

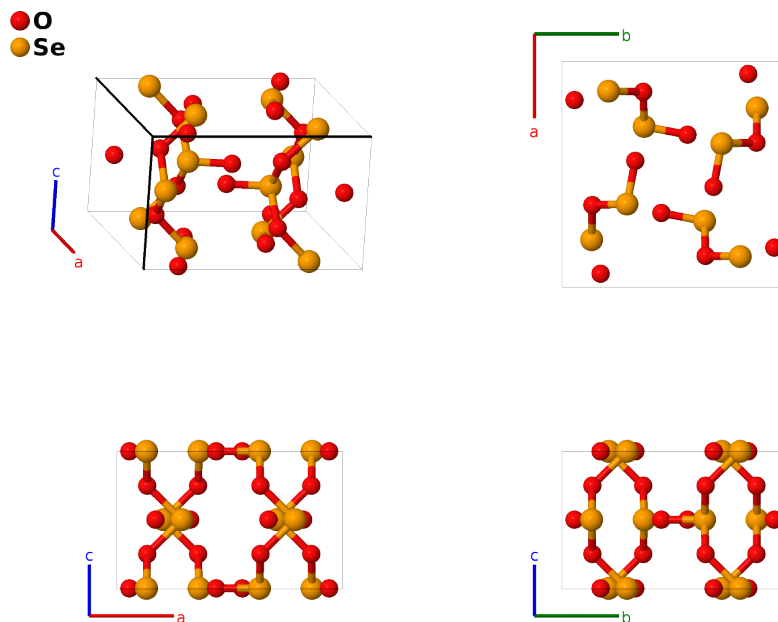
Downeyite (α -SeO₂, *C*47) Structure: A2B_tP24_135_gh_h-001

This structure originally had the label [A2B_tP24_135_gh_h](#). Calls to that address will be redirected here.

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

https://aflow.org/p/A2B_tP24_135_gh_h-001



Prototype	O ₂ Se
AFLOW prototype label	A2B_tP24_135_gh_h-001
<i>Strukturbericht</i> designation	<i>C</i> 47
Mineral name	downeyite
ICSD	72367
Pearson symbol	tP24
Space group number	135
Space group symbol	<i>P</i> 4 ₂ / <i>mbc</i>
AFLOW prototype command	<code>aflow --proto=A2B_tP24_135_gh_h-001 --params=a, c/a, x₁, x₂, y₂, x₃, y₃</code>

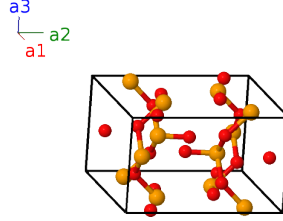
- SeO₂ has been observed in three phases (Orosel, 2004):
 - Downeyite, α -SeO₂, *Strukturbericht C*47, the ground state (this structure),

- β -SeO₂, and
- γ -SeO₂.

- 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 this structure was taken at 139K.

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	$= x_1 \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_3	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_4	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_5	$= -x_1 \mathbf{a}_1 - (x_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - a(x_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_6	$= x_1 \mathbf{a}_1 + (x_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + a(x_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_7	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_8	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + x_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(8g)	O I
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}}$	(8h)	O II
\mathbf{B}_{10}	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}}$	(8h)	O II
\mathbf{B}_{11}	$= -y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
\mathbf{B}_{12}	$= y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
\mathbf{B}_{13}	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	O II
\mathbf{B}_{14}	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	O II
\mathbf{B}_{15}	$= (y_2 + \frac{1}{2}) \mathbf{a}_1 + (x_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
\mathbf{B}_{16}	$= -(y_2 - \frac{1}{2}) \mathbf{a}_1 - (x_2 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} - a(x_2 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	O II
\mathbf{B}_{17}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ay_3 \hat{\mathbf{y}}$	(8h)	Se I
\mathbf{B}_{18}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ay_3 \hat{\mathbf{y}}$	(8h)	Se I
\mathbf{B}_{19}	$= -y_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ay_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	Se I
\mathbf{B}_{20}	$= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ay_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	Se I
\mathbf{B}_{21}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(y_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Se I
\mathbf{B}_{22}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(y_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(8h)	Se I
\mathbf{B}_{23}	$= (y_3 + \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(y_3 + \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(8h)	Se I

$$\mathbf{B}_{24} = -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 = -a\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2}c\hat{\mathbf{z}} \quad (8h) \quad \text{Se I}$$

References

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