

Fe₃GeTe₂ Structure:

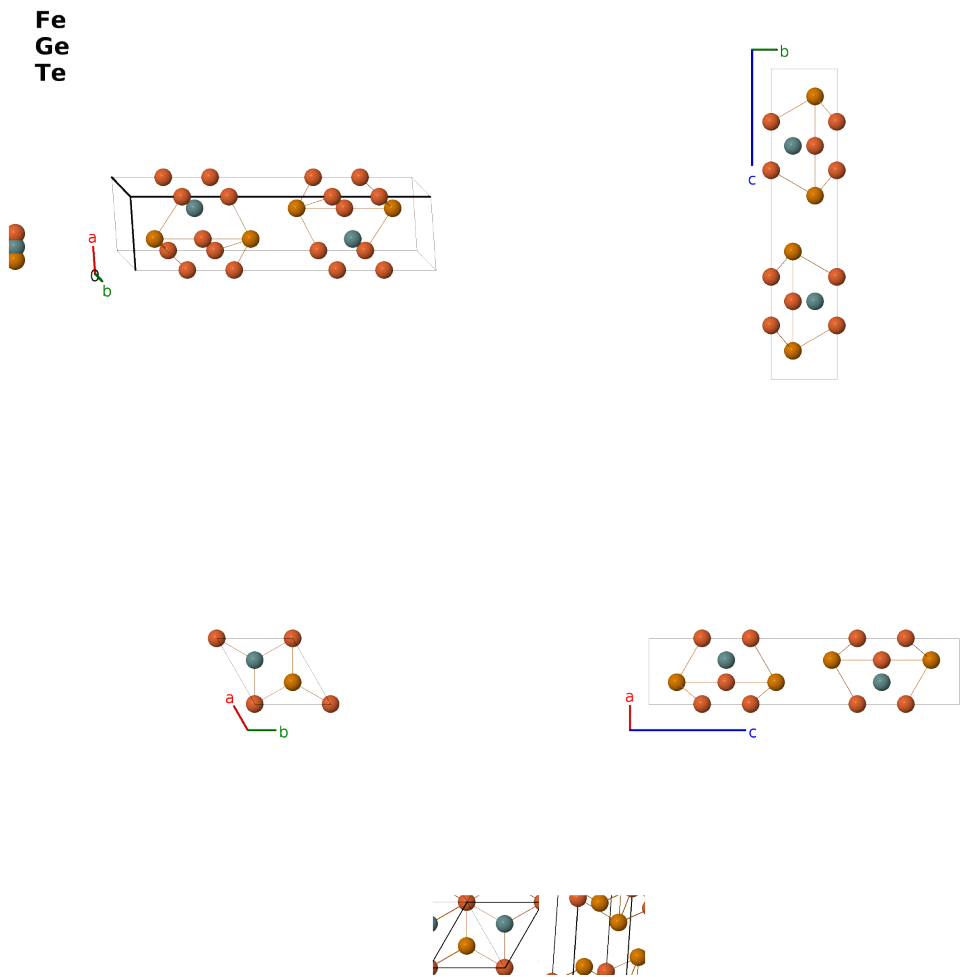
A3BC2_hP12_194_ce_d_f-001

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

https://aflow.org/prototype-encyclopedia/A3BC2_hP12_194_ce_d_f-001



Prototype	Fe ₃ GeTe ₂
AFLOW prototype label	A3BC2_hP12_194_ce_d_f-001
ICSD	415616
CCDC	1729580
Pearson symbol	hP12
Space group number	194
Space group symbol	$P6_3/mmc$

AFLOW prototype command `aflow --proto=A3BC2_hP12_194_ce_d_f-001`
 `--params=a, c/a, z3, z4`

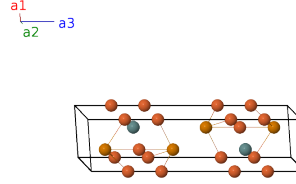
Other compounds with this structure

Fe₃GaTe₂, Ni₃GeTe₂

- (Deiseroth, 2006) note that the Fe (2c) site has 83% occupancy, and Ge (2d) 99%. The nearly isostructural compound Ni₃GeTe₂ is identical to the parent structure with nickel on the iron sites, except that the Ni (2c) site is split: the (2c) site is 70% occupied, and the (2a) (0,0,0) site contains 25% nickel.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Fe I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Fe I
$\mathbf{B}_3$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2d)	Ge I
$\mathbf{B}_4$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2d)	Ge I
$\mathbf{B}_5$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_6$	$= \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_7$	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_8$	$= -\left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B}_9$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4f)	Te I
$\mathbf{B}_{10}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c \left(z_4 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(4f)	Te I
$\mathbf{B}_{11}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4f)	Te I
$\mathbf{B}_{12}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c \left(z_4 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(4f)	Te I

References

- [1] H. Deiseroth, K. Aleksandrov, C. Reiner, L. Kienle, and R. K. Kremer, *Fe₃GeTe₂ and Ni₃GeTe₂ - Two New Layered Transition-Metal Compounds: Crystal Structures, HRTEM Investigations, and Magnetic and Electrical Properties*, Eur. J. Inorg. Chem. **2006**, 1561–1567 (2006), doi:10.1002/ejic.200501020.

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