

0201 [(La,Ba)₂CuO₄] High-*T_c* Structure: AB2C4_tI14_139_a_e_ce-001

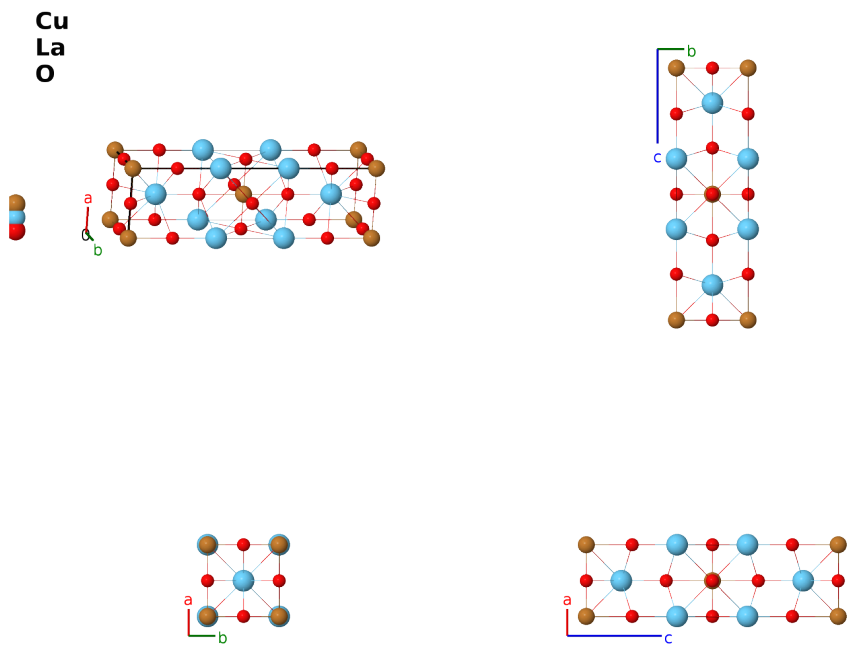
This structure previously used the label(s) **AB2C4_tI14_139_a_e_ce**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/V35A>

https://aflow.org/prototype-encyclopedia/AB2C4_tI14_139_a_e_ce-001



Prototype	Ba ₂ CuO ₄
AFLOW prototype label	AB2C4_tI14_139_a_e_ce-001
ICSD	68379
CCDC	1630306
Pearson symbol	tI14
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=AB2C4_tI14_139_a_e_ce-001</code> <code>--params=a, c/a, z₃, z₄</code>

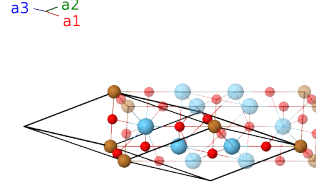
Other compounds with this structure

$\text{Ba}_2\text{CuO}_{3+\delta}$

- 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

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



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 $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$* , 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).

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