# FeNNi Structure: ABC_tP3_123_c_a_b-001

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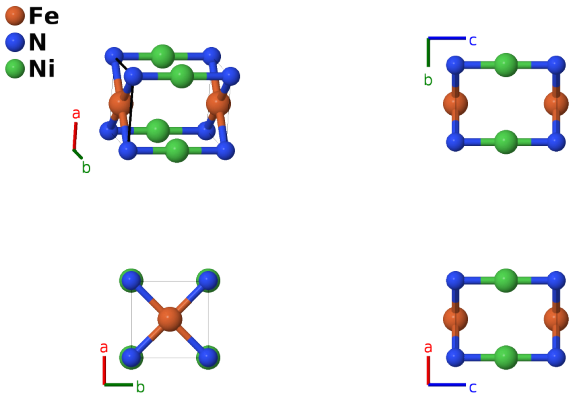
https://aflow.org/p/C14E

https://aflow.org/p/ABC_tP3_123_c_a_b-001

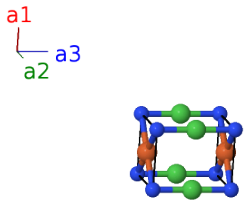



| | |
|---|---|
| **Prototype** | FeNNi |
| **AFLOW prototype label** | ABC_tP3_123_c_a_b-001 |
| **ICSD** | 53505 |
| **Pearson symbol** | tP3 |
| **Space group number** | 123 |
| **Space group symbol** | $P4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=ABC_tP3_123_c_a_b-001 --params=`$a, c/a$ |

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

**Simple Tetragonal primitive vectors**

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




**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | N I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (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. Arnott 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.