

Face-Centered Orthorhombic La_2CuO_4 Structure:

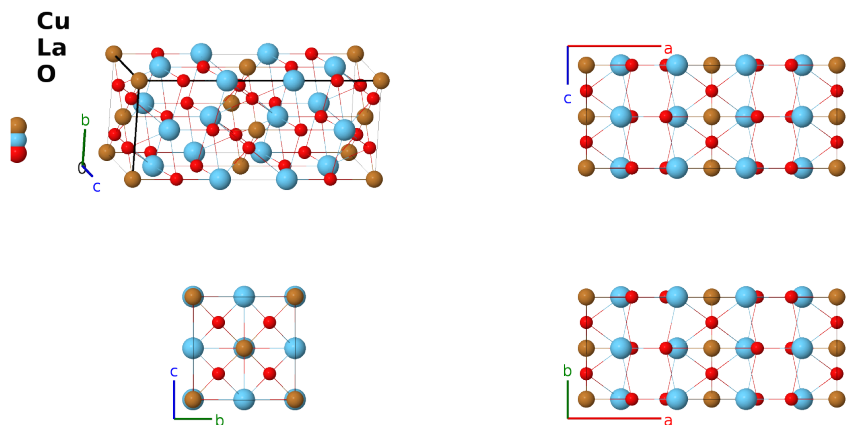
AB2C4_oF28_69_a_g_cg-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, 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. Osas, 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/LB5P>

https://aflow.org/prototype-encyclopedia/AB2C4_oF28_69_a_g_cg-001



Prototype	CuLa_2O_4
AFLOW prototype label	AB2C4_oF28_69_a_g_cg-001
ICSD	19003
CCDC	1597781
Pearson symbol	oF28
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	<code>aflow --proto=AB2C4_oF28_69_a_g_cg-001</code> <code>--params=a, b/a, c/a, x3, x4</code>

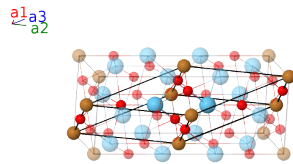
- We have found three possible structures for La_2CuO_4 , the parent compound of the high-temperature cuprate superconductors. All are distortions of the tetragonal $\text{K}_2\text{NiF}_4/0201$ $[(\text{La},\text{Ba})_2\text{CuO}_4]$ High- T_c Structure, and reduce to that structure with doping of the lanthanum site:
 - (Longo, 1973) proposed an face-centered orthorhombic structure (this structure).
 - Later other workers, including (Reehuis, 2006) and references therein, proposed a base-centered orthorhombic structure.
 - (Reehuis, 2006) found that a base-centered monoclinic structure was a better fit to their neutron diffraction data.
- As the two orthorhombic structures are both referenced in the literature, we present them, as well as the more recent monoclinic structure.

Face-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}b\hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}c\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}b\hat{\mathbf{y}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(4a) Cu I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1$	=	$\frac{1}{4}b\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8c) O I
$\mathbf{B}_3$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}b\hat{\mathbf{y}} + \frac{1}{4}c\hat{\mathbf{z}}$	(8c) O I
$\mathbf{B}_4$	=	$-x_3\mathbf{a}_1 + x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	=	$ax_3\hat{\mathbf{x}}$	(8g) La I
$\mathbf{B}_5$	=	$x_3\mathbf{a}_1 - x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	=	$-ax_3\hat{\mathbf{x}}$	(8g) La I
$\mathbf{B}_6$	=	$-x_4\mathbf{a}_1 + x_4\mathbf{a}_2 + x_4\mathbf{a}_3$	=	$ax_4\hat{\mathbf{x}}$	(8g) O II
$\mathbf{B}_7$	=	$x_4\mathbf{a}_1 - x_4\mathbf{a}_2 - x_4\mathbf{a}_3$	=	$-ax_4\hat{\mathbf{x}}$	(8g) O II

References

- [1] J. M. Longo and P. M. Raccach, *The structure of La_2CuO_4 and LaSrVO_4* , J. Solid State Chem. **6**, 526–531 (1973), doi:10.1016/S0022-4596(73)80010-6.
- [2] M. Reehuis, C. Ulrich, K. Prokeš, A. Gozar, G. Blumberg, S. Komiya, Y. Ando, P. Pattison, and B. Keimer, *Crystal structure and high-field magnetism of La_2CuO_4* , Phys. Rev. B **73**, 144513 (2006), doi:10.1103/PhysRevB.73.144513.

First cited in

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.