

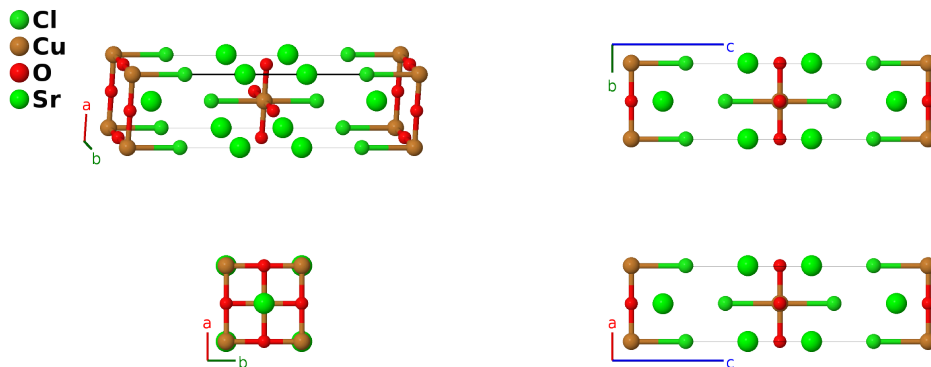
Sr₂CuO₂Cl₂ Structure:

A2BC2D2_tI14_139_e_a_c_e-001

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<https://afLOW.org/p/0HCF>

https://afLOW.org/p/A2BC2D2_tI14_139_e_a_c_e-001



Prototype	Cl ₂ CuO ₂ Sr ₂
AFLOW prototype label	A2BC2D2_tI14_139_e_a_c_e-001
ICSD	67067
Pearson symbol	tI14
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>afLOW --proto=A2BC2D2_tI14_139_e_a_c_e-001 --params=a, c/a, z₃, z₄</code>

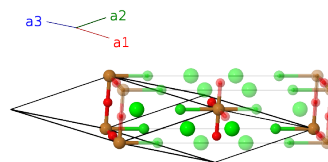
Other compounds with this structure

Ca₂CuO₂Cl₂, Na₂Fe₂Se₂O, Na₂Ti₂As₂O, Na₂Ti₂Sb₂O

- This is the quaternary form of the K₂NiF₄ structure.

Body-centered Tetragonal primitive vectors

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



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) Cl I
\mathbf{B}_5	=	$-z_3 \mathbf{a}_1 - z_3 \mathbf{a}_2$	=	$-cz_3 \hat{\mathbf{z}}$	(4e) Cl I
\mathbf{B}_6	=	$z_4 \mathbf{a}_1 + z_4 \mathbf{a}_2$	=	$cz_4 \hat{\mathbf{z}}$	(4e) Sr I
\mathbf{B}_7	=	$-z_4 \mathbf{a}_1 - z_4 \mathbf{a}_2$	=	$-cz_4 \hat{\mathbf{z}}$	(4e) Sr I

References

- [1] L. L. Miller, X. L. Wang, S. X. Wang, C. Stassis, D. C. Johnston, J. J. Faber, and C.-K. Loongo, *Synthesis, structure, and properties of $\text{Sr}_2\text{CuO}_2\text{Cl}_2$* , Phys. Rev. B **41**, 1921–1925 (1990), doi:10.1103/PhysRevB.41.1921.