

FePSe₃ Structure:

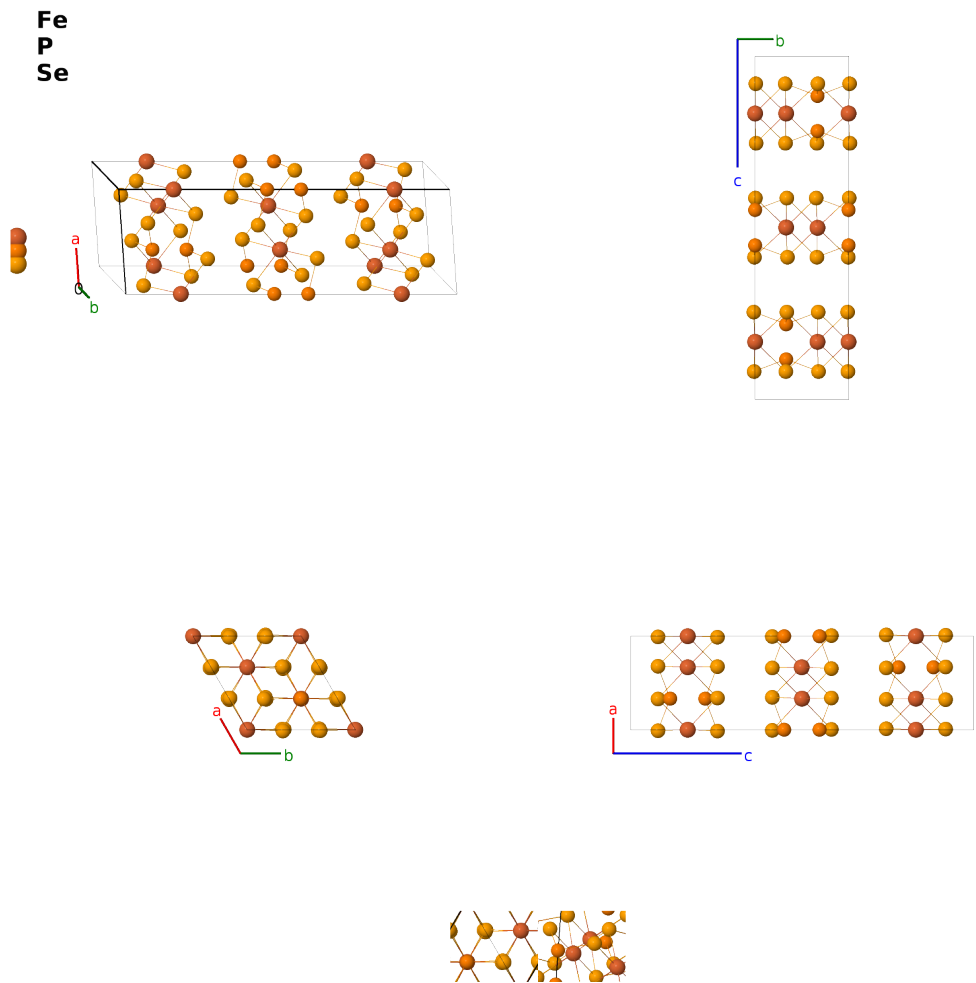
ABC3_hR10_148_c_c_f-001

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/CFP9>

https://aflow.org/prototype-encyclopedia/ABC3_hR10_148_c_c_f-001



Prototype	FePSe ₃
AFLOW prototype label	ABC3_hR10_148_c_c_f-001
ICSD	86272
CCDC	1646161
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, x1, x2, x3, y3, z3`

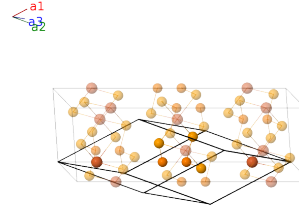
Other compounds with this structure

CrGeTe₃, CrSiTe₃, MnPSe₃

- 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 *R*3 #146.
 - For quaternary compounds in this structure, see Li₂ZrTeO₆.
 - 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)	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

- [1] A. Wiedenmann, J. Rossat-Mignod, A. Louisy, R. Brec, and J. Rouxel, *Neutron diffraction study of the layered compounds MnPSe₃ and FePSe₃*, Solid State Commun. **40**, 1067–1072 (1981), doi:10.1016/0038-1098(81)90253-2.

- [2] W. Klingen, G. Eulenberger, and H. Hahn, *Über die Kristallstrukturen von $Fe_2P_2Se_6$ und $Fe_2P_2S_6$* , Z. Anorganische und Allgemeine Chemie **401**, 97–112 (1973), doi:10.1002/zaac.19734010113.

Found in

- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

First cited in

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.