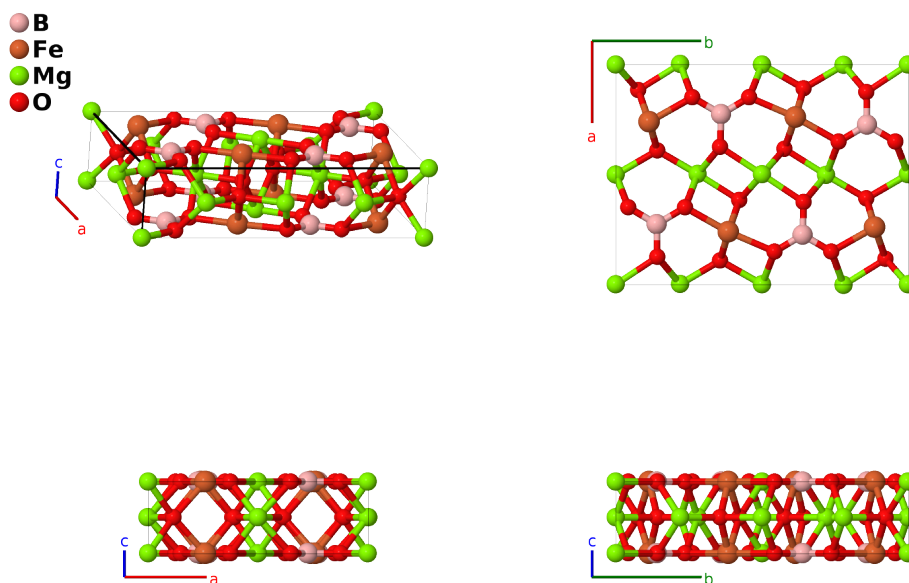


Ludwigite (Mg_2FeBO_5) Structure: ABC2D5_oP36_55_g_g_adh_3g2h-001

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<https://aflow.org/p/A5YT>

https://aflow.org/p/ABC2D5_oP36_55_g_g_adh_3g2h-001



Prototype	BFeMg_2O_5
AFLOW prototype label	ABC2D5_oP36_55_g_g_adh_3g2h-001
Mineral name	ludwigite
ICSD	87761
Pearson symbol	oP36
Space group number	55
Space group symbol	$Pbam$
AFLOW prototype command	<pre>aflow --proto=ABC2D5_oP36_55_g_g_adh_3g2h-001 --params=a, b/a, c/a, x3, y3, x4, y4, x5, y5, x6, y6, x7, y7, x8, y8, x9, y9, x10, y10</pre>

Other compounds with this structure

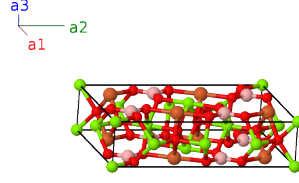
Cu_2AlBO_5 , Cu_2GaBO_5 , Co_2AlBO_5 , Co_2SnBO_5 , Co_3BO_5 , Fe_3BO_5 , Mg_2InBO_5 , Mg_2MnBO_5 , Mn_2CoBO_5 , Ni_2CrBO_5 , Ni_2FeBO_5 (bonaccordite), Ni_2SnBO_5 , Ni_2VBO_5

- The stoichiometry of the metallic atoms should not be taken as exact, *e.g.*, the actual composition of the reference compound is $\text{Mg}_{1.76}\text{Fe}_{1.22}\text{Al}_{0.02}\text{BO}_5$. (Irwin, 1999)

- The Mg-I (2a) site has the composition $\text{Mg}_{0.99}\text{Fe}_{0.01}$, the Mg-II (2d) site $\text{Fe}_{0.557}\text{Mg}_{0.443}$, the Mg-III (2g) site $\text{Mg}_{0.99}\text{Fe}_{0.01}$, and the Fe-I (4h) site $\text{Fe}_{0.92}\text{Al}_{0.08}$.

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= 0$	$=$	0	(2a)	Mg I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}}$	(2a)	Mg I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2d)	Mg II
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2d)	Mg II
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}}$	(4g)	B I
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}}$	(4g)	B I
\mathbf{B}_7	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	B I
\mathbf{B}_8	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	B I
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}}$	(4g)	Fe I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}}$	(4g)	Fe I
\mathbf{B}_{11}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Fe I
\mathbf{B}_{12}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	Fe I
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}}$	(4g)	O I
\mathbf{B}_{14}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}}$	(4g)	O I
\mathbf{B}_{15}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O I
\mathbf{B}_{16}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O I
\mathbf{B}_{17}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}}$	(4g)	O II
\mathbf{B}_{18}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2$	$=$	$-ax_6 \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}}$	(4g)	O II
\mathbf{B}_{19}	$= -(x_6 - \frac{1}{2}) \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O II
\mathbf{B}_{20}	$= (x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O II
\mathbf{B}_{21}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}}$	(4g)	O III
\mathbf{B}_{22}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2$	$=$	$-ax_7 \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}}$	(4g)	O III
\mathbf{B}_{23}	$= -(x_7 - \frac{1}{2}) \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O III
\mathbf{B}_{24}	$= (x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}}$	(4g)	O III
\mathbf{B}_{25}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Mg III
\mathbf{B}_{26}	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Mg III
\mathbf{B}_{27}	$= -(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4h)	Mg III

$$\begin{aligned}
\mathbf{B}_{28} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{Mg III} \\
\mathbf{B}_{29} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{30} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{31} &= -(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{32} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O IV} \\
\mathbf{B}_{33} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O V} \\
\mathbf{B}_{34} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O V} \\
\mathbf{B}_{35} &= -(x_{10} - \frac{1}{2}) \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O V} \\
\mathbf{B}_{36} &= (x_{10} + \frac{1}{2}) \mathbf{a}_1 - (y_{10} - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = a(x_{10} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{10} - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} & (4h) & \text{O V}
\end{aligned}$$

References

- [1] M. B. Irwin and R. C. Peterson, *The Crystal Structure of Ludwigite*, Can. Mineral. **37**, 939–943 (1999).