Barringerite (Revised Fe_2P, $C22$) Crystal Structure: A2B_hP9_189_fg_ad-001

This structure originally had the label `A2B_hP9_189_fg_bc`. Calls to that address will be redirected here.

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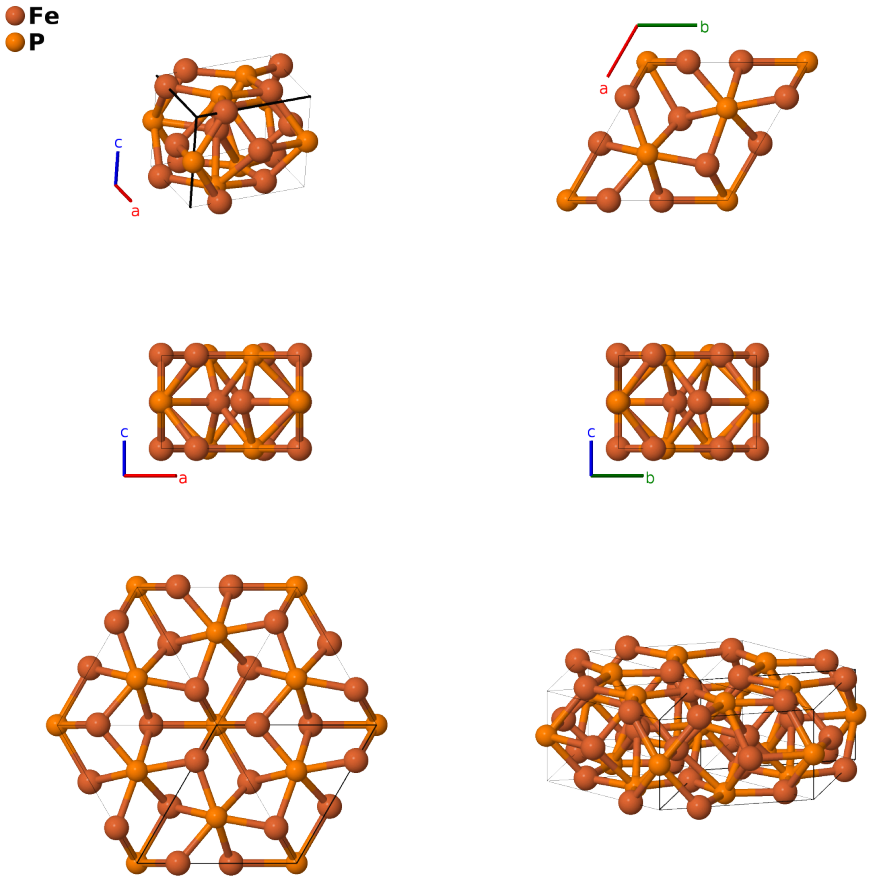
https://aflow.org/p/6UK2

https://aflow.org/p/A2B_hP9_189_fg_ad-001



Prototype	Fe_2P
AFLOW prototype label	A2B_hP9_189_fg_ad-001
***Strukturbericht* designation**	$C22$
Mineral name	barringerite
ICSD	200529
Pearson symbol	hP9
Space group number	189
Space group symbol	$P\bar{6}2m$

AFLOW prototype command `aflow --proto=A2B_hP9_189_fg_ad-001 --params=`$a, c/a, x_3, x_4$

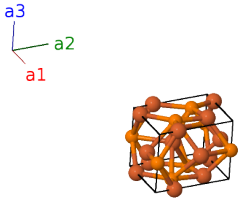
Other compounds with this structure

Co_2As, Mg_2In, Mn_2P, Ni_2P, Pd_2As, Pd_2Ge, Pd_2Si, Pt_2Ge, Pt_2Si (HT)

- This is not the structure given in (Hermann, 1937) *Strukturbericht* Vol. II, 95. As noted by (Wyckoff, 1963), that structure was "generally accepted for years, [but] has recently been shown to be incorrect." This is the corrected structure, as given in Wyckoff and (Villars, 1991). See the original Fe_2P ($C22$) page for the *Strukturbericht* version of this crystal.
- This is the binary version of the structure. The two iron sites are independent, and can be replaced by different atoms. We put the resulting ternary structures under the ZrNiAl prototype.

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
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	P II
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	P II
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Fe I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_2$	=	$\frac{1}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}}$	(3f)	Fe I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}}$	(3f)	Fe I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Fe II
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Fe II
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Fe II

References

[1] H. Fujii, S. Komura, T. Takeda, T. Okamoto, Y. Ito, and J. Akimitsu, *Polarized Neutron Diffraction Study of Fe_2P Single Crystal*, J. Phys. Soc. Jpn. **46**, 1616–1621 (1979), doi:10.1143/JPSJ.46.1616.

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

[3] 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] R. G. W. Wyckoff, *Crystal Structure*, vol. 1 (Interscience, New York, London, Sydney, 1963).