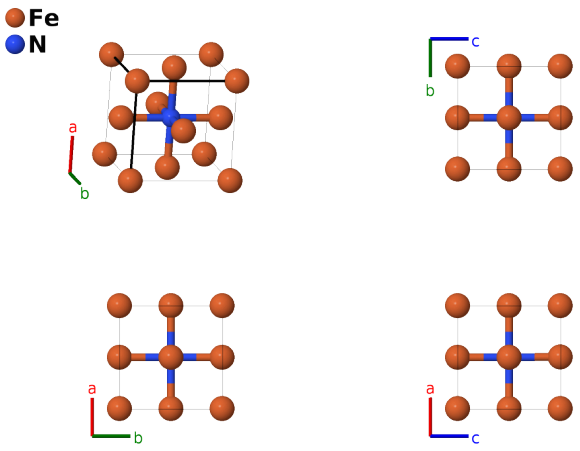
γ'-Fe_4N ($L'1_0$) Structure: A4B_cP5_221_ac_b-002

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/TEA9

https://aflow.org/p/A4B_cP5_221_ac_b-002



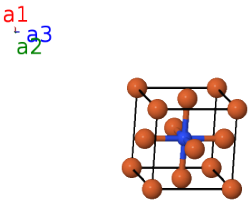
Prototype	Fe_4N
AFLOW prototype label	A4B_cP5_221_ac_b-002
***Strukturbericht* designation**	$L'1_0$
ICSD	79980
Pearson symbol	cP5
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A4B_cP5_221_ac_b-002 --params=`a

Other compounds with this structure
Mn_4Ni

- This is the correct structure for γ'-Fe_4N. For our earlier erroneous attempt, see A4B_cP5_221_bc_a-001.
- This is a binary form of the cubic perovskite structure (AB3C_cP5_221_a_c_b), *Strukturbericht* designation $E2_1$.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Fe I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	N I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Fe II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	Fe II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	Fe II

References

[1] H. Jacobs, R. Rechenbach, and U. Zachwieja, *Structure determination of γ'-Fe_4N and ϵ-Fe_3Na*, J. Alloys Compd. **227**, 10–17 (1995), doi:10.1016/0925-8388(95)01610-4.