$GeSb_2Te_4$ Structure: AB2C4_hR7_166_a_c_2c-002

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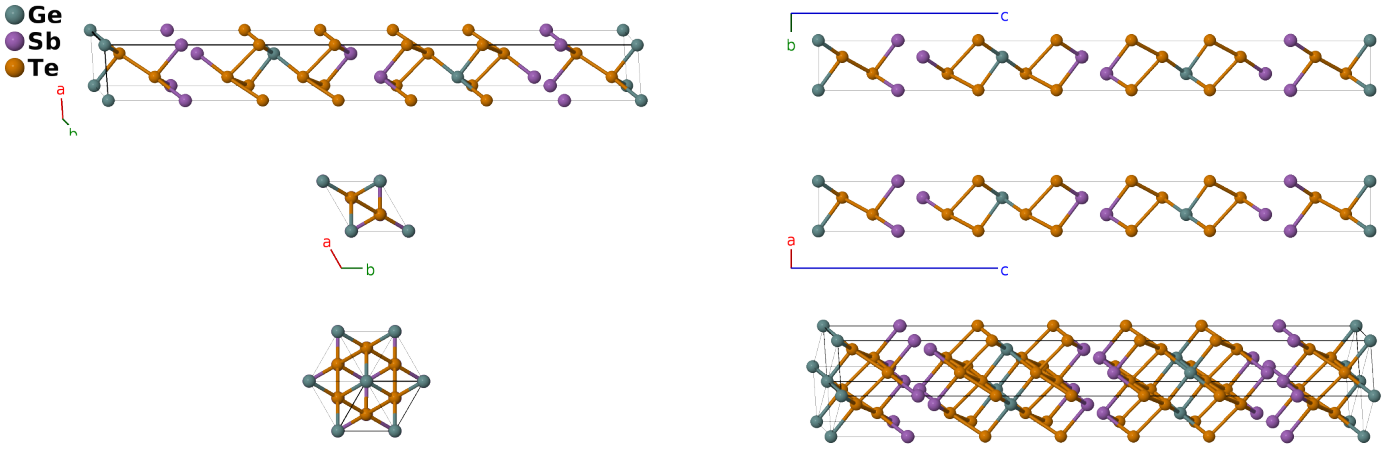
https://aflow.org/p/5J2E

https://aflow.org/p/AB2C4_hR7_166_a_c_2c-002



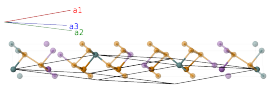
Prototype	$GeSb_2Te_4$
AFLOW prototype label	AB2C4_hR7_166_a_c_2c-002
ICSD	30393
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB2C4_hR7_166_a_c_2c-002 --params=`$a, c/a, x_2, x_3, x_4$

Other compounds with this structure
$GeBi_2Te_4$, $PbSb_2Te_4$, $SnSb_2Te_4$

- This structure is nearly identical to $MnBi_2Te_4$, but the assumed ordering of the tellurium atoms is different in the two cases.
- We use the data from (Agaev, 1966) as reported by (Matsunaga, 2004), however the ICSD entry states that all of the (2c) sites have occupancy $Te_{0.66}Sb_{33}$. We follow (Matsunaga, 2004) and label the first (2c) site as Sb with the other two Te, preserving the stiochiometry.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ge I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Sb I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Sb I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Te II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Te II

References

[1] T. Matsunaga and N. Yamada, *Structural investigation of $GeSb_2Te_4$:A high-speed phase-change material*, Phys. Rev. B **69**, 104111 (2004), doi:10.1103/PhysRevB.69.104111.

[2] K. A. Agaev and A. G. Talybov, *Electron-diffraction analysis of structure of $GeSb_2Te_4$*, Sov. Phys. Crystallogr. **11**, 400 (1966).