

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

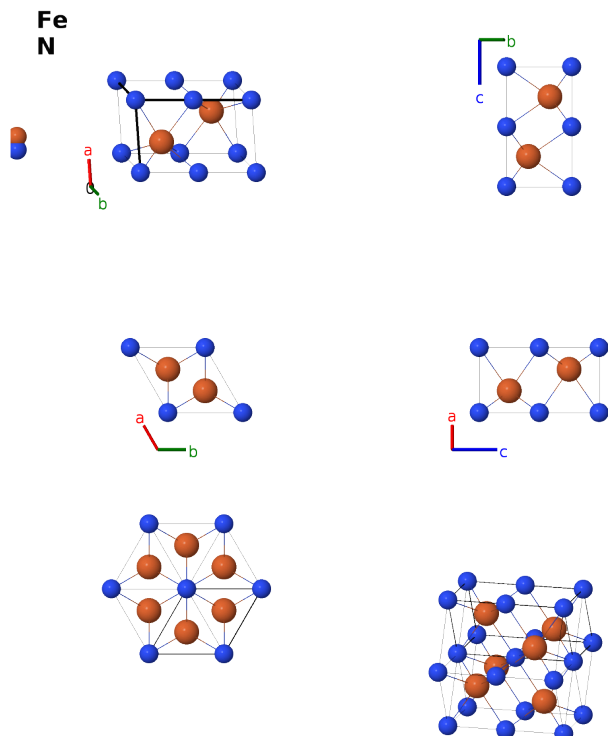
This structure previously used the label(s) `AB_hP4_194_c_a.Fe2N`. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/Q425>

https://aflow.org/prototype-encyclopedia/AB_hP4_194_c_a-003



Prototype	Fe_2N
AFLOW prototype label	AB_hP4_194_c_a-003
<i>Strukturbericht</i> designation	$L'3_0$
Pearson symbol	hP4
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	<code>aflow --proto=AB_hP4_194_c_a-003 --params=a, c/a</code>

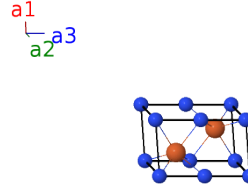
Other compounds with this structure

β -CTa₂, CV₂, γ -CW₂, Mn₂N, Nb₂N, Ta₂N

- 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 -Fe₂N, which has the β -V₂N $L'3_2$ structure.
- We take the lattice constants for this structure from the Fe-Fe distances in ϵ -Fe₂N 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 -V₂N, it is likely that this structure is only an approximation to the correct structure for these compounds as well.
- Fe₂N is also observed in the ζ -Fe₂N 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

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\hat{\mathbf{y}} \\ \mathbf{a}_3 &= c\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	(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, Frankfurt, 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. Kesting, *The Crystal Structure of Fe₂P, Fe₂N, Fe₃N and FeB*, Z. kristallogr. **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).

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