

GeTe Structure:

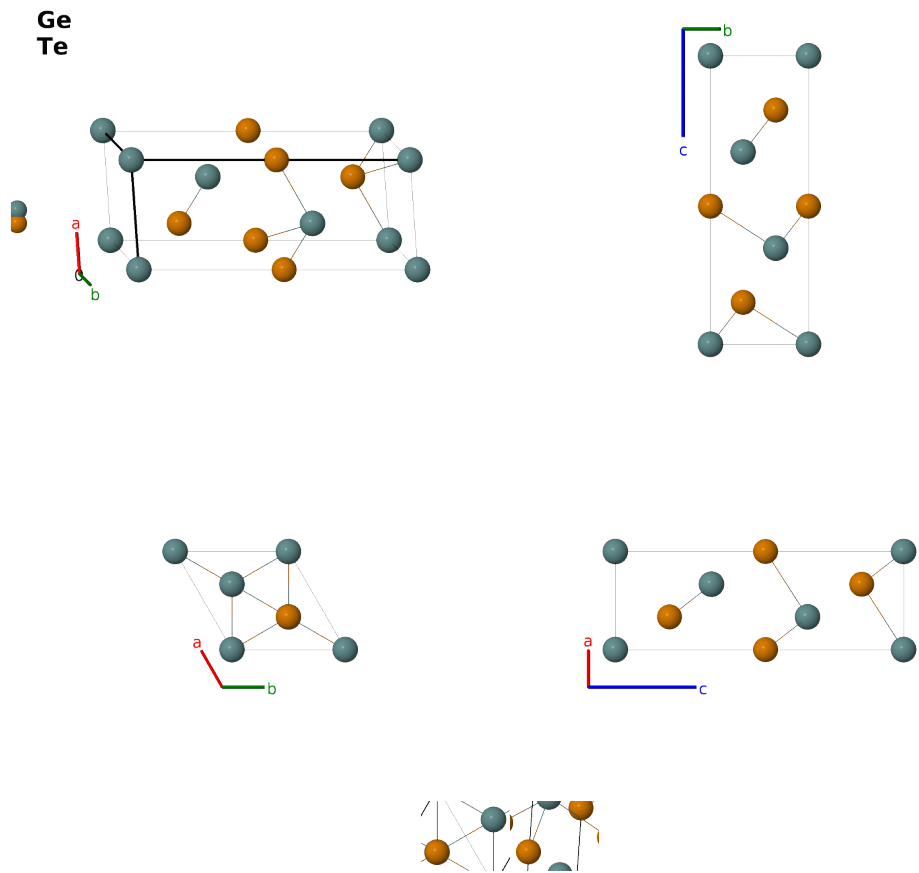
AB_hR2_160_a_a-002

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<https://aflow.org/prototype-encyclopedia/8379>

https://aflow.org/prototype-encyclopedia/AB_hR2_160_a_a-002

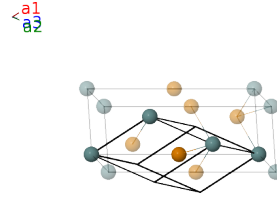


Prototype	GeTe
AFLOW prototype label	AB_hR2_160_a_a-002
ICSD	159907
CCDC	1676329
Pearson symbol	hR2
Space group number	160
Space group symbol	$R\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB_hR2_160_a_a-002</code> <code>--params=a, c/a, x₁, x₂</code>

- This is a distortion of the rock salt ($B1$) structure, and GeTe undergoes a phase transition to the rock salt structure above 300°C . When $\alpha = 60^\circ$ ($c/a = \sqrt{6}$) and $z_2 - z_1 = 1/2$ this becomes the rock salt structure.
- Space group $R3m$ #160 does not specify the origin of the z -axis. Here we arbitrarily set $z_1 = 0$.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	$=$	$cx_1 \hat{\mathbf{z}}$	(1a) Ge I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(1a) Te I

References

- [1] T. Nonaka, G. Ohbayashi, Y. Toriumi, Y. Mori, and H. Hashimoto, *Crystal structure of GeTe and $\text{Ge}_2\text{Sb}_2\text{Te}_5$ meta-stable phase*, Thin Solid Films **370**, 258–261 (2000), doi:10.1016/S0040-6090(99)01090-1.

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