

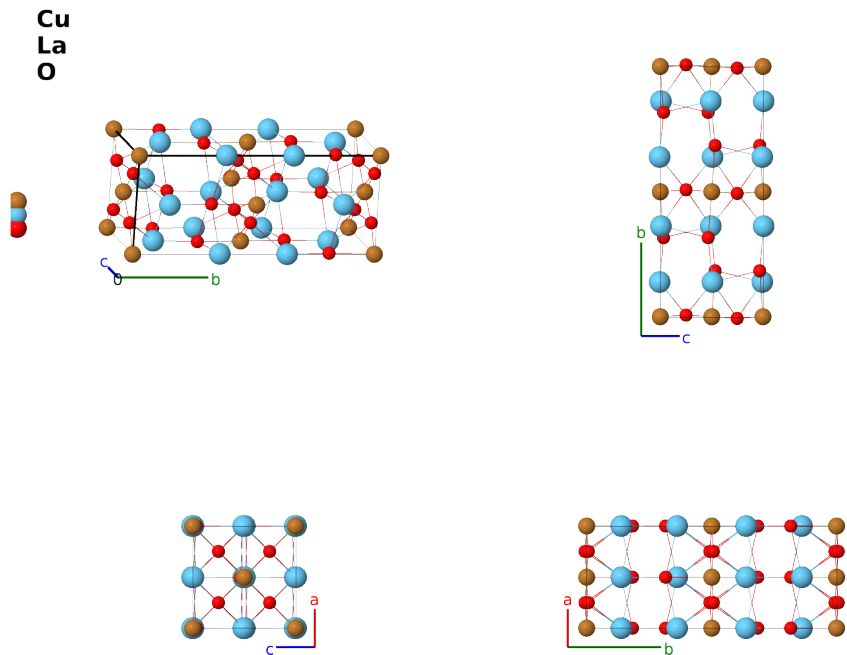
Base-Centered Orthorhombic La_2CuO_4 Structure: AB2C4_oC28_64_a_f_ef-003

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. 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/Y6BX>

https://aflow.org/prototype-encyclopedia/AB2C4_oC28_64_a_f_ef-003



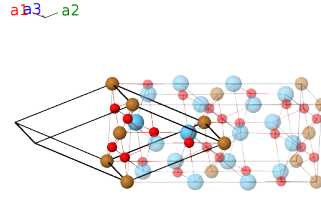
Prototype	CuLa_2O_4
AFLOW prototype label	AB2C4_oC28_64_a_f_ef-003
ICSD	155496
CCDC	1672107
Pearson symbol	oC28
Space group number	64
Space group symbol	$Cmce$
AFLOW prototype command	<code>aflow --proto=AB2C4_oC28_64_a_f_ef-003</code> <code>--params=a, b/a, c/a, y2, y3, z3, y4, z4</code>

Other compounds with this structure
 La_2NiO_4 , Nd_2CeO_4 , $\text{Sc}_2(\text{La}, \text{Sr})\text{O}_4$

- 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 $\text{K}_2\text{NiF}_4/0201$ $[(\text{La},\text{Ba})_2\text{CuO}_4]$ High- T_c Structure, and reduce to that structure with doping of the lanthanum site:
 - (Longo, 1973) proposed a face-centered orthorhombic structure.
 - Later other workers, including (Reehuis, 2006) and references therein, proposed a base-centered orthorhombic structure (this 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.
- (Reehuis, 2006) gave the structure of the base-centered phase in the $Bmab$ setting of space group #64. We used FINDSYM to transform it to the standard $Cmca$ setting.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= 0$	$=$	0	(4a)	Cu I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B}_3$	$= -\left(y_2 - \frac{1}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_4$	$= \left(y_2 + \frac{1}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_5$	$= \left(y_2 + \frac{3}{4}\right) \mathbf{a}_1 - \left(y_2 - \frac{3}{4}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_6$	$= -\left(y_2 - \frac{3}{4}\right) \mathbf{a}_1 + \left(y_2 + \frac{3}{4}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B}_7$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_8$	$= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_9$	$= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_{10}$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8f)	La I
$\mathbf{B}_{11}$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B}_{12}$	$= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8f)	O II

$$\mathbf{B}_{13} = -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \begin{matrix} \\ (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

$$\mathbf{B}_{14} = y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 = -by_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} \quad (8f) \quad \text{O II}$$

References

- [1] 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.
- [2] 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.

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.