

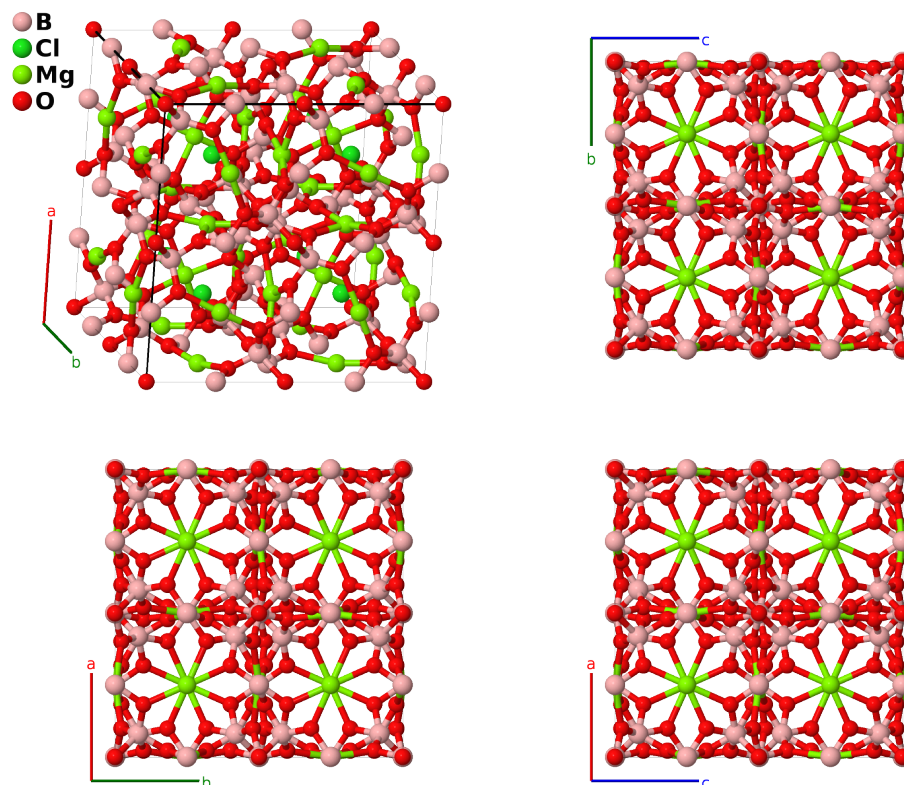
Boracite ($\text{Mg}_3\text{B}_7\text{ClO}_{13}$) Structure: A7BC3D13_cF192_219_ce_a_d_bh-001

This structure originally had the label A7BC3D13_cF192_219_de.b_c_ah. Calls to that address will be redirected here.

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<https://aflow.org/p/0WNV>

https://aflow.org/p/A7BC3D13_cF192_219_ce_a_d_bh-001



Prototype	$\text{B}_7\text{ClMg}_3\text{O}_{13}$
AFLOW prototype label	A7BC3D13_cF192_219_ce_a_d_bh-001
Mineral name	boracite
ICSD	22009
Pearson symbol	cF192
Space group number	219
Space group symbol	$F\bar{4}3c$
AFLOW prototype command	<pre>aflow --proto=A7BC3D13_cF192_219_ce_a_d_bh-001 --params=a, x5, x6, y6, z6</pre>

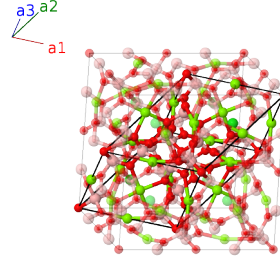
Other compounds with this structure

$\text{Cr}_3\text{B}_7\text{BrO}_{13}$, $\text{Cr}_3\text{B}_7\text{ClO}_{13}$, $\text{Cr}_3\text{B}_7\text{IO}_{13}$, $\text{Fe}_3\text{B}_7\text{BrO}_{13}$, $\text{Fe}_3\text{B}_7\text{ClO}_{13}$, $\text{Fe}_3\text{B}_7\text{IO}_{13}$, $\text{Mg}_3\text{B}_7\text{BrO}_{13}$, $\text{Mg}_3\text{B}_7\text{ClO}_{13}$, $\text{Mg}_3\text{B}_7\text{IO}_{13}$, $\text{Mn}_3\text{B}_7\text{BrO}_{13}$, $\text{Mn}_3\text{B}_7\text{ClO}_{13}$, $\text{Mn}_3\text{B}_7\text{IO}_{13}$

- Experimental data was obtained at 400°C.

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)	Cl 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)	Cl 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)	O I
\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)	O I
\mathbf{B}_5	$= \frac{1}{2}\mathbf{a}_1$	$=$	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	B I
\mathbf{B}_6	$= \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	B I
\mathbf{B}_7	$= \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	B I
\mathbf{B}_8	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24c)	B I
\mathbf{B}_9	$= \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(24c)	B I
\mathbf{B}_{10}	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24c)	B I
\mathbf{B}_{11}	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	Mg I
\mathbf{B}_{12}	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	Mg I
\mathbf{B}_{13}	$= \frac{1}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	Mg I
\mathbf{B}_{14}	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(24d)	Mg I
\mathbf{B}_{15}	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(24d)	Mg I
\mathbf{B}_{16}	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(24d)	Mg I
\mathbf{B}_{17}	$= x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} + ax_5\hat{\mathbf{y}} + ax_5\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{18}	$= x_5\mathbf{a}_1 + x_5\mathbf{a}_2 - 3x_5\mathbf{a}_3$	$=$	$-ax_5\hat{\mathbf{x}} - ax_5\hat{\mathbf{y}} + ax_5\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{19}	$= x_5\mathbf{a}_1 - 3x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$-ax_5\hat{\mathbf{x}} + ax_5\hat{\mathbf{y}} - ax_5\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{20}	$= -3x_5\mathbf{a}_1 + x_5\mathbf{a}_2 + x_5\mathbf{a}_3$	$=$	$ax_5\hat{\mathbf{x}} - ax_5\hat{\mathbf{y}} - ax_5\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{21}	$= (x_5 + \frac{1}{2})\mathbf{a}_1 + (x_5 + \frac{1}{2})\mathbf{a}_2 + (x_5 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2})\hat{\mathbf{x}} + a(x_5 + \frac{1}{2})\hat{\mathbf{y}} + a(x_5 + \frac{1}{2})\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{22}	$= (x_5 + \frac{1}{2})\mathbf{a}_1 + (x_5 + \frac{1}{2})\mathbf{a}_2 - (3x_5 - \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2})\hat{\mathbf{x}} - a(x_5 - \frac{1}{2})\hat{\mathbf{y}} + a(x_5 + \frac{1}{2})\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{23}	$= -(3x_5 - \frac{1}{2})\mathbf{a}_1 + (x_5 + \frac{1}{2})\mathbf{a}_2 + (x_5 + \frac{1}{2})\mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2})\hat{\mathbf{x}} - a(x_5 - \frac{1}{2})\hat{\mathbf{y}} - a(x_5 - \frac{1}{2})\hat{\mathbf{z}}$	(32e)	B II
\mathbf{B}_{24}	$= (x_5 + \frac{1}{2})\mathbf{a}_1 - (3x_5 - \frac{1}{2})\mathbf{a}_2 + (x_5 + \frac{1}{2})\mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2})\hat{\mathbf{x}} + a(x_5 + \frac{1}{2})\hat{\mathbf{y}} - a(x_5 - \frac{1}{2})\hat{\mathbf{z}}$	(32e)	B II

$$\begin{aligned}
\mathbf{B}_{25} &= \begin{pmatrix} (-x_6 + y_6 + z_6) \mathbf{a}_1 + \\ (x_6 - y_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6 - z_6) \mathbf{a}_3 \end{pmatrix} = ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{26} &= \begin{pmatrix} (x_6 - y_6 + z_6) \mathbf{a}_1 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_2 - \\ (x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = -ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{27} &= \begin{pmatrix} (x_6 + y_6 - z_6) \mathbf{a}_1 - \\ (x_6 + y_6 + z_6) \mathbf{a}_2 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = -ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{28} &= \begin{pmatrix} -(x_6 + y_6 + z_6) \mathbf{a}_1 + \\ (x_6 + y_6 - z_6) \mathbf{a}_2 + \\ (x_6 - y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = ax_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{29} &= \begin{pmatrix} (x_6 + y_6 - z_6) \mathbf{a}_1 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_2 + \\ (x_6 - y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{30} &= \begin{pmatrix} -(x_6 + y_6 + z_6) \mathbf{a}_1 + \\ (x_6 - y_6 + z_6) \mathbf{a}_2 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = az_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{31} &= \begin{pmatrix} (-x_6 + y_6 + z_6) \mathbf{a}_1 + \\ (x_6 + y_6 - z_6) \mathbf{a}_2 - \\ (x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = -az_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{32} &= \begin{pmatrix} (x_6 - y_6 + z_6) \mathbf{a}_1 - \\ (x_6 + y_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6 - z_6) \mathbf{a}_3 \end{pmatrix} = -az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{33} &= \begin{pmatrix} (x_6 - y_6 + z_6) \mathbf{a}_1 + \\ (x_6 + y_6 - z_6) \mathbf{a}_2 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{34} &= \begin{pmatrix} (-x_6 + y_6 + z_6) \mathbf{a}_1 - \\ (x_6 + y_6 + z_6) \mathbf{a}_2 + \\ (x_6 - y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = -ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{35} &= \begin{pmatrix} -(x_6 + y_6 + z_6) \mathbf{a}_1 + \\ (-x_6 + y_6 + z_6) \mathbf{a}_2 + \\ (x_6 + y_6 - z_6) \mathbf{a}_3 \end{pmatrix} = ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{36} &= \begin{pmatrix} (x_6 + y_6 - z_6) \mathbf{a}_1 + \\ (x_6 - y_6 + z_6) \mathbf{a}_2 - \\ (x_6 + y_6 + z_6) \mathbf{a}_3 \end{pmatrix} = -ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{37} &= \begin{pmatrix} (x_6 - y_6 + z_6 + \frac{1}{2}) \mathbf{a}_1 + \\ (-x_6 + y_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_6 + y_6 - z_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{38} &= \begin{pmatrix} (-x_6 + y_6 + z_6 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_6 - y_6 + z_6 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_6 + y_6 + z_6 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{39} &= \begin{pmatrix} -(x_6 + y_6 + z_6 - \frac{1}{2}) \mathbf{a}_1 + \\ (x_6 + y_6 - z_6 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_6 + y_6 + z_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{40} &= \begin{pmatrix} (x_6 + y_6 - z_6 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_6 + y_6 + z_6 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_6 - y_6 + z_6 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}} & (96h) & \text{O II}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{41} &= \begin{pmatrix} -x_6 + y_6 + z_6 + \frac{1}{2} \\ x_6 + y_6 - z_6 + \frac{1}{2} \\ x_6 - y_6 + z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{42} &= \begin{pmatrix} x_6 - y_6 + z_6 + \frac{1}{2} \\ x_6 + y_6 + z_6 - \frac{1}{2} \\ -x_6 + y_6 + z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{43} &= \begin{pmatrix} x_6 + y_6 - z_6 + \frac{1}{2} \\ -x_6 + y_6 + z_6 + \frac{1}{2} \\ x_6 + y_6 + z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= -a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{44} &= \begin{pmatrix} -(x_6 + y_6 + z_6 - \frac{1}{2}) \\ x_6 - y_6 + z_6 + \frac{1}{2} \\ x_6 + y_6 - z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{45} &= \begin{pmatrix} x_6 + y_6 - z_6 + \frac{1}{2} \\ x_6 - y_6 + z_6 + \frac{1}{2} \\ -x_6 + y_6 + z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{46} &= \begin{pmatrix} -(x_6 + y_6 + z_6 - \frac{1}{2}) \\ -x_6 + y_6 + z_6 + \frac{1}{2} \\ x_6 - y_6 + z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{47} &= \begin{pmatrix} -x_6 + y_6 + z_6 + \frac{1}{2} \\ x_6 + y_6 + z_6 - \frac{1}{2} \\ x_6 + y_6 - z_6 + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - &= -a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_6 - \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II} \\
\mathbf{B}_{48} &= \begin{pmatrix} x_6 - y_6 + z_6 + \frac{1}{2} \\ x_6 + y_6 - z_6 + \frac{1}{2} \\ x_6 + y_6 + z_6 - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + &= -a \left(z_6 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_6 - \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (96h) & \text{O II}
\end{aligned}$$

References

- [1] S. Sueno, J. R. Clark, J. J. Papike, and J. A. Konnert, *Crystal-Structure Refinement of Cubic Boracite*, Am. Mineral. **58**, 691–697 (1973).