

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

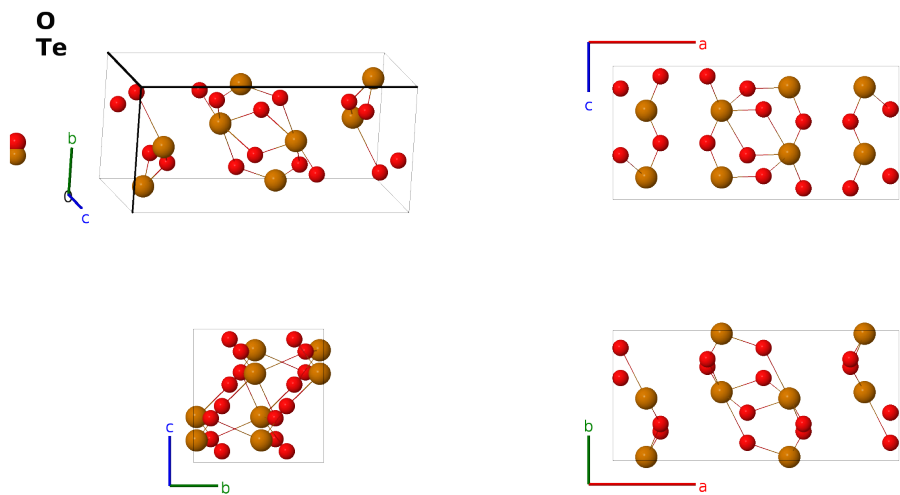
This structure previously used the label(s) **A2B_oP24_61_2c_c.TeO2**. Calls to these addresses will be redirected here.

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- 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/GK2A>

https://aflow.org/prototype-encyclopedia/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
CCDC	1602223
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</code> <code>--params=a,b/a,c/a,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃</code>

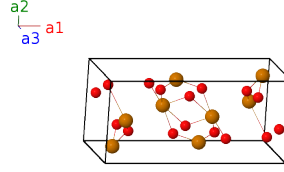
Other compounds with this structure

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.
- TeO_2 has been observed in three different forms (Ceriotti, 2006; Liu, 2016):
 - α - TeO_2 , paratellurite is the ground state
 - β - TeO_2 , tellurite (this structure) is stable under ambient conditions and is the most commonly observed phase
 - γ - TeO_2 is metastable, and forms at 663K in the β - SnF_2 structure.
- Pararammelsbergite (NiAs_2), tellurite and brookite ($C21$, TiO_2) 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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_6$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_8$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(8c)	O I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{10}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{12}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{14}$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{16}$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8c)	O II
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8c)	Te I

$$\begin{aligned}
\mathbf{B}_{18} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) &\text{Te I} \\
\mathbf{B}_{19} &= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 &= -ax_3 \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) &\text{Te I} \\
\mathbf{B}_{20} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3 &= a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} &(8c) &\text{Te I} \\
\mathbf{B}_{21} &= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3 &= -ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}} &(8c) &\text{Te I} \\
\mathbf{B}_{22} &= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) &\text{Te I} \\
\mathbf{B}_{23} &= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3 &= ax_3 \hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}} &(8c) &\text{Te I} \\
\mathbf{B}_{24} &= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 + z_3 \mathbf{a}_3 &= -a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}} &(8c) &\text{Te I}
\end{aligned}$$

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. Mashimo¹, N. Kawai¹, 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.

First cited in

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