

CaCuO₂ Structure:

ABC2_tP4_123_a_d_e-001

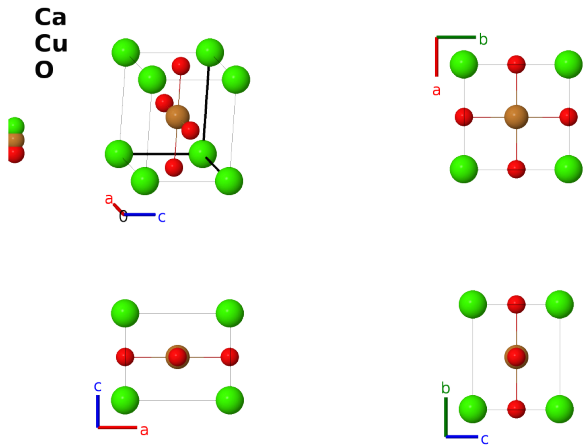
This structure previously used the label(s) **ABC2_tP4_123_d_a_f**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/ABC2_tP4_123_a_d_e-001



Prototype	CaCuO ₂
AFLOW prototype label	ABC2_tP4_123_a_d_e-001
ICSD	65066
CCDC	1627216
Pearson symbol	tP4
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	<code>aflow --proto=ABC2_tP4_123_a_d_e-001 --params=a, c/a</code>

Other compounds with this structure

(Ba, Sr)CuO₂, (Sr, La)CuO₂, (Sr, Ca)CuO₂, LaNiO₂, NdNiO₂, CsNiF₂, KNiF₂, LiNiF₂, NaNiF₂, RbNiF₂

- As noted in (Siegrist, 1988) this is the parent structure of the high-temperature cuprate superconductors.
- (Siegrist, 1988) give the composition of the Ca (1a) site as Ca_{0.86}Sr_{0.14}.
- We have shifted the origin from the Cu site to the Ca site.

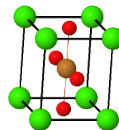
Simple Tetragonal primitive vectors

a2
a1 a3

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) Ca I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(1d) Cu I
$\mathbf{B}_3$	=	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e) O I
$\mathbf{B}_4$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} c \hat{\mathbf{z}}$	(2e) O I

References

- [1] T. Siegrist, S. M. Zahurak, D. W. Murphy, and R. S. Roth, *The parent structure of the layered high-temperature superconductors*, Nature **334**, 231–232 (1988), doi:10.1038/334231a0.

First cited in

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