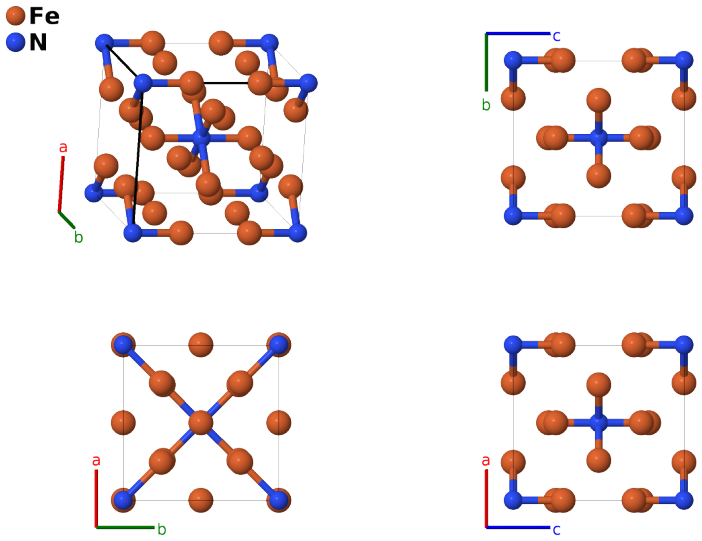
Fe_8N ($D2_g$) Structure: A8B_tI18_139_deh_a-001

This structure originally had the label `A8B_tI18_139_deh_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

https://aflow.org/p/6VR8

https://aflow.org/p/A8B_tI18_139_deh_a-001

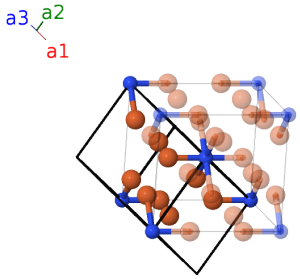


Prototype	Fe_8N
AFLOW prototype label	A8B_tI18_139_deh_a-001
***Strukturbericht* designation**	$D2_g$
ICSD	654562
Pearson symbol	tI18
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A8B_tI18_139_deh_a-001 --params=`$a, c/a, z_3, x_4$

- (Jack, 1951) and others refer to this structure as α''-$Fe_{16}N_2$.
- (Yamashita, 2012) determined the structure by examining crystals containing various amounts of α''-$Fe_{16}N_2$ and α-Fe (bcc iron). We use their data from the sample that was 90% α''-$Fe_{16}N_2$. Their measurements were confirmed by first principles calculations and are in agreement with the first principles calculations of (Sims, 2012).
- The ICSD entry is from (Jack, 1951).

Body-centered Tetragonal primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	N I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Fe I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Fe II
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + 2x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Fe III
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - 2x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Fe III
$\mathbf{B_8}$	=	$x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Fe III
$\mathbf{B_9}$	=	$-x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Fe III

References

[1] S. Yamashita, Y. Masubuchi, Y. Nakazawa, T. Okayama, M. Tsuchiya, and S. Kikkawa, *Crystal structure and magnetic properties of "α″-$Fe_{16}N_2$" containing residual α-Fe prepared by low-temperature ammonia nitridation*, J. Solid State Chem. **194**, 76–79 (2012), doi:10.1016/j.jssc.2012.07.025.

[2] K. H. Jack, *The occurrence and the crystal structure of α″-iron nitride; a new type of interstitial alloy formed during the tempering of nitrogen-martensite*, Proc. R. Soc. A Math. Phys. Eng. Sci. **208**, 216–217 (1951), doi:10.1098/rspa.1951.0155.

[3] H. Sims, W. H. Butler, M. Richter, K. Koepernik, E. Şaşioğlu, C. Friedrich, and S. Blügel, *Theoretical investigation into the possibility of very large moments in $Fe_{16}N_2$*, Phys. Rev. B **86**, 174422 (2012), doi:10.1103/PhysRevB.86.174422.