Face-Centered Orthorhombic La_2CuO_4 Structure: AB2C4_oF28_69_a_g_cg-001

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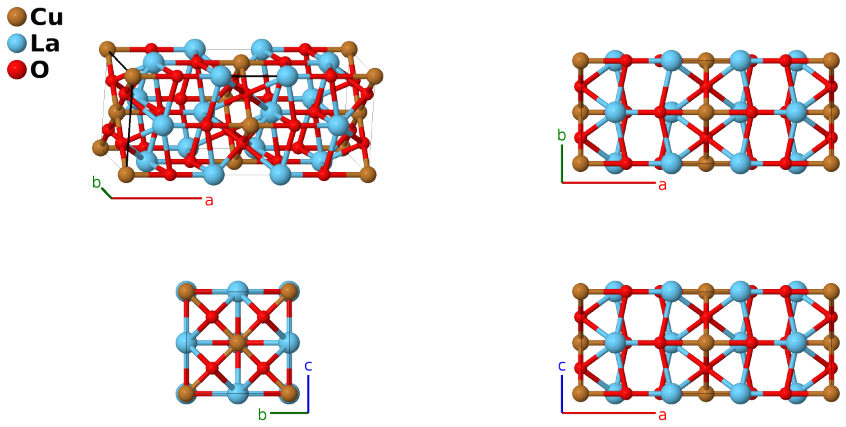
https://aflow.org/p/LB5P

https://aflow.org/p/AB2C4_oF28_69_a_g_cg-001

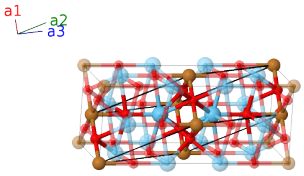


Prototype	$CuLa_2O_4$
AFLOW prototype label	AB2C4_oF28_69_a_g_cg-001
ICSD	19003
Pearson symbol	oF28
Space group number	69
Space group symbol	$Fmmm$
AFLOW prototype command	`aflow --proto=AB2C4_oF28_69_a_g_cg-001 --params=`$a, b/a, c/a, x_3, x_4$

- 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 K_2NiF_4/0201 [$(La,Ba)_2CuO_4$] 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. Raccah, *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.