Original Fe_2P ($C22$) Structure: A2B_hP9_150_ef_ad-001

This structure originally had the label `A2B_hP9_150_ef_bd`. Calls to that address will be redirected here.

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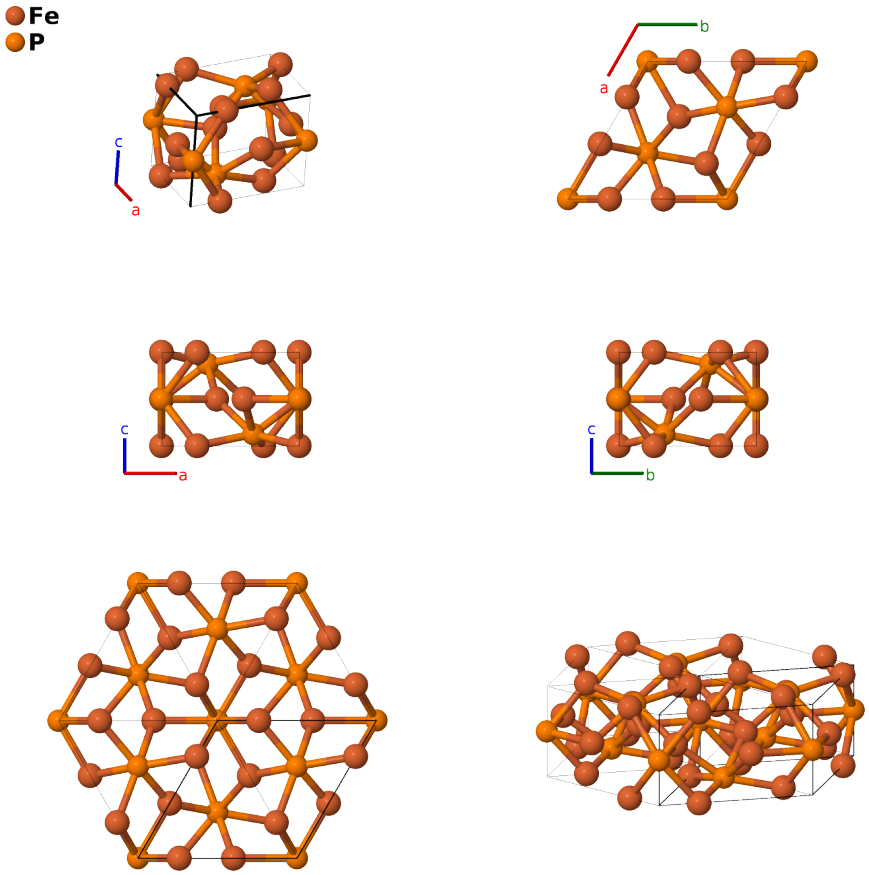
https://aflow.org/p/6CGG

https://aflow.org/p/A2B_hP9_150_ef_ad-001

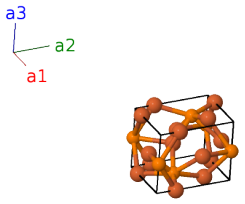


Prototype	Fe_2P
AFLOW prototype label	A2B_hP9_150_ef_ad-001
***Strukturbericht* designation**	$C22$
ICSD	none
Pearson symbol	hP9
Space group number	150
Space group symbol	$P321$
AFLOW prototype command	`aflow --proto=A2B_hP9_150_ef_ad-001 --params=`$a, c/a, z_2, x_3, x_4$

- 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 Fe_2P page. When z_2 is set to zero this structure reverts to the revised Fe_2P structure.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



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. Kosting, *The Crystal Structure of Fe_2P, Fe_2N, Fe_3N 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 RXn, RnMX2, RnMX3*, 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).