

GeSb₂Te₄ Structure:

AB2C4_hR7_166_a_c_2c-002

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<https://aflow.org/prototype-encyclopedia/5J2E>

https://aflow.org/prototype-encyclopedia/AB2C4_hR7_166_a_c_2c-002

Prototype	GeSb ₂ Te ₄
AFLOW prototype label	AB2C4_hR7_166_a_c_2c-002
ICSD	30393
CCDC	1604732
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB2C4_hR7_166_a_c_2c-002 --params=a, c/a, x₂, x₃, x₄</code>

Other compounds with this structure

GeAs₂Te₄, GeBi₂Te₄, PbBi₂Te₄, PbSb₂Te₄, SnBi₂Te₄, SnSb₂Te₄, TeS₂Bi₄, BiSbSnTe₄, Bi₂Sb₂Te₃

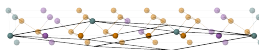
- This structure is nearly identical to MnBi₂Te₄, but the assumed ordering of the tellurium atoms is different in the two cases.
- We use the data from (Agaev, 1966) as reported by (Matsunaga, 2004), however the ICSD entry states that all of the (2c) sites have occupancy Te_{0.66}Sb_{0.33}. We follow (Matsunaga, 2004) and label the first (2c) site as Sb with the other two Te, preserving the stoichiometry.
- The binary form of this structure is Sn₄P₃.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

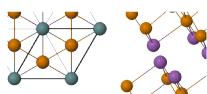
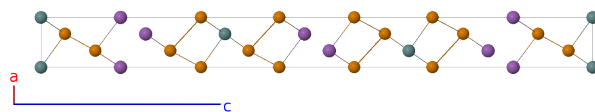
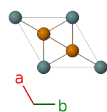
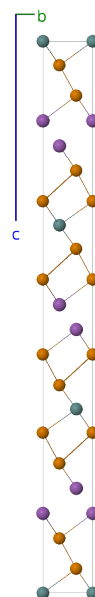
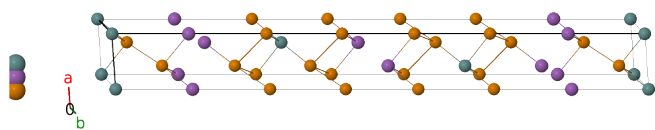
$$\mathbf{a}_1 = \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$$

$$\mathbf{a}_2 = \frac{1}{\sqrt{3}}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$$

$$\mathbf{a}_3 = -\frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\hat{\mathbf{y}} + \frac{1}{3}c\hat{\mathbf{z}}$$



Ge
Sb
Te



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).

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