

Original Fe₂P (*C*22) Structure: A2B_hP9_150_ef_ad-001

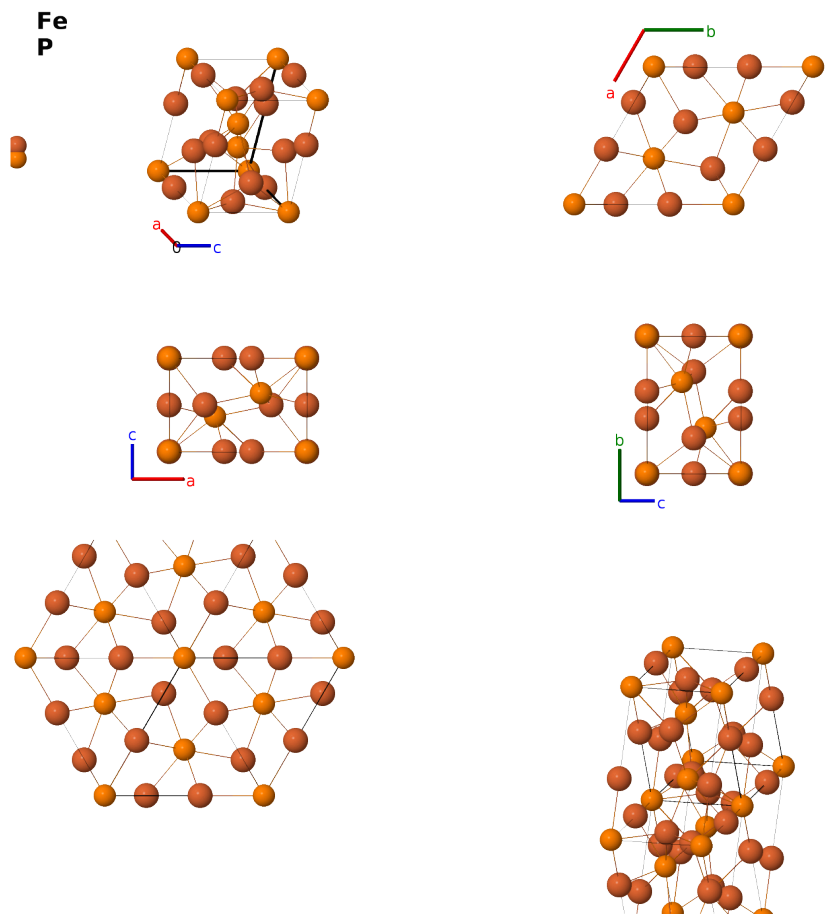
This structure previously used the label(s) **A2B_hP9_150_ef_bd**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/6CGG>

https://aflow.org/prototype-encyclopedia/A2B_hP9_150_ef_ad-001

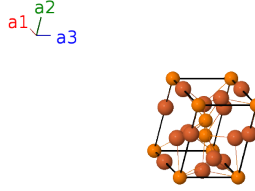


Prototype	Fe ₂ P
AFLOW prototype label	A2B_hP9_150_ef_ad-001
<i>Strukturbericht</i> designation	<i>C</i> 22
Pearson symbol	hP9
Space group number	150
Space group symbol	<i>P</i> 321

AFLOW prototype command `aflow --proto=A2B_hP9_150_ef_ad-001`
 `--params=a, c/a, z2, x3, x4`

- This is the structure given in *Strukturbericht* Vol. II, apparently from (Friauf, 1930), which we have not been able to locate. As noted by Wyckoff, the structure, which was “generally accepted for years, has recently been shown to be incorrect.” (Vol I., 360, also in Hendricks, 1930). The corrected structure, as given in Pearson’s Handbook, is given in the revised Fe₂P page. When z_2 is set to zero this structure reverts to the revised Fe₂P structure.

Trigonal (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
$\mathbf{B}_2$	=	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2d) P II
$\mathbf{B}_3$	=	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(2d) P II
$\mathbf{B}_4$	=	$x_3 \mathbf{a}_1$	=	$\frac{1}{2}ax_3 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(3e) Fe I
$\mathbf{B}_5$	=	$x_3 \mathbf{a}_2$	=	$\frac{1}{2}ax_3 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3 \hat{\mathbf{y}}$	(3e) Fe I
$\mathbf{B}_6$	=	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}}$	(3e) Fe I
$\mathbf{B}_7$	=	$x_4 \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}ax_4 \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f) Fe II
$\mathbf{B}_8$	=	$x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}ax_4 \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4 \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f) Fe II
$\mathbf{B}_9$	=	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$-ax_4 \hat{\mathbf{x}} + \frac{1}{2}c \hat{\mathbf{z}}$	(3f) Fe II

References

- [1] J. B. Friauf, , Trans. Amer. Soc. Steel Treat. **17**, 499–508 (1930).
- [2] S. B. Hendricks and P. R. Kesting, *The Crystal Structure of Fe₂P, Fe₂N, Fe₃N and FeB*, Z. Kristallogr. **74**, 511–533 (1930), doi:10.1524/zkri.1930.74.1.511.
- [3] R. G. W. Wyckoff, *Crystal Structures, Inorganic Compounds RX_n, R_nMX₂, R_nMX₃*, vol. 2 (Wiley, 1964).
- [4] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

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