Calaverite ($AuTe_2$, $C34$) Structure: AB2_mC6_12_a_i-001

This structure previously used the label(s) `AB2_mC6_12_a_i`. Calls to these addresses will be redirected here.

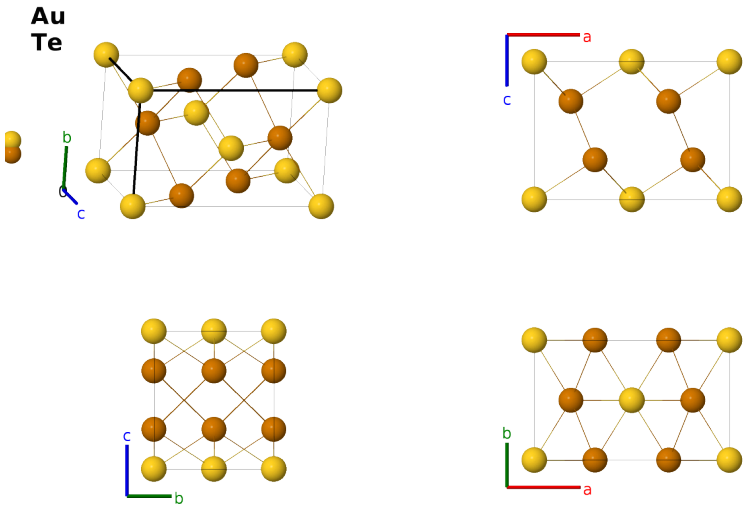
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/1QX2

https://aflow.org/prototype-encyclopedia/AB2_mC6_12_a_i-001



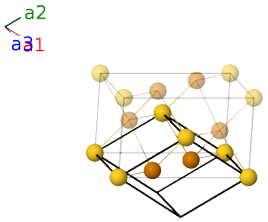
Prototype	$AuTe_2$
AFLOW prototype label	AB2_mC6_12_a_i-001
***Strukturbericht* designation**	$C34$
Mineral name	calaverite
ICSD	72434
CCDC	1633294
Pearson symbol	mC6
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=AB2_mC6_12_a_i-001 --params=`$a, b/a, c/a, \beta, x_2, z_2$

Other compounds with this structure
$Au_{10}Se_3Te_{17}$

- This structure was given the $C34$ designation by (Gottfried, 1937). (Pertlik, 1984) put calverite in space group Pc #7.
- $AuTe_2$ can also be found as krennerite ($C46$).
- $C34$ Calverite (this structure), α-HgO2, and NiO_2 have the same AFLOW prototype label, AB2_mC6_12_a_i. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Base-centered Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Au I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	Te I

References

[1] K. Reithmayer, W. Steurer, H. Schulz, and J. L. de Boer, *High-pressure single-crystal structure study on calaverite, $AuTe_2$*, Acta Crystallogr. Sect. B **49**, 6–11 (1993), doi:10.1107/S0108768192007286.

[2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

[3] F. Pertlik, *Kristallchemie natülicher Telluride III: Die Kristallstruktur des Minerals Calaverit, $AuTe_2$*, Z. Kristallogr. **169**, 227–236 (1984), doi:10.1524/zkri.1984.169.1-4.227.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017