

SrCuO₂ Structure:

AB2C_oC16_63_c_2c_c-001

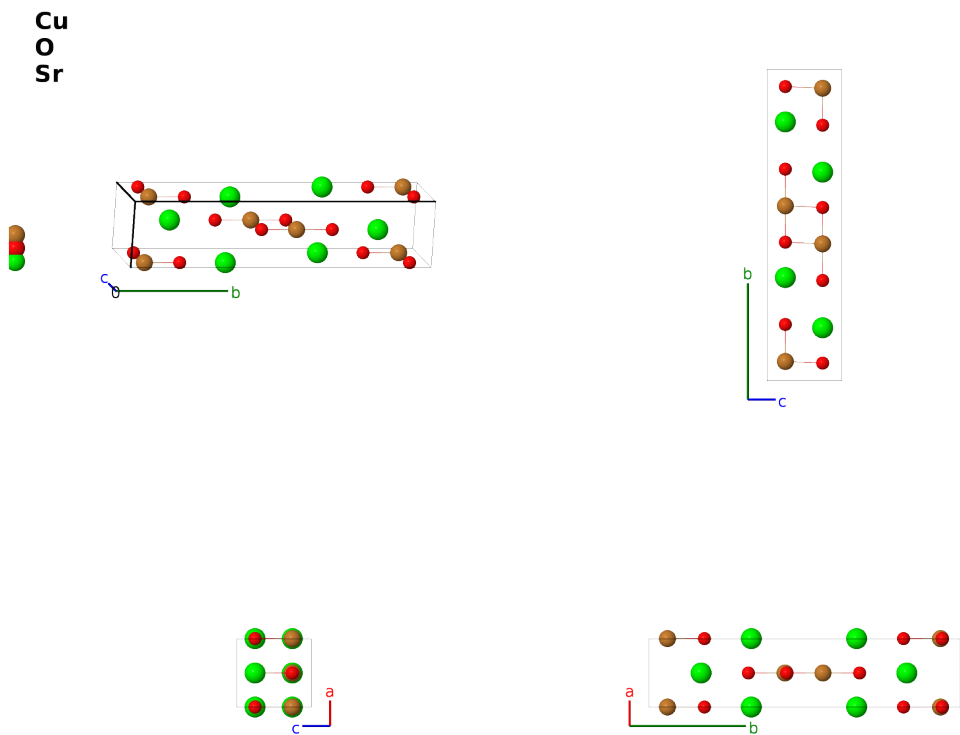
This structure previously used the label(s) **AB2C_oC16_63_c_2c_c**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/WL5U>

https://aflow.org/prototype-encyclopedia/AB2C_oC16_63_c_2c_c-001



Prototype	CuO ₂ Sr
AFLOW prototype label	AB2C_oC16_63_c_2c_c-001
ICSD	77291
CCDC	1637732
Pearson symbol	oC16
Space group number	63
Space group symbol	<i>Cmcm</i>

AFLOW prototype command `aflow --proto=AB2C_oC16_63_c_2c_c-001`
 `--params=a,b/a,c/a,y1,y2,y3,y4`

Other compounds with this structure

BCMo₂

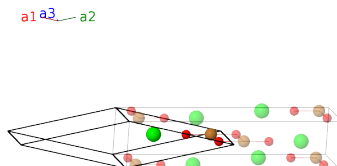
- We use the data from (Matsushita, 1994), but the ICSD is from (Heinau, 1994).
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Base-centered Orthorhombic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}}$$

$$\mathbf{a}_2 = \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}}$$

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Cu I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B}_5$	$= -y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_6$	$= y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B}_7$	$= -y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Sr I
$\mathbf{B}_8$	$= y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Sr I

References

- [1] Y. Matsushita, Y. Oyama, M. Hasegawa, and H. Takei, *Growth and Structural Refinement of Orthorhombic SrCuO₂ Crystals*, J. Solid State Chem. **114**, 289–293 (1994), doi:10.1006/jssc.1995.1043.
- [2] M. Heinau, J. R. Baumann, B. Nick, M. Hartweg, and L. Walz, *Single crystal refinements of seven Sr_{1-x}Ca_xCuO₂ structures (x=0-0.573) and of Ca_{2-y}Sr_yCuO₃*, Z. Krystallogr. **209**, 418–421 (1994), doi:10.1524/zkri.1994.209.5.418.

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