

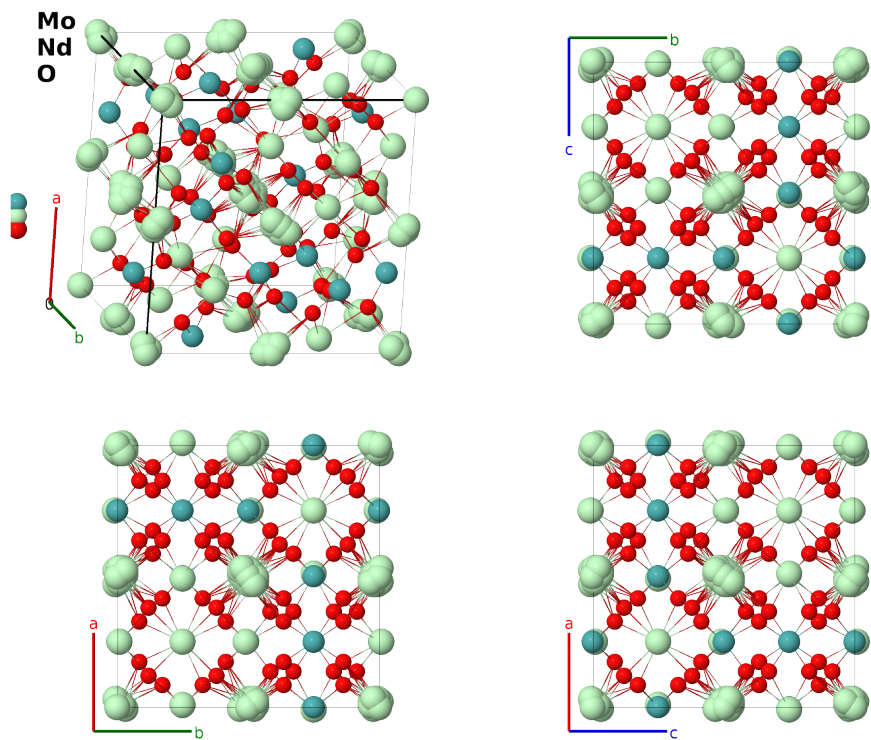
Nd₅Mo₃O₁₆ Structure: A3B17C16_cP144_222_d_cei-fi-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, 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/5VRX>

https://aflow.org/prototype-encyclopedia/A3B17C16_cP144_222_d_cei-fi-001

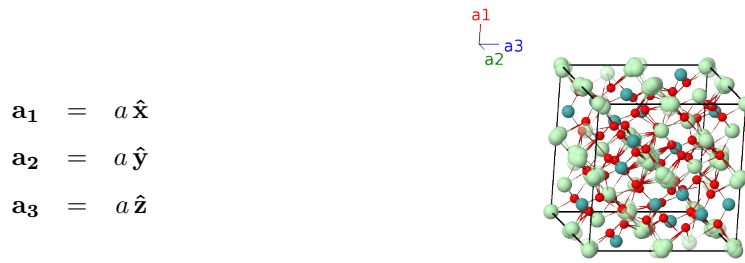


Prototype	Mo ₃ Nd ₅ O ₁₆
AFLOW prototype label	A3B17C16_cP144_222_d_cei-fi-001
ICSD	424717
CCDC	1735410
Pearson symbol	cP144
Space group number	222
Space group symbol	$Pn\bar{3}n$
AFLOW prototype command	<pre>aflow --proto=A3B17C16_cP144_222_d_cei-fi-001 --params=a, x₃, x₄, x₅, y₅, z₅, x₆, y₆, z₆</pre>

- There is considerable disorder in this structure.

- The Nd I (2c) site is occupied 92.7% of the time, while the Nd III (48i) site is occupied 1.21% of the time. These atoms nearly overlap, so we can think of them as forming an Nd I/III complex, where most of the time the (2c) site is occupied, but on rare occasions the atom occupies one of the (48i) sites. For modeling purposes it is easier to assume the (2c) sites are fully occupied and the (48i) sites are vacant, with the (2c) atoms having a very large thermal parameter U .
 - The Mo I (2d) site is occupied 96.4% of the time.
 - 95.2% of the O II (48i) sites are filled.
 - The Nd II (12d) and O I (16f) sites are fully occupied.
- These occupancies make the observed stoichiometry $\text{Nd}_{5.19}\text{Mg}_3\text{O}_{14.96}$. If we ignore the Nd III atoms and fully occupy the other sites we have $\text{Nd}_5\text{Mg}_3\text{O}_{16}$, the claimed stoichiometry, and the structure would be nearly identical to $\text{Ce}_5\text{Mo}_3\text{O}_{16}$.
 - We use the data taken at 110K.

Simple Cubic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(8c)	Nd I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(8c)	Nd I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(8c)	Nd I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(8c)	Nd I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	(8c)	Nd I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(8c)	Nd I
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	(8c)	Nd I
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	(8c)	Nd I
$\mathbf{B}_9$	$= \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{11}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{12}$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{13}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}}$	(12d)	Mo I
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{17}$	$= \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d)	Mo I
$\mathbf{B}_{18}$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(12d)	Mo I

$\mathbf{B}_{88} =$	$(y_5 + \frac{1}{2}) \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(y_5 + \frac{1}{2}) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} - az_5 \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{89} =$	$-x_5 \mathbf{a}_1 - z_5 \mathbf{a}_2 + (y_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{90} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - z_5 \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - az_5 \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{91} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 + (y_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{92} =$	$-x_5 \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_2 - y_5 \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + a(z_5 + \frac{1}{2}) \hat{\mathbf{y}} - ay_5 \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{93} =$	$-z_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{94} =$	$-z_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$-az_5 \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{95} =$	$(z_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a(z_5 + \frac{1}{2}) \hat{\mathbf{x}} - ay_5 \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{96} =$	$(z_5 + \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 + (x_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(z_5 + \frac{1}{2}) \hat{\mathbf{x}} + a(y_5 + \frac{1}{2}) \hat{\mathbf{y}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	Nd III
$\mathbf{B}_{97} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{98} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{99} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 + y_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{100} =$	$x_6 \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{101} =$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{102} =$	$z_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{103} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{104} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{105} =$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{106} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + z_6 \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{107} =$	$y_6 \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{108} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{109} =$	$y_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{110} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{111} =$	$y_6 \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{112} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{113} =$	$x_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(48i)	O II
$\mathbf{B}_{114} =$ </					

$$\begin{aligned}
\mathbf{B}_{121} &= -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}} - az_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{122} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{123} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{124} &= -x_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{125} &= -z_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= -az_6 \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{126} &= -z_6 \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -az_6 \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{127} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 - y_6 \mathbf{a}_3 &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{128} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 - x_6 \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{129} &= -y_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= -ay_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{130} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{131} &= -y_6 \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -ay_6 \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{132} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 - x_6 \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{133} &= -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}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{134} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{135} &= -y_6 \mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_2 - z_6 \mathbf{a}_3 &= -ay_6 \hat{\mathbf{x}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{136} &= \left(y_6 + \frac{1}{2}\right) \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3 &= a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{137} &= -x_6 \mathbf{a}_1 - z_6 \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{138} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 - z_6 \mathbf{a}_2 - y_6 \mathbf{a}_3 &= a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{139} &= \left(x_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_3 &= 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}} & (48i) & \text{O II} \\
\mathbf{B}_{140} &= -x_6 \mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right) \mathbf{a}_2 - y_6 \mathbf{a}_3 &= -ax_6 \hat{\mathbf{x}} + a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{141} &= -z_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= -az_6 \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + a \left(x_6 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{142} &= -z_6 \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 - x_6 \mathbf{a}_3 &= -az_6 \hat{\mathbf{x}} + a \left(y_6 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{143} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 - y_6 \mathbf{a}_2 - x_6 \mathbf{a}_3 &= a \left(z_6 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}} & (48i) & \text{O II} \\
\mathbf{B}_{144} &= \left(z_6 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_6 + \frac{1}{2}\right) \mathbf{a}_3 &= 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}} & (48i) & \text{O II}
\end{aligned}$$

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).