# Tetragonal $FeNb_2O_6$ Structure: AB2C6_tP18_113_c_2c_3e-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

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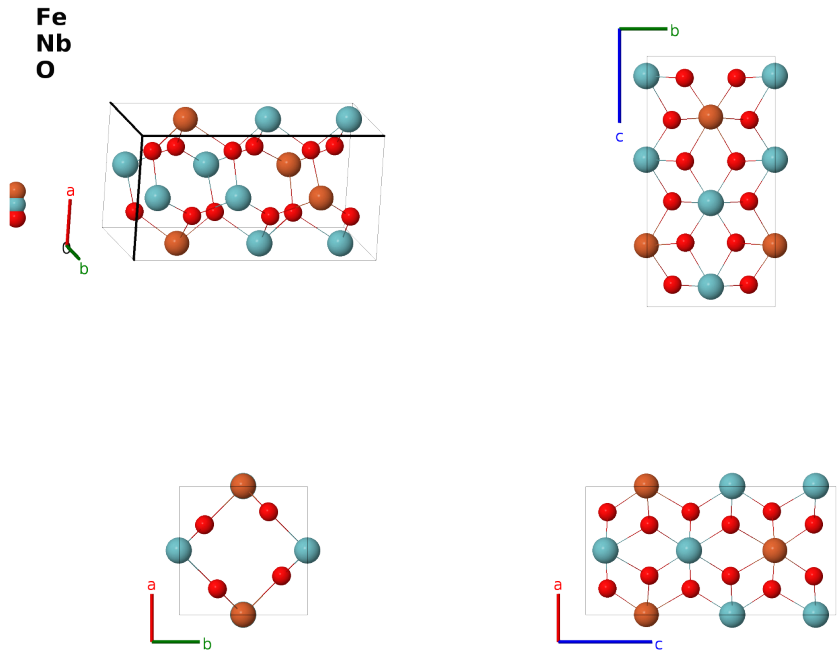
https://aflow.org/prototype-encyclopedia/31E6

https://aflow.org/prototype-encyclopedia/AB2C6_tP18_113_c_2c_3e-001




| | |
|---|---|
| **Prototype** | $FeNb_2O_6$ |
| **AFLOW prototype label** | AB2C6_tP18_113_c_2c_3e-001 |
| **ICSD** | 47187 |
| **CCDC** | 1614495 |
| **Pearson symbol** | tP18 |
| **Space group number** | 113 |
| **Space group symbol** | $P\bar{4}2_1m$ |
| **AFLOW prototype command** | `aflow --proto=AB2C6_tP18_113_c_2c_3e-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4, x_5, z_5, x_6, z_6$ |

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**Other compounds with this structure**
Li(Nb, W)$O_6$

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- $FeNb_2O_6$ can also be found as columbite, $E5_1$.
- The (2c) sites are all combinations of iron and niobium with compositions $Fe_{0.43}Nb_{57}$, $Fe_{0.39}Nb_{0.61}$ and $Fe_{0.18}Nb_{0.82}$, respectively. We arbitrarily list the first one as Fe and the second and third as Nb to preserve the stoichiometry.

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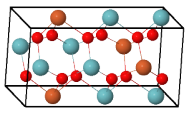
**Simple Tetragonal primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (2c) | Fe I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_1\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_1\,\hat{\mathbf{z}}$ | (2c) | Fe I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2c) | Nb I |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_2\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_2\,\hat{\mathbf{z}}$ | (2c) | Nb I |
| $\mathbf{B_5}$ | = | $\frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2c) | Nb II |
| $\mathbf{B_6}$ | = | $\frac{1}{2}\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$ | (2c) | Nb II |
| $\mathbf{B_7}$ | = | $x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4e) | O I |
| $\mathbf{B_8}$ | = | $-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (4e) | O I |
| $\mathbf{B_9}$ | = | $\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4e) | O I |
| $\mathbf{B_{10}}$ | = | $-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$ | = | $-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (4e) | O I |
| $\mathbf{B_{11}}$ | = | $x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4e) | O II |
| $\mathbf{B_{12}}$ | = | $-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$ | = | $-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$ | (4e) | O II |
| $\mathbf{B_{13}}$ | = | $\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$ | = | $a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (4e) | O II |
| $\mathbf{B_{14}}$ | = | $-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$ | = | $-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$ | (4e) | O II |
| $\mathbf{B_{15}}$ | = | $x_6\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $ax_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (4e) | O III |
| $\mathbf{B_{16}}$ | = | $-x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$ | = | $-ax_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (4e) | O III |
| $\mathbf{B_{17}}$ | = | $\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (4e) | O III |
| $\mathbf{B_{18}}$ | = | $-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$ | = | $-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (4e) | O III |

**References**


[1] A. Aruga, E. Tokizaki, I. Nakai, and Y. Sugitani, *Structure of iron diniobium hexaoxide, $FeNb_2O_6$: an example of metal-disordered trirutile structure*, Acta Crystallogr. Sect. C **41**, 663–665 (1985), doi:10.1107/S0108270185005029.


**First cited in**

N. Anderson, M. J. Mehl, H. Eckert, S. Divilov, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 5*. Submitted to Computational Materials Science (2026).