$Fe_{5-\delta}GeTe_2$ Structure: A5BC2_hR8_160_5a_a_2a-001

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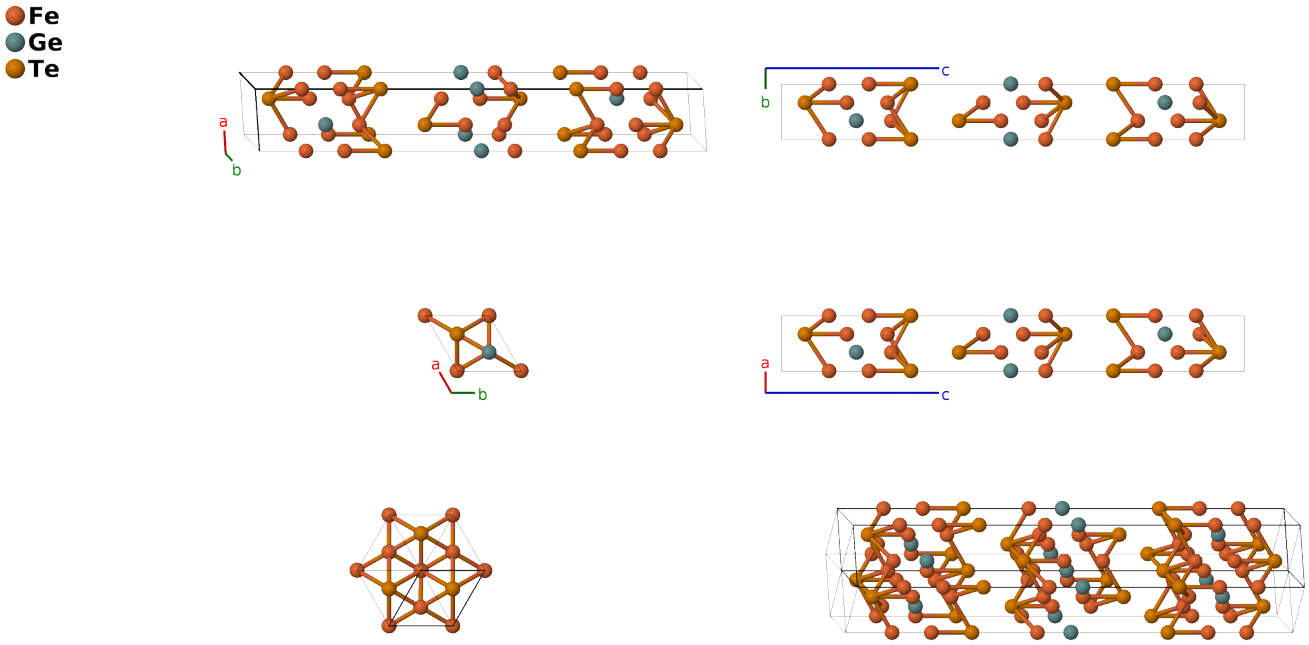
https://aflow.org/p/6V4S

https://aflow.org/p/A5BC2_hR8_160_5a_a_2a-001

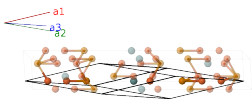


Prototype	Fe_5GeTe_2
AFLOW prototype label	A5BC2_hR8_160_5a_a_2a-001
ICSD	130074
Pearson symbol	hR8
Space group number	160
Space group symbol	$R3m$
AFLOW prototype command	`aflow --proto=A5BC2_hR8_160_5a_a_2a-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8$

- The Fe-III and Fe-V sites are partially occupied, with 89.8% and 72.5% filling, respectively, so that $\delta = 0.377$. The iron atoms may also be replaced by nickel.
- (Stahl, 2018) found that the germanium atoms actually half-fill two sites, one with $z = 0.48493$ and the other with $z = 0.50663$. In the diagram these two sites will overlap, so we replaced them by a single averaged site.
- 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)	Fe 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)	Fe II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(1a)	Fe III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(1a)	Fe IV
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(1a)	Fe V
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$cx_6\,\hat{\mathbf{z}}$	(1a)	Ge I
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$cx_7\,\hat{\mathbf{z}}$	(1a)	Te I
$\mathbf{B_8}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + x_8\,\mathbf{a}_3$	=	$cx_8\,\hat{\mathbf{z}}$	(1a)	Te II

References

[1] J. Stahl, E. Shlaen, and D. Johrendt, *The van der Waals Ferromagnets $Fe_{5-\delta}GeTe_2$ and $Fe_{5-\delta-x}Ni_xGeTe_2$ - Crystal Structure, Stacking Faults, and Magnetic Properties*, Z. Anorganische und Allgemeine Chemie **644**, 1923–1929 (2018), doi:10.1002/zaac.201800456.