# $Ti_5Te_4$ Structure: A4B5_tI18_87_h_ah-001

This structure originally had the label `A4B5_tI18_87_h_ah`. Calls to that address will be redirected here.

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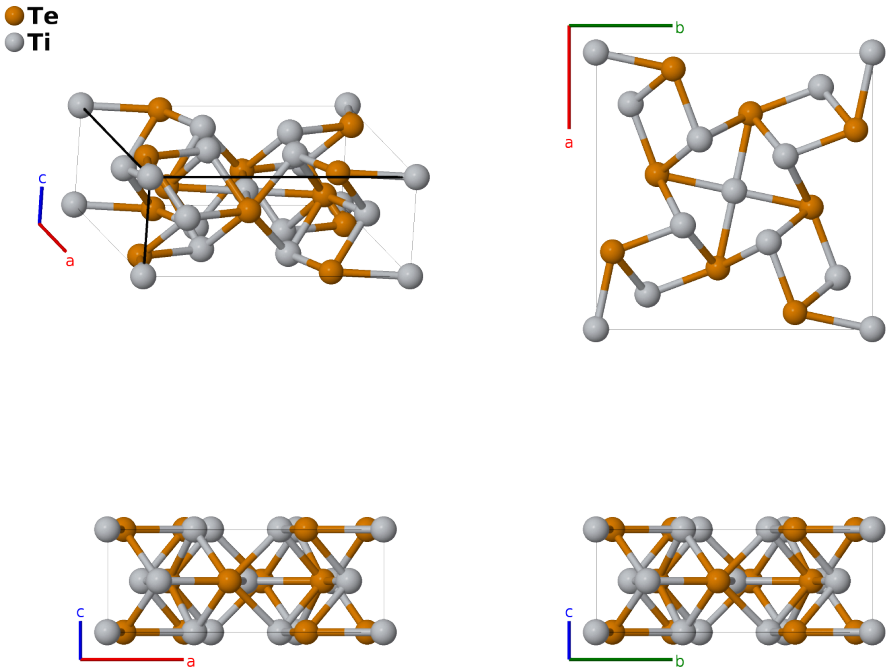
https://aflow.org/p/E7DL

https://aflow.org/p/A4B5_tI18_87_h_ah-001



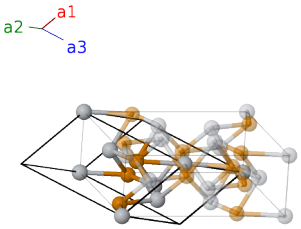

| | |
|---|---|
| **Prototype** | $Te_4Ti_5$ |
| **AFLOW prototype label** | A4B5_tI18_87_h_ah-001 |
| **ICSD** | 15451 |
| **Pearson symbol** | tI18 |
| **Space group number** | 87 |
| **Space group symbol** | $I4/m$ |
| **AFLOW prototype command** | `aflow --proto=A4B5_tI18_87_h_ah-001 --params=`$a, c/a, x_2, y_2, x_3, y_3$ |

**Other compounds with this structure**

$Mo_5As_4$, $Nb_5Sb_4$, $Nb_5Se_4$, $Nb_5Te_4$, $Ta_5Sb_4$, $V_5S_4$, $V_5Se_4$

**Body-centered Tetragonal primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Ti I |
| $\mathbf{B_2}$ | = | $y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + (x_2+y_2)\,\mathbf{a}_3$ | = | $ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}}$ | (8h) | Te I |
| $\mathbf{B_3}$ | = | $-y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - (x_2+y_2)\,\mathbf{a}_3$ | = | $-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}}$ | (8h) | Te I |
| $\mathbf{B_4}$ | = | $x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + (x_2-y_2)\,\mathbf{a}_3$ | = | $-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$ | (8h) | Te I |
| $\mathbf{B_5}$ | = | $-x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - (x_2-y_2)\,\mathbf{a}_3$ | = | $ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$ | (8h) | Te I |
| $\mathbf{B_6}$ | = | $y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$ | = | $ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$ | (8h) | Ti II |
| $\mathbf{B_7}$ | = | $-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$ | = | $-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$ | (8h) | Ti II |
| $\mathbf{B_8}$ | = | $x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$ | = | $-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$ | (8h) | Ti II |
| $\mathbf{B_9}$ | = | $-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$ | = | $ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$ | (8h) | Ti II |

**References**


[1] F. Gr, A. Kjekshus, and F. Raaum, *The crystal structure of $Ti_5Te_4$*, Acta Cryst. **14**, 930–934 (1961), doi:10.1107/S0365110X61002722.


**Found in**


[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.