# $Au_2Nb_3$ Structure: A2B3_tI10_139_e_ae-001

This structure originally had the label `A2B3_tI10_139_e_ae`. Calls to that address will be redirected here.

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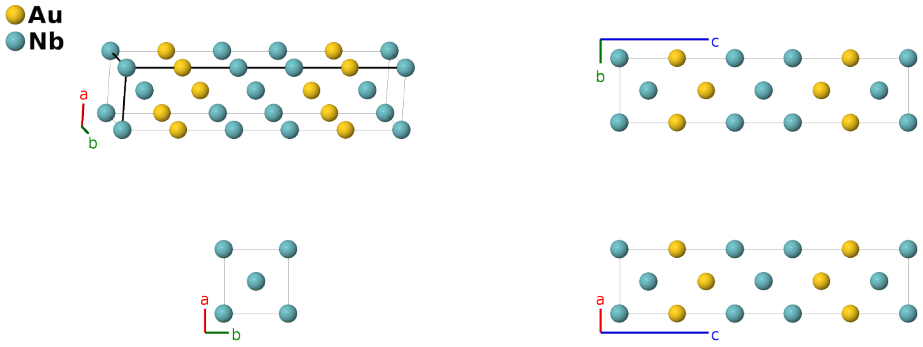
https://aflow.org/p/5STC

https://aflow.org/p/A2B3_tI10_139_e_ae-001



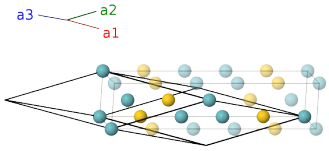

| | |
|---|---|
| **Prototype** | $Au_2Nb_3$ |
| **AFLOW prototype label** | A2B3_tI10_139_e_ae-001 |
| **ICSD** | 58559 |
| **Pearson symbol** | tI10 |
| **Space group number** | 139 |
| **Space group symbol** | $I4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=A2B3_tI10_139_e_ae-001 --params=`$a, c/a, z_2, z_3$ |

**Other compounds with this structure**
$Os_2Al_3$, $Ti_2Cu_3$

- (Schubert, 1960) listed the lattice constants in "kX" units. We used the conversion factor 1.00207789 to convert their units into Ångstroms (Arblaster, 1997). (We had previously (Hicks, 2021) divided instead of multiplied. This has been corrected.)
- When $c/a = 5, z_2 = 1/5$ and $z_3 = 2/5$, the atoms are on the sites of a body-centered cubic lattice.

**Body-centered Tetragonal primitive vectors**

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



**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Nb I |
| $\mathbf{B_2}$ | = | $z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$ | = | $cz_2\,\hat{\mathbf{z}}$ | (4e) | Au I |
| $\mathbf{B_3}$ | = | $-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$ | = | $-cz_2\,\hat{\mathbf{z}}$ | (4e) | Au I |
| $\mathbf{B_4}$ | = | $z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$ | = | $cz_3\,\hat{\mathbf{z}}$ | (4e) | Nb II |
| $\mathbf{B_5}$ | = | $-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$ | = | $-cz_3\,\hat{\mathbf{z}}$ | (4e) | Nb II |

**References**


[1] K. Schubert, T. R. Anantharaman, H. O. K. Ata, H. G. Meissner, M. Pötzschke, W. Rossteutscher, and E. Stolz, *Einige strukturelle Ergebnisse an metallischen Phasen (6)*, Naturwissenschaften **47**, 512 (1960), doi:10.1007/BF00641115.

[2] J. W. Arblaster, *Crystallographic Properties of Platinum*, Platinum Metals Rev. **41**, 12–21 (1997).

[3] 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.


**Found in**


[1] L.-E. Edshammar, *The Crystal Structures of $Os_2Al_3$ and $OsAl_2$*, Acta Chem. Scand. **19**, 871–874 (1965), doi:10.3891/acta.chem.scand.19-0871.