Base-Centered Orthorhombic La_2CuO_4 Structure: AB2C4_oC28_64_a_f_ef-003

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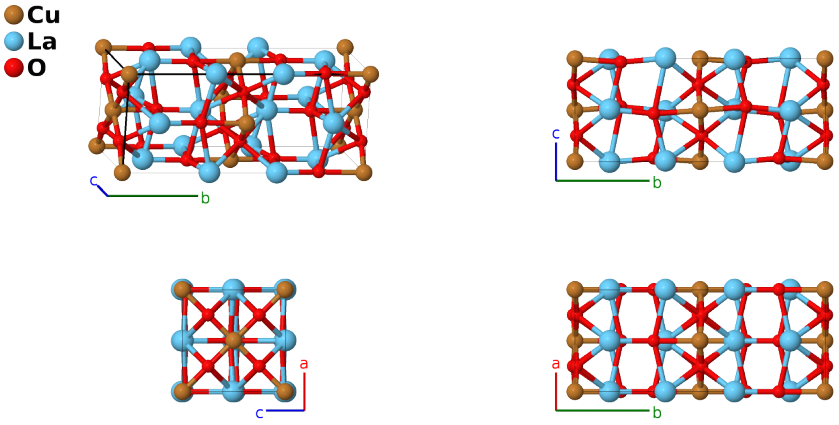
https://aflow.org/p/AB2C4_oC28_64_a_f_ef-003



Prototype	$CuLa_2O_4$
AFLOW prototype label	AB2C4_oC28_64_a_f_ef-003
ICSD	155496
Pearson symbol	oC28
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=AB2C4_oC28_64_a_f_ef-003 --params=`$a, b/a, c/a, y_2, y_3, z_3, y_4, z_4$

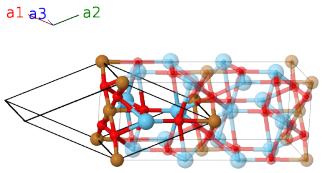
Other compounds with this structure
La_2NiO_4, Nd_2CeO_4

- 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 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

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



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
$\mathbf{B_{13}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{14}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	O II

References

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[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.