$FePSe_3$ Structure: ABC3_hR10_148_c_c_f-001

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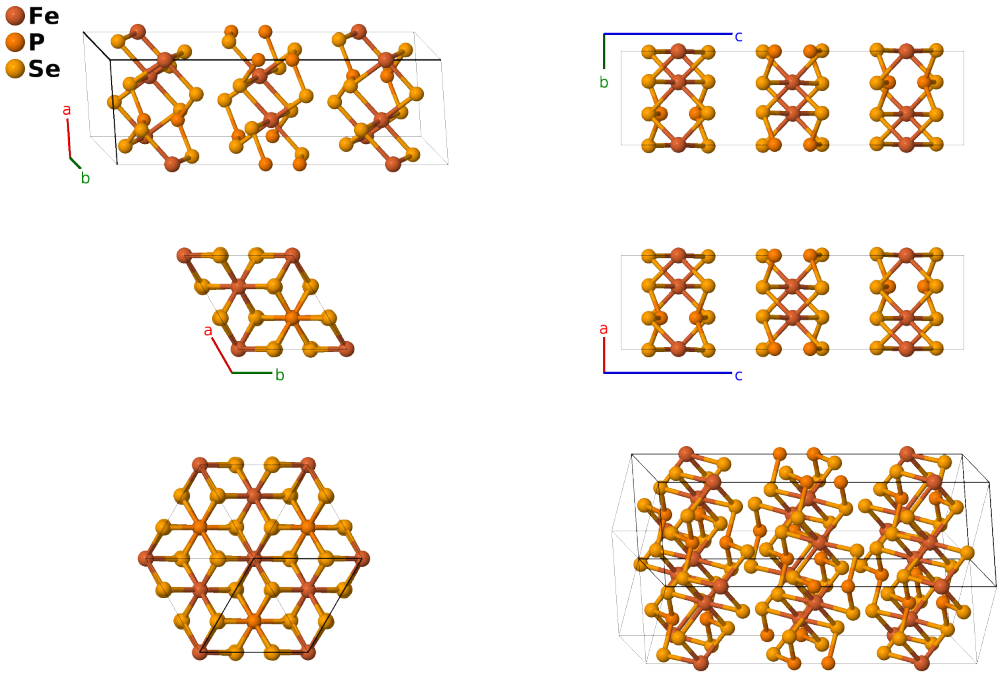
https://aflow.org/p/CFP9

https://aflow.org/p/ABC3_hR10_148_c_c_f-001



Prototype	$FePSe_3$
AFLOW prototype label	ABC3_hR10_148_c_c_f-001
ICSD	86272
Pearson symbol	hR10
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	`aflow --proto=ABC3_hR10_148_c_c_f-001 --params=`$a, c/a, x_1, x_2, x_3, y_3, z_3$

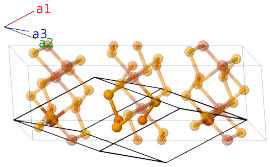
Other compounds with this structure
$CrGeTe_3$, $CrSiTe_3$, $MnPSe_3$

- We use the data taken by (Wiedenmann, 1981) at 15K, while the ICSD entry used their data at 154K.
- (Klingen, 1973) placed this structure in the non-centrosymmetric space group $R3$ #146.
- For quaternary compounds in this structure, see Li_2ZrTeO_6.

- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \tfrac{1}{3}c\,\hat{\mathbf{z}}
\end{aligned}$$



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)	Fe 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)	Fe 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)	P I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	P I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_6}$	=	$z_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + y_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_7}$	=	$y_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_3 - z_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 - 2y_3 + z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_9}$	=	$-z_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - y_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(y_3 - z_3)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(2x_3 - y_3 - z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Se I
$\mathbf{B_{10}}$	=	$-y_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_3 - y_3)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_3 + y_3 - 2z_3)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(x_3 + y_3 + z_3)\,\hat{\mathbf{z}}$	(6f)	Se I

References

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[2] W. Klingen, G. Eulenberger, and H. Hahn, *Uber die Kristallstrukturen von Fe_2P_2Se6 und $Fe_2P_2S_6$*, Z. Anorganische und Allgemeine Chemie **401**, 97–112 (1973), doi:10.1002/zaac.19734010113.

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