

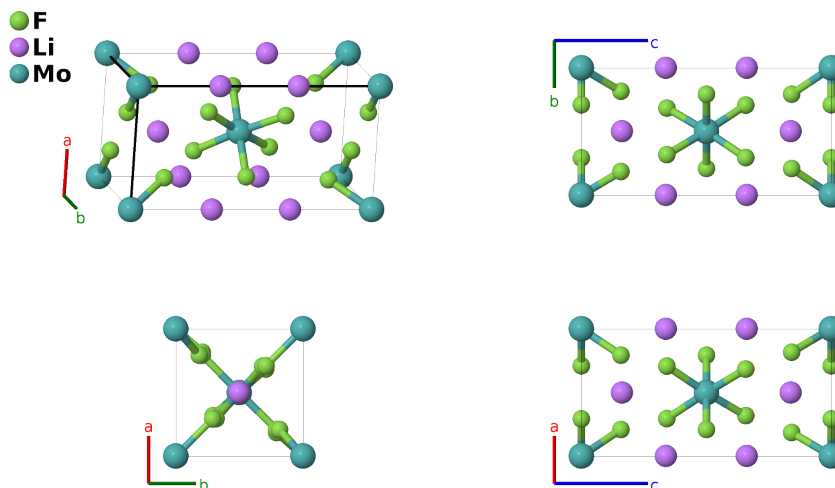
Li₂MoF₆ Structure: A6B2C_tP18_94_eg_c_a-001

This structure originally had the label A6B2C_tP18_94_eg_c_a. Calls to that address will be redirected here.

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<https://aflow.org/p/1ZGT>

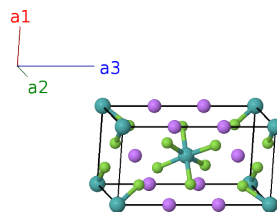
https://aflow.org/p/A6B2C_tP18_94_eg_c_a-001



Prototype	F ₆ Li ₂ Mo
AFLOW prototype label	A6B2C_tP18_94_eg_c_a-001
ICSD	23173
Pearson symbol	tP18
Space group number	94
Space group symbol	<i>P</i> 4 ₂ 2 ₁ 2
AFLOW prototype command	aflow --proto=A6B2C_tP18_94_eg_c_a-001 --params= <i>a</i> , <i>c/a</i> , <i>z</i> ₂ , <i>x</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄

Simple Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates	=	Cartesian coordinates	=	Wyckoff position	Atom type
\mathbf{B}_1	=	0	=	0	(2a)	Mo I
\mathbf{B}_2	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Mo I
\mathbf{B}_3	=	$z_2 \mathbf{a}_3$	=	$cz_2 \hat{\mathbf{z}}$	(4c)	Li I
\mathbf{B}_4	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Li I
\mathbf{B}_5	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Li I
\mathbf{B}_6	=	$-z_2 \mathbf{a}_3$	=	$-cz_2 \hat{\mathbf{z}}$	(4c)	Li I
\mathbf{B}_7	=	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4e)	F I
\mathbf{B}_8	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4e)	F I
\mathbf{B}_9	=	$-(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	F I
\mathbf{B}_{10}	=	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4e)	F I
\mathbf{B}_{11}	=	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{12}	=	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{13}	=	$-(y_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$-a(y_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{14}	=	$(y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$a(y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{15}	=	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{16}	=	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{17}	=	$y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	F II
\mathbf{B}_{18}	=	$-y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(8g)	F II

References

- [1] G. Brunton, *The Crystal Structure of Li_2MoF_6* , Mater. Res. Bull. **6**, 555–560 (1971), doi:10.1016/0025-5408(71)90004-3.

Found in

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