Li_2WO_4 (II) Structure: A2B4C_tI112_141_fg_2hi_h-001

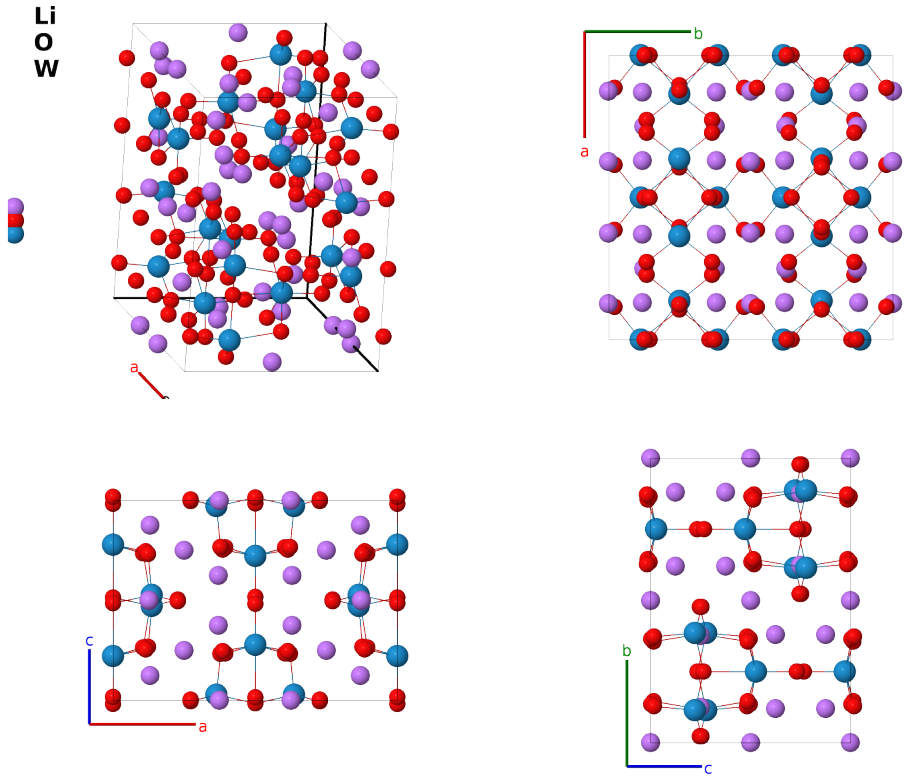
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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. 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/M4CM

https://aflow.org/prototype-encyclopedia/A2B4C_tI112_141_fg_2hi_h-001

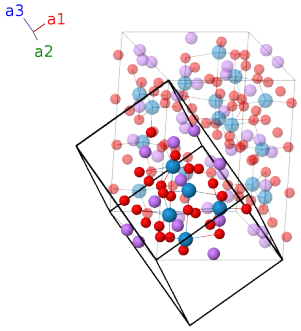


Prototype	Li_2O_4W
AFLOW prototype label	A2B4C_tI112_141_fg_2hi_h-001
ICSD	10479
CCDC	1595311
Pearson symbol	tI112
Space group number	141
Space group symbol	$I4_1/amd$
AFLOW prototype command	`aflow --proto=A2B4C_tI112_141_fg_2hi_h-001 --params=`$a, c/a, x_1, x_2, y_3, z_3, y_4, z_4, y_5, z_5, x_6, y_6, z_6$

- Li_2WO_4 is found in a variety of phases at different pressures and temperatures (Yamaoka, 1973; Pistorius, 1975):
- Li_2WO_4(I), which is in the Phenakite ($S1_3$) structure, is stable at low pressures and temperatures above 300°C.
- Tetragonal Li_2WO_4(II) (this structure) is the ground state, and is stable below a line from (300°C, 0 kBar) to (650°C, 2 kBar) to (550°C, 12 kBar) to (380°C, 15 kBar).
- Orthorhombic Li_2WO_4(III) is the high temperature structure for all pressures above phases II and IV. Its exact crystal structure has not been determined. It has been conjectured to be in space group $Pna2_1$ #33, $Pnnm$ #58 or $Cmmm$ #65.
- Monoclinic Li_2WO_4(IV), stable at pressures higher than phase II and temperatures lower than phase III.
- Later (Hämmer, 2022) determined the structure of triclinic Li_2WO_4 (V) (this structure), which may be the phase (Belyaev, 1961) observed at ambient pressure above 660°C.
- (Horiuchi, 1979) state that this structure is similar to spinel ($H1_4$).
- The ICSD assigns this structure to the Bi_2CdO_4 prototype, but these structures do not even have the same sets of occupied Wyckoff positions, so we give Li_2WO_4 (II) its own prototype.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(16f)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(16f)	Li I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	Li I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_1 - \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	Li I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(16f)	Li I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(16f)	Li I
$\mathbf{B_7}$	=	$-x_1\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	Li I
$\mathbf{B_8}$	=	$x_1\,\mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + a\left(x_1 + \frac{1}{4}\right)\,\hat{\mathbf{y}} - \frac{1}{4}c\,\hat{\mathbf{z}}$	(16f)	Li I
$\mathbf{B_9}$	=	$\left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_2 + \left(2x_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_2 - \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16g)	Li II
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_2 + \frac{1}{4}\right)\,\hat{\mathbf{y}} + \frac{3}{8}c\,\hat{\mathbf{z}}$	(16g)	Li II
$\mathbf{B_{11}}$	=	$\left(x_2 + \frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	Li II
$\mathbf{B_{12}}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{8}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	Li II
$\mathbf{B_{13}}$	=	$-\left(x_2 - \frac{7}{8}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{8}\right)\,\mathbf{a}_2 - \left(2x_2 - \frac{3}{4}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{3}{4}\right)\,\hat{\mathbf{y}} + \frac{1}{8}c\,\hat{\mathbf{z}}$	(16g)	Li II

$$\mathbf{B_{14}} = \left(x_2+\tfrac{7}{8}\right)\mathbf{a}_1+\left(x_2+\tfrac{1}{8}\right)\mathbf{a}_2+\left(2x_2+\tfrac{3}{4}\right)\mathbf{a}_3 = ax_2\,\hat{\mathbf{x}}+a\left(x_2+\tfrac{3}{4}\right)\hat{\mathbf{y}}+\tfrac{1}{8}c\,\hat{\mathbf{z}} \quad (16g) \quad \text{Li II}$$

$$\mathbf{B_{15}} = -\left(x_2-\tfrac{1}{8}\right)\mathbf{a}_1+\left(x_2+\tfrac{7}{8}\right)\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3 = a\left(x_2+\tfrac{1}{2}\right)\hat{\mathbf{x}}-a\left(x_2+\tfrac{1}{4}\right)\hat{\mathbf{y}}+\tfrac{3}{8}c\,\hat{\mathbf{z}} \quad (16g) \quad \text{Li II}$$

$$\mathbf{B_{16}} = \left(x_2+\tfrac{1}{8}\right)\mathbf{a}_1-\left(x_2-\tfrac{7}{8}\right)\mathbf{a}_2+\tfrac{1}{4}\mathbf{a}_3 = -a\left(x_2-\tfrac{1}{2}\right)\hat{\mathbf{x}}+a\left(x_2-\tfrac{1}{4}\right)\hat{\mathbf{y}}+\tfrac{3}{8}c\,\hat{\mathbf{z}} \quad (16g) \quad \text{Li II}$$

$$\mathbf{B_{17}} = (y_3+z_3)\,\mathbf{a}_1+z_3\,\mathbf{a}_2+y_3\,\mathbf{a}_3 = ay_3\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{18}} = \left(-y_3+z_3+\tfrac{1}{2}\right)\mathbf{a}_1+z_3\,\mathbf{a}_2-\left(y_3-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_3-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{19}} = z_3\,\mathbf{a}_1+\left(-y_3+z_3+\tfrac{1}{2}\right)\mathbf{a}_2-y_3\,\mathbf{a}_3 = -a\left(y_3-\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_3+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{20}} = z_3\,\mathbf{a}_1+(y_3+z_3)\,\mathbf{a}_2+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_3-\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{21}} = \left(y_3-z_3+\tfrac{1}{2}\right)\mathbf{a}_1-z_3\,\mathbf{a}_2+\left(y_3+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_3+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{22}} = -(y_3+z_3)\,\mathbf{a}_1-z_3\,\mathbf{a}_2-y_3\,\mathbf{a}_3 = -ay_3\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{23}} = -z_3\,\mathbf{a}_1+\left(y_3-z_3+\tfrac{1}{2}\right)\mathbf{a}_2+y_3\,\mathbf{a}_3 = a\left(y_3+\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_3-\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{24}} = -z_3\,\mathbf{a}_1-(y_3+z_3)\,\mathbf{a}_2-\left(y_3-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_3-\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_3+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O I}$$

$$\mathbf{B_{25}} = (y_4+z_4)\,\mathbf{a}_1+z_4\,\mathbf{a}_2+y_4\,\mathbf{a}_3 = ay_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{26}} = \left(-y_4+z_4+\tfrac{1}{2}\right)\mathbf{a}_1+z_4\,\mathbf{a}_2-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_4-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{27}} = z_4\,\mathbf{a}_1+\left(-y_4+z_4+\tfrac{1}{2}\right)\mathbf{a}_2-y_4\,\mathbf{a}_3 = -a\left(y_4-\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_4+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{28}} = z_4\,\mathbf{a}_1+(y_4+z_4)\,\mathbf{a}_2+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_4+\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_4-\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{29}} = \left(y_4-z_4+\tfrac{1}{2}\right)\mathbf{a}_1-z_4\,\mathbf{a}_2+\left(y_4+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_4+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{30}} = -(y_4+z_4)\,\mathbf{a}_1-z_4\,\mathbf{a}_2-y_4\,\mathbf{a}_3 = -ay_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{31}} = -z_4\,\mathbf{a}_1+\left(y_4-z_4+\tfrac{1}{2}\right)\mathbf{a}_2+y_4\,\mathbf{a}_3 = a\left(y_4+\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4-\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{32}} = -z_4\,\mathbf{a}_1-(y_4+z_4)\,\mathbf{a}_2-\left(y_4-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_4-\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_4+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{O II}$$

$$\mathbf{B_{33}} = (y_5+z_5)\,\mathbf{a}_1+z_5\,\mathbf{a}_2+y_5\,\mathbf{a}_3 = ay_5\,\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{34}} = \left(-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_1+z_5\,\mathbf{a}_2-\left(y_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_5-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_5\,\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{35}} = z_5\,\mathbf{a}_1+\left(-y_5+z_5+\tfrac{1}{2}\right)\mathbf{a}_2-y_5\,\mathbf{a}_3 = -a\left(y_5-\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{36}} = z_5\,\mathbf{a}_1+(y_5+z_5)\,\mathbf{a}_2+\left(y_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_5+\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{4}a\,\hat{\mathbf{y}}+c\left(z_5-\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{37}} = \left(y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_1-z_5\,\mathbf{a}_2+\left(y_5+\tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_5+\tfrac{1}{2}\right)\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{38}} = -(y_5+z_5)\,\mathbf{a}_1-z_5\,\mathbf{a}_2-y_5\,\mathbf{a}_3 = -ay_5\,\hat{\mathbf{y}}-cz_5\,\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{39}} = -z_5\,\mathbf{a}_1+\left(y_5-z_5+\tfrac{1}{2}\right)\mathbf{a}_2+y_5\,\mathbf{a}_3 = a\left(y_5+\tfrac{1}{4}\right)\hat{\mathbf{x}}-\tfrac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_5-\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{40}} = -z_5\,\mathbf{a}_1-(y_5+z_5)\,\mathbf{a}_2-\left(y_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_5-\tfrac{1}{4}\right)\hat{\mathbf{x}}+\tfrac{1}{4}a\,\hat{\mathbf{y}}-c\left(z_5+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (16h) \quad \text{W I}$$

$$\mathbf{B_{41}} = (y_6+z_6)\,\mathbf{a}_1+(x_6+z_6)\,\mathbf{a}_2+(x_6+y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}}+ay_6\,\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{42}} = \left(-y_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_1-(x_6-z_6)\,\mathbf{a}_2-\left(x_6+y_6-\tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}}-a\left(y_6-\tfrac{1}{2}\right)\hat{\mathbf{y}}+cz_6\,\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{43}} = (x_6+z_6)\,\mathbf{a}_1+\left(-y_6+z_6+\tfrac{1}{2}\right)\mathbf{a}_2+(x_6-y_6)\,\mathbf{a}_3 = -a\left(y_6-\tfrac{1}{4}\right)\hat{\mathbf{x}}+a\left(x_6-\tfrac{1}{4}\right)\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{4}\right)\hat{\mathbf{z}} \quad (32i) \quad \text{O III}$$

$$\mathbf{B_{44}} = -(x_6 - z_6)\,\mathbf{a}_1 + (y_6 + z_6)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_6 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_6 - \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_6 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{45}} = \left(y_6 - z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + a\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{46}} = -(y_6 + z_6)\,\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{47}} = (x_6 - z_6)\,\mathbf{a}_1 + \left(y_6 - z_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3 = a\left(y_6 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_6 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{48}} = -(x_6 + z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 - \left(x_6 + y_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_6 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_6 - \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_6 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{49}} = -(y_6 + z_6)\,\mathbf{a}_1 - (x_6 + z_6)\,\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{50}} = \left(y_6 - z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_6 - z_6)\,\mathbf{a}_2 + \left(x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} + a\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{51}} = -(x_6 + z_6)\,\mathbf{a}_1 + \left(y_6 - z_6 + \tfrac{1}{2}\right)\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3 = a\left(y_6 + \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_6 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{52}} = (x_6 - z_6)\,\mathbf{a}_1 - (y_6 + z_6)\,\mathbf{a}_2 + \left(x_6 - y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = -a\left(y_6 - \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_6 + \tfrac{1}{4}\right)\hat{\mathbf{y}} - c\left(z_6 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{53}} = \left(-y_6 + z_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + \left(x_6 - y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = ax_6\,\hat{\mathbf{x}} - a\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{54}} = (y_6 + z_6)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - (x_6 - y_6)\,\mathbf{a}_3 = -ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{55}} = -(x_6 - z_6)\,\mathbf{a}_1 + \left(-y_6 + z_6 + \tfrac{1}{2}\right)\mathbf{a}_2 - (x_6 + y_6)\,\mathbf{a}_3 = -a\left(y_6 - \tfrac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_6 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

$$\mathbf{B_{56}} = (x_6 + z_6)\,\mathbf{a}_1 + (y_6 + z_6)\,\mathbf{a}_2 + \left(x_6 + y_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = a\left(y_6 + \tfrac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_6 + \tfrac{1}{4}\right)\hat{\mathbf{y}} + c\left(z_6 - \tfrac{1}{4}\right)\hat{\mathbf{z}} \quad \text{(32i)} \quad \text{O III}$$

References

[1] H. Horiuchi, N. Morimoto, and S. Yamaoka, *The crystal structure of Li2WO4II: A structure related to spinel*, J. Solid State Chem. **30**, 129–135 (1979), doi:10.1016/0022-4596(79)90094-X.

[2] S. Yamaoka, O. Fukunaga, T. Ono, E. Iizuka, and S. Asami, *Phase Transformations of Li_2WO_4 at High Pressure*, J. Solid State Chem. **6**, 280–285 (1973), doi:10.1016/0022-4596(73)90191-6.

[3] C. W. F. T. Pistorius, *Phase Behavior of Li_2WO_4 at High Pressures and Temperatures*, J. Solid State Chem. **13**, 325–329 (1975), doi:10.1016/0022-4596(75)90147-4.

[4] M. Hämmer and H. A. Höppe, *New Insights into Alkali Metal Tungstates: The High Temperature Polymorphism of Na_2WO_4, the New Polymorph Li_2WO_4-V and the Redetermined Crystal Structure of $Li_2W_2O_7$*, Z. Anorganische und Allgemeine Chemie **648**, 202100373 (2022), doi:10.1002/zaac.202100373.

[5] I. N. Belyaev, , Russ. J. Inorg. Chem. **6**, 602 (1961).

Found in

[1] H. Horiuchi, N. Morimoto, and S. Yamaoka, *The crystal structure of Li_2WO_4(IV) and its relation to the wolframite-type structure*, J. Solid State Chem. **35**, 115–119 (1980), doi:10.1016/0022-4596(80)90554-X.

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).