Fe_4GeTe_2 Structure: A3BC_hR10_166_3c_c_c-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

---

https://aflow.org/prototype-encyclopedia/FR7H

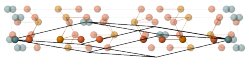
https://aflow.org/prototype-encyclopedia/A3BC_hR10_166_3c_c_c-001

Prototype	Fe_4GeTe_2
AFLOW prototype label	A3BC_hR10_166_3c_c_c-001
Pearson symbol	hR10
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3BC_hR10_166_3c_c_c-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5$

- Like Fe_3GeTe_2 and Fe_5GeTe_2 this is a layered van der Waals material.
- (Bera, 2023) give the occupation of the Fe I site as 27.5% and the Ge I site as 72.5%. This does not agree with their claimed stoichiometry $Fe_{4.2}Ge_{0.8}Te_2$. We suspect that this is the occupation for two sites, in which case the occupations for Fe I and Ge I should be 13.75% and 36.25%, respectively, for a final stoichiometry of $Fe_{4.275}Ge_{0.725}Te_2$, much closer to the claimed value.
- The ideal Fe_4GeTe_2 structure can be obtained by eliminating the Fe I atom and replacing the (2c) Ge I sites with a (1a) (0 0 0) site fully occupied by germanium. Such a structure would have the AFLOW label A4BC2_hR7_166_2c_a_c.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

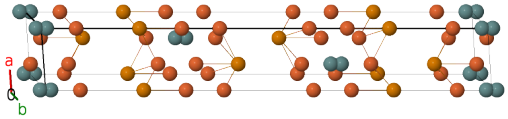
Rhombohedral primitive vectors

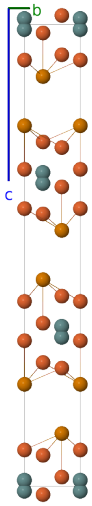
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}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

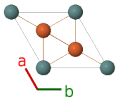


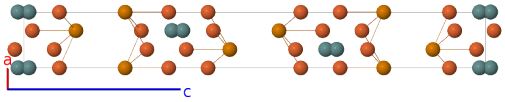
Basis vectors

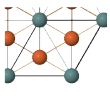
Fe
Ge
Te











		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(2c)	Fe I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-cx_1\,\hat{\mathbf{z}}$	(2c)	Fe 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)	Fe II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Fe II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Fe III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	Fe III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Ge I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Ge I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(2c)	Te I
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	Te I

References

[1] S. Bera, S. K. Pradhan, M. S. Khan, R. Pal, B. Pal, S. Kalimuddin, A. Bera, B. Das, A. N. Pal, and M. Mondal, *Unravelling the nature of spin reorientation transition in quasi-2D vdW magnetic material, Fe_4GeTe_2*, J. Magn. Magn. Mater. **565**, 170257 (2023), doi:10.1016/j.jmmm.2022.170257.

First cited in

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5.* Submitted to Computational Materials Science (2026).