Predicted Li_3AlP_2 Structure: AB3C2_oI96_73_f_3f_acde-001

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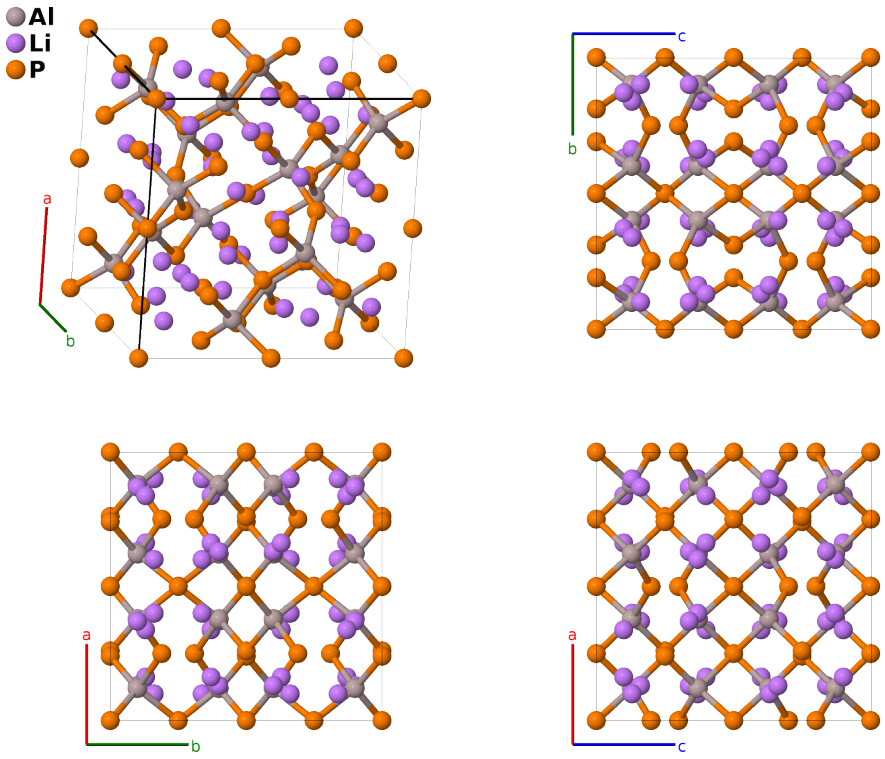
https://aflow.org/p/QKN5

https://aflow.org/p/AB3C2_oI96_73_f_3f_acde-001



Prototype	$AlLi_3P_2$
AFLOW prototype label	AB3C2_oI96_73_f_3f_acde-001
ICSD	186820
Pearson symbol	oI96
Space group number	73
Space group symbol	*Ibca*
AFLOW prototype command	`aflow --proto=AB3C2_oI96_73_f_3f_acde-001 --params=`$a, b/a, c/a, x_2, y_3, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

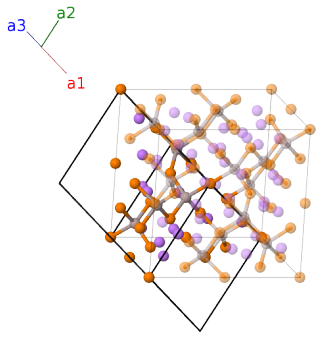
Other compounds with this structure
Li_3AlAs_2, Li_3Ga_2

- The first experimental information we have for this structure is from (Juza, 1952), who placed the system in space group *Ibca* #71 bu could not locate the lithium atoms, except to note that they are on a (16f) site.

- (Dadsetani, 2011) used this work as the starting point for first-principles calculations to minimize the total energy of the structure, including the positions of the lithium atoms, keeping the structure in space group *Ibca*, shown here.
- (Restle, 2020) used ball milling and annealing to produce samples of Li_3AlP_2 and Li_3GaP_2 and found them to be in space group *Cmce* #64. While we believe that this work is correct, we present both structures.
- (Dadsetani, 2011) only gave one (16f) position for the lithium atoms, so we generated the other two sets by taking $x \to y \to z \to x$.
- ICSD entry 186820 is no longer in the database. This suggests that this structure was withdrawn, but we have no confirmation of that.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(8a)	P I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(8a)	P I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(8a)	P I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(8a)	P I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	P II
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	P II
$\mathbf{B_7}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{3}{4}\right)\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8c)	P II
$\mathbf{B_8}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{3}{4}\right)\,\mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8c)	P II
$\mathbf{B_9}$	=	$y_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(8d)	P III
$\mathbf{B_{10}}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	P III
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}}$	(8d)	P III
$\mathbf{B_{12}}$	=	$\left(y_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8d)	P III
$\mathbf{B_{13}}$	=	$\left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_4\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8e)	P IV
$\mathbf{B_{14}}$	=	$-\left(z_4 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8e)	P IV
$\mathbf{B_{15}}$	=	$-\left(z_4 - \frac{3}{4}\right)\,\mathbf{a}_1 - z_4\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}b\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8e)	P IV
$\mathbf{B_{16}}$	=	$\left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8e)	P IV
$\mathbf{B_{17}}$	=	$(y_5 + z_5)\,\mathbf{a}_1 + (x_5 + z_5)\,\mathbf{a}_2 + (x_5 + y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16f)	Al I
$\mathbf{B_{18}}$	=	$\left(-y_5 + z_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_5 - z_5)\,\mathbf{a}_2 - \left(x_5 + y_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(16f)	Al I

$$\mathbf{B_{19}} = (y_5 - z_5)\,\mathbf{a}_1 - \left(x_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_5 + y_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16f) \quad \text{Al I}$$

$$\mathbf{B_{20}} = -\left(y_5 + z_5 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_5 - z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_5 - y_5)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (16f) \quad \text{Al I}$$

$$\mathbf{B_{21}} = -(y_5 + z_5)\,\mathbf{a}_1 - (x_5 + z_5)\,\mathbf{a}_2 - (x_5 + y_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16f) \quad \text{Al I}$$

$$\mathbf{B_{22}} = \left(y_5 - z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_5 - z_5)\,\mathbf{a}_2 + \left(x_5 + y_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = ax_5\,\hat{\mathbf{x}} + b\left(y_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}} \quad (16f) \quad \text{Al I}$$

$$\mathbf{B_{23}} = -(y_5 - z_5)\,\mathbf{a}_1 + \left(x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(x_5 - y_5 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}} \quad (16f) \quad \text{Al I}$$

$$\mathbf{B_{24}} = \left(y_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_5 + z_5 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_5 - y_5)\,\mathbf{a}_3 = -ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (16f) \quad \text{Al I}$$

$$\mathbf{B_{25}} = (y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{26}} = \left(-y_6 + z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - \left(x_6 + y_6 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{27}} = (y_6 - z_6)\,\mathbf{a}_1 - \left(x_6 + z_6 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{28}} = -\left(y_6 + z_6 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 - z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{29}} = -(y_6 + z_6)\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{30}} = \left(y_6 - z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + \left(x_6 + y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + b\left(y_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{31}} = -(y_6 - z_6)\,\mathbf{a}_1 + \left(x_6 + z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(x_6 - y_6 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{32}} = \left(y_6 + z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_6 + z_6 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li I}$$

$$\mathbf{B_{33}} = (y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{34}} = \left(-y_7 + z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - \left(x_7 + y_7 - \tfrac{1}{2}\right)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{35}} = (y_7 - z_7)\,\mathbf{a}_1 - \left(x_7 + z_7 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = -a\left(x_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{36}} = -\left(y_7 + z_7 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 - z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{37}} = -(y_7 + z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{38}} = \left(y_7 - z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + \left(x_7 + y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = ax_7\,\hat{\mathbf{x}} + b\left(y_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{39}} = -(y_7 - z_7)\,\mathbf{a}_1 + \left(x_7 + z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(x_7 - y_7 + \tfrac{1}{2}\right)\,\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$$\mathbf{B_{40}} = \left(y_7 + z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_7 + z_7 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\,\hat{\mathbf{z}} \quad (16f) \quad \text{Li II}$$

$\mathbf{B_{41}}$	=	$(y_8+z_8)\,\mathbf{a}_1+(x_8+z_8)\,\mathbf{a}_2+(x_8+y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{42}}$	=	$\left(-y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_1-(x_8-z_8)\,\mathbf{a}_2-\left(x_8+y_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-b\left(y_8-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{43}}$	=	$(y_8-z_8)\,\mathbf{a}_1-\left(x_8+z_8-\frac{1}{2}\right)\,\mathbf{a}_2+\left(-x_8+y_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8-\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{44}}$	=	$-\left(y_8+z_8-\frac{1}{2}\right)\,\mathbf{a}_1+\left(x_8-z_8+\frac{1}{2}\right)\,\mathbf{a}_2+(x_8-y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{45}}$	=	$-(y_8+z_8)\,\mathbf{a}_1-(x_8+z_8)\,\mathbf{a}_2-(x_8+y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{46}}$	=	$\left(y_8-z_8+\frac{1}{2}\right)\,\mathbf{a}_1+(x_8-z_8)\,\mathbf{a}_2+\left(x_8+y_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+b\left(y_8+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{47}}$	=	$-(y_8-z_8)\,\mathbf{a}_1+\left(x_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_2+\left(x_8-y_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_8+\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(16f)	Li III
$\mathbf{B_{48}}$	=	$\left(y_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_1+\left(-x_8+z_8+\frac{1}{2}\right)\,\mathbf{a}_2-(x_8-y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(16f)	Li III

References

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