

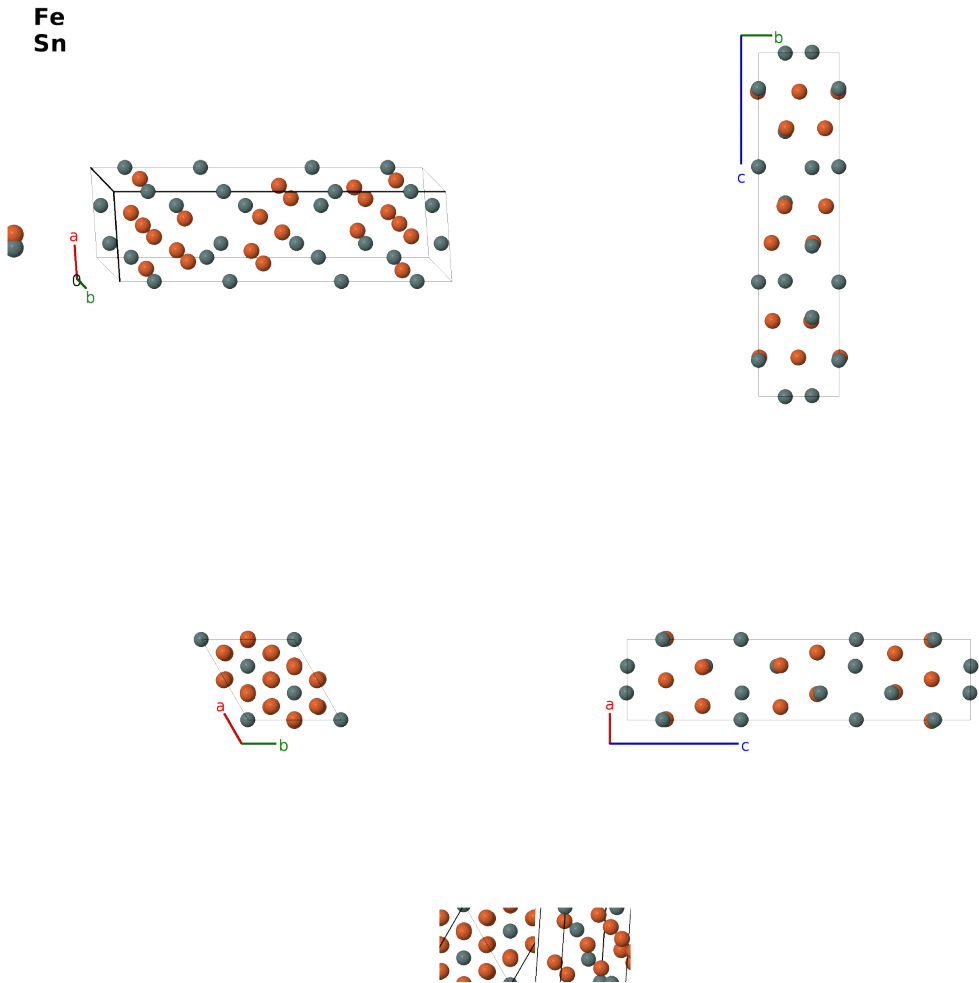
Fe₃Sn₂ Structure: A3B2_hR10_166_h_2c-001

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

https://aflow.org/prototype-encyclopedia/A3B2_hR10_166_h_2c-001



Prototype	Fe ₃ Sn ₂
AFLOW prototype label	A3B2_hR10_166_h_2c-001
ICSD	71
CCDC	1590696
Pearson symbol	hR10
Space group number	166
Space group symbol	$R\bar{3}m$

AFLOW prototype command `aflow --proto=A3B2_hR10_166_h_2c-001`
 `--params=a,c/a,x1,x2,x3,z3`

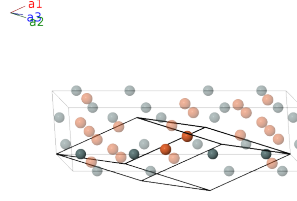
Other compounds with this structure

V₃Sb₂

- There is no ICSD entry for (Dally, 2021), so we use the one from the earlier work of (Malaman, 1976).
 - 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

	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)	Sn 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)	Sn 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)	Sn 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)	Sn II
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Fe I
$\mathbf{B}_6$	$= z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Fe I
$\mathbf{B}_7$	$= x_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Fe I
$\mathbf{B}_8$	$= -z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Fe I
$\mathbf{B}_9$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Fe I
$\mathbf{B}_{10}$	$= -x_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{\sqrt{3}}a(x_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(2x_3 + z_3) \hat{\mathbf{z}}$	(6h)	Fe I

References

- [1] R. L. Dally, D. Phelan, N. Bishop, N. J. Ghimire, and J. W. Lynn, *Isotropic Nature of the Metallic Kagome Ferromagnet Fe₃Sn₂ at High Temperatures*, Crystals **11**, 307 (2021), doi:10.3390/cryst11030307.
- [2] B. Malaman, B. Roques, A. Courtois, and J. Protas, *Structure cristalline du stannure de fer Fe₃Sn₂*, Acta Crystallographica B **32**, 1348–1351 (1976), doi:10.1107/S0567740876005323.

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