

Au₂Nb₃ Structure:

A2B3_tI10_139_e_ae-001

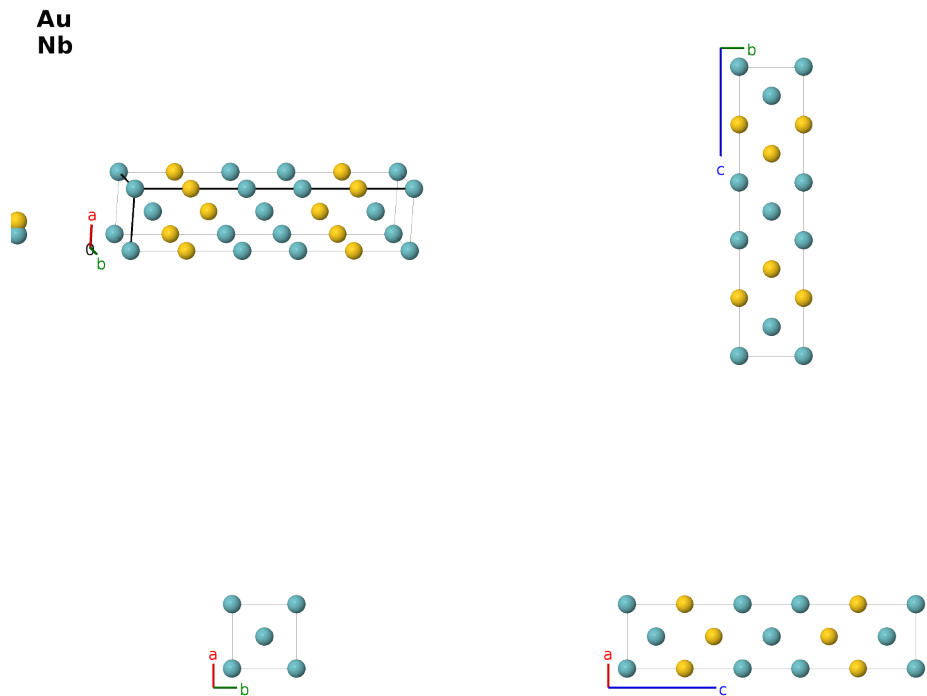
This structure previously used the label(s) **A2B3_tI10_139_e_ae**. Calls to these addresses will be redirected here.

Cite this page as:

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<https://aflow.org/prototype-encyclopedia/5STC>

https://aflow.org/prototype-encyclopedia/A2B3_tI10_139_e_ae-001



Prototype	Au ₂ Nb ₃
AFLOW prototype label	A2B3_tI10_139_e_ae-001
ICSD	58559
CCDC	1622570
Pearson symbol	tI10
Space group number	139
Space group symbol	<i>I4/mmm</i>
AFLOW prototype command	<code>aflow --proto=A2B3_tI10_139_e_ae-001</code> <code>--params=a, c/a, z₂, z₃</code>

Other compounds with this structure

Os₂Al₃, Ti₂Cu₃

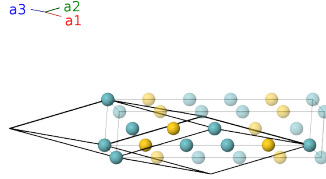
- (Schubert, 1960) listed the lattice constants in “kX” units. We used the conversion factor 1.00207789 to convert their units into Ångstroms (Arblaster, 1997). (We had previously (Hicks, 2021) divided instead of multiplied. This has been corrected.)
- When $c/a = 5$, $z_2 = 1/5$ and $z_3 = 2/5$, the 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 Os₂Al₃ and OsAl₂*, Acta Chem. Scand. **19**, 871–874 (1965), doi:10.3891/acta.chem.scand.19-0871.

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