$FePSe_3$ Structure: ABC3_hR10_146_2a_2a_2b-001

This structure originally had the label `ABC3_hR10_146_2a_2a_2b`. Calls to that address will be redirected here.

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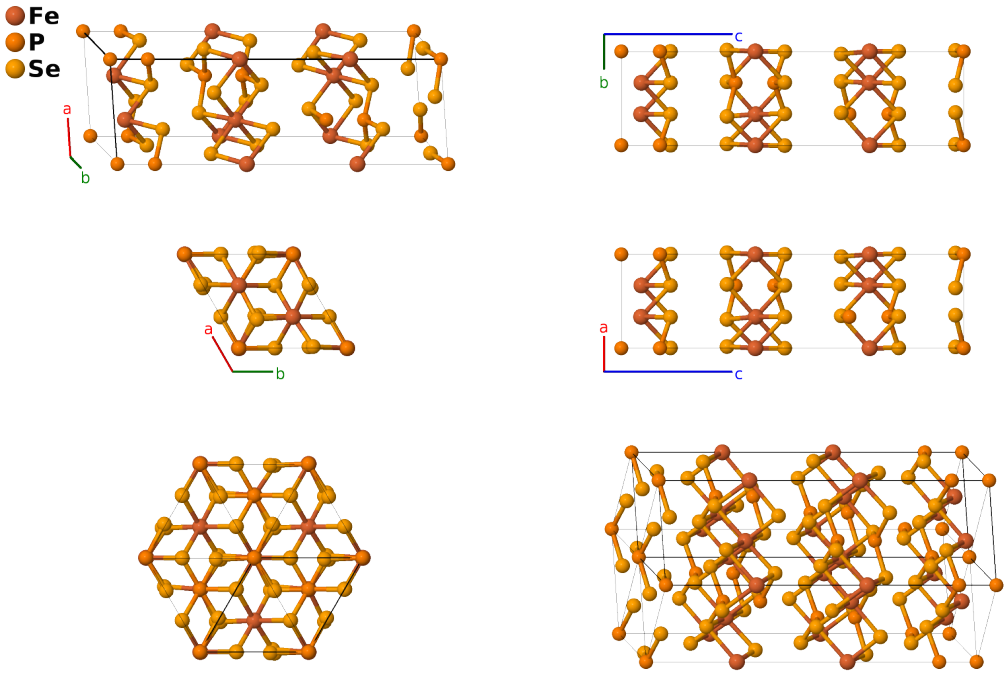
https://aflow.org/p/EARG

https://aflow.org/p/ABC3_hR10_146_2a_2a_2b-001

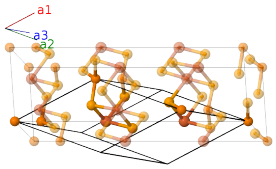


Prototype	$FePSe_3$
AFLOW prototype label	ABC3_hR10_146_2a_2a_2b-001
ICSD	16246
Pearson symbol	hR10
Space group number	146
Space group symbol	$R3$
AFLOW prototype command	`aflow --proto=ABC3_hR10_146_2a_2a_2b-001 --params=`$a, c/a, x_1, x_2, x_3, x_4, x_5, y_5, z_5, x_6, y_6, z_6$

- (Klingen, 1973) also considered the possibility that this structure could be in the centrosymmetric space group $R\bar{3}$ #148. That structure was refined by (Wiedenmann, 1981).

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$cx_1\,\hat{\mathbf{z}}$	(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)	P I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(1a)	P II
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_5 - z_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 - 2y_5 + z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(3b)	Se I
$\mathbf{B_6}$	=	$z_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + y_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_5 - z_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_5 - y_5 - z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(3b)	Se I
$\mathbf{B_7}$	=	$y_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_5 + y_5 - 2z_5)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_5 + y_5 + z_5)\,\hat{\mathbf{z}}$	(3b)	Se I
$\mathbf{B_8}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - 2y_6 + z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(3b)	Se II
$\mathbf{B_9}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + y_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(y_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(2x_6 - y_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(3b)	Se II
$\mathbf{B_{10}}$	=	$y_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 + y_6 - 2z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(x_6 + y_6 + z_6)\,\hat{\mathbf{z}}$	(3b)	Se II

References

[1] 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.

[2] A. Wiedenmann, J. Rossat-Mignod, A. Louisy, R. Brec, and J. Rouxel, *Neutron diffraction study of the layered compounds $MnPSe_3$ and $FePSe_3$*, Solid State Commun. **40**, 1067–1072 (1981), doi:10.1016/0038-1098(81)90253-2.

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