Base-Centered Monoclinic La_2CuO_4 Structure: AB2C4_mC28_8_2a_4a_4a2b-001

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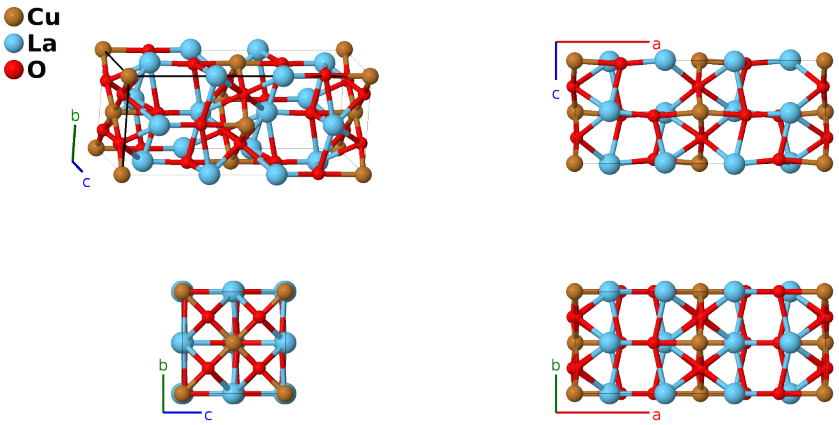
https://aflow.org/p/AB2C4_mC28_8_2a_4a_4a2b-001



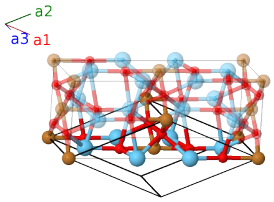
Prototype	$CuLa_2O_4$
AFLOW prototype label	AB2C4_mC28_8_2a_4a_4a2b-001
ICSD	155497
Pearson symbol	mC28
Space group number	8
Space group symbol	Cm
AFLOW prototype command	`aflow --proto=AB2C4_mC28_8_2a_4a_4a2b-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}$

- 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 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 $\alpha = 90°$, 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

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



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. 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.