

FePSe₃ Structure:

ABC3_hR10_146_2a_2a_2b-001

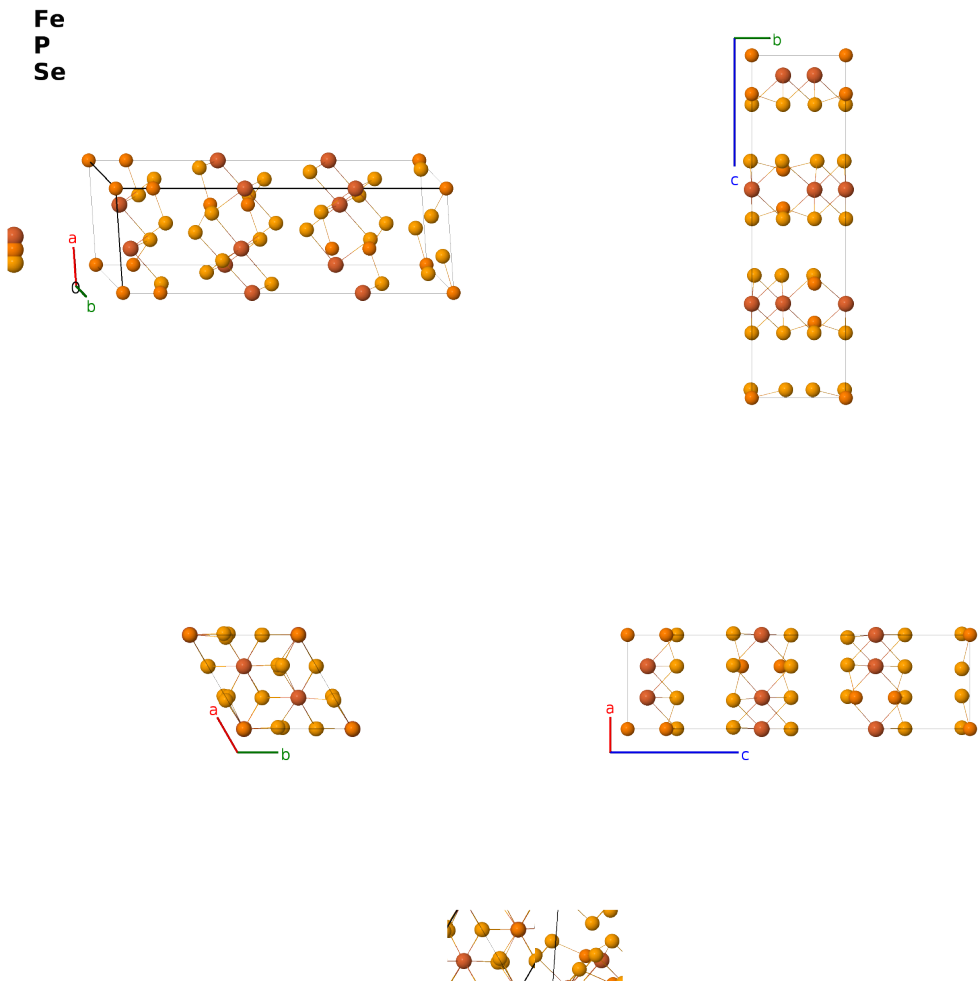
This structure previously used the label(s) **ABC3_hR10_146_2a_2a_2b**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/prototype-encyclopedia/ABC3_hR10_146_2a_2a_2b-001



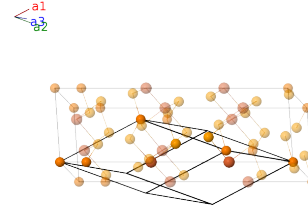
Prototype	FePSe ₃
AFLOW prototype label	ABC3_hR10_146_2a_2a_2b-001
ICSD	16246
CCDC	1596847
Pearson symbol	hR10

Space group number	146
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=ABC3_hR10_146_2a_2a_2b-001</code> <code>--params=a, c/a, x₁, x₂, x₃, x₄, x₅, y₅, z₅, x₆, y₆, z₆</code>

- (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

$$\begin{aligned}
\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\
\mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + x_1 \mathbf{a}_2 + x_1 \mathbf{a}_3$	=	$cx_1 \hat{\mathbf{z}}$	(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, *Über die Kristallstrukturen von $\text{Fe}_2\text{P}_2\text{Se}_6$ und $\text{Fe}_2\text{P}_2\text{S}_6$* , 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.

Found in

- [1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.

First cited in

D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043