CuAu(I) ($L1_0$) Structure: AB_tP2_123_a_d-001

This structure originally had the label `AB_tP2_123_a_d`. Calls to that address will be redirected here.

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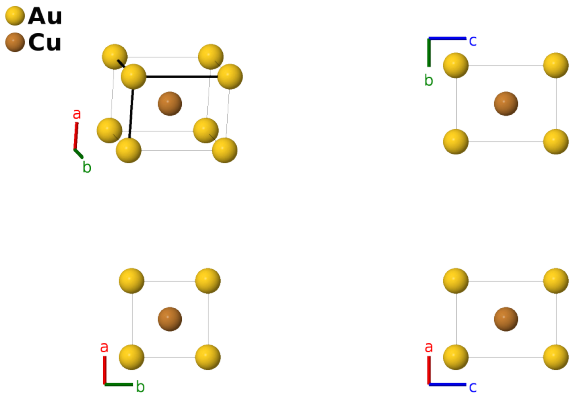
https://aflow.org/p/9JUZ

https://aflow.org/p/AB_tP2_123_a_d-001



Prototype	AuCu
AFLOW prototype label	AB_tP2_123_a_d-001
***Strukturbericht* designation**	$L1_0$
ICSD	42574
Pearson symbol	tP2
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=AB_tP2_123_a_d-001 --params=`$a, c/a$

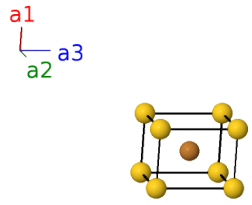
Other compounds with this structure
FePt, (Ni, Fe)Pt, (Cu, Fe)Pt, AgTi, AlTi, BiLi, BiNa, CoPt, EuIn, FePd, FePt, GaTi, HgPt, HgTi, HgZr, InPu, IrMn, IrNb, IrTi, IrV, MnNi, MnPt, MnRh, NiZn, NpSb, NiPt, PtV, PtZn, PuSb, RhTi, RuTa

- There can be considerable disorder in CuAu(I), as it can exist as $Cu_{1-x}Au_x$ with $0.44 < x < 0.56$. (Pearson, 1958; Bjerkelund, 1967)
- For $x > 0.5$ this transforms to the CuAu(II) phase above 390°C. This phase is orthorhombic with a and c only changing slightly but $b \approx 10a$. This phase also exists at 200°C for $0.33 < x < 0.65$, excluding the range where CuAu(I) forms. (Pearson, 1958)
- (Ewald, 1931) and later (Pearson, 1958) both doubled the unit cell and gave this structure the Pearson symbol $tP4$.

- $L1_0$ has $c/a \approx \sqrt{2}$, characteristic of face-centered cubic ordering, while $L2_a$ has $c/a \approx 1$, a body-centered cubic-like system. This structure has the same AFLOW designation, AB_tP2_123_a_d, as δ-CuTi ($L2_a$). The only difference in the structures is the c/a ratio. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We previously used the data from (Bayless, 1990), but we switched to (Bjerkelund, 1967) to match the ICSD entry.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Au I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Cu I

References

[1] E. Bjerkelund, W. B. Pearson, K. Selte, and A. Kjekshus, *Lattice Parameters of the CuAu(I) Phase*, Acta Chem. Scand. **21**, 2900–2901 (1967), doi:10.3891/acta.chem.scand.21-2900.

[2] P. Bayliss, *Revised Unit-Cell Dimensions, Space Group, and Chemical Formula of Some Metallic Materials*, Can. Mineral. **28**, 751–755 (1990).

[3] W. B. Pearson, *A Handbook of Lattice Spacings and Structures of Metals and Alloys*, *International Series of Monographs on Metal Physics and Physical Metallurgy*, vol. 4 (Pergamon Press, Oxford, London, Edinburgh, New York, Paris, Frankfort, 1958), 1964 reprint with corrections edn.

[4] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).