

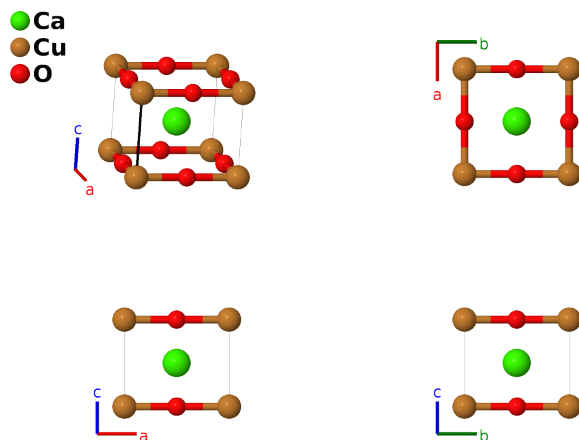
CaCuO₂ Structure: ABC2_tP4_123_a_d_e-001

This structure originally had the label ABC2_tP4_123_d_a_f. Calls to that address will be redirected here.

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<https://aflow.org/p/ACQJ>

https://aflow.org/p/ABC2_tP4_123_a_d_e-001



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

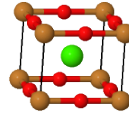
Other compounds with this structure

(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

a3
a2
a1



$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$

Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	=	0	(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.