Wodginite (LiFe(WO$_4$)$_2$) Structure: ABC8D2_mC48_15_e_e_4f_f-001
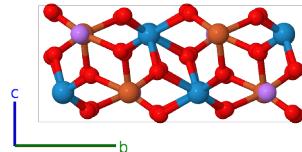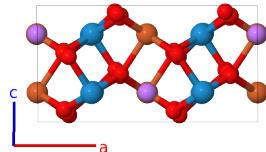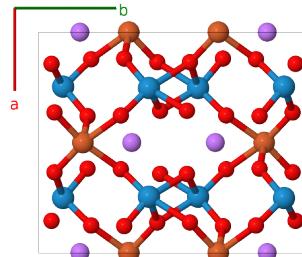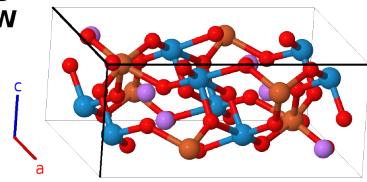
Prototype	FeLiO$_8$W$_2$
AFLOW prototype label	ABC8D2_mC48_15_e_e_4f_f-001
Mineral name	wodginite
ICSD	262314
Pearson symbol	mC48
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	aflow --proto=ABC8D2_mC48_15_e_e_4f_f-001
	--params=$a, b/a, c/a, \beta, y_1, y_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7$

Other compounds with this structure

MnSn(TaO$_4$)$_2$ (wodginite)

- We use the structural data taken by (Biesenkamp, 2021) at 38K.

- The ICSD entry is from the earlier work of (Albinao, 2012).

- We use this as an example of the mineral wodginite. As with all such minerals there is a wide range of disorder on the metallic sites. For more information on wodginite see (Ercit, 1992) and the papers immediately following it in the *Canadian Mineralogist*.

Base-centered Monoclinic primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
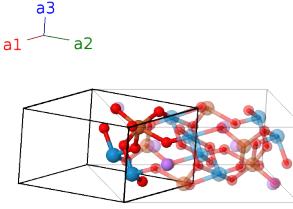
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a_1} + y_1\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	=	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_2}$	=	$y_1\,\mathbf{a_1} - y_1\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	=	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Fe I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a_1} + y_2\,\mathbf{a_2} + \tfrac{1}{4}\,\mathbf{a_3}$	=	$\tfrac{1}{4}c\cos\beta\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + \tfrac{1}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Li I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a_1} - y_2\,\mathbf{a_2} + \tfrac{3}{4}\,\mathbf{a_3}$	=	$\tfrac{3}{4}c\cos\beta\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + \tfrac{3}{4}c\sin\beta\,\hat{\mathbf{z}}$	(4e)	Li I
$\mathbf{B_5}$	=	$(x_3 - y_3)\,\mathbf{a_1} + (x_3 + y_3)\,\mathbf{a_2} + z_3\,\mathbf{a_3}$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_6}$	=	$-(x_3 + y_3)\,\mathbf{a_1} - (x_3 - y_3)\,\mathbf{a_2} - \left(z_3 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_3 + c\left(z_3 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_7}$	=	$-(x_3 - y_3)\,\mathbf{a_1} - (x_3 + y_3)\,\mathbf{a_2} - z_3\,\mathbf{a_3}$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_8}$	=	$(x_3 + y_3)\,\mathbf{a_1} + (x_3 - y_3)\,\mathbf{a_2} + \left(z_3 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_3 + c\left(z_3 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O I
$\mathbf{B_9}$	=	$(x_4 - y_4)\,\mathbf{a_1} + (x_4 + y_4)\,\mathbf{a_2} + z_4\,\mathbf{a_3}$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{10}}$	=	$-(x_4 + y_4)\,\mathbf{a_1} - (x_4 - y_4)\,\mathbf{a_2} - \left(z_4 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_4 + c\left(z_4 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{11}}$	=	$-(x_4 - y_4)\,\mathbf{a_1} - (x_4 + y_4)\,\mathbf{a_2} - z_4\,\mathbf{a_3}$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a_1} + (x_4 - y_4)\,\mathbf{a_2} + \left(z_4 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_4 + c\left(z_4 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	=	$(x_5 - y_5)\,\mathbf{a_1} + (x_5 + y_5)\,\mathbf{a_2} + z_5\,\mathbf{a_3}$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{14}}$	=	$-(x_5 + y_5)\,\mathbf{a_1} - (x_5 - y_5)\,\mathbf{a_2} - \left(z_5 - \tfrac{1}{2}\right)\mathbf{a_3}$	=	$-\left(ax_5 + c\left(z_5 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - c\left(z_5 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{15}}$	=	$-(x_5 - y_5)\,\mathbf{a_1} - (x_5 + y_5)\,\mathbf{a_2} - z_5\,\mathbf{a_3}$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{16}}$	=	$(x_5 + y_5)\,\mathbf{a_1} + (x_5 - y_5)\,\mathbf{a_2} + \left(z_5 + \tfrac{1}{2}\right)\mathbf{a_3}$	=	$\left(ax_5 + c\left(z_5 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	O III
$\mathbf{B_{17}}$	=	$(x_6 - y_6)\,\mathbf{a_1} + (x_6 + y_6)\,\mathbf{a_2} + z_6\,\mathbf{a_3}$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8f)	O IV

$$\mathbf{B_{18}} = -(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - \left(z_6 - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_6 + c\left(z_6 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - c\left(z_6 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{O IV}$$

$$\mathbf{B_{19}} = -(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -\left(ax_6 + cz_6\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{O IV}$$

$$\mathbf{B_{20}} = (x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \left(z_6 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_6 + c\left(z_6 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + c\left(z_6 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{O IV}$$

$$\mathbf{B_{21}} = (x_7 - y_7)\,\mathbf{a}_1 + (x_7 + y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \left(ax_7 + cz_7\cos\beta\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{W I}$$

$$\mathbf{B_{22}} = -(x_7 + y_7)\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - \left(z_7 - \tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_7 + c\left(z_7 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - c\left(z_7 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{W I}$$

$$\mathbf{B_{23}} = -(x_7 - y_7)\,\mathbf{a}_1 - (x_7 + y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\left(ax_7 + cz_7\cos\beta\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{W I}$$

$$\mathbf{B_{24}} = (x_7 + y_7)\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + \left(z_7 + \tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_7 + c\left(z_7 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + c\left(z_7 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \qquad \text{(8f)} \qquad \text{W I}$$

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[3] T. S. Ercit, F. C. Hawthorne, and P. Černý, *The wodginite group. I. Structural crystallography*, Can. Mineral. **30**, 597–611 (1992).