

Li₂CuO₂ Structure:

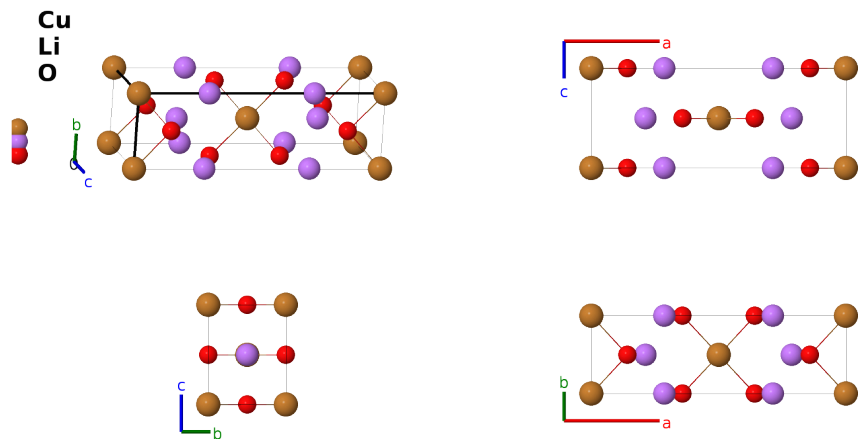
AB2C2_oI10_71_a_e_f-002

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<https://aflow.org/prototype-encyclopedia/7P5Q>

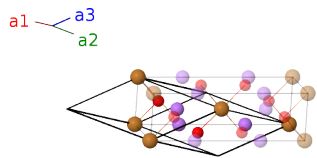
https://aflow.org/prototype-encyclopedia/AB2C2_oI10_71_a_e_f-002



Prototype	CuLi ₂ O ₂
AFLOW prototype label	AB2C2_oI10_71_a_e_f-002
ICSD	67204
CCDC	1629222
Pearson symbol	oI10
Space group number	71
Space group symbol	<i>Immm</i>
AFLOW prototype command	<code>aflow --proto=AB2C2_oI10_71_a_e_f-002</code> <code>--params=a,b/a,c/a,x₂,x₃</code>

Body-centered Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= -\frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} - \frac{1}{2}b\hat{y} + \frac{1}{2}c\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}b\hat{y} - \frac{1}{2}c\hat{z} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	Cu I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}}$	Li I
$\mathbf{B}_3$	$=$	$-x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}}$	Li I
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + x_3 \mathbf{a}_2 + (x_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	O I
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1 - x_3 \mathbf{a}_2 - (x_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$	O I

References

- [1] F. Sapina, J. Rodríguez-Carvajal, M. J. Sanchis, R. Ibáñez, A. Beltrán, and D. Beltrán, *Crystal and magnetic structure of Li_2CuO_2* , Solid State Commun. **74**, 779–784 (1990), doi:10.1016/0038-1098(90)90934-4.

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