$L'3_0$ (approximate Fe_2N) Structure: AB_hP4_194_c_a-003

This structure originally had the label `AB_hP4_194_c_a.Fe2N`. Calls to that address will be redirected here.

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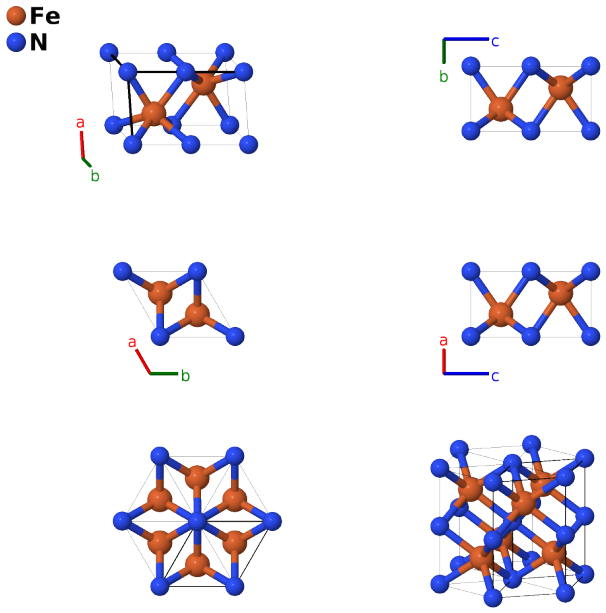
https://aflow.org/p/Q425

https://aflow.org/p/AB_hP4_194_c_a-003



Prototype	Fe_2N
AFLOW prototype label	AB_hP4_194_c_a-003
***Strukturbericht* designation**	$L'3_0$
ICSD	none
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=AB_hP4_194_c_a-003 --params=`$a, c/a$

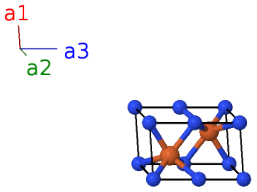
Other compounds with this structure
β-CTa_2, CV_2, CW_2, Mn_2N, Nb_2N, $Ta_{\approx 2}N$

- The $L'3_0$ designation is only found in (Smithells, 1955) and (Pearson, 1958), as well as their following volumes.
- Smithells gives two possible positions of the nitrogen atoms. We use the one that matches Pearson, which (Parthé, 1993) notes is equivalent to the NiAs $B8_1$ structure, but here the (2a) nitrogen site is only half-filled to maintain stoichiometry.

- Neither of the defining references gives a source for the structure.
- It is likely an approximation to ϵ-Fe_2N, which has the β-V_2N $L'3_2$ structure.
- We take the lattice constants for this structure from the Fe-Fe distances in ϵ-Fe_2N provided by (Hendricks, 1930), though this is *not* the structure described by Hendricks.
- The similar compounds list is taken from (Pearson, 1967). As it is quite similar to the list for β-V_2N, it is likely that this structure is only an approximation to the correct structure for these compounds as well.
- Fe_2N is also observed in the ζ-Fe_2N structure.
- This structure has the same AFLOW designation, AB_hP4_194_c_a_Fe2N, as $B8_1$. The two structures differ by their lattice constants and the half-occupancy of the (2a) site in $L'3_0$.

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	(2a)	N I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Fe I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(2c)	Fe I

References

[1] C. J. Smithells, *Metals Reference Book* (Butterworths Scientific, London, 1955), second edn.

[2] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.

[3] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

[4] S. B. Hendricks and P. R. Kosting, *The Crystal Structure of Fe_2P, Fe_2N, Fe_3N and FeB*, Z. ristallogr. **74**, 511–533 (1930), doi:10.1524/zkri.1930.74.1.511.

[5] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys, Volume 2*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 8 (Pergamon Press, Oxford, London, Edinburgh, New York, Toronto, Sydney, Paris, Braunschweig, 1967).