Weberite (Na_2MgAlF_7) Structure: AB7CD2_oI44_24_a_c3d_b_ab-001

This structure originally had the label `AB7CD2_oI44_24_a_b3d_c_ac`. Calls to that address will be redirected here.

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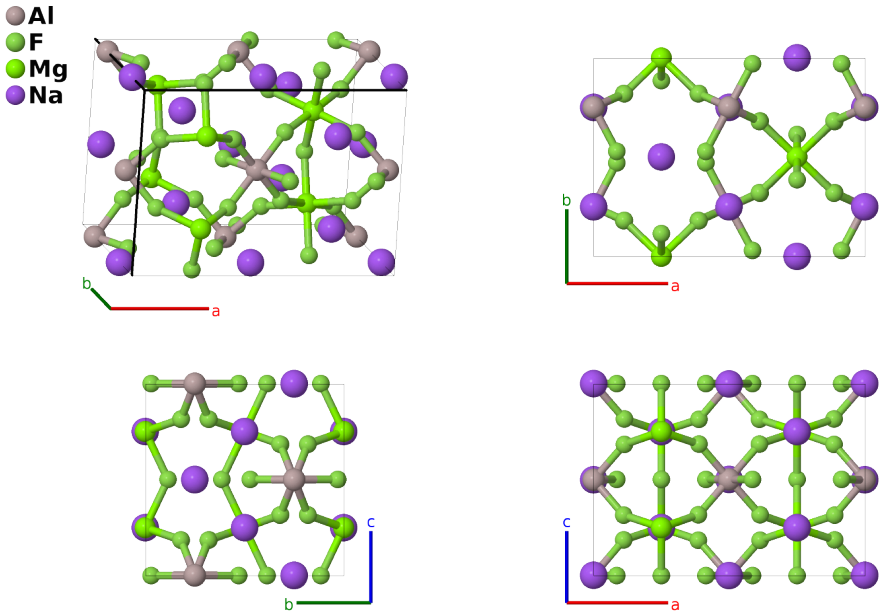
https://aflow.org/p/Q6TN

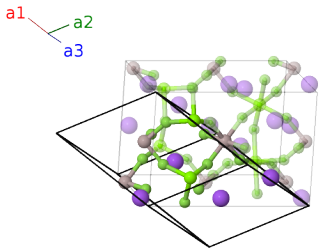
https://aflow.org/p/AB7CD2_oI44_24_a_c3d_b_ab-001



Prototype	AlF_7MgNa_2
AFLOW prototype label	AB7CD2_oI44_24_a_c3d_b_ab-001
Mineral name	weberite
ICSD	33512
Pearson symbol	oI44
Space group number	24
Space group symbol	$I2_12_12_1$
AFLOW prototype command	`aflow --proto=AB7CD2_oI44_24_a_c3d_b_ab-001 --params=`$a, b/a, c/a, x_1, x_2, y_3, y_4, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_1 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_1 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Al I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \left(x_2 + \frac{1}{4}\right)\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 - \left(x_2 - \frac{1}{4}\right)\,\mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Na I
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}}$	(4b)	Mg I
$\mathbf{B_6}$	=	$-\left(y_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Mg I
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \left(y_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}}$	(4b)	Na II
$\mathbf{B_8}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - \left(y_4 - \frac{1}{4}\right)\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4b)	Na II
$\mathbf{B_9}$	=	$\left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}b\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B_{10}}$	=	$-\left(z_5 - \frac{1}{4}\right)\,\mathbf{a}_1 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(4c)	F I
$\mathbf{B_{11}}$	=	$(y_6 + z_6)\,\mathbf{a}_1 + (x_6 + z_6)\,\mathbf{a}_2 + (x_6 + y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	F II
$\mathbf{B_{12}}$	=	$\left(-y_6 + z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_6 - z_6)\,\mathbf{a}_2 - \left(x_6 + y_6 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8d)	F II
$\mathbf{B_{13}}$	=	$(y_6 - z_6)\,\mathbf{a}_1 - \left(x_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_6 + y_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8d)	F II
$\mathbf{B_{14}}$	=	$-\left(y_6 + z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_6 - z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_6 - y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	F II
$\mathbf{B_{15}}$	=	$(y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	F III
$\mathbf{B_{16}}$	=	$\left(-y_7 + z_7 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - \left(x_7 + y_7 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8d)	F III
$\mathbf{B_{17}}$	=	$(y_7 - z_7)\,\mathbf{a}_1 - \left(x_7 + z_7 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_7 + y_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_7 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8d)	F III
$\mathbf{B_{18}}$	=	$-\left(y_7 + z_7 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_7 - z_7 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	F III
$\mathbf{B_{19}}$	=	$(y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8d)	F IV
$\mathbf{B_{20}}$	=	$\left(-y_8 + z_8 + \frac{1}{2}\right)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - \left(x_8 + y_8 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8d)	F IV

$\mathbf{B_{21}}$	=	$(y_8 - z_8)\,\mathbf{a}_1 - \left(x_8 + z_8 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_8 + y_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_8 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8d)	F IV
$\mathbf{B_{22}}$	=	$-\left(y_8 + z_8 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_8 - z_8 + \frac{1}{2}\right)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	F IV

References

[1] O. Knop, T. S. Cameron, and K. Jochem, *What is the True Space Group of Weberite?*, J. Solid State Chem. **43**, 213–221 (1982), doi:10.1016/0022-4596(82)90231-6.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.