

Cubic Cu₂OSeO₃ Structure:

A2B4C_cP56_198_ab_2a2b_2a-001

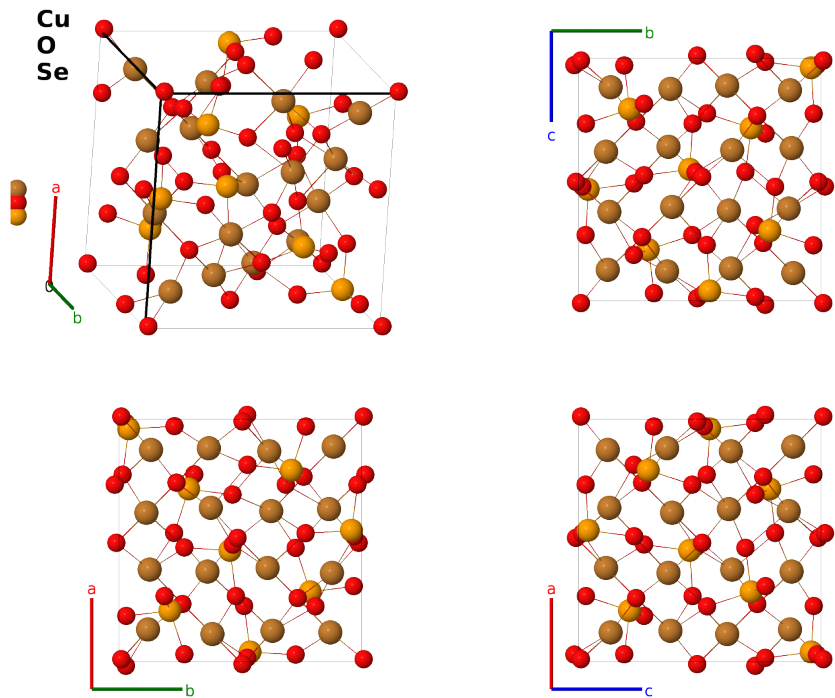
This structure previously used the label(s) **A2B4C.cP56_198_ab_2a2b_2a**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/PZ2V>

https://aflow.org/prototype-encyclopedia/A2B4C_cP56_198_ab_2a2b_2a-001



Prototype	Cu ₂ O ₄ Se
AFLOW prototype label	A2B4C_cP56_198_ab_2a2b_2a-001
ICSD	60652
CCDC	1624228
Pearson symbol	cP56
Space group number	198
Space group symbol	<i>P</i> 2 ₁ 3
AFLOW prototype command	<pre>aflow --proto=A2B4C_cP56_198_ab_2a2b_2a-001 --params=a, x₁, x₂, x₃, x₄, x₅, x₆, y₆, z₆, x₇, y₇, z₇, x₈, y₈, z₈</pre>

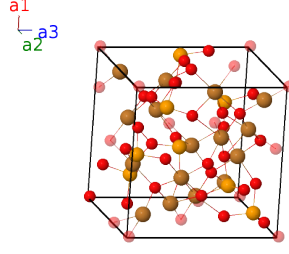
- This is the cubic phase of Cu₂OSeO₃. There is also a monoclinic phase.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + ax_1 \hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - x_1 \mathbf{a}_2 +$ $\left(x_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 - x_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_1 \hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + ax_2 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - x_2 \mathbf{a}_2 +$ $\left(x_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_2 \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + ax_3 \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - x_3 \mathbf{a}_2 +$ $\left(x_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{11}$	$= -x_3 \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{12}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_3 \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{13}$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} + ax_4 \hat{\mathbf{z}}$	(4a)	Se I
$\mathbf{B}_{14}$	$= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - x_4 \mathbf{a}_2 +$ $\left(x_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se I
$\mathbf{B}_{15}$	$= -x_4 \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se I
$\mathbf{B}_{16}$	$= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 - x_4 \mathbf{a}_3$	$=$	$a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_4 \hat{\mathbf{z}}$	(4a)	Se I
$\mathbf{B}_{17}$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + x_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + ax_5 \hat{\mathbf{z}}$	(4a)	Se II
$\mathbf{B}_{18}$	$= -\left(x_5 - \frac{1}{2}\right) \mathbf{a}_1 - x_5 \mathbf{a}_2 +$ $\left(x_5 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se II
$\mathbf{B}_{19}$	$= -x_5 \mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right) \mathbf{a}_2 -$ $\left(x_5 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4a)	Se II
$\mathbf{B}_{20}$	$= \left(x_5 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right) \mathbf{a}_2 - x_5 \mathbf{a}_3$	$=$	$a\left(x_5 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_5 \hat{\mathbf{z}}$	(4a)	Se II

$\mathbf{B}_{21} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + ay_6 \hat{\mathbf{y}} + az_6 \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{22} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - ay_6 \hat{\mathbf{y}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{23} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_6 \hat{\mathbf{x}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{24} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - az_6 \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{25} =$	$z_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + y_6 \mathbf{a}_3$	$=$	$az_6 \hat{\mathbf{x}} + ax_6 \hat{\mathbf{y}} + ay_6 \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{26} =$	$(z_6 + \frac{1}{2}) \mathbf{a}_1 - (x_6 - \frac{1}{2}) \mathbf{a}_2 - y_6 \mathbf{a}_3$	$=$	$a(z_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{y}} - ay_6 \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{27} =$	$-(z_6 - \frac{1}{2}) \mathbf{a}_1 - x_6 \mathbf{a}_2 + (y_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_6 - \frac{1}{2}) \hat{\mathbf{x}} - ax_6 \hat{\mathbf{y}} + a(y_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{28} =$	$-z_6 \mathbf{a}_1 + (x_6 + \frac{1}{2}) \mathbf{a}_2 - (y_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_6 \hat{\mathbf{x}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{29} =$	$y_6 \mathbf{a}_1 + z_6 \mathbf{a}_2 + x_6 \mathbf{a}_3$	$=$	$ay_6 \hat{\mathbf{x}} + az_6 \hat{\mathbf{y}} + ax_6 \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{30} =$	$-y_6 \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_2 - (x_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_6 \hat{\mathbf{x}} + a(z_6 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{31} =$	$(y_6 + \frac{1}{2}) \mathbf{a}_1 - (z_6 - \frac{1}{2}) \mathbf{a}_2 - x_6 \mathbf{a}_3$	$=$	$a(y_6 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_6 - \frac{1}{2}) \hat{\mathbf{y}} - ax_6 \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{32} =$	$-(y_6 - \frac{1}{2}) \mathbf{a}_1 - z_6 \mathbf{a}_2 + (x_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_6 - \frac{1}{2}) \hat{\mathbf{x}} - az_6 \hat{\mathbf{y}} + a(x_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	Cu II
$\mathbf{B}_{33} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + ay_7 \hat{\mathbf{y}} + az_7 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{34} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - ay_7 \hat{\mathbf{y}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{35} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_7 \hat{\mathbf{x}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{36} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - az_7 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{37} =$	$z_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + y_7 \mathbf{a}_3$	$=$	$az_7 \hat{\mathbf{x}} + ax_7 \hat{\mathbf{y}} + ay_7 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{38} =$	$(z_7 + \frac{1}{2}) \mathbf{a}_1 - (x_7 - \frac{1}{2}) \mathbf{a}_2 - y_7 \mathbf{a}_3$	$=$	$a(z_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{y}} - ay_7 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{39} =$	$-(z_7 - \frac{1}{2}) \mathbf{a}_1 - x_7 \mathbf{a}_2 + (y_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(z_7 - \frac{1}{2}) \hat{\mathbf{x}} - ax_7 \hat{\mathbf{y}} + a(y_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{40} =$	$-z_7 \mathbf{a}_1 + (x_7 + \frac{1}{2}) \mathbf{a}_2 - (y_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-az_7 \hat{\mathbf{x}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{41} =$	$y_7 \mathbf{a}_1 + z_7 \mathbf{a}_2 + x_7 \mathbf{a}_3$	$=$	$ay_7 \hat{\mathbf{x}} + az_7 \hat{\mathbf{y}} + ax_7 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{42} =$	$-y_7 \mathbf{a}_1 + (z_7 + \frac{1}{2}) \mathbf{a}_2 - (x_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_7 \hat{\mathbf{x}} + a(z_7 + \frac{1}{2}) \hat{\mathbf{y}} - a(x_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{43} =$	$(y_7 + \frac{1}{2}) \mathbf{a}_1 - (z_7 - \frac{1}{2}) \mathbf{a}_2 - x_7 \mathbf{a}_3$	$=$	$a(y_7 + \frac{1}{2}) \hat{\mathbf{x}} - a(z_7 - \frac{1}{2}) \hat{\mathbf{y}} - ax_7 \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{44} =$	$-(y_7 - \frac{1}{2}) \mathbf{a}_1 - z_7 \mathbf{a}_2 + (x_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_7 - \frac{1}{2}) \hat{\mathbf{x}} - az_7 \hat{\mathbf{y}} + a(x_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O III
$\mathbf{B}_{45} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + ay_8 \hat{\mathbf{y}} + az_8 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{46} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} + a(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{47} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_8 \hat{\mathbf{x}} + a(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - a(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{48} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - az_8 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{49} =$	$z_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + y_8 \mathbf{a}_3$	$=$	$az_8 \hat{\mathbf{x}} + ax_8 \hat{\mathbf{y}} + ay_8 \hat{\mathbf{z}}$	(12b)	O IV
$\mathbf{B}_{50} =$	$(z_8 + \frac{1}{2}) \mathbf{a}_1 - (x_8 - \frac{1}{2}) \mathbf{a}_2 - y_8 \mathbf{a}_3$	$=$	$a(z_8 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_8 - \frac{1}{2}) \hat{\mathbf{y}} - ay_8 \hat{\mathbf{z}}$	(12b)	O IV

$$\begin{aligned}
\mathbf{B}_{51} &= -\left(z_8 - \frac{1}{2}\right) \mathbf{a}_1 - x_8 \mathbf{a}_2 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - ax_8 \hat{\mathbf{y}} + a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O IV} \\
\mathbf{B}_{52} &= -z_8 \mathbf{a}_1 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_3 &= -az_8 \hat{\mathbf{x}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O IV} \\
\mathbf{B}_{53} &= y_8 \mathbf{a}_1 + z_8 \mathbf{a}_2 + x_8 \mathbf{a}_3 &= ay_8 \hat{\mathbf{x}} + az_8 \hat{\mathbf{y}} + ax_8 \hat{\mathbf{z}} &(12b) &\quad \text{O IV} \\
\mathbf{B}_{54} &= -y_8 \mathbf{a}_1 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_8 - \frac{1}{2}\right) \mathbf{a}_3 &= -ay_8 \hat{\mathbf{x}} + a\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O IV} \\
\mathbf{B}_{55} &= \left(y_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_2 - x_8 \mathbf{a}_3 &= a\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} &(12b) &\quad \text{O IV} \\
\mathbf{B}_{56} &= -\left(y_8 - \frac{1}{2}\right) \mathbf{a}_1 - z_8 \mathbf{a}_2 + \left(x_8 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - az_8 \hat{\mathbf{y}} + a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{z}} &(12b) &\quad \text{O IV}
\end{aligned}$$

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- [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

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First cited in

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