

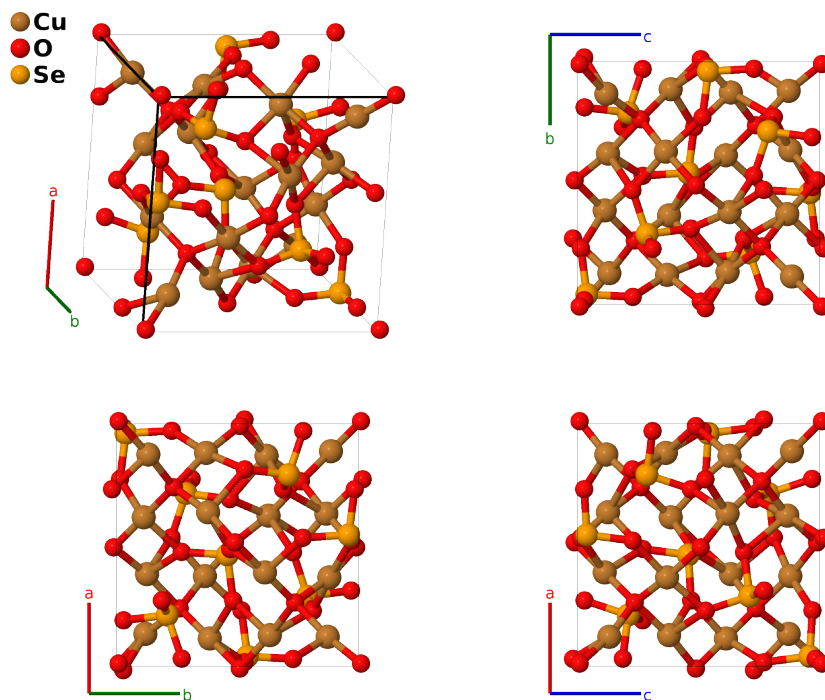
Cubic Cu_2OSeO_3 Structure: A2B4C_cP56_198_ab_2a2b_2a-001

This structure originally had the label A2B4C_cP56_198_ab_2a2b_2a. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/PZ2V>

https://aflow.org/p/A2B4C_cP56_198_ab_2a2b_2a-001

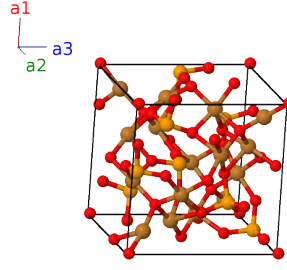


Prototype	$\text{Cu}_2\text{O}_4\text{Se}$
AFLOW prototype label	A2B4C_cP56_198_ab_2a2b_2a-001
ICSD	60652
Pearson symbol	cP56
Space group number	198
Space group symbol	$P2_13$
AFLOW prototype command	<code>aflow --proto=A2B4C_cP56_198_ab_2a2b_2a-001</code> <code>--params=a, x1, x2, x3, x4, x5, x6, y6, z6, x7, y7, z7, x8, y8, z8</code>

- This is the cubic phase of Cu_2OSeO_3 . There is also a monoclinic phase.

Simple Cubic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + a x_1 \hat{\mathbf{y}} + a x_1 \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_1 \hat{\mathbf{y}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_1 \hat{\mathbf{z}}$	(4a)	Cu I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + a x_2 \hat{\mathbf{y}} + a x_2 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_6	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_2 \hat{\mathbf{y}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_7	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_8	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_2 \hat{\mathbf{z}}$	(4a)	O I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + a x_3 \hat{\mathbf{y}} + a x_3 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{10}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{11}	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{12}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_3 \hat{\mathbf{z}}$	(4a)	O II
\mathbf{B}_{13}	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$a x_4 \hat{\mathbf{x}} + a x_4 \hat{\mathbf{y}} + a x_4 \hat{\mathbf{z}}$	(4a)	Se I
\mathbf{B}_{14}	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_4 \hat{\mathbf{y}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se I
\mathbf{B}_{15}	$= -x_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_4 \hat{\mathbf{x}} + a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se I
\mathbf{B}_{16}	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$a \left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_4 \hat{\mathbf{z}}$	(4a)	Se I
\mathbf{B}_{17}	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$a x_5 \hat{\mathbf{x}} + a x_5 \hat{\mathbf{y}} + a x_5 \hat{\mathbf{z}}$	(4a)	Se II
\mathbf{B}_{18}	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - a x_5 \hat{\mathbf{y}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se II
\mathbf{B}_{19}	$= -x_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_5 \hat{\mathbf{x}} + a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se II
\mathbf{B}_{20}	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a \left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - a x_5 \hat{\mathbf{z}}$	(4a)	Se II
\mathbf{B}_{21}	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$a x_6 \hat{\mathbf{x}} + a y_6 \hat{\mathbf{y}} + a z_6 \hat{\mathbf{z}}$	(12b)	Cu II

$$\mathbf{B}_{52} = \begin{matrix} -z_8 \mathbf{a}_1 + (x_8 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_8 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -az_8 \hat{\mathbf{x}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B}_{53} = y_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3 = ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B}_{54} = \begin{matrix} -y_8 \mathbf{a}_1 + (z_8 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_8 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ay_8 \hat{\mathbf{x}} + a(z_8 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B}_{55} = (y_8 + \frac{1}{2}) \mathbf{a}_1 - (z_8 - \frac{1}{2}) \mathbf{a}_2 - x_8 \mathbf{a}_3 = a(y_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_8 - \frac{1}{2}) \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

$$\mathbf{B}_{56} = \begin{matrix} -(y_8 - \frac{1}{2}) \mathbf{a}_1 - z_8 \mathbf{a}_2 + \\ (x_8 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(y_8 - \frac{1}{2}) \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + a(x_8 + \frac{1}{2}) \hat{\mathbf{z}} \quad (12b) \quad \text{O IV}$$

References

- [1] H. Effenberger and F. Pertlik, *Die Kristallstrukturen der Kupfer(II)-oxo-selenite $\text{Cu}_2\text{O}(\text{SeO}_3)$ (kubisch und monoklin) und $\text{Cu}_4\text{O}(\text{SeO}_3)_3$ (monoklin und triklin)*, *Monatsh. Chem.* **117**, 887–896 (1986), doi:10.1007/BF00811258.

Found in

- [1] P. Y. Portnichenko, J. Romhányi, Y. A. Onykienko, A. Henschel, M. Schmidt, A. S. Cameron, M. A. Surmach, J. A. Lim, J. T. Park, A. Schneidewind, D. L. A. 6, H. Rosner, J. van den Brink, and D. S. Inosov, *Magnon spectrum of the helimagnetic insulator Cu_2OSeO_3* , *Nature Comm.* **7**, 10725 (2016), doi:10.1038/ncomms10725.