Au_2V Structure: A2B_oC12_38_de_ab-001

This structure originally had the label `A2B_oC12_38_de_ab`. Calls to that address will be redirected here.

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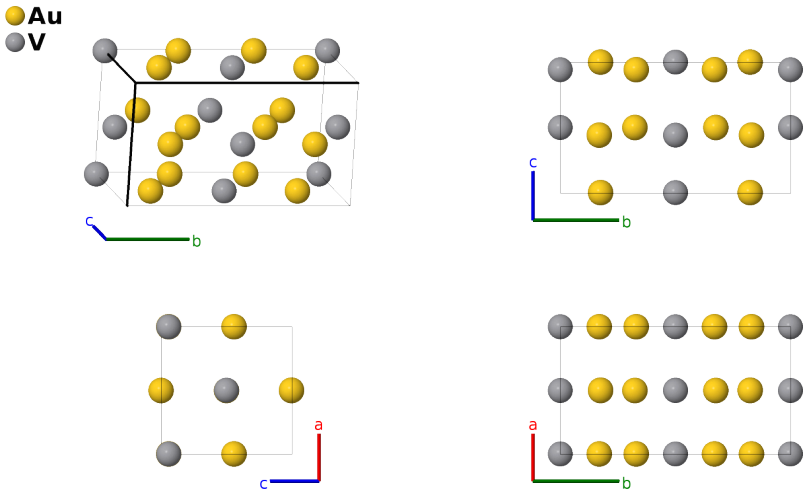
https://aflow.org/p/PCHF

https://aflow.org/p/A2B_oC12_38_de_ab-001



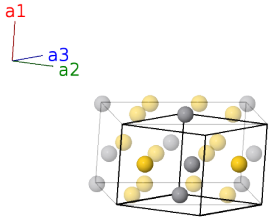
Prototype	Au_2V
AFLOW prototype label	A2B_oC12_38_de_ab-001
ICSD	58614
Pearson symbol	oC12
Space group number	38
Space group symbol	$Amm2$
AFLOW prototype command	`aflow --proto=A2B_oC12_38_de_ab-001 --params=`$a, b/a, c/a, z_1, z_2, y_3, z_3, y_4, z_4$

Other compounds with this structure
Cu_2Ti, Pt_2Ta

- 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 cordinate. 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

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



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.