

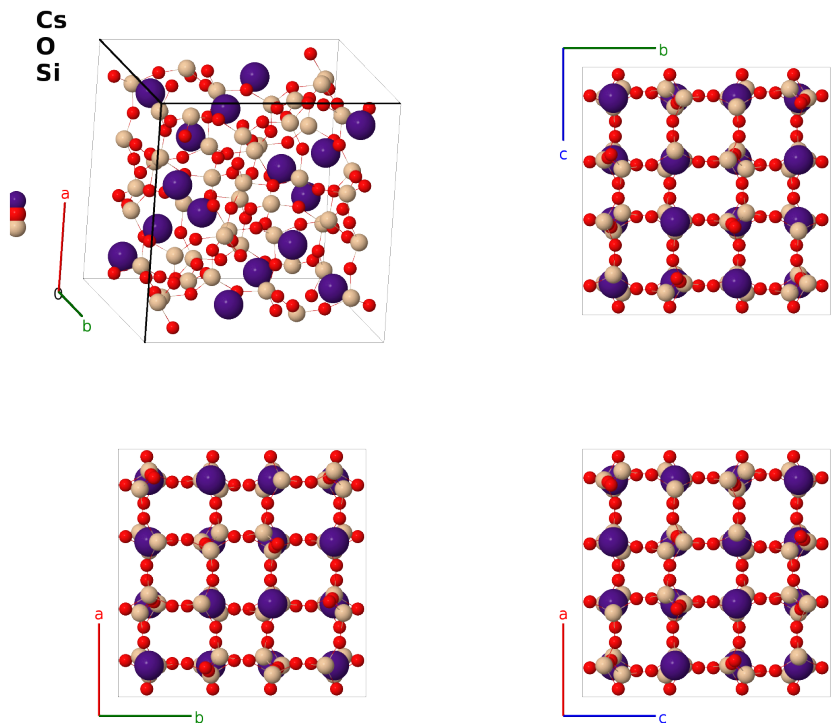
Boropollucite [Cs(Si₂B)O₆] Structure: AB6C3_cI160_230_b_h_g-001

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- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/C3ND>

https://aflow.org/prototype-encyclopedia/AB6C3_cI160_230_b_h_g-001

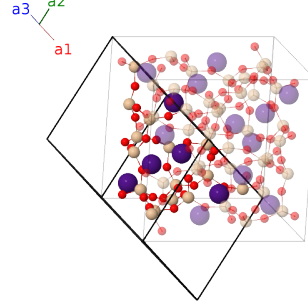


Prototype	BCsO ₆ Si ₂
AFLOW prototype label	AB6C3_cI160_230_b_h_g-001
Mineral name	boropollucite
ICSD	413224
CCDC	1728269
Pearson symbol	cI160
Space group number	230
Space group symbol	$Ia\bar{3}d$
AFLOW prototype command	<code>aflow --proto=AB6C3_cI160_230_b_h_g-001 --params=a, y₂, x₃, y₃, z₃</code>

- According to (Bubnova, 2004) the Cs (16b) site is 81.4% filled, and the Si (48g) site is 65.9% silicon and 36.5% boron. This gives the final stoichiometry of $\text{Cs}_{0.814}\text{B}_{1.095}\text{Si}_{1.977}\text{O}_6$
- Other entries in the ICSD show that the Cs site may also contain calcium.
- The Wyckoff labels listed in Table 3 of (Bubnova, 2004) are incorrect. They are corrected in the ICSD entry.
- The Wyckoff positions in the ICSD differ slightly from the published values. We use the values from the ICSD CIF.

Body-centered Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_2$	$= \frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_3$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_3$	$= \frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} - \frac{1}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_4$	$= \frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_5$	$= \frac{3}{4}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{\mathbf{x}} + \frac{3}{8}a\hat{\mathbf{y}} + \frac{3}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_6$	$= \frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + \frac{5}{8}a\hat{\mathbf{y}} - \frac{1}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_7$	$= \frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{5}{8}a\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_8$	$= \frac{3}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + \frac{5}{8}a\hat{\mathbf{z}}$	(16b)	Cs I
$\mathbf{B}_9$	$= \frac{1}{4}\mathbf{a}_1 - (y_2 - \frac{3}{8})\mathbf{a}_2 + (y_2 + \frac{1}{8})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} + ay_2\hat{\mathbf{y}} - a(y_2 - \frac{1}{4})\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{10}$	$= -(2y_2 - \frac{3}{4})\mathbf{a}_1 - (y_2 - \frac{1}{8})\mathbf{a}_2 - (y_2 - \frac{3}{8})\mathbf{a}_3$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} - a(y_2 - \frac{1}{2})\hat{\mathbf{y}} - a(y_2 - \frac{1}{4})\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{11}$	$= (2y_2 + \frac{3}{4})\mathbf{a}_1 + (y_2 + \frac{1}{8})\mathbf{a}_2 + (y_2 + \frac{3}{8})\mathbf{a}_3$	$=$	$-\frac{1}{8}a\hat{\mathbf{x}} + a(y_2 + \frac{1}{2})\hat{\mathbf{y}} + a(y_2 + \frac{1}{4})\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{12}$	$= \frac{1}{4}\mathbf{a}_1 + (y_2 + \frac{3}{8})\mathbf{a}_2 - (y_2 - \frac{1}{8})\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{\mathbf{x}} - ay_2\hat{\mathbf{y}} + a(y_2 + \frac{1}{4})\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{13}$	$= (y_2 + \frac{1}{8})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 - (y_2 - \frac{3}{8})\mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} + ay_2\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{14}$	$= -(y_2 - \frac{3}{8})\mathbf{a}_1 - (2y_2 - \frac{3}{4})\mathbf{a}_2 - (y_2 - \frac{1}{8})\mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} - a(y_2 - \frac{1}{2})\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{15}$	$= (y_2 + \frac{3}{8})\mathbf{a}_1 + (2y_2 + \frac{3}{4})\mathbf{a}_2 + (y_2 + \frac{1}{8})\mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4})\hat{\mathbf{x}} - \frac{1}{8}a\hat{\mathbf{y}} + a(y_2 + \frac{1}{2})\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{16}$	$= -(y_2 - \frac{1}{8})\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + (y_2 + \frac{3}{8})\mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{4})\hat{\mathbf{x}} + \frac{1}{8}a\hat{\mathbf{y}} - ay_2\hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{17}$	$= -(y_2 - \frac{3}{8})\mathbf{a}_1 + (y_2 + \frac{1}{8})\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	$=$	$ay_2\hat{\mathbf{x}} - a(y_2 - \frac{1}{4})\hat{\mathbf{y}} + \frac{1}{8}a\hat{\mathbf{z}}$	(48g)	Si I

$\mathbf{B}_{18} =$	$-(y_2 - \frac{1}{8}) \mathbf{a}_1 - (y_2 - \frac{3}{8}) \mathbf{a}_2 -$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} - \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Si I
	$(2y_2 - \frac{3}{4}) \mathbf{a}_3$				
$\mathbf{B}_{19} =$	$(y_2 + \frac{1}{8}) \mathbf{a}_1 + (y_2 + \frac{3}{8}) \mathbf{a}_2 +$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} - \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Si I
	$(2y_2 + \frac{3}{4}) \mathbf{a}_3$				
$\mathbf{B}_{20} =$	$(y_2 + \frac{3}{8}) \mathbf{a}_1 - (y_2 - \frac{1}{8}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{1}{8}a \hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{21} =$	$\frac{3}{4} \mathbf{a}_1 + (y_2 + \frac{5}{8}) \mathbf{a}_2 - (y_2 - \frac{7}{8}) \mathbf{a}_3$	$=$	$\frac{3}{8}a \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{22} =$	$(2y_2 + \frac{1}{4}) \mathbf{a}_1 + (y_2 + \frac{7}{8}) \mathbf{a}_2 +$	$=$	$\frac{5}{8}a \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Si I
	$(y_2 + \frac{5}{8}) \mathbf{a}_3$				
$\mathbf{B}_{23} =$	$-(2y_2 - \frac{1}{4}) \mathbf{a}_1 - (y_2 - \frac{7}{8}) \mathbf{a}_2 -$	$=$	$\frac{5}{8}a \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Si I
	$(y_2 - \frac{5}{8}) \mathbf{a}_3$				
$\mathbf{B}_{24} =$	$\frac{3}{4} \mathbf{a}_1 - (y_2 - \frac{5}{8}) \mathbf{a}_2 + (y_2 + \frac{7}{8}) \mathbf{a}_3$	$=$	$\frac{3}{8}a \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{25} =$	$-(y_2 - \frac{7}{8}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 +$	$=$	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Si I
	$(y_2 + \frac{5}{8}) \mathbf{a}_3$				
$\mathbf{B}_{26} =$	$(y_2 + \frac{5}{8}) \mathbf{a}_1 + (2y_2 + \frac{1}{4}) \mathbf{a}_2 +$	$=$	$a(y_2 + \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8}a \hat{\mathbf{y}} + ay_2 \hat{\mathbf{z}}$	(48g)	Si I
	$(y_2 + \frac{7}{8}) \mathbf{a}_3$				
$\mathbf{B}_{27} =$	$-(y_2 - \frac{5}{8}) \mathbf{a}_1 - (2y_2 - \frac{1}{4}) \mathbf{a}_2 -$	$=$	$-a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{5}{8}a \hat{\mathbf{y}} - ay_2 \hat{\mathbf{z}}$	(48g)	Si I
	$(y_2 - \frac{7}{8}) \mathbf{a}_3$				
$\mathbf{B}_{28} =$	$(y_2 + \frac{7}{8}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - (y_2 - \frac{5}{8}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{4}) \hat{\mathbf{x}} + \frac{3}{8}a \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{29} =$	$(y_2 + \frac{5}{8}) \mathbf{a}_1 - (y_2 - \frac{7}{8}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}}$	(48g)	Si I
$\mathbf{B}_{30} =$	$(y_2 + \frac{7}{8}) \mathbf{a}_1 + (y_2 + \frac{5}{8}) \mathbf{a}_2 +$	$=$	$ay_2 \hat{\mathbf{x}} + a(y_2 + \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8}a \hat{\mathbf{z}}$	(48g)	Si I
	$(2y_2 + \frac{1}{4}) \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$-(y_2 - \frac{7}{8}) \mathbf{a}_1 - (y_2 - \frac{5}{8}) \mathbf{a}_2 -$	$=$	$-ay_2 \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{5}{8}a \hat{\mathbf{z}}$	(48g)	Si I
	$(2y_2 - \frac{1}{4}) \mathbf{a}_3$				
$\mathbf{B}_{32} =$	$-(y_2 - \frac{5}{8}) \mathbf{a}_1 + (y_2 + \frac{7}{8}) \mathbf{a}_2 +$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{4}) \hat{\mathbf{y}} + \frac{3}{8}a \hat{\mathbf{z}}$	(48g)	Si I
	$\frac{3}{4} \mathbf{a}_3$				
$\mathbf{B}_{33} =$	$(y_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 +$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(96h)	O I
	$(x_3 + y_3) \mathbf{a}_3$				
$\mathbf{B}_{34} =$	$(-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 -$	$=$	$-ax_3 \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + az_3 \hat{\mathbf{z}}$	(96h)	O I
	$(x_3 - z_3) \mathbf{a}_2 - (x_3 + y_3 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$(y_3 - z_3) \mathbf{a}_1 - (x_3 + z_3 - \frac{1}{2}) \mathbf{a}_2 +$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} - az_3 \hat{\mathbf{z}}$	(96h)	O I
	$(-x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$-(y_3 + z_3 - \frac{1}{2}) \mathbf{a}_1 +$	$=$	$ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} - a(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	O I
	$(x_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - y_3) \mathbf{a}_3$				
$\mathbf{B}_{37} =$	$(x_3 + y_3) \mathbf{a}_1 + (y_3 + z_3) \mathbf{a}_2 +$	$=$	$az_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}}$	(96h)	O I
	$(x_3 + z_3) \mathbf{a}_3$				
$\mathbf{B}_{38} =$	$-(x_3 + y_3 - \frac{1}{2}) \mathbf{a}_1 +$	$=$	$az_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(96h)	O I
	$(-y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2$				

$\mathbf{B}_{43}$	$=$	$\begin{aligned} & -\left(x_3+z_3-\frac{1}{2}\right) \mathbf{a}_1+ \\ & \left(-x_3+y_3+\frac{1}{2}\right) \mathbf{a}_2+\left(y_3-z_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$a y_3 \hat{\mathbf{x}}-a z_3 \hat{\mathbf{y}}-a\left(x_3-\frac{1}{2}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{44}$	$=$	$\begin{aligned} & \left(x_3-z_3+\frac{1}{2}\right) \mathbf{a}_1+ \\ & \left(x_3-y_3\right) \mathbf{a}_2-\left(y_3+z_3-\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a y_3 \hat{\mathbf{x}}-a\left(z_3-\frac{1}{2}\right) \hat{\mathbf{y}}+a x_3 \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{45}$	$=$	$\begin{aligned} & \left(x_3-z_3+\frac{1}{2}\right) \mathbf{a}_1+ \\ & \left(y_3-z_3\right) \mathbf{a}_2+\left(x_3+y_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{x}}+a\left(x_3+\frac{1}{4}\right) \hat{\mathbf{y}}-a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{46}$	$=$	$\begin{aligned} & -\left(x_3+z_3-\frac{1}{2}\right) \mathbf{a}_1- \\ & \left(y_3+z_3-\frac{1}{2}\right) \mathbf{a}_2- \\ & \left(x_3+y_3-\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{y}}-a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{47}$	$=$	$\begin{aligned} & -\left(x_3-z_3\right) \mathbf{a}_1+\left(y_3+z_3\right) \mathbf{a}_2+ \\ & \left(-x_3+y_3+\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(y_3+\frac{1}{4}\right) \hat{\mathbf{x}}-a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{y}}+a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{48}$	$=$	$\begin{aligned} & \left(x_3+z_3\right) \mathbf{a}_1+ \\ & \left(-y_3+z_3+\frac{1}{2}\right) \mathbf{a}_2+\left(x_3-y_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{x}}+a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{y}}+a\left(z_3+\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{49}$	$=$	$\begin{aligned} & \left(-y_3+z_3+\frac{1}{2}\right) \mathbf{a}_1+ \\ & \left(x_3-y_3\right) \mathbf{a}_2+\left(x_3+z_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{x}}+a\left(z_3+\frac{1}{4}\right) \hat{\mathbf{y}}-a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{50}$	$=$	$\begin{aligned} & \left(y_3+z_3\right) \mathbf{a}_1+ \\ & \left(-x_3+y_3+\frac{1}{2}\right) \mathbf{a}_2-\left(x_3-z_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{x}}+a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{y}}+a\left(y_3+\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{51}$	$=$	$\begin{aligned} & -\left(y_3+z_3-\frac{1}{2}\right) \mathbf{a}_1- \\ & \left(x_3+y_3-\frac{1}{2}\right) \mathbf{a}_2- \\ & \left(x_3+z_3-\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{x}}-a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{y}}-a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{52}$	$=$	$\begin{aligned} & \left(y_3-z_3\right) \mathbf{a}_1+\left(x_3+y_3\right) \mathbf{a}_2+ \\ & \left(x_3-z_3+\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(x_3+\frac{1}{4}\right) \hat{\mathbf{x}}-a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{y}}+a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{53}$	$=$	$\begin{aligned} & \left(-x_3+y_3+\frac{1}{2}\right) \mathbf{a}_1- \\ & \left(x_3-z_3\right) \mathbf{a}_2+\left(y_3+z_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{x}}+a\left(y_3+\frac{1}{4}\right) \hat{\mathbf{y}}-a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{54}$	$=$	$\begin{aligned} & \left(x_3-y_3\right) \mathbf{a}_1+\left(x_3+z_3\right) \mathbf{a}_2+ \\ & \left(-y_3+z_3+\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(z_3+\frac{1}{4}\right) \hat{\mathbf{x}}-a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{y}}+a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{55}$	$=$	$\begin{aligned} & \left(x_3+y_3\right) \mathbf{a}_1+ \\ & \left(x_3-z_3+\frac{1}{2}\right) \mathbf{a}_2+\left(y_3-z_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{x}}+a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{y}}+a\left(x_3+\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{56}$	$=$	$\begin{aligned} & -\left(x_3+y_3-\frac{1}{2}\right) \mathbf{a}_1- \\ & \left(x_3+z_3-\frac{1}{2}\right) \mathbf{a}_2- \\ & \left(y_3+z_3-\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a\left(z_3-\frac{1}{4}\right) \hat{\mathbf{x}}-a\left(y_3-\frac{1}{4}\right) \hat{\mathbf{y}}-a\left(x_3-\frac{1}{4}\right) \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{57}$	$=$	$\begin{aligned} & -\left(y_3+z_3\right) \mathbf{a}_1-\left(x_3+z_3\right) \mathbf{a}_2- \\ & \left(x_3+y_3\right) \mathbf{a}_3 \end{aligned}$	$=$	$-a x_3 \hat{\mathbf{x}}-a y_3 \hat{\mathbf{y}}-a z_3 \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{58}$	$=$	$\begin{aligned} & \left(y_3-z_3+\frac{1}{2}\right) \mathbf{a}_1+ \\ & \left(x_3-z_3\right) \mathbf{a}_2+\left(x_3+y_3+\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$a x_3 \hat{\mathbf{x}}+a\left(y_3+\frac{1}{2}\right) \hat{\mathbf{y}}-a z_3 \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{59}$	$=$	$\begin{aligned} & -\left(y_3-z_3\right) \mathbf{a}_1+ \\ & \left(x_3+z_3+\frac{1}{2}\right) \mathbf{a}_2+ \\ & \left(x_3-y_3+\frac{1}{2}\right) \mathbf{a}_3 \end{aligned}$	$=$	$a\left(x_3+\frac{1}{2}\right) \hat{\mathbf{x}}-a y_3 \hat{\mathbf{y}}+a z_3 \hat{\mathbf{z}}$	$(96h)$	O I
$\mathbf{B}_{60}$	$=$	$\begin{aligned} & \left(y_3+z_3+\frac{1}{2}\right) \mathbf{a}_1+ \\ & \left(-x_3+z_3+\frac{1}{2}\right) \mathbf{a}_2-\left(x_3-y_3\right) \mathbf{a}_3 \end{aligned$				

$$\begin{aligned}
\mathbf{B}_{64} &= \begin{pmatrix} -(x_3 - y_3) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(z_3 + \frac{1}{2} \right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + ay_3 \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{65} &= \begin{pmatrix} -(x_3 + z_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - \\ (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{66} &= \begin{pmatrix} (x_3 - z_3) \mathbf{a}_1 + (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(y_3 + \frac{1}{2} \right) \hat{\mathbf{x}} - az_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{67} &= \begin{pmatrix} (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = -ay_3 \hat{\mathbf{x}} + az_3 \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{68} &= \begin{pmatrix} (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - y_3) \mathbf{a}_2 + (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = ay_3 \hat{\mathbf{x}} + a \left(z_3 + \frac{1}{2} \right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{69} &= \begin{pmatrix} (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (y_3 - z_3) \mathbf{a}_2 - (x_3 + y_3) \mathbf{a}_3 \end{pmatrix} = -a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{70} &= \begin{pmatrix} (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{71} &= \begin{pmatrix} (x_3 - z_3) \mathbf{a}_1 - (y_3 + z_3) \mathbf{a}_2 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(y_3 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{72} &= \begin{pmatrix} -(x_3 + z_3) \mathbf{a}_1 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_2 - (x_3 - y_3) \mathbf{a}_3 \end{pmatrix} = a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(z_3 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{73} &= \begin{pmatrix} (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_1 - \\ (x_3 - y_3) \mathbf{a}_2 - (x_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(z_3 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{74} &= \begin{pmatrix} -(y_3 + z_3) \mathbf{a}_1 + \\ (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_2 + (x_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(y_3 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{75} &= \begin{pmatrix} (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{76} &= \begin{pmatrix} -(y_3 - z_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(x_3 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{77} &= \begin{pmatrix} (x_3 - y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 - z_3) \mathbf{a}_2 - (y_3 + z_3) \mathbf{a}_3 \end{pmatrix} = -a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(y_3 - \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{78} &= \begin{pmatrix} -(x_3 - y_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2 + \\ (y_3 - z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = -a \left(z_3 - \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{79} &= \begin{pmatrix} -(x_3 + y_3) \mathbf{a}_1 + \\ (-x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3 \end{pmatrix} = a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{x}} - a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I} \\
\mathbf{B}_{80} &= \begin{pmatrix} (x_3 + y_3 + \frac{1}{2}) \mathbf{a}_1 + \\ (x_3 + z_3 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_3 + z_3 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \left(z_3 + \frac{1}{4} \right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{4} \right) \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{4} \right) \hat{\mathbf{z}} & (96h) & \text{O I}
\end{aligned}$$

References

- [1] R. S. Bubnova, N. K. Stepanov, A. A. Levin, S. K. Filatov, P. Paufler, and D. C. Meyer, *Crystal structure and thermal behaviour of boropollucite CsBSi₂O₆*, Solid State Sci. **6**, 629–637 (2004), doi:10.1016/j.solidstatesciences.2004.03.015.

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