Si_3Cl_8 Structure: A8B3_cF176_219_eh_abe-001

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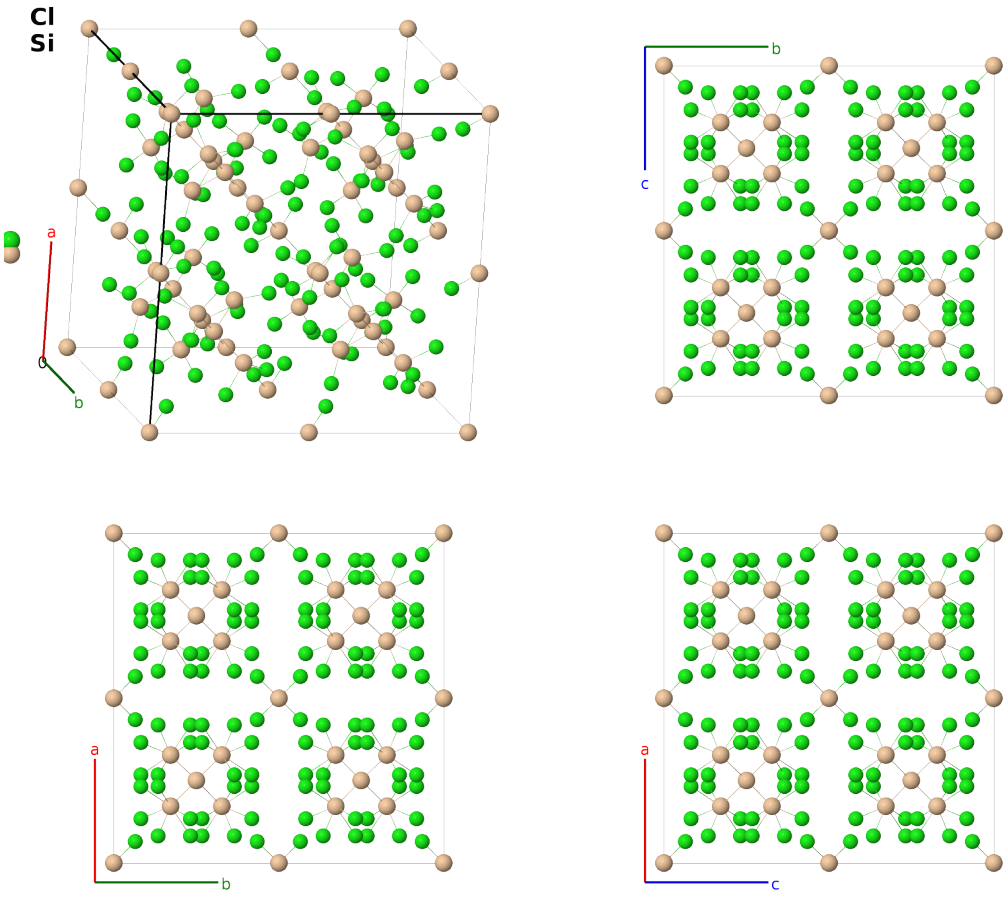
https://aflow.org/prototype-encyclopedia/ZRK3

https://aflow.org/prototype-encyclopedia/A8B3_cF176_219_eh_abe-001

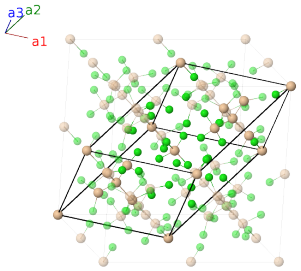


Prototype	Cl_8Si_3
AFLOW prototype label	A8B3_cF176_219_eh_abe-001
ICSD	2767
CCDC	1592571
Pearson symbol	cF176
Space group number	219
Space group symbol	$F\bar{4}3c$

AFLOW prototype command `aflow --proto=A8B3_cF176_219_eh_abe-001 --params=`$a, x_3, x_4, x_5, y_5, z_5$

Face-centered Cubic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(8a)	Si I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(8a)	Si I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8b)	Si II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - 3x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - 3x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_8}$	=	$-3x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_9}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_{10}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(3x_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_{11}}$	=	$-\left(3x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_{12}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(3x_3-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{14}}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - 3x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{15}}$	=	$x_4\,\mathbf{a}_1 - 3x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{16}}$	=	$-3x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{17}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{18}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2 - \left(3x_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{19}}$	=	$-\left(3x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B_{20}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - \left(3x_4-\frac{1}{2}\right)\,\mathbf{a}_2 + \left(x_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(32e)	Si III

$\mathbf{B_{21}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1+$ $(x_5-y_5+z_5)\,\mathbf{a}_2+$ $(x_5+y_5-z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{22}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1+$ $(-x_5+y_5+z_5)\,\mathbf{a}_2-$ $(x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+az_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{23}}$	=	$(x_5+y_5-z_5)\,\mathbf{a}_1-$ $(x_5+y_5+z_5)\,\mathbf{a}_2+$ $(-x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{24}}$	=	$-(x_5+y_5+z_5)\,\mathbf{a}_1+$ $(x_5+y_5-z_5)\,\mathbf{a}_2+$ $(x_5-y_5+z_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}-az_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{25}}$	=	$(x_5+y_5-z_5)\,\mathbf{a}_1+$ $(-x_5+y_5+z_5)\,\mathbf{a}_2+$ $(x_5-y_5+z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{26}}$	=	$-(x_5+y_5+z_5)\,\mathbf{a}_1+$ $(x_5-y_5+z_5)\,\mathbf{a}_2+$ $(-x_5+y_5+z_5)\,\mathbf{a}_3$	=	$az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{27}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1+$ $(x_5+y_5-z_5)\,\mathbf{a}_2-$ $(x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+ay_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{28}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1-$ $(x_5+y_5+z_5)\,\mathbf{a}_2+$ $(x_5+y_5-z_5)\,\mathbf{a}_3$	=	$-az_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}-ay_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{29}}$	=	$(x_5-y_5+z_5)\,\mathbf{a}_1+$ $(x_5+y_5-z_5)\,\mathbf{a}_2+$ $(-x_5+y_5+z_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{30}}$	=	$(-x_5+y_5+z_5)\,\mathbf{a}_1-$ $(x_5+y_5+z_5)\,\mathbf{a}_2+$ $(x_5-y_5+z_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{31}}$	=	$-(x_5+y_5+z_5)\,\mathbf{a}_1+$ $(-x_5+y_5+z_5)\,\mathbf{a}_2+$ $(x_5+y_5-z_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}-ax_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{32}}$	=	$(x_5+y_5-z_5)\,\mathbf{a}_1+$ $(x_5-y_5+z_5)\,\mathbf{a}_2-$ $(x_5+y_5+z_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}-az_5\,\hat{\mathbf{y}}+ax_5\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{33}}$	=	$\left(x_5-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+$ $\left(-x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2+$ $\left(x_5+y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{34}}$	=	$\left(-x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_1+$ $\left(x_5-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_2-$ $\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}+a\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{35}}$	=	$-\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_1+$ $\left(x_5+y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_2+$ $\left(-x_5+y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{x}}-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96h)	Cl II
$\mathbf{B_{36}}$	=	$\left(x_5+y_5-z_5+\frac{1}{2}\right)\,\mathbf{a}_1-$ $\left(x_5+y_5+z_5-\frac{1}{2}\right)\,\mathbf{a}_2+$ $\left(x_5-y_5+z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{x}}+a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{y}}-a\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(96h)	Cl II

$$\mathbf{B_{37}} = \left(-x_5+y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_5+y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_5-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{38}} = \left(x_5-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_1-\left(x_5+y_5+z_5-\tfrac{1}{2}\right)\mathbf{a}_2+\left(-x_5+y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{y}}-a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{39}} = \left(x_5+y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_5+y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_2-\left(x_5+y_5+z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{40}} = -\left(x_5+y_5+z_5-\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_5-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_5+y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{y}}-a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{41}} = \left(x_5+y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_5-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(-x_5+y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{42}} = -\left(x_5+y_5+z_5-\tfrac{1}{2}\right)\mathbf{a}_1+\left(-x_5+y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_5-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(z_5+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}}-a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{43}} = \left(-x_5+y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_1-\left(x_5+y_5+z_5-\tfrac{1}{2}\right)\mathbf{a}_2+\left(x_5+y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}}-a\left(x_5-\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

$$\mathbf{B_{44}} = \left(x_5-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_1+\left(x_5+y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_2-\left(x_5+y_5+z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(z_5-\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}}+a\left(x_5+\tfrac{1}{2}\right)\hat{\mathbf{z}}$$ (96h) Cl II

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