α-Tl_2TeO_3 Structure: A3BC2_oP48_50_3m_m_2m-001

This structure originally had the label `A3BC2_oP48_50_3m_m_2m`. Calls to that address will be redirected here.

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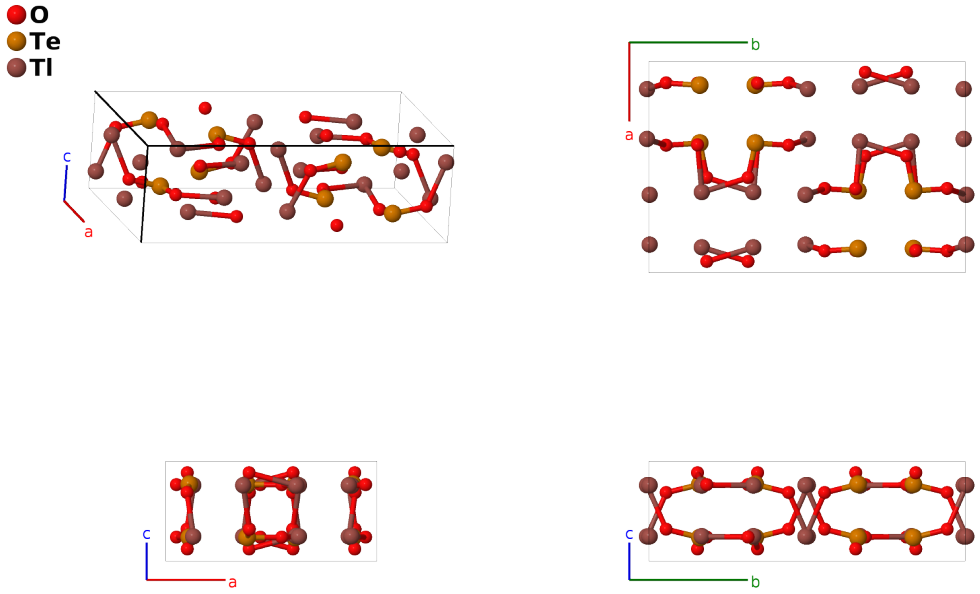
https://aflow.org/p/06EV

https://aflow.org/p/A3BC2_oP48_50_3m_m_2m-001

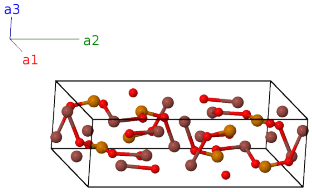


Prototype	O_3TeTl_2
AFLOW prototype label	A3BC2_oP48_50_3m_m_2m-001
ICSD	240675
Pearson symbol	oP48
Space group number	50
Space group symbol	*Pban*
AFLOW prototype command	`aflow --proto=A3BC2_oP48_50_3m_m_2m-001 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- This is the high-temperature structure of Tl_2TeO_3. Below 440°C it transforms into the monoclinic βTl_2TeO_3 structure, but remains metastable at 25°C, where this data was taken. (Rieger, 2007).

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_2}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_3}$	=	$-\left(x_1-\frac{1}{2}\right)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-a\left(x_1-\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - \left(y_1-\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - b\left(y_1-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_6}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_7}$	=	$\left(x_1+\frac{1}{2}\right)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$a\left(x_1+\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_8}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1+\frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + b\left(y_1+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8m)	O I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{10}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{11}}$	=	$-\left(x_2-\frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-a\left(x_2-\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{12}}$	=	$x_2\,\mathbf{a}_1 - \left(y_2-\frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{14}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{15}}$	=	$\left(x_2+\frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$a\left(x_2+\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{16}}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2+\frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8m)	O II
$\mathbf{B_{17}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{18}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{19}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{20}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3-\frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} - b\left(y_3-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{21}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{22}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{23}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{24}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3+\frac{1}{2}\right)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + b\left(y_3+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8m)	O III
$\mathbf{B_{25}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{26}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{27}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{28}}$	=	$x_4\,\mathbf{a}_1 - \left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8m)	Te I

$\mathbf{B_{29}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{30}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{31}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{32}}$	=	$-x_4\,\mathbf{a}_1 + \left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8m)	Te I
$\mathbf{B_{33}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{34}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{35}}$	=	$-\left(x_5-\frac{1}{2}\right)\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-a\left(x_5-\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{36}}$	=	$x_5\,\mathbf{a}_1 - \left(y_5-\frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} - b\left(y_5-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{37}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{38}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{39}}$	=	$\left(x_5+\frac{1}{2}\right)\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5+\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{40}}$	=	$-x_5\,\mathbf{a}_1 + \left(y_5+\frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + b\left(y_5+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8m)	Tl I
$\mathbf{B_{41}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{42}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{43}}$	=	$-\left(x_6-\frac{1}{2}\right)\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-a\left(x_6-\frac{1}{2}\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{44}}$	=	$x_6\,\mathbf{a}_1 - \left(y_6-\frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} - b\left(y_6-\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{45}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{46}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{47}}$	=	$\left(x_6+\frac{1}{2}\right)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6+\frac{1}{2}\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II
$\mathbf{B_{48}}$	=	$-x_6\,\mathbf{a}_1 + \left(y_6+\frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} + b\left(y_6+\frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8m)	Tl II

References

[1] F. Rieger and A.-V. Mudring, *Phase Transition in Tl_2TeO_3: Influence and Origin of the Thallium Lone Pair Distortion*, Inorg. Chem. **46**, 446–452 (2007), doi:10.1021/ic061273j.

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[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.