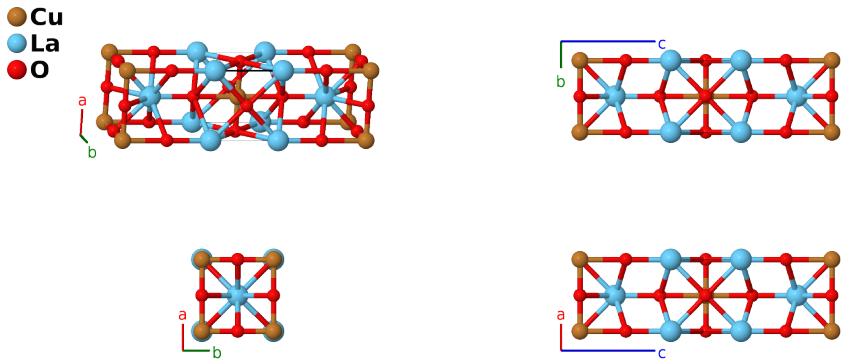
0201 [$(La,Ba)_2CuO_4$] High-T_c Structure: AB2C4_tI14_139_a_e_ce-001

This structure originally had the label `AB2C4_tI14_139_a_e_ce`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/V35A

https://aflow.org/p/AB2C4_tI14_139_a_e_ce-001



Prototype	Ba_2CuO_4
AFLOW prototype label	AB2C4_tI14_139_a_e_ce-001
ICSD	68379
Pearson symbol	tI14
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB2C4_tI14_139_a_e_ce-001 --params=`$a, c/a, z_3, z_4$

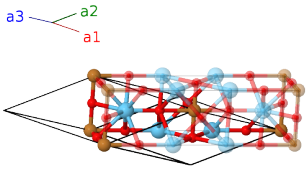
Other compounds with this structure

$Ba_2CuO_{3+\delta}$

- The original "high"-temperature (30K) superconductor found by Bednorz and Mueller. Lanthanum (92.5%) and barium (7.5%) atoms are distributed randomly on the lanthanum sublattice. The ground state structure of the parent compound, La_2CuO_4, is a face-centered orthorhombic, base-centered orthorhombic, or base-centered monoclinic distortion of this structure.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	O I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	La I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	La I
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	O II

References

[1] J. D. Jorgensen, H.-B. Schüttler, D. G. Hinks, I. D. W. Capone, K. Zhang, and M. B. Brodsky, *Lattice instability and high-T_c superconductivity in $La_{2-x}Ba_xCuO_4$*, Phys. Rev. Lett. **58**, 1024–1029 (1987), doi:10.1103/PhysRevLett.58.1024.

Found in

[1] H. Shaked, P. M. Keane, J. C. Rodrigues, F. F. Owen, R. L. Hitterman, and J. D. Jorgensen, *Crystal Structures of the High-T_c Superconducting Copper Oxides*, Elsevier Science B. V., Amsterdam (1994).