# ZrTaNO Structure: ABCD_hP4_187_c_b_a_f-001

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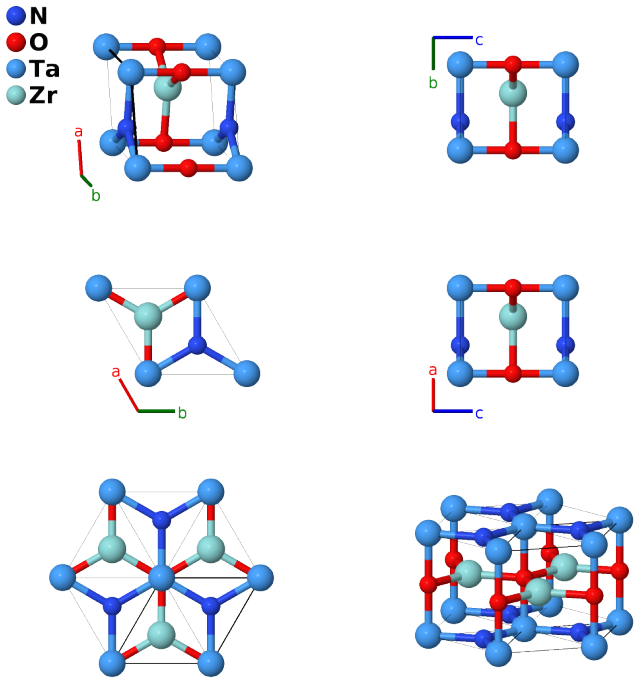
https://aflow.org/p/84DL

https://aflow.org/p/ABCD_hP4_187_c_b_a_f-001

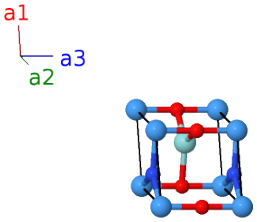



| | |
|---|---|
| **Prototype** | NOTaZr |
| **AFLOW prototype label** | ABCD_hP4_187_c_b_a_f-001 |
| **ICSD** | 76012 |
| **Pearson symbol** | hP4 |
| **Space group number** | 187 |
| **Space group symbol** | $P\bar{6}m2$ |
| **AFLOW prototype command** | `aflow --proto=ABCD_hP4_187_c_b_a_f-001 --params=`$a, c/a$ |

- We have shifted the origin of (Schönberg, 1954) to give the smallest possible Wyckoff indicies.

**Hexagonal primitive vectors**

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (1a) | Ta I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (1b) | O I |
| $\mathbf{B_3}$ | = | $\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$ | (1c) | N I |
| $\mathbf{B_4}$ | = | $\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (1f) | Zr I |

**References**


[1] N. Schönberg, *The Structure of the Metallic Quaternary Phase ZrTaNO*, Acta Chem. Scand. **8**, 627–629 (1954), doi:10.3891/acta.chem.scand.08-0627.