

γ -SeO₂ Structure:

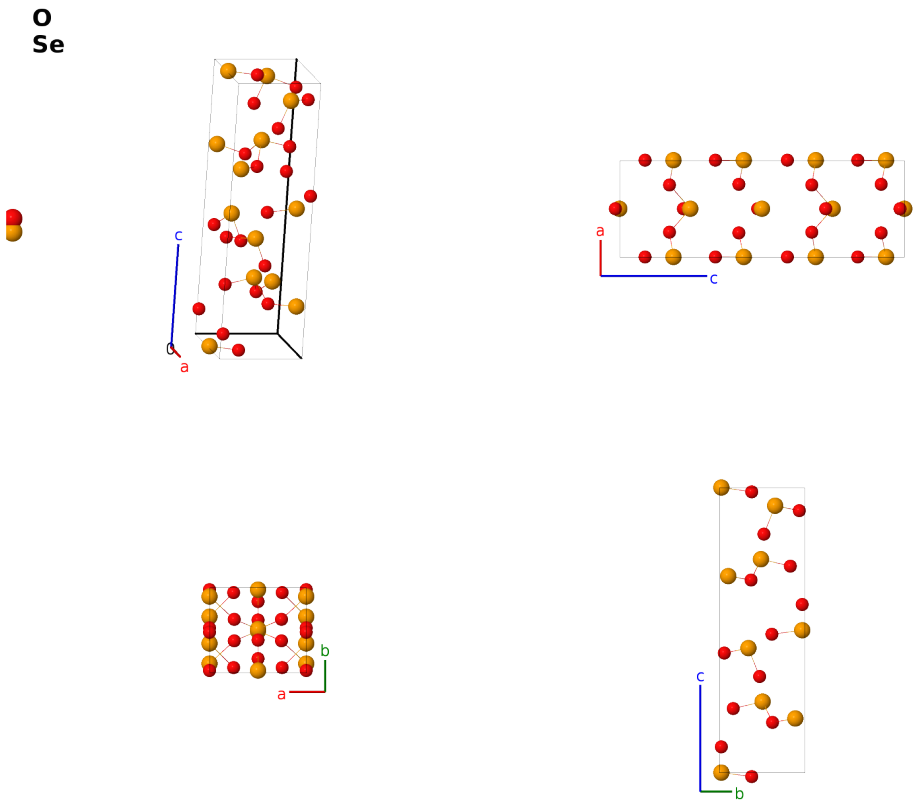
A2B_oP24_26_2a2b2c_2a2b-001

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/PVJF>

https://aflow.org/prototype-encyclopedia/A2B_oP24_26_2a2b2c_2a2b-001

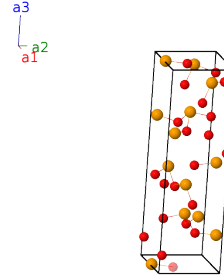


Prototype	O ₂ Se
AFLOW prototype label	A2B_oP24_26_2a2b2c_2a2b-001
ICSD	99465
CCDC	1658691
Pearson symbol	oP24
Space group number	26
Space group symbol	<i>Pmc</i> 2 ₁
AFLOW prototype command	<code>aflow --proto=A2B_oP24_26_2a2b2c_2a2b-001</code> <code>--params=a, b/a, c/a, y₁, z₁, y₂, z₂, y₃, z₃, y₄, z₄, y₅, z₅, y₆, z₆, y₇, z₇, y₈, z₈, x₉, y₉, z₉, x₁₀, y₁₀, z₁₀</code>

- SeO₂ has been observed in three phases (Orosel, 2004):
 - Downeyite, α -SeO₂, *Strukturbericht C47*, the ground state,
 - β -SeO₂, and
 - γ -SeO₂ (this structure).
- The later two phases form at high pressures (up to 15GPa and 820°C) but upon quenching and slowly reducing the pressure they remain metastable under ambient conditions.
- Data for γ -SeO₂ was taken at 200K using powder diffraction data.
- Space group $Pmc2_1$ #26 allows an arbitrary choice for the origin of the z -axis. Here we follow (Orosel, 2004) and set $z_7 = 0$ for the Se III (2b) site.

Simple Orthorhombic primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$-y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_4$	$-y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_5$	$y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B}_6$	$-y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B}_7$	$y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(2a)	Se II
$\mathbf{B}_8$	$-y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	Se II
$\mathbf{B}_9$	$\frac{1}{2} \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(2b)	O III
$\mathbf{B}_{10}$	$\frac{1}{2} \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O III
$\mathbf{B}_{11}$	$\frac{1}{2} \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(2b)	O IV
$\mathbf{B}_{12}$	$\frac{1}{2} \mathbf{a}_1 - y_6 \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O IV
$\mathbf{B}_{13}$	$\frac{1}{2} \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(2b)	Se III
$\mathbf{B}_{14}$	$\frac{1}{2} \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Se III
$\mathbf{B}_{15}$	$\frac{1}{2} \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(2b)	Se IV
$\mathbf{B}_{16}$	$\frac{1}{2} \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	Se IV
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4c)	O V

$$\begin{aligned}
\mathbf{B}_{18} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{O V} \\
\mathbf{B}_{19} &= x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c \left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{O V} \\
\mathbf{B}_{20} &= -x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= -ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} &(4c) &\text{O V} \\
\mathbf{B}_{21} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(4c) &\text{O VI} \\
\mathbf{B}_{22} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{O VI} \\
\mathbf{B}_{23} &= x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c \left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} &(4c) &\text{O VI} \\
\mathbf{B}_{24} &= -x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= -ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} &(4c) &\text{O VI}
\end{aligned}$$

References

- [1] D. Orosel, O. Leynaud, P. Balog, and M. Jansen, *Pressure–temperature phase diagram of SeO₂. Characterization of new phases*, J. Solid State Chem. **177**, 1631–1638 (2004), doi:10.1016/j.jssc.2003.12.028.

Found in

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

First cited in

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.