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

This structure previously used the label(s) `A2B_hP9_189_fg_bc`. Calls to these addresses will be redirected here.

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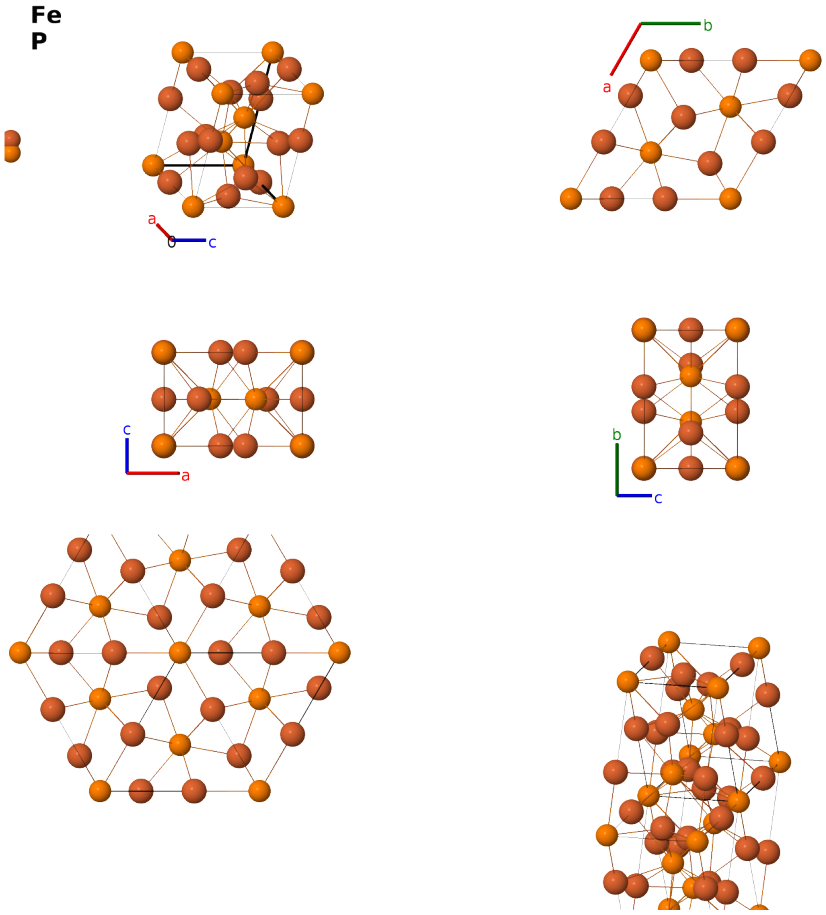
https://aflow.org/prototype-encyclopedia/6UK2

https://aflow.org/prototype-encyclopedia/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
CCDC	1705425
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=`$a, c/a, x_3, x_4$

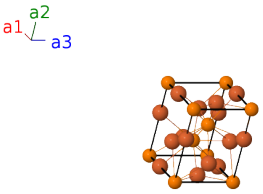
Other compounds with this structure

Co_2As, Cr_2As, Mg_2In, Mn_2P, Ni_2P, Pd_2As, Pd_2Ge, Pd_2Si, Pt_2Ge, Pt_2Si (HT), S_2U

- 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. There are two possible tenary versions:
  - The two iron sites are independent, and can be replaced by different atoms. We put the resulting ternary structures under the ZrNiAl prototype.
  - The two potassium sites are also independent, that ternary structure can be represented by Zr_6CoAs_2.
- The quaternary version of this structure has different species on all four Wyckoff sites. We represent this by the $Tb_3Mn_3Ga_2Si$ structure.

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).

First cited in

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