

Fe_{5-δ}GeTe₂ Structure:

A5BC2_hR8_160_5a_a_2a-001

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<https://aflow.org/prototype-encyclopedia/6V4S>

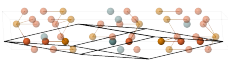
https://aflow.org/prototype-encyclopedia/A5BC2_hR8_160_5a_a_2a-001

Prototype	Fe ₅ GeTe ₂
AFLOW prototype label	A5BC2_hR8_160_5a_a_2a-001
ICSD	130074
CCDC	1874246
Pearson symbol	hR8
Space group number	160
Space group symbol	<i>R</i> 3 <i>m</i>
AFLOW prototype command	<code>aflow --proto=A5BC2_hR8_160_5a_a_2a-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄, x₅, x₆, x₇, x₈</code>

- 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. (This structure would have the AFLOW prototype label A5BC2_hR8_160_5a_a_2a.)
- Hexagonal settings of this structure can be obtained with the option `--hex`.

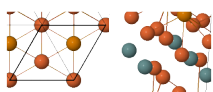
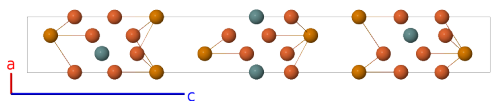
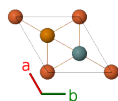
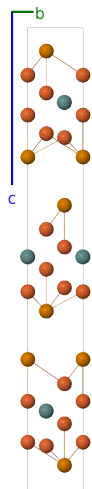
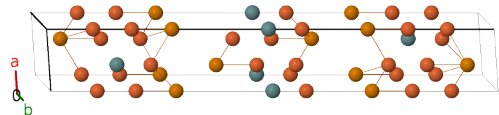
Rhombohedral primitive vectors

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



Basis vectors

Fe
Ge
Te



		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$cx_1 \hat{\mathbf{z}}$	(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.

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