

Li₂WO₄ (V) Structure:

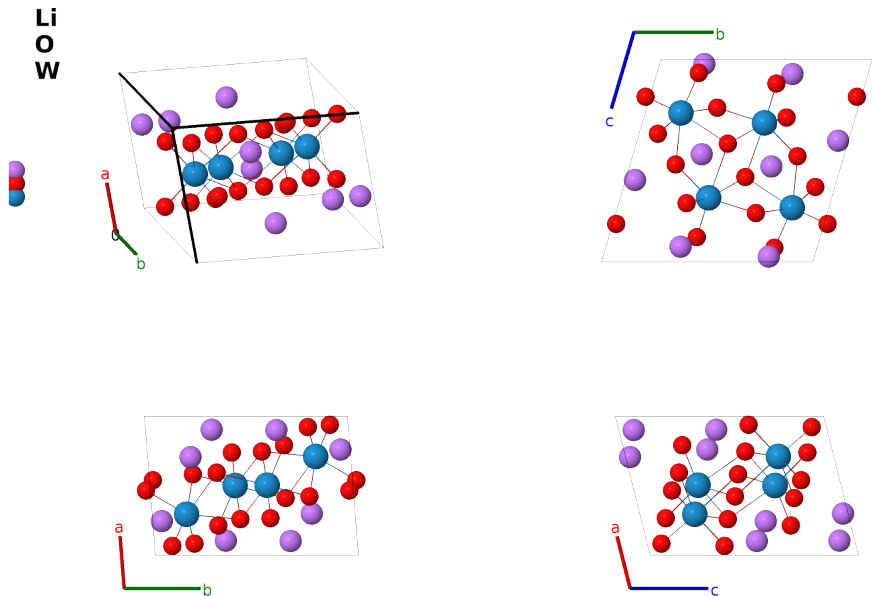
A2B4C_aP28_2_4i_8i_2i-001

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/X8JU>

https://aflow.org/prototype-encyclopedia/A2B4C_aP28_2_4i_8i_2i-001



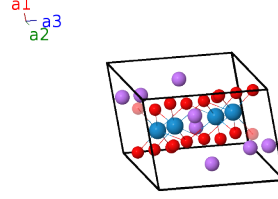
Prototype	Li ₂ O ₄ W
AFLOW prototype label	A2B4C_aP28_2_4i_8i_2i-001
ICSD	46287
CCDC	2126944
Pearson symbol	aP28
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=A2B4C_aP28_2_4i_8i_2i-001 --params=a,b/a,c/a,α,β,γ,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆, z₆,x₇,y₇,z₇,x₈,y₈,z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄</pre>

- Li₂WO₄ is found in a variety of phases at different pressures and temperatures (Yamaoka, 1973; Pistorius, 1975):
- Li₂WO₄(I), which is in the Phenakite (S_{13}) structure, is stable at low pressures and temperatures above 300°C.

- Tetragonal $\text{Li}_2\text{WO}_4(\text{II})$ 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 $\text{Li}_2\text{WO}_4(\text{III})$ 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 $\text{Li}_2\text{WO}_4(\text{IV})$, 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.

Triclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= a \hat{\mathbf{x}} \\
\mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
c_x &= c \cos \beta \\
c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(2i)	Li I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} - (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} - c_z z_1 \hat{\mathbf{z}}$	(2i)	Li I
$\mathbf{B}_3$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(2i)	Li II
$\mathbf{B}_4$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} - (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} - c_z z_2 \hat{\mathbf{z}}$	(2i)	Li II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	Li III
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	Li III
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	Li IV
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	Li IV
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	O I
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	O II
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(2i)	O III

$\mathbf{B}_{14}$	$=$	$-x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$	(2i)	O III
$\mathbf{B}_{15}$	$=$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B}_{16}$	$=$	$-x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}}$	(2i)	O IV
$\mathbf{B}_{17}$	$=$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B}_{18}$	$=$	$-x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}}$	(2i)	O V
$\mathbf{B}_{19}$	$=$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(2i)	O VI
$\mathbf{B}_{20}$	$=$	$-x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} - (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} - c_z z_{10} \hat{\mathbf{z}}$	(2i)	O VI
$\mathbf{B}_{21}$	$=$	$x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}}$	(2i)	O VII
$\mathbf{B}_{22}$	$=$	$-x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} - (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} - c_z z_{11} \hat{\mathbf{z}}$	(2i)	O VII
$\mathbf{B}_{23}$	$=$	$x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} + (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} + c_z z_{12} \hat{\mathbf{z}}$	(2i)	O VIII
$\mathbf{B}_{24}$	$=$	$-x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} - (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} - c_z z_{12} \hat{\mathbf{z}}$	(2i)	O VIII
$\mathbf{B}_{25}$	$=$	$x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} + (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} + c_z z_{13} \hat{\mathbf{z}}$	(2i)	W I
$\mathbf{B}_{26}$	$=$	$-x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} - (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} - c_z z_{13} \hat{\mathbf{z}}$	(2i)	W I
$\mathbf{B}_{27}$	$=$	$x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} + (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} + c_z z_{14} \hat{\mathbf{z}}$	(2i)	W II
$\mathbf{B}_{28}$	$=$	$-x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} - (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} - c_z z_{14} \hat{\mathbf{z}}$	(2i)	W II

References

- [1] M. Hämmer and H. A. Höpfe, *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 $\text{Li}_2\text{W}_2\text{O}_7$* , Z. Anorganische und Allgemeine Chemie **648**, 202100373 (2022), doi:10.1002/zaac.202100373.
- [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] I. N. Belyaev, , Russ. J. Inorg. Chem. **6**, 602 (1961).

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).