Pinnoite ($MgB_2O[OH]_6$) Structure: A2B6CD7_tP64_77_2d_6d_d_ab6d-001

This structure originally had the label `A2B6CD7_tP64_77_2d_6d_d_ab6d`. Calls to that address will be redirected here.

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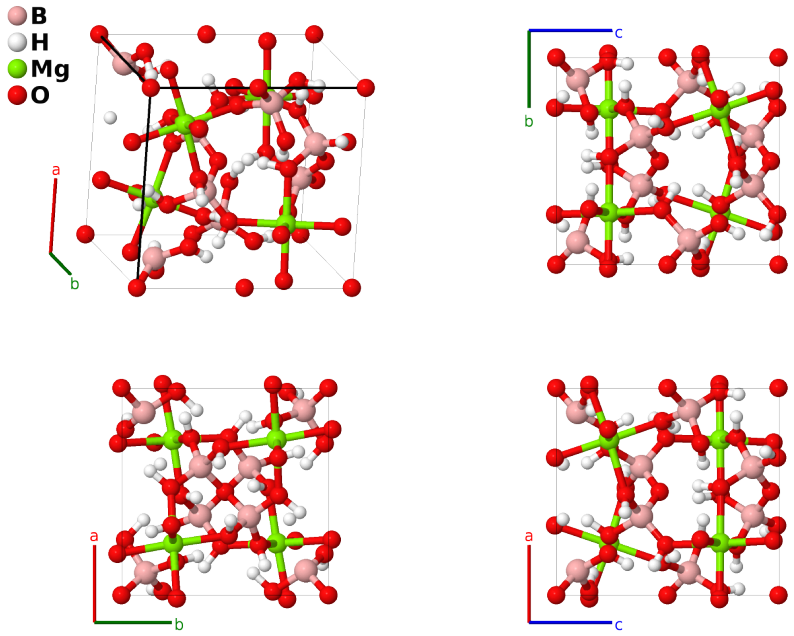
https://aflow.org/p/Z918

https://aflow.org/p/A2B6CD7_tP64_77_2d_6d_d_ab6d-001

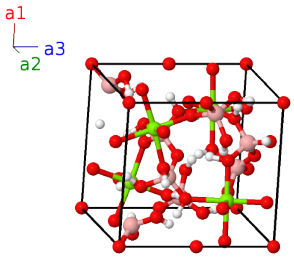


Prototype	$B_2H_6MgO_7$
AFLOW prototype label	A2B6CD7_tP64_77_2d_6d_d_ab6d-001
Mineral name	pinnoite
ICSD	20662
Pearson symbol	tP64
Space group number	77
Space group symbol	$P4_2$
AFLOW prototype command	`aflow --proto=A2B6CD7_tP64_77_2d_6d_d_ab6d-001 --params=`$a, c/a, z_1, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}$

- (Genkina, 1983) state that their Wyckoff positions were to be multiplied by 10^{-4}. This is not the case for the z-coordinates and the x- and y-coordinates of the hydrogen atoms: those coordinates should be multiplied by 10^{-3}. This confusion led to incorrect hydrogen-oxygen distances in both our original page (Hicks, 2019) and in (Villars, 2016). We believe the current interpretation is correct, as our Mg-O and B-O distances agree with (Genkina, 1983) and all of our O-H bonds are on the order of 1Å. The ICSD CIF also interprets the coordinates in this fashion.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1+\frac{1}{2}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{1}{2}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1+y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}+ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1-y_3\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}-ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1+x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}}+ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B_8}$	=	$y_3\,\mathbf{a}_1-x_3\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}}-ax_3\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	B I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1+x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}}+ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B_{12}}$	=	$y_4\,\mathbf{a}_1-x_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}}-ax_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	B II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1+y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}}+ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1-y_5\,\mathbf{a}_2+z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}}-ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B_{15}}$	=	$-y_5\,\mathbf{a}_1+x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}}+ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B_{16}}$	=	$y_5\,\mathbf{a}_1-x_5\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}}-ax_5\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H I
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1+y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1-y_6\,\mathbf{a}_2+z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}}-ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_{19}}$	=	$-y_6\,\mathbf{a}_1+x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}}+ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_{20}}$	=	$y_6\,\mathbf{a}_1-x_6\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}}-ax_6\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1+y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}}+ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B_{22}}$	=	$-x_7\,\mathbf{a}_1-y_7\,\mathbf{a}_2+z_7\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}}-ay_7\,\hat{\mathbf{y}}+cz_7\,\hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B_{23}}$	=	$-y_7\,\mathbf{a}_1+x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}}+ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B_{24}}$	=	$y_7\,\mathbf{a}_1-x_7\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}}-ax_7\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H III
$\mathbf{B_{25}}$	=	$x_8\,\mathbf{a}_1+y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B_{26}}$	=	$-x_8\,\mathbf{a}_1-y_8\,\mathbf{a}_2+z_8\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-ay_8\,\hat{\mathbf{y}}+cz_8\,\hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B_{27}}$	=	$-y_8\,\mathbf{a}_1+x_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B_{28}}$	=	$y_8\,\mathbf{a}_1-x_8\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4d)	H IV
$\mathbf{B_{29}}$	=	$x_9\,\mathbf{a}_1+y_9\,\mathbf{a}_2+z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(4d)	H V

$$
\begin{aligned}
\mathbf{B_{30}} &= -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 &&= -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} && \text{(4d)} && \text{H V}\\
\mathbf{B_{31}} &= -y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{H V}\\
\mathbf{B_{32}} &= y_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + \left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + c\left(z_9+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{H V}\\
\mathbf{B_{33}} &= x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 &&= ax_{10}\,\hat{\mathbf{x}} + ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} && \text{(4d)} && \text{H VI}\\
\mathbf{B_{34}} &= -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 &&= -ax_{10}\,\hat{\mathbf{x}} - ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} && \text{(4d)} && \text{H VI}\\
\mathbf{B_{35}} &= -y_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{H VI}\\
\mathbf{B_{36}} &= y_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + \left(z_{10}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{H VI}\\
\mathbf{B_{37}} &= x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 &&= ax_{11}\,\hat{\mathbf{x}} + ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} && \text{(4d)} && \text{Mg I}\\
\mathbf{B_{38}} &= -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 &&= -ax_{11}\,\hat{\mathbf{x}} - ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} && \text{(4d)} && \text{Mg I}\\
\mathbf{B_{39}} &= -y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{Mg I}\\
\mathbf{B_{40}} &= y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + \left(z_{11}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{Mg I}\\
\mathbf{B_{41}} &= x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 &&= ax_{12}\,\hat{\mathbf{x}} + ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O III}\\
\mathbf{B_{42}} &= -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 &&= -ax_{12}\,\hat{\mathbf{x}} - ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O III}\\
\mathbf{B_{43}} &= -y_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{12}\,\hat{\mathbf{x}} + ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O III}\\
\mathbf{B_{44}} &= y_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + \left(z_{12}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{12}\,\hat{\mathbf{x}} - ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O III}\\
\mathbf{B_{45}} &= x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 &&= ax_{13}\,\hat{\mathbf{x}} + ay_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O IV}\\
\mathbf{B_{46}} &= -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 &&= -ax_{13}\,\hat{\mathbf{x}} - ay_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O IV}\\
\mathbf{B_{47}} &= -y_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + \left(z_{13}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{13}\,\hat{\mathbf{x}} + ax_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O IV}\\
\mathbf{B_{48}} &= y_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 + \left(z_{13}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{13}\,\hat{\mathbf{x}} - ax_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O IV}\\
\mathbf{B_{49}} &= x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 &&= ax_{14}\,\hat{\mathbf{x}} + ay_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O V}\\
\mathbf{B_{50}} &= -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 &&= -ax_{14}\,\hat{\mathbf{x}} - ay_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O V}\\
\mathbf{B_{51}} &= -y_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{14}\,\hat{\mathbf{x}} + ax_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O V}\\
\mathbf{B_{52}} &= y_{14}\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 + \left(z_{14}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{14}\,\hat{\mathbf{x}} - ax_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O V}\\
\mathbf{B_{53}} &= x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 &&= ax_{15}\,\hat{\mathbf{x}} + ay_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O VI}\\
\mathbf{B_{54}} &= -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 &&= -ax_{15}\,\hat{\mathbf{x}} - ay_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O VI}\\
\mathbf{B_{55}} &= -y_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{15}\,\hat{\mathbf{x}} + ax_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O VI}\\
\mathbf{B_{56}} &= y_{15}\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 + \left(z_{15}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{15}\,\hat{\mathbf{x}} - ax_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O VI}\\
\mathbf{B_{57}} &= x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 &&= ax_{16}\,\hat{\mathbf{x}} + ay_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O VII}\\
\mathbf{B_{58}} &= -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 &&= -ax_{16}\,\hat{\mathbf{x}} - ay_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O VII}\\
\mathbf{B_{59}} &= -y_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{16}\,\hat{\mathbf{x}} + ax_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O VII}\\
\mathbf{B_{60}} &= y_{16}\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 + \left(z_{16}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{16}\,\hat{\mathbf{x}} - ax_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O VII}\\
\mathbf{B_{61}} &= x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 &&= ax_{17}\,\hat{\mathbf{x}} + ay_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O VIII}\\
\mathbf{B_{62}} &= -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 &&= -ax_{17}\,\hat{\mathbf{x}} - ay_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} && \text{(4d)} && \text{O VIII}\\
\mathbf{B_{63}} &= -y_{17}\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + \left(z_{17}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= -ay_{17}\,\hat{\mathbf{x}} + ax_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O VIII}\\
\mathbf{B_{64}} &= y_{17}\,\mathbf{a}_1 - x_{17}\,\mathbf{a}_2 + \left(z_{17}+\tfrac{1}{2}\right)\mathbf{a}_3 &&= ay_{17}\,\hat{\mathbf{x}} - ax_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\tfrac{1}{2}\right)\hat{\mathbf{z}} && \text{(4d)} && \text{O VIII}
\end{aligned}
$$

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[2] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

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