

Base-Centered Monoclinic La_2CuO_4 Structure:

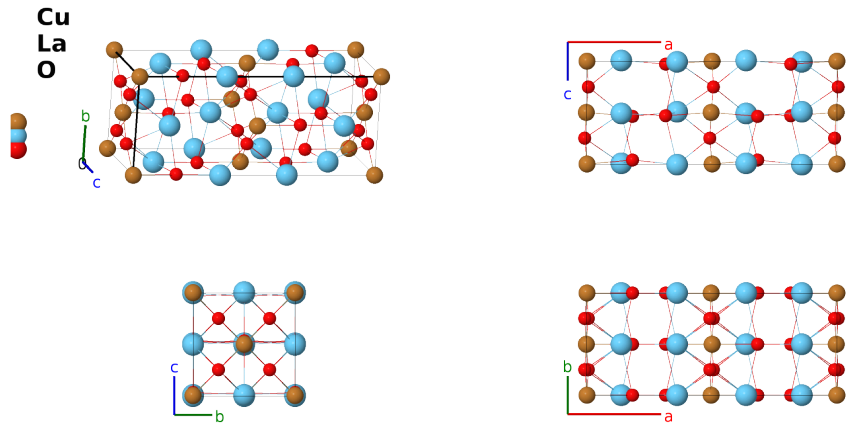
AB2C4_mC28_8_2a_4a_4a2b-001

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. Osos, 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/T7TZ>

https://aflow.org/prototype-encyclopedia/AB2C4_mC28_8_2a_4a_4a2b-001



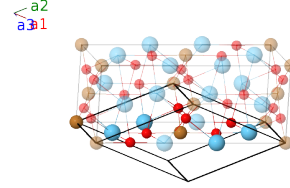
Prototype	CuLa_2O_4
AFLOW prototype label	AB2C4_mC28_8_2a_4a_4a2b-001
ICSD	155497
CCDC	1672108
Pearson symbol	mC28
Space group number	8
Space group symbol	Cm
AFLOW prototype command	<pre>aflow --proto=AB2C4_mC28_8_2a_4a_4a2b-001 --params=a,b/a,c/a,beta,x1,z1,x2,z2,x3,z3,x4,z4,x5,z5,x6,z6,x7,z7,x8,z8,x9,z9,x10, z10,x11,y11,z11,x12,y12,z12</pre>

- 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 $\text{K}_2\text{NiF}_4/0201$ $[(\text{La,Ba})_2\text{CuO}_4]$ 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.
 - (Reehuis, 2006) found that this 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 monoclinic phase in the Bm , unique axis a , setting of space group #8. We used FINDSYM to transform it to the standard Cm , unique axis b setting. Although they never give a value, we assume $\alpha = 90^\circ$, as the other lattice parameters are the same as in the $Cmca$ phase.
- (Rehuis, 2006) made several mistakes in the labeling of the Wyckoff positions in the $Bm11$ section of Table I:
 - The copper sites labeled (4a) are actually (2a).
 - The oxygen sites labeled (4a) are actually (4b).

Base-centered Monoclinic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B}_2$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Cu II
$\mathbf{B}_3$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	La I
$\mathbf{B}_4$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	La II
$\mathbf{B}_5$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	La III
$\mathbf{B}_6$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	La IV
$\mathbf{B}_7$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_8$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_9$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{10}$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{11}$	$(x_{11} - y_{11}) \mathbf{a}_1 +$ $(x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4b)	O V
$\mathbf{B}_{12}$	$(x_{11} + y_{11}) \mathbf{a}_1 +$ $(x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	=	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4b)	O V
$\mathbf{B}_{13}$	$(x_{12} - y_{12}) \mathbf{a}_1 +$ $(x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4b)	O VI
$\mathbf{B}_{14}$	$(x_{12} + y_{12}) \mathbf{a}_1 +$ $(x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	=	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(4b)	O VI

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.