

Downeyite (α -SeO₂, C47) Structure: A2B_tP24_135_gh_h-001

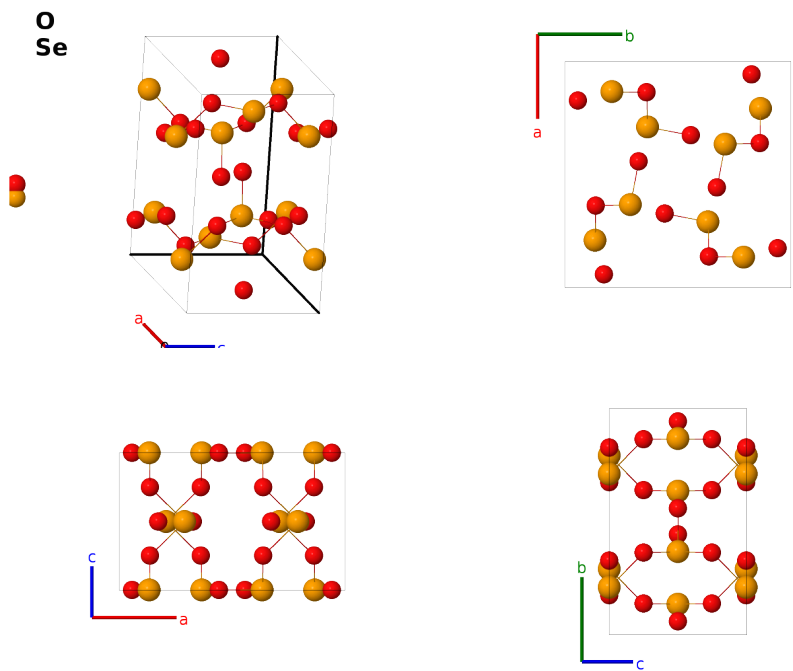
This structure previously used the label(s) **A2B_tP24_135_gh_h**. Calls to these addresses will be redirected here.

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

https://aflow.org/prototype-encyclopedia/A2B_tP24_135_gh_h-001



Prototype	O ₂ Se
AFLOW prototype label	A2B_tP24_135_gh_h-001
<i>Strukturbericht</i> designation	C47
Mineral name	downeyite
ICSD	72367
CCDC	1633231
Pearson symbol	tP24
Space group number	135
Space group symbol	$P4_2/mbc$
AFLOW prototype command	<pre>aflow --proto=A2B_tP24_135_gh_h-001 --params=a, c/a, x₁, x₂, y₂, x₃, y₃</pre>

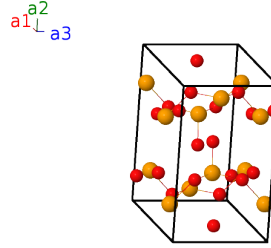
- SeO₂ has been observed in three phases (Orosel, 2004):
 - Downeyite, α -SeO₂, *Strukturbericht C47*, the ground state (this structure),
 - β -SeO₂, and
 - γ -SeO₂.
- The later two phases form at high pressures (up to 15GPa and 820°C) but upon quenching and slowly reducing the pressure they remain metastable under ambient conditions.
- Data for this structure was taken at 139K.

Simple Tetragonal primitive vectors

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

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

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



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

$$\begin{aligned}
\mathbf{B}_{20} &= y_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a y_3 \hat{\mathbf{x}} - a x_3 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8h) &\text{Se I} \\
\mathbf{B}_{21} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 &= -a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} &(8h) &\text{Se I} \\
\mathbf{B}_{22} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 &= a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} &(8h) &\text{Se I} \\
\mathbf{B}_{23} &= \left(y_3 + \frac{1}{2}\right) \mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= a \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8h) &\text{Se I} \\
\mathbf{B}_{24} &= -\left(y_3 - \frac{1}{2}\right) \mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3 &= -a \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}} &(8h) &\text{Se I}
\end{aligned}$$

References

- [1] K. Ståhl, J. P. Legros, and J. Galy, *The crystal structure of SeO₂ at 139 and 286 K*, Z. Krystallogr. **202**, 99–107 (1992), doi:10.1524/zkri.1992.202.14.99.
- [2] 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] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).

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