β-SeTl ($B37$) Structure: AB_tI16_140_ab_h-001

This structure originally had the label `AB_tI16_140_ab_h`. Calls to that address will be redirected here.

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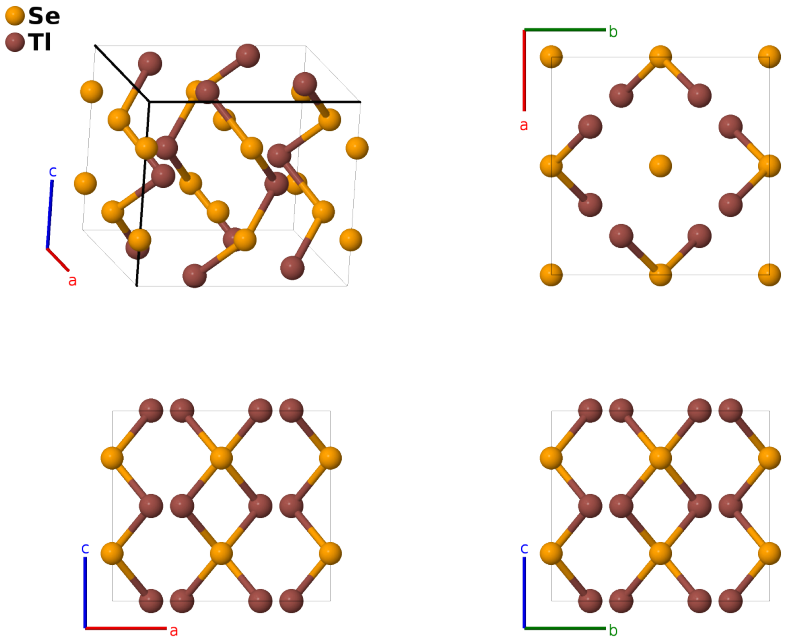
https://aflow.org/p/BFE0

https://aflow.org/p/AB_tI16_140_ab_h-001



Prototype	SeTl
AFLOW prototype label	AB_tI16_140_ab_h-001
***Strukturbericht* designation**	$B37$
ICSD	30219
Pearson symbol	tI16
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=AB_tI16_140_ab_h-001 --params=`$a, c/a, x_3$

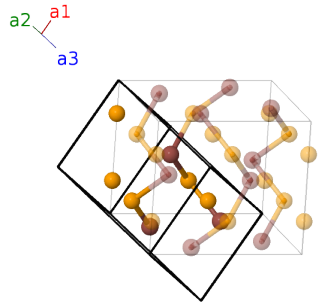
Other compounds with this structure
InTe, STl, $AlKTe_2$, $AlNaSe_2$, $AlNaTe_2$, $GaNaTe_2$, $GaTe_2Tl$, $InKTe_2$, $InNaTe_2$, InS_2Te

- When $c = a$ and $x = 1/4$ the atoms are at the positions of the body-centered cubic (A2) lattice.

- (Okamoto, 2011) identifies this as β-SeTl, stable from 188°C to the melting point at approximately 350°C. No crystallographic information on the ground-state α phase has been found.
- The lattice constants presented here are from (Yadav, 1976), while the atomic positions and the ICSD entry are from (Ketelaar, 1939).

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	Se I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	Se I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Se II
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Se II
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Tl I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Tl I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Tl I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Tl I

References

[1] J. A. A. Ketelaar, W. H. t'Hart, M. Moerel, and D. Polder, *The Crystal Structure of TlSe, Thallous Thallic or Thallosic Selenide*, Z. Krystallogr. **101**, 396–406 (1939), doi:10.1524/zkri.1939.101.1.396.

[2] R. Yadav, R. P. Ram, and S. Bhan, *On the Thallium-Selenium-Tellurium System*, Z. Metallkd. **67**, 173–177 (1976), doi:10.1515/ijmr-1976-670308.

[3] H. Okamoto, *Se-Tl (Selenium-Thallium)*, J. Phase Eq. Diff. **32**, 570–571 (2011), doi:10.1007/s11669-011-9954-2.

Found in

[1] P. Villars, *TlSe Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.