

Au₂V Structure:

A2B_oC12_38_de_ab-001

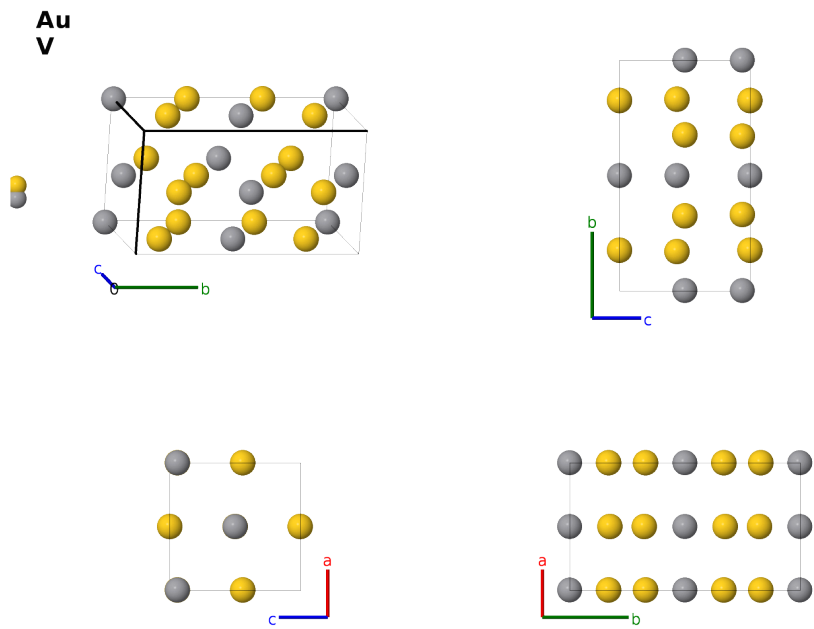
This structure previously used the label(s) **A2B_oC12_38_de_ab**. Calls to these addresses will be redirected here.

Cite this page as:

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- 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.

<https://aflow.org/prototype-encyclopedia/PCHF>

https://aflow.org/prototype-encyclopedia/A2B_oC12_38_de_ab-001



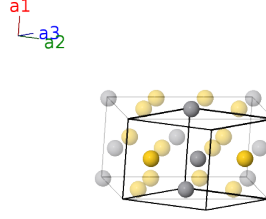
Prototype	Au ₂ V
AFLOW prototype label	A2B_oC12_38_de_ab-001
ICSD	58614
CCDC	1622620
Pearson symbol	oC12
Space group number	38
Space group symbol	<i>Amm</i> 2
AFLOW prototype command	<code>aflow --proto=A2B_oC12_38_de_ab-001</code> <code>--params=a, b/a, c/a, z₁, z₂, y₃, z₃, y₄, z₄</code>

Other compounds with this structure
Cu₂Ti, Pt₂Ta

- The published atomic positions put the system in the $Cmcm$ #65 space group, despite the authors' statement that the system is in the $Amm2$ #38. We forced this system into $Amm2$ by slightly shifting the y_4 coordinate. If $y_3 = y_4$ then the space group becomes $Cmcm$.
- Space group $Amm2$ #38 allows an arbitrary choice of the origin of the z -axis. Here we follow (Stolz, 1962) and set $z_2 = 0$ for the Au-II position.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= \frac{1}{2}b \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}b \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= -z_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$cz_1 \hat{\mathbf{z}}$	(2a)	V I
$\mathbf{B}_2$	$= \frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + cz_2 \hat{\mathbf{z}}$	(2b)	V II
$\mathbf{B}_3$	$= (y_3 - z_3) \mathbf{a}_2 + (y_3 + z_3) \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4d)	Au I
$\mathbf{B}_4$	$= -(y_3 + z_3) \mathbf{a}_2 - (y_3 - z_3) \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4d)	Au I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + (y_4 - z_4) \mathbf{a}_2 + (y_4 + z_4) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	Au II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 - (y_4 + z_4) \mathbf{a}_2 - (y_4 - z_4) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4e)	Au II

References

- [1] E. Stolz and K. Schubert, *Strukturuntersuchungen in einigen zu T^4 - B^1 homologen und quasihomologen Systemen*, Z. Metallkd. **53**, 433–444 (1962), doi:10.1515/ijmr-1962-530701.

Found in

- [1] P. Villars, *Au₂V Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.

First cited in

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