$SrCuO_2$ Structure: AB2C_oC16_63_c_2c_c-001

This structure originally had the label `AB2C_oC16_63_c_2c_c`. Calls to that address will be redirected here.

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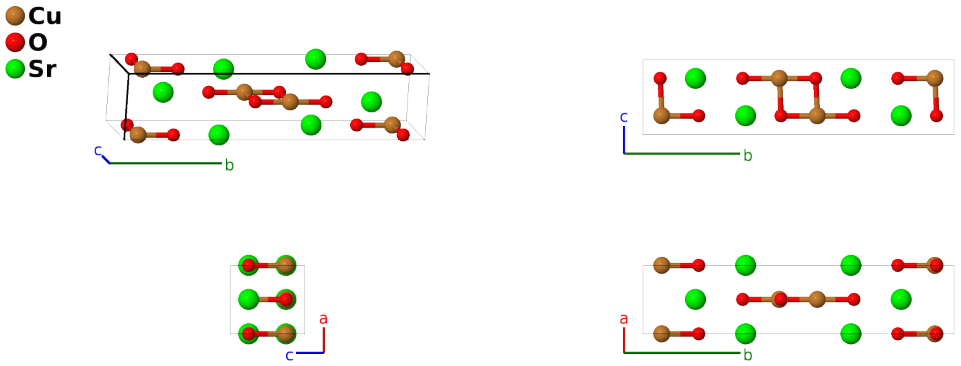
https://aflow.org/p/WL5U

https://aflow.org/p/AB2C_oC16_63_c_2c_c-001



Prototype	CuO_2Sr
AFLOW prototype label	AB2C_oC16_63_c_2c_c-001
ICSD	77291
Pearson symbol	oC16
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=AB2C_oC16_63_c_2c_c-001 --params=`$a, b/a, c/a, y_1, y_2, y_3, y_4$

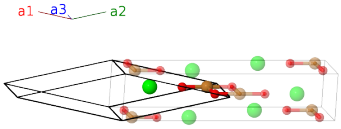
Other compounds with this structure

$BCMo_2$

- We use the data from (Matsushita, 1994), but the ICSD is from (Heinau, 1994).

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 $SrCuO_2$ 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 $Sr_{1-x}Ca_xCuO_2$ structures (x=0-0.573) and of $Ca_{2-y}Sr_yCuO_3$*, Z. Krystallogr. **209**, 418–421 (1994), doi:10.1524/zkri.1994.209.5.418.