θ-AlF_3 Structure: AB3_tP64_129_2cdi_2cfhijk-001

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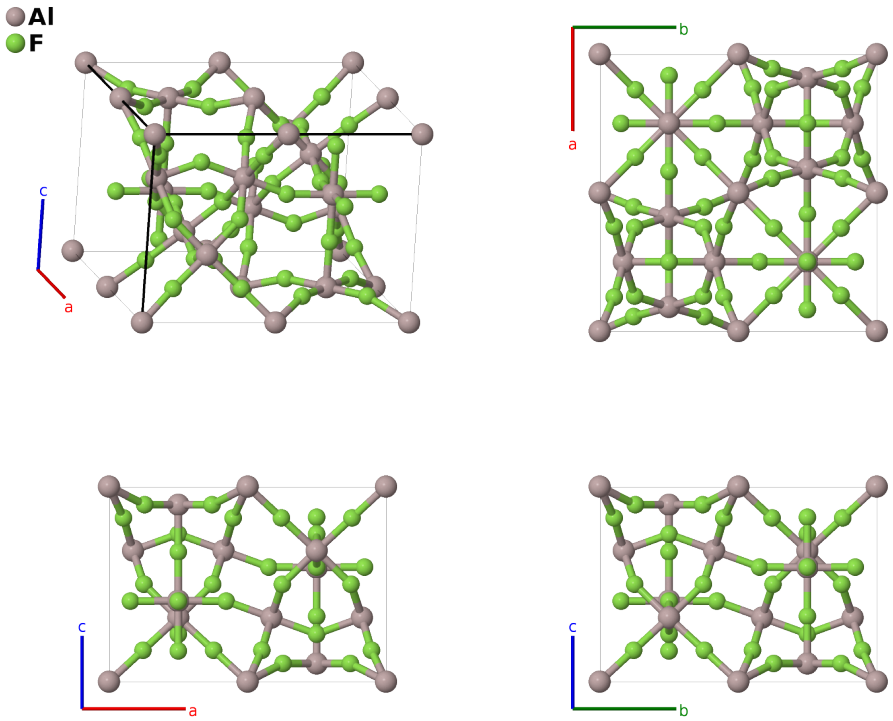
https://aflow.org/p/HQ3Z

https://aflow.org/p/AB3_tP64_129_2cdi_2cfhijk-001



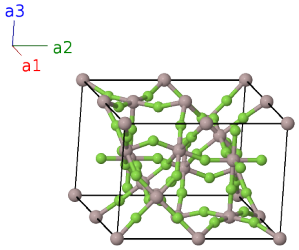
Prototype	AlF_3
AFLOW prototype label	AB3_tP64_129_2cdi_2cfhijk-001
ICSD	79814
Pearson symbol	tP64
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=AB3_tP64_129_2cdi_2cfhijk-001 --params=`$a, c/a, z_1, z_2, z_3, z_4, z_6, x_7, y_8, z_8, y_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}$

- AlF_3 has a variety of polymorphs (Le Bail, 2006) including:
  - α-AlF_3, which takes the rhombohedral FeF_3 ($D0_{12}$) structure.
  - β-AlF_3 has a body-centered orthorhombic structure.
  - η-AlF_3 has the β-AlH_3 structure.

– κ-AlF_3 is tetragonal structure.
– θ-AlF_3 (this structure), also known as τ-AlF_3, is a larger tetragonal structure.
– Above 713K AlF_3 transforms into the cubic ReO_3 ($D0_9$) 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
$\mathbf{B_{22}}$	=	$\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B_{23}}$	=	$-\left(x_7-\frac{1}{2}\right)\,\mathbf{a}_1-x_7\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_7-\frac{1}{2}\right)\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B_{24}}$	=	$x_7\,\mathbf{a}_1+\left(x_7+\frac{1}{2}\right)\,\mathbf{a}_2+\frac{1}{2}\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+a\left(x_7+\frac{1}{2}\right)\,\hat{\mathbf{y}}+\frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	F IV
$\mathbf{B_{25}}$	=	$\frac{1}{4}\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(8i)	Al IV

$$
\begin{array}{lcccccc}
\mathbf{B_{26}} & = & \frac{1}{4}\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & \frac{1}{4}a\,\hat{\mathbf{x}} - a\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & \text{(8i)} & \text{Al IV} \\
\mathbf{B_{27}} & = & -\left(y_8 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 & = & -a\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{Al IV} \\
\mathbf{B_{29}} & = & \frac{3}{4}\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 & = & \frac{3}{4}a\,\hat{\mathbf{x}} + a\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{Al IV} \\
\mathbf{B_{31}} & = & \left(y_8 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 & = & a\left(y_8 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{F V} \\
\mathbf{B_{34}} & = & \frac{1}{4}\,\mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & \frac{1}{4}a\,\hat{\mathbf{x}} - a\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & \text{(8i)} & \text{F V} \\
\mathbf{B_{35}} & = & -\left(y_9 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 & = & -a\left(y_9 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{F V} \\
\mathbf{B_{37}} & = & \frac{3}{4}\,\mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 & = & \frac{3}{4}a\,\hat{\mathbf{x}} + a\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{F V} \\
\mathbf{B_{39}} & = & \left(y_9 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 & = & a\left(y_9 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} & \text{(8i)} & \text{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}} & \text{(8i)} & \text{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}} & \text{(8j)} & \text{F VI} \\
\mathbf{B_{42}} & = & -\left(x_{10} - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right)\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & -a\left(x_{10} - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_{10} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & \text{(8j)} & \text{F VI} \\
\mathbf{B_{43}} & = & -\left(x_{10} - \frac{1}{2}\right)\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & -a\left(x_{10} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & \text{(8j)} & \text{F VI} \\
\mathbf{B_{44}} & = & x_{10}\,\mathbf{a}_1 - \left(x_{10} - \frac{1}{2}\right)\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} - a\left(x_{10} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & \text{(8j)} & \text{F VI} \\
\mathbf{B_{45}} & = & -x_{10}\,\mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} + a\left(x_{10} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & \text{(8j)} & \text{F VI} \\
\mathbf{B_{46}} & = & \left(x_{10} + \frac{1}{2}\right)\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & a\left(x_{10} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & \text{(8j)} & \text{F VI} \\
\mathbf{B_{47}} & = & \left(x_{10} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_{10} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 & = & a\left(x_{10} + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_{10} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}} & \text{(8j)} & \text{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}} & \text{(8j)} & \text{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}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{50}} & = & -\left(x_{11} - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_{11} - \frac{1}{2}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & -a\left(x_{11} - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_{11} - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{51}} & = & -\left(y_{11} - \frac{1}{2}\right)\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & -a\left(y_{11} - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{52}} & = & 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}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{53}} & = & -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}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{54}} & = & \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}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{55}} & = & \left(y_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_{11} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & 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}} & \text{(16k)} & \text{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}} & \text{(16k)} & \text{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}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{58}} & = & \left(x_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_{11} + \frac{1}{2}\right)\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & a\left(x_{11} + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_{11} + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} & \text{(16k)} & \text{F VII} \\
\mathbf{B_{59}} & = & \left(y_{11} + \frac{1}{2}\right)\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 & = & a\left(y_{11} + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} - cz_{11}\,\hat{\mathbf{z}} & \text{(16k)} & \text{F VII} \\
\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}} & \text{(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}} & \text{(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}} & \text{(16k)} & \text{F VII}
\end{array}
$$

$\mathbf{B_{63}}$	=	$-\left(y_{11}-\frac{1}{2}\right)\,\mathbf{a}_1-\left(x_{11}-\frac{1}{2}\right)\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$-a\left(y_{11}-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_{11}-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(16k)	F VII
$\mathbf{B_{64}}$	=	$y_{11}\,\mathbf{a}_1+x_{11}\,\mathbf{a}_2+z_{11}\,\mathbf{a}_3$	=	$ay_{11}\,\hat{\mathbf{x}}+ax_{11}\,\hat{\mathbf{y}}+cz_{11}\,\hat{\mathbf{z}}$	(16k)	F VII

References

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