

SeO₃ Structure:

A3B_tP32_114_3e_e-001

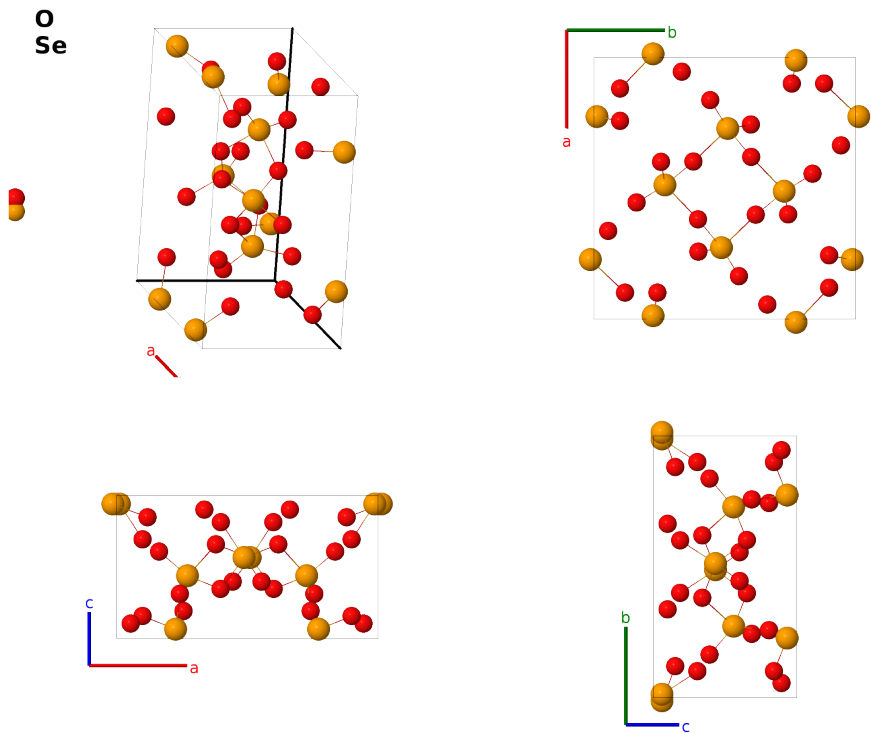
This structure previously used the label(s) **A3B_tP32_114_3e_e**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/U620>

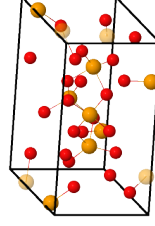
https://aflow.org/prototype-encyclopedia/A3B_tP32_114_3e_e-001



Prototype	O ₃ Se
AFLOW prototype label	A3B_tP32_114_3e_e-001
Pearson symbol	tP32
Space group number	114
Space group symbol	$P\bar{4}_21c$
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

a1 a2 a3



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

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) &\quad \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) &\quad \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) &\quad \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) &\quad \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) &\quad \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) &\quad \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) &\quad \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) &\quad \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) &\quad \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) &\quad \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.

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