

FeNNi Structure:

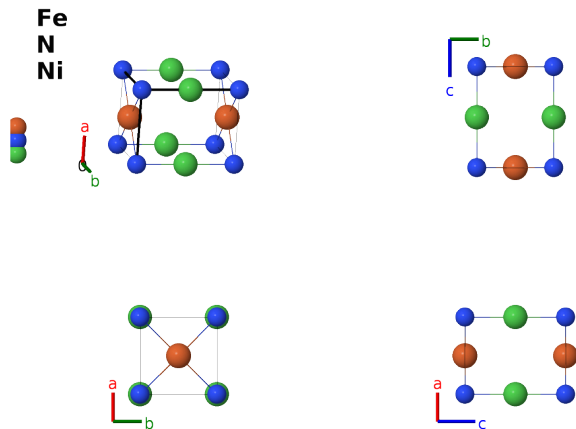
ABC_tP3_123_c_a_b-001

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<https://aflow.org/prototype-encyclopedia/C14E>

https://aflow.org/prototype-encyclopedia/ABC_tP3_123_c_a_b-001

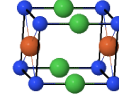


Prototype	FeNNi
AFLOW prototype label	ABC_tP3_123_c_a_b-001
ICSD	53505
CCDC	1618182
Pearson symbol	tP3
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	<code>aflow --proto=ABC_tP3_123_c_a_b-001</code> <code>--params=a, c/a</code>

- The structure is inferred from comments made in (Arnott, 1960).

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) N I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} c \hat{\mathbf{z}}$	(1b) Ni I
$\mathbf{B}_3$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(1c) Fe I

References

- [1] R. J. Arnett and A. Wold, *The preparation and crystallography of FeNiN and the series Fe_{4-x}Ni_xN*, J. Phys.: Conf. Ser. **15**, 152–156 (1960), doi:10.1016/0022-3697(60)90113-X.

Found in

- [1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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