text{F VII} \\
&\quad z_{11} \mathbf{a}_3 \\
\mathbf{B}_{64} &= y_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3 &= ay_{11} \hat{\mathbf{x}} + ax_{11} \hat{\mathbf{y}} + cz_{11} \hat{\mathbf{z}} &(16k) &\text{F VII}
\end{aligned}$$

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