Li_2MoF_6 Structure: A6B2C_tP18_94_eg_c_a-001

This structure previously used the label(s) `A6B2C_tP18_94_eg_c_a`. Calls to these addresses will be redirected here.

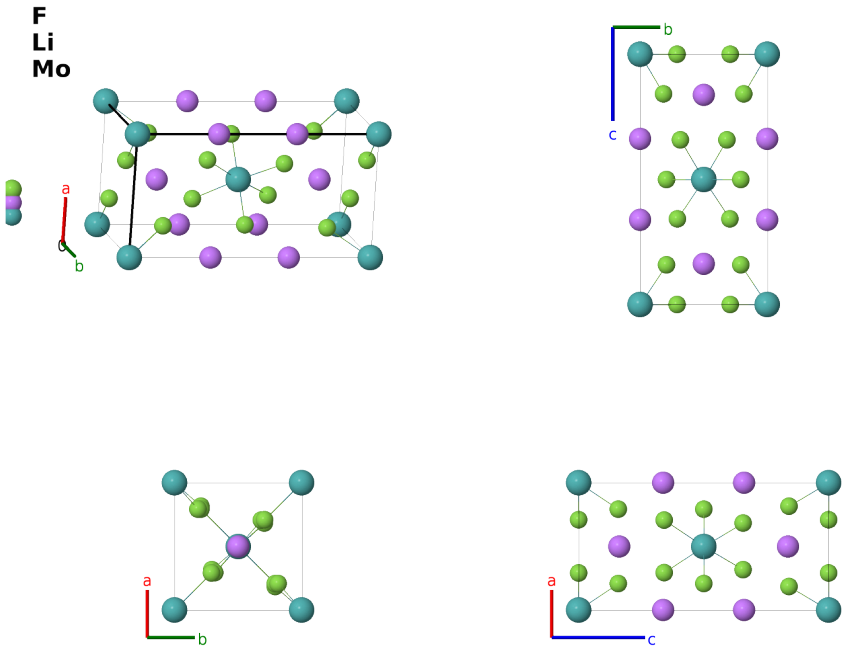
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, 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. Oses, 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/1ZGT

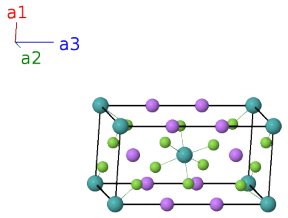
https://aflow.org/prototype-encyclopedia/A6B2C_tP18_94_eg_c_a-001



Prototype	F_6Li_2Mo
AFLOW prototype label	A6B2C_tP18_94_eg_c_a-001
ICSD	23173
CCDC	1599316
Pearson symbol	tP18
Space group number	94
Space group symbol	$P4_22_12$
AFLOW prototype command	`aflow --proto=A6B2C_tP18_94_eg_c_a-001 --params=`$a, c/a, z_2, x_3, x_4, y_4, z_4$

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Li I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_9}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4e)	F I
$\mathbf{B_{10}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{13}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{14}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{15}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8g)	F II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043