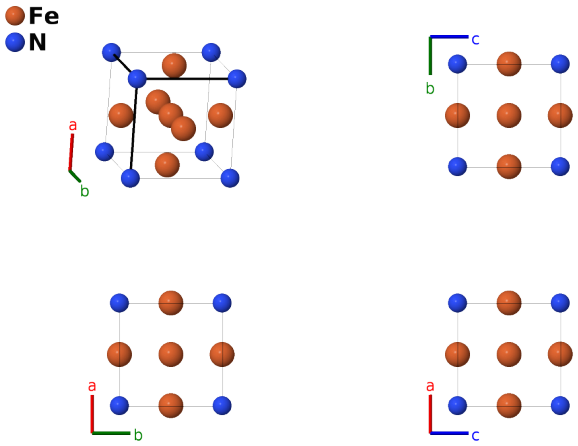
Erroneous $L'1_0$ Structure: A4B_cP5_221_bc_a-001

This structure originally had the label `A4B_cP5_221_bc_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/Q52R

https://aflow.org/p/A4B_cP5_221_bc_a-001

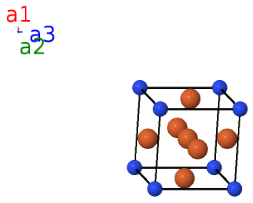


Prototype	Fe_4N
AFLOW prototype label	A4B_cP5_221_bc_a-001
***Strukturbericht* designation**	$L'1_0$
ICSD	none
Pearson symbol	cP5
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A4B_cP5_221_bc_a-001 --params=`a

- We (Hicks, 2019) accidentally misplaced the nickel atom in the $L'1_0$ structure. The correct structure can be found at γ'-Fe_4N $L'1_0$ page.
- Despite our error, 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)	N 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)	Fe 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.

[2] 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.