

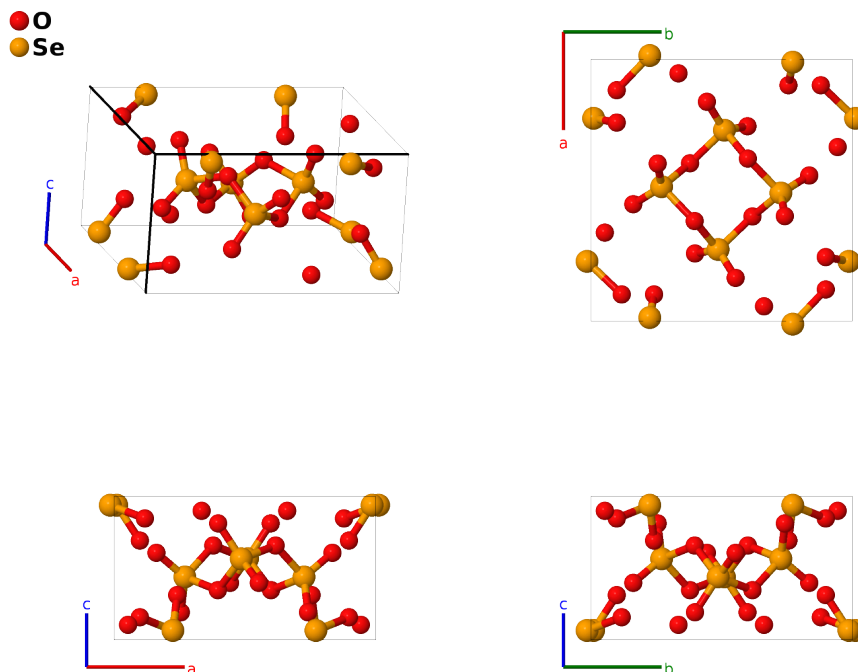
SeO₃ Structure: A3B_tP32_114_3e_e-001

This structure originally had the label A3B_tP32_114_3e_e. Calls to that address will be redirected here.

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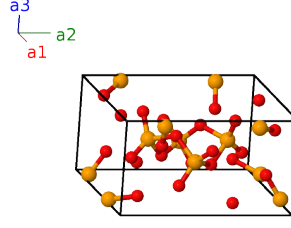
<https://aflow.org/p/U620>

https://aflow.org/p/A3B_tP32_114_3e_e-001



| | |
|-------------------------|--|
| Prototype | O ₃ Se |
| AFLOW prototype label | A3B_tP32_114_3e_e-001 |
| ICSD | none |
| Pearson symbol | tP32 |
| Space group number | 114 |
| Space group symbol | $P\bar{4}2_1c$ |
| AFLOW prototype command | <code>aflow --proto=A3B_tP32_114_3e_e-001</code> <code>--params=a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃, x₄, y₄, z₄</code> |

Simple Tetragonal primitive vectors



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

Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|--|-----|---|------------------|-----------|
| \mathbf{B}_1 | $= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $ax_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_2 | $= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $-ax_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_3 | $= y_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$ | $=$ | $ay_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_4 | $= -y_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$ | $=$ | $-ay_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_5 | $= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_6 | $= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_7 | $= -\left(y_1 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_8 | $= \left(y_1 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $a\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O I |
| \mathbf{B}_9 | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{10} | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{11} | $= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$ | $=$ | $ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{12} | $= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$ | $=$ | $-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{13} | $= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{14} | $= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{15} | $= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{16} | $= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O II |
| \mathbf{B}_{17} | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (8e) | O III |
| \mathbf{B}_{18} | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (8e) | O III |
| \mathbf{B}_{19} | $= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$ | (8e) | O III |
| \mathbf{B}_{20} | $= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$ | (8e) | O III |
| \mathbf{B}_{21} | $= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O III |
| \mathbf{B}_{22} | $= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$ | $=$ | $a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$ | (8e) | O III |

$$\begin{aligned}
\mathbf{B}_{23} &= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{O III} \\
\mathbf{B}_{24} &= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{O III} \\
\mathbf{B}_{25} &= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= ax_4 \hat{\mathbf{x}} + ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{26} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3 &= -ax_4 \hat{\mathbf{x}} - ay_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{27} &= y_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= ay_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{28} &= -y_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -ay_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{29} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{30} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{31} &= -\left(y_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{Se I} \\
\mathbf{B}_{32} &= \left(y_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8e) & \text{Se I}
\end{aligned}$$

References

- [1] F. C. Mijlhoff and C. H. MacGillavry, *Symmetry and unit-cell dimensions of selenium trioxide*, Acta Cryst. **15**, 620 (1962), doi:10.1107/S0365110X62001644.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.