GeTe Structure: AB_hR2_160_a_a-002

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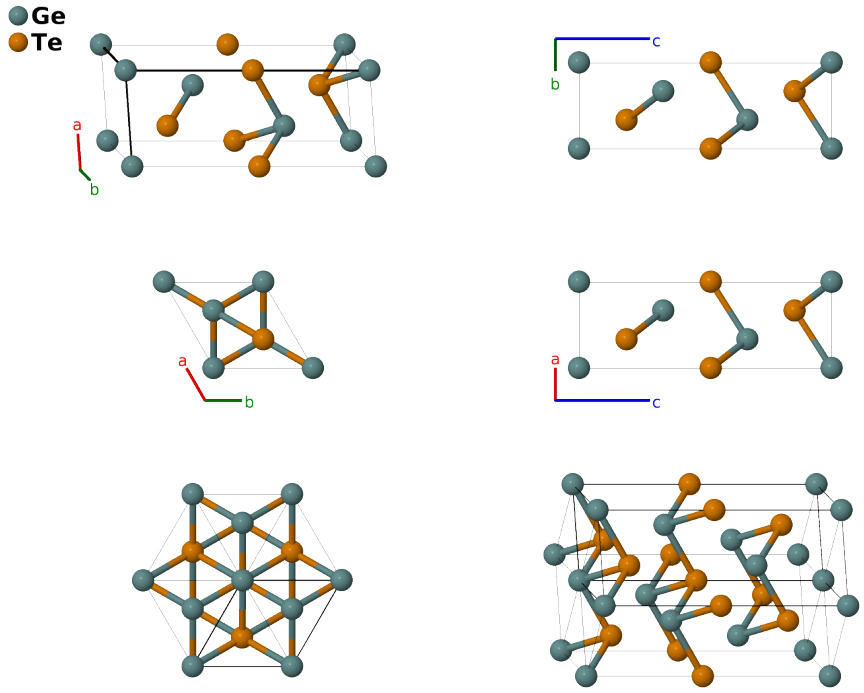
https://aflow.org/p/8379

https://aflow.org/p/AB_hR2_160_a_a-002

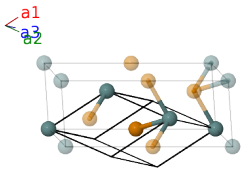


Prototype	GeTe
AFLOW prototype label	AB_hR2_160_a_a-002
ICSD	159907
Pearson symbol	hR2
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=AB_hR2_160_a_a-002 --params=`$a, c/a, x_1, x_2$

- 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 $\alpha = 60°(c/a = \sqrt{6})$ 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

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



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 $Ge_2Sb_2Te_5$ meta-stable phase*, Thin Solid Films **370**, 258–261 (2000), doi:10.1016/S0040-6090(99)01090-1.