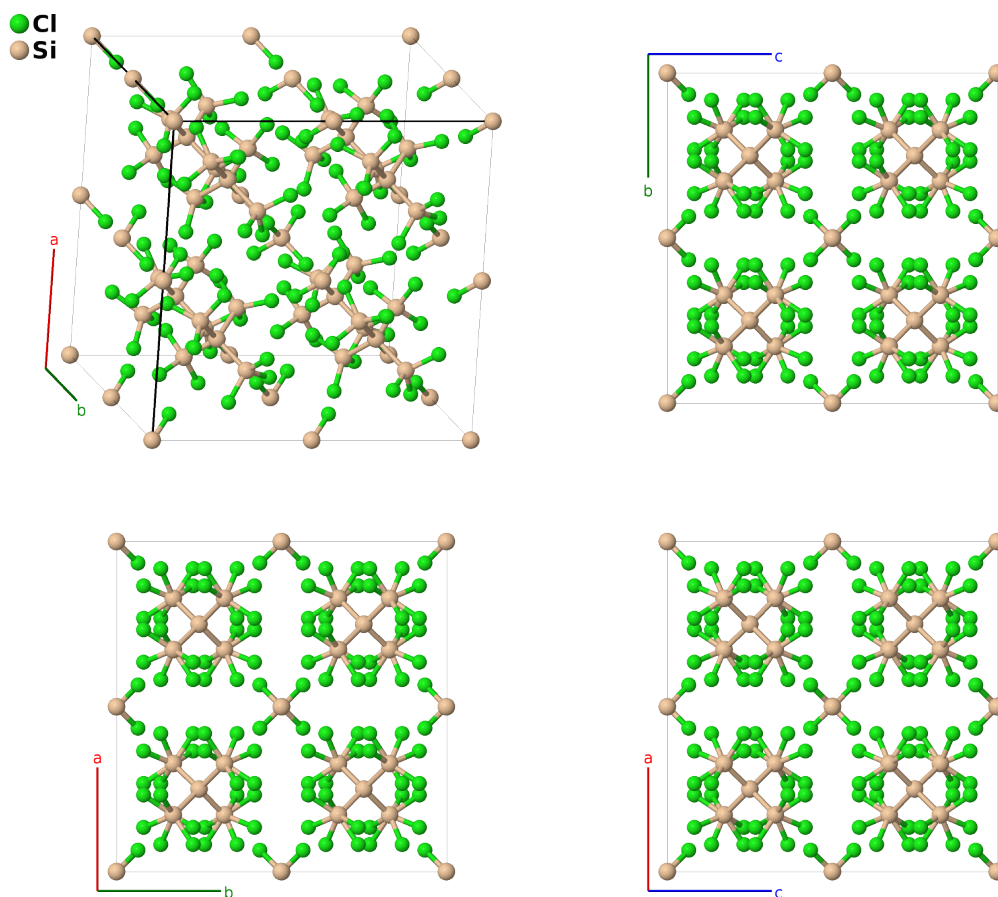


# Si<sub>3</sub>Cl<sub>8</sub> Structure: A8B3\_cF176\_219\_eh\_abe-001

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<https://aflow.org/p/ZRK3>

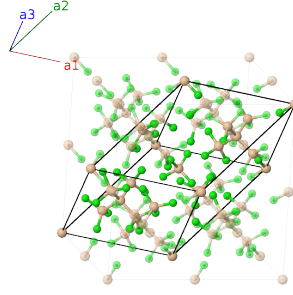
[https://aflow.org/p/A8B3\\_cF176\\_219\\_eh\\_abe-001](https://aflow.org/p/A8B3_cF176_219_eh_abe-001)



Prototype	Cl <sub>8</sub> Si <sub>3</sub>
AFLOW prototype label	A8B3_cF176_219_eh_abe-001
ICSD	2767
Pearson symbol	cF176
Space group number	219
Space group symbol	$F\bar{4}3c$
AFLOW prototype command	<code>aflow --proto=A8B3_cF176_219_eh_abe-001 --params=a, x<sub>3</sub>, x<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub></code>

Face-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}a \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}} \\
\mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}}
\end{aligned}$$



## 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
$\mathbf{B}_9$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B}_{10}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 - (3x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B}_{11}$	$-(3x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(32e)	Cl I
$\mathbf{B}_{12}$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (3x_3 - \frac{1}{2}) \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(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
$\mathbf{B}_{17}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B}_{18}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 - (3x_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B}_{19}$	$-(3x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(32e)	Si III
$\mathbf{B}_{20}$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (3x_4 - \frac{1}{2}) \mathbf{a}_2 + (x_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(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

$$\begin{aligned}
\mathbf{B}_{22} &= \begin{pmatrix} (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 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + az_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{23} &= \begin{pmatrix} (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 \end{pmatrix} = -ax_5 \hat{\mathbf{x}} + ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{24} &= \begin{pmatrix} -(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 \end{pmatrix} = ax_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{25} &= \begin{pmatrix} (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 \end{pmatrix} = az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{26} &= \begin{pmatrix} -(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 \end{pmatrix} = az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{27} &= \begin{pmatrix} (-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 \end{pmatrix} = -az_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + ay_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{28} &= \begin{pmatrix} (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 \end{pmatrix} = -az_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{29} &= \begin{pmatrix} (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 \end{pmatrix} = ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{30} &= \begin{pmatrix} (-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 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} + az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{31} &= \begin{pmatrix} -(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 \end{pmatrix} = ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{32} &= \begin{pmatrix} (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 \end{pmatrix} = -ay_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{33} &= \begin{pmatrix} (x_5 - y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (-x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_5 + y_5 - z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{34} &= \begin{pmatrix} (-x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 - y_5 + z_5 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_5 + y_5 + z_5 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{35} &= \begin{pmatrix} -(x_5 + y_5 + z_5 - \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 + y_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{36} &= \begin{pmatrix} (x_5 + y_5 - z_5 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_5 + y_5 + z_5 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_5 - y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_5 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{37} &= \begin{pmatrix} (-x_5 + y_5 + z_5 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_5 + y_5 - z_5 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_5 - y_5 + z_5 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{Cl II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{38} &= \begin{pmatrix} x_5 - y_5 + z_5 + \frac{1}{2} \\ x_5 + y_5 + z_5 - \frac{1}{2} \\ -x_5 + y_5 + z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= -a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{39} &= \begin{pmatrix} x_5 + y_5 - z_5 + \frac{1}{2} \\ -x_5 + y_5 + z_5 + \frac{1}{2} \\ x_5 + y_5 + z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= -a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{40} &= \begin{pmatrix} -x_5 + y_5 + z_5 - \frac{1}{2} \\ x_5 - y_5 + z_5 + \frac{1}{2} \\ x_5 + y_5 - z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{41} &= \begin{pmatrix} x_5 + y_5 - z_5 + \frac{1}{2} \\ x_5 - y_5 + z_5 + \frac{1}{2} \\ -x_5 + y_5 + z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{42} &= \begin{pmatrix} -x_5 + y_5 + z_5 - \frac{1}{2} \\ -x_5 + y_5 + z_5 + \frac{1}{2} \\ x_5 - y_5 + z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(z_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{43} &= \begin{pmatrix} -x_5 + y_5 + z_5 + \frac{1}{2} \\ x_5 + y_5 + z_5 - \frac{1}{2} \\ x_5 + y_5 - z_5 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= -a \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II} \\
\mathbf{B}_{44} &= \begin{pmatrix} x_5 - y_5 + z_5 + \frac{1}{2} \\ x_5 + y_5 - z_5 + \frac{1}{2} \\ x_5 + y_5 + z_5 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= -a \left(z_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_5 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{Cl II}
\end{aligned}$$

## References

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