

Paratellurite (α TeO₂) Structure: A2B_tP12_92_b_a-002

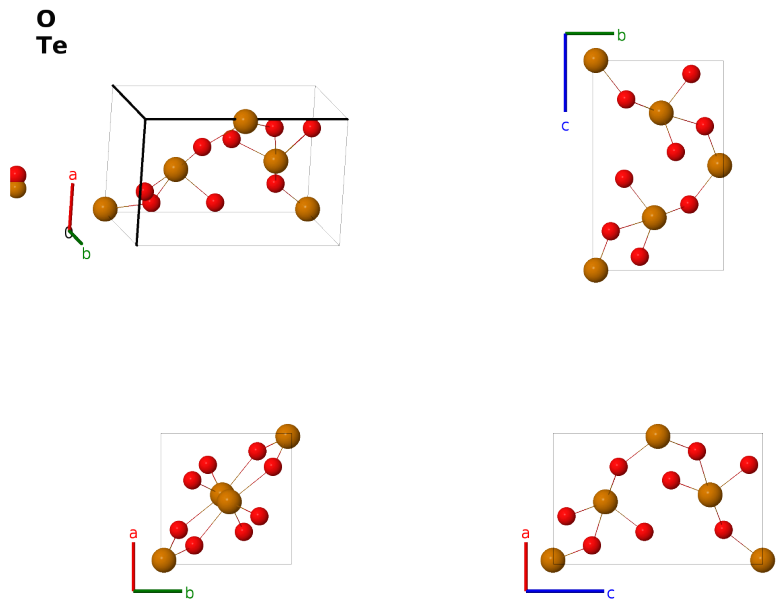
This structure previously used the label(s) **A2B_tP12_92_b_a.Te02**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/6BKE>

https://aflow.org/prototype-encyclopedia/A2B_tP12_92_b_a-002



Prototype	O ₂ Te
AFLOW prototype label	A2B_tP12_92_b_a-002
Mineral name	paratellurite
ICSD	202792
CCDC	1707357
Pearson symbol	tP12
Space group number	92
Space group symbol	<i>P</i> 4 ₁ 2 ₁ 2
AFLOW prototype command	<code>aflow --proto=A2B_tP12_92_b_a-002</code> <code>--params=a, c/a, x₁, x₂, y₂, z₂</code>

Other compounds with this structure

γ -SnF₂

- TeO₂ has been observed in three different forms (Ceriotti, 2006; Liu, 2016):
 - α -TeO₂, paratellurite (this structure) is the ground state
 - β -TeO₂, tellurite 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.
- Paratellurite and α -cristobalite (C30) have the same AFLOW prototype label, A2B_tP12.92_b.a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Tetragonal primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2$	$=$	$ax_1 \hat{\mathbf{x}} + ax_1 \hat{\mathbf{y}}$	(4a)	Te I
$\mathbf{B}_2$	$= -x_1 \mathbf{a}_1 - x_1 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - ax_1 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4a)	Te I
$\mathbf{B}_3$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_1 + \frac{1}{2}\right) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{1}{4} c \hat{\mathbf{z}}$	(4a)	Te I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_1 - \frac{1}{2}\right) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + \frac{3}{4} c \hat{\mathbf{z}}$	(4a)	Te I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_6$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_7$	$= -\left(y_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_8$	$= \left(y_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_2 + \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_9$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{4}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{4}\right) \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_{10}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{3}{4}\right) \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{3}{4}\right) \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_{11}$	$= y_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{x}} + ax_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(8b)	O I
$\mathbf{B}_{12}$	$= -y_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{x}} - ax_2 \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8b)	O I

References

- [1] P. A. Thomas, *The crystal structure and absolute optical chirality of paratellurite, α -TeO₂*, J. Phys. C: Solid State Phys. **21**, 4611–4627 (1988), doi:10.1016/S0022-3697(00)00012-3.
- [2] X. Liu, T. Mashimo¹, N. Kawai¹, T. Sekine, Z. Zeng, and X. Zhou, *Phase transition and equation of state of paratellurite (TeO₂) under high pressure*, Mater. Res. Express **3**, 076206 (2016), doi:10.1088/2053-1591/3/7/076206.

Found in

- [1] M. Ceriotti, F. Pietrucci, and M. Bernasconi, *Ab initio study of the vibrational properties of crystalline TeO_2 : The α , β , and γ phases*, Phys. Rev. B **73**, 104304 (2006), doi:10.1103/PhysRevB.73.104304.

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