

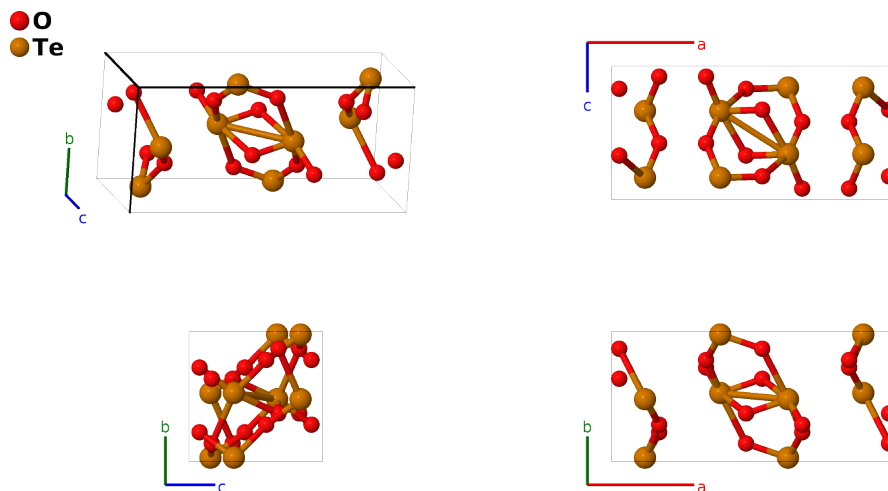
Tellurite (β -TeO₂, *C*52) Structure: A2B_oP24_61_2c_c-002

This structure originally had the label **A2B_oP24_61_2c_c.Te02**. Calls to that address will be redirected here.

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<https://afLOW.org/p/GK2A>

https://afLOW.org/p/A2B_oP24_61_2c_c-002



Prototype	O ₂ Te
AFLOW prototype label	A2B_oP24_61_2c_c-002
<i>Strukturbericht</i> designation	<i>C</i> 52
Mineral name	tellurite
ICSD	26844
Pearson symbol	oP24
Space group number	61
Space group symbol	<i>Pbca</i>
AFLOW prototype command	<code>afLOW --proto=A2B_oP24_61_2c_c-002 --params=a, b/a, c/a, x₁, y₁, z₁, x₂, y₂, z₂, x₃, y₃, z₃</code>

Other compounds with this structure

γ -SnF₂

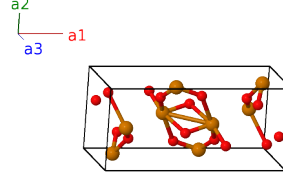
- The original version of this page (Hicks, 2021) used a lattice constant $a = 15.035\text{\AA}$. The correct value is $a = 12.035\text{\AA}$, and we use that here.
- TeO₂ has been observed in three different forms (Ceriotti, 2006; Liu, 2016):
 - α -TeO₂, paratellurite is the ground state

- β -TeO₂, tellurite (this structure) is stable under ambient conditions and is the most commonly observed phase
- γ -TeO₂ is metastable, and forms at 663K in the β -SnF₂ structure.

- Pararammelsbergite (NiAs₂), tellurite and brookite (C21, TiO₂) have the same AFLOW prototype label, A2B_oP24_61_2c.c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_2	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_3	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_4	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_5	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_6	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_7	$= x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_8	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	O I
\mathbf{B}_9	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{10}	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{11}	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{12}	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{13}	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{14}	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{15}	$= x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{16}	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	O II
\mathbf{B}_{17}	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8c)	Te I
\mathbf{B}_{18}	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Te I
\mathbf{B}_{19}	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Te I
\mathbf{B}_{20}	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8c)	Te I

$$\begin{aligned}
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} & (8c) & \text{Te I} \\
\mathbf{B}_{22} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 &= a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Te I} \\
\mathbf{B}_{23} &= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_3 \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Te I} \\
\mathbf{B}_{24} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + &= -a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} & (8c) & \text{Te I} \\
& \quad z_3 \mathbf{a}_3 & & &
\end{aligned}$$

References

- [1] H. Beyer, *Verfeinerung der Kristallstruktur von Tellurit, dem rhombischen TeO_2* , Z. Kristallgr. **124**, 228–237 (1967), doi:10.1524/zkri.1967.124.3.228.
- [2] X. Liu, T. Mashimo, N. Kawai, T. Sekine, Z. Zeng, and X. Zhou, *Phase transition and equation of state of paratellurite (TeO_2) under high pressure*, Mater. Res. Express **3**, 076206 (2016), doi:10.1088/2053-1591/3/7/076206.