

Fe₁₂Zr₂P₇ Structure:

A12B7C2_hP21_174_2j2k_ajk_cf-001

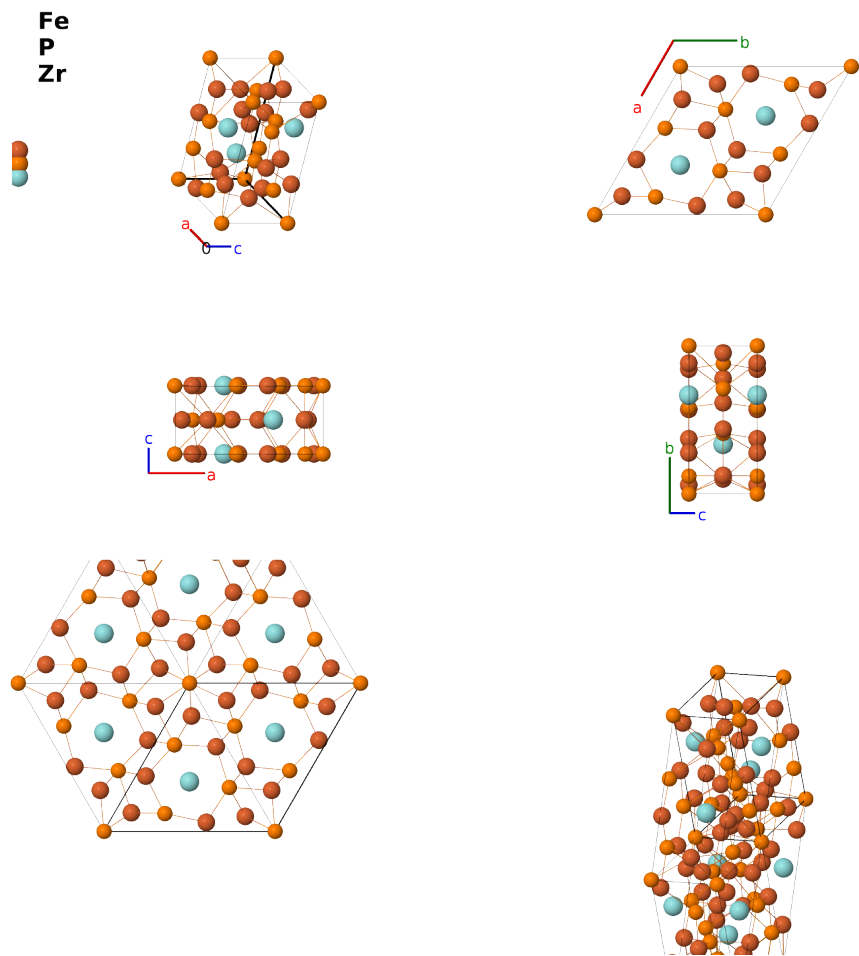
This structure previously used the label(s) **A12B7C2_hP21_174_2j2k_ajk_cf**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/EE97>

https://aflow.org/prototype-encyclopedia/A12B7C2_hP21_174_2j2k_ajk_cf-001

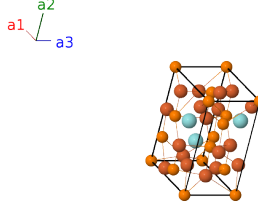


Prototype	Fe ₁₂ P ₇ Zr ₂
AFLOW prototype label	A12B7C2_hP21_174_2j2k_ajk_cf-001
ICSD	25757
CCDC	1601400
Pearson symbol	hP21
Space group number	174

Space group symbol $P\bar{6}$

AFLOW prototype command `aflow --proto=A12B7C2_hP21_174_2j2k_ajk_cf-001`
`--params=a, c/a, x4, y4, x5, y5, x6, y6, x7, y7, x8, y8, x9, y9`

Hexagonal primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	0	$=$	0	(1a)	P I
$\mathbf{B}_2$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}}$	(1c)	Zr I
$\mathbf{B}_3$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(1f)	Zr II
$\mathbf{B}_4$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_4 + y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_4 - y_4) \hat{\mathbf{y}}$	(3j)	Fe I
$\mathbf{B}_5$	$-y_4 \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_4 - 2y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}}$	(3j)	Fe I
$\mathbf{B}_6$	$-(x_4 - y_4) \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4 \hat{\mathbf{y}}$	(3j)	Fe I
$\mathbf{B}_7$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_5 + y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_5 - y_5) \hat{\mathbf{y}}$	(3j)	Fe II
$\mathbf{B}_8$	$-y_5 \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_5 - 2y_5) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5 \hat{\mathbf{y}}$	(3j)	Fe II
$\mathbf{B}_9$	$-(x_5 - y_5) \mathbf{a}_1 - x_5 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_5 - y_5) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5 \hat{\mathbf{y}}$	(3j)	Fe II
$\mathbf{B}_{10}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 + y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_6 - y_6) \hat{\mathbf{y}}$	(3j)	P II
$\mathbf{B}_{11}$	$-y_6 \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2$	$=$	$\frac{1}{2}a (x_6 - 2y_6) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6 \hat{\mathbf{y}}$	(3j)	P II
$\mathbf{B}_{12}$	$-(x_6 - y_6) \mathbf{a}_1 - x_6 \mathbf{a}_2$	$=$	$-\frac{1}{2}a (2x_6 - y_6) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6 \hat{\mathbf{y}}$	(3j)	P II
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_7 + y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_7 - y_7) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Fe III
$\mathbf{B}_{14}$	$-y_7 \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_7 - 2y_7) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Fe III
$\mathbf{B}_{15}$	$-(x_7 - y_7) \mathbf{a}_1 - x_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_7 - y_7) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Fe III
$\mathbf{B}_{16}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_8 + y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_8 - y_8) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Fe IV
$\mathbf{B}_{17}$	$-y_8 \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_8 - 2y_8) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Fe IV
$\mathbf{B}_{18}$	$-(x_8 - y_8) \mathbf{a}_1 - x_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_8 - y_8) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	Fe IV
$\mathbf{B}_{19}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_9 + y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a (x_9 - y_9) \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	P III
$\mathbf{B}_{20}$	$-y_9 \mathbf{a}_1 + (x_9 - y_9) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}a (x_9 - 2y_9) \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	P III
$\mathbf{B}_{21}$	$-(x_9 - y_9) \mathbf{a}_1 - x_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-\frac{1}{2}a (2x_9 - y_9) \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3k)	P III

References

- [1] E. Ganglberger, *Die Kristallstruktur von Fe₁₂Zr₂P₇*, Mh. Chem. **99**, 557–565 (1968), doi:10.1007/BF00901204.

Found in

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

First cited in

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