β-SeO_2 Structure: A2B_oP12_26_abc_ab-002

This structure originally had the label `A2B_oP12_26_abc_ab.SeO2`. Calls to that address will be redirected here.

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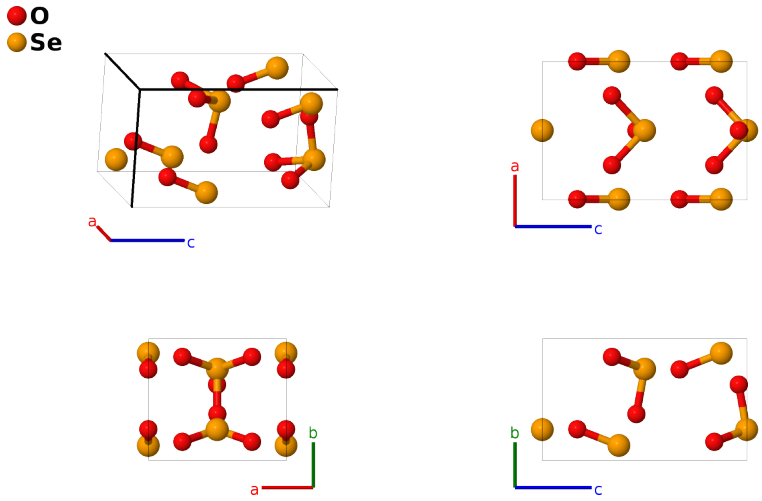
https://aflow.org/p/2MYY

https://aflow.org/p/A2B_oP12_26_abc_ab-002

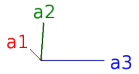


Prototype	O_2Se
AFLOW prototype label	A2B_oP12_26_abc_ab-002
ICSD	99464
Pearson symbol	oP12
Space group number	26
Space group symbol	$Pmc2_1$
AFLOW prototype command	`aflow --proto=A2B_oP12_26_abc_ab-002 --params=`$a, b/a, c/a, y_1, z_1, y_2, z_2, y_3, z_3, y_4, z_4, x_5, y_5, z_5$

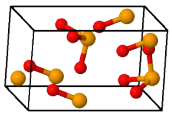
- SeO_2 has been observed in three phases (Orosel, 2004):
  - Downeyite, α-SeO_2, *Strukturbericht* $C47$, the ground state,
  - β-SeO_2 (this structure), and
  - γ-SeO_2.
- The later two phases form at high pressures (up to 15GPa and 820°C) but upon quenching and slowly reducing the pressure they remain metastable under ambient conditions.
- Data for β-SeO_2 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 $z_4 = 0$ for the Se II (2b) site.

- β-SeO_2 has the same AFLOW label as 70 GPa H_2S, A2B_oP12_26_abc_ab. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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
$\mathbf{B_2}$	=	$-y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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)	Se I
$\mathbf{B_4}$	=	$-y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	Se I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2b)	Se II
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Se II
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{11}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B_{12}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4c)	O III

References

[1] D. Orosel, O. Leynaud, P. Balog, and M. Jansen, *Pressure–temperature phase diagram of SeO_2. 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.