Fe_3Sn_2 Structure: A3B2_hR10_166_h_2c-001

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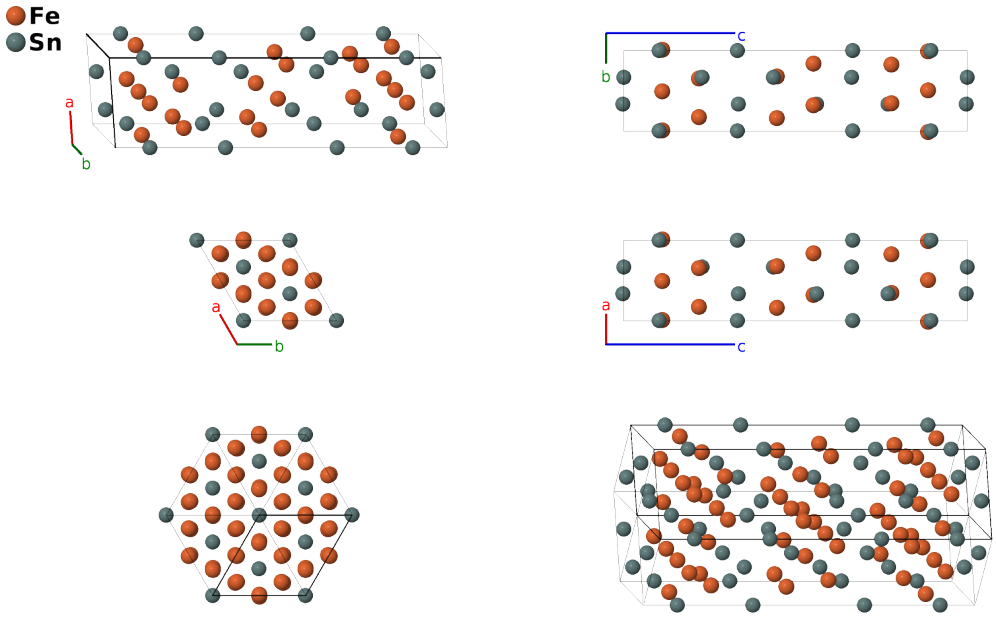
https://aflow.org/p/KQQW

https://aflow.org/p/A3B2_hR10_166_h_2c-001



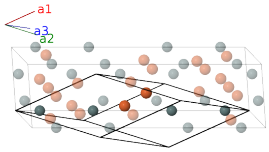
Prototype	Fe_3Sn_2
AFLOW prototype label	A3B2_hR10_166_h_2c-001
ICSD	71
Pearson symbol	hR10
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B2_hR10_166_h_2c-001 --params=`$a, c/a, x_1, x_2, x_3, z_3$

Other compounds with this structure
V_3Sb_2

- 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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(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 Fe_3Sn_2 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 Fe_3Sn_2*, Acta Crystallographica B **32**, 1348–1351 (1976), doi:10.1107/S0567740876005323.