# TaMoN Structure: ABC_tP6_129_c_c_c-002

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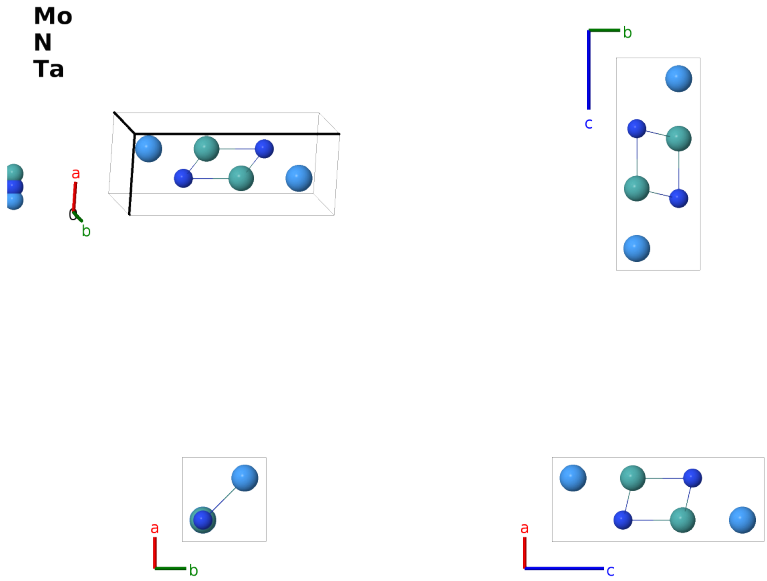
https://aflow.org/prototype-encyclopedia/MURN

https://aflow.org/prototype-encyclopedia/ABC_tP6_129_c_c_c-002




| | |
|---|---|
| **Prototype** | MoNTa |
| **AFLOW prototype label** | ABC_tP6_129_c_c_c-002 |
| **ICSD** | 100437 |
| **CCDC** | 1659571 |
| **Pearson symbol** | tP6 |
| **Space group number** | 129 |
| **Space group symbol** | $P4/nmm$ |
| **AFLOW prototype command** | `aflow --proto=ABC_tP6_129_c_c_c-002 --params=`$a, c/a, z_1, z_2, z_3$ |

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**Other compounds with this structure**
CrNbN, MoNbN, ReAlSi, ReGaSi

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- There are two prototypes with the AFLOW label ABC_tP6_129_c_c_c:

  - CaGaN, with c/a $\approx$ 2.1, and
  - TaMoN (this structure), with c/a $\approx$ 2.5.

- The ICSD lists TaMoN and similar structures under prototype CaGaN, but the sharp difference in c/a between the two structures is significant enough to warrant a new prototype.
- (Vendl, 1978) gives the atomic coordinates in setting 1 of space group $P4/nmm$ #129. We shifted the origin to place the system in our standard setting 2.

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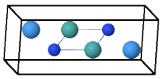
**Simple Tetragonal primitive vectors**


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



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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$ | (2c) | Mo I |
| $\mathbf{B_2}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$ | (2c) | Mo I |
| $\mathbf{B_3}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$ | (2c) | N I |
| $\mathbf{B_4}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$ | (2c) | N I |
| $\mathbf{B_5}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2c) | Ta I |
| $\mathbf{B_6}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2c) | Ta I |

**References**


[1] A. Vendl, *Die Kristallstruktur des Komplexnitrides TaMoN*, Monatsh. Chem. **109**, 1001–1004 (1978), doi:10.1007/BF00907321.


**Found in**


[1] *Inorganic Crystal Structure Database*. Entry 100437 (TaMoN).


**First cited in**


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