

Bogdanovite (Cu₃Au, *L*1₂) Structure: AB3_cP4_221_a_c-001

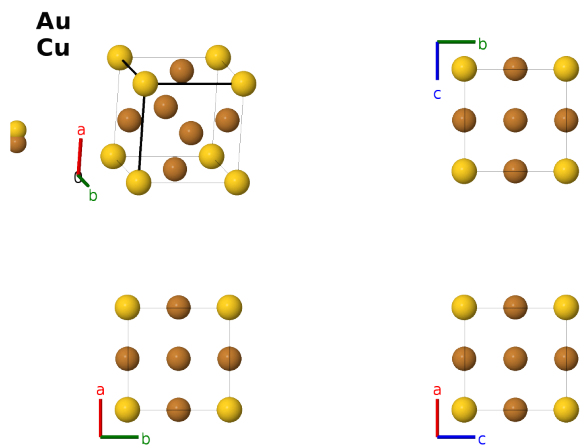
This structure previously used the label(s) **AB3_cP4_221_a_c**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/NK1T>

https://aflow.org/prototype-encyclopedia/AB3_cP4_221_a_c-001



Prototype	AuCu ₃
AFLOW prototype label	AB3_cP4_221_a_c-001
<i>Strukturbericht</i> designation	<i>L</i> 1 ₂
Mineral name	bogdanovite
ICSD	42587
CCDC	1612239
Pearson symbol	cP4
Space group number	221
Space group symbol	<i>Pm</i> $\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB3_cP4_221_a_c-001 --params=a</code>

Other compounds with this structure

Al₃Er, Al₃Li (metastable), Al₃Np, Al₃Tm, Al₃U, Br₃Sr, Ca₃Pb, Fe₃Ga, Fe₃Ge, Fe₃Pt, Ga₃Er, Ga₃Ho, Ga₃Lu, Ga₃Tm, Ga₃U, Ge₃U, Hg₃Zr, In₃Dy, In₃Er, In₃Gd, In₃Ho, In₃Lu, In₃Pu, In₃Tb, In₃Th, In₃U, In₃Y, In₃Yb, Ir₃Cr, Ir₃Nb, Ir₃Tl, Ir₃U, Ir₃V, Ir₃Zr, La₃Al, La₃In, Mn₃Ir, Mn₃Pt, Mn₃Rh, Ni₃Al, Ni₃Fe, Ni₃Ga, Ni₃Ge, Ni₃Mn, Ni₃Si, Pb₃Ca, Pb₃Gd, Pb₃Gd, Pb₃La, Pb₃Nd, Pb₃Pr, Pb₃Pu, Pb₃Y, Pd₃Ce, Pd₃Dy, Pd₃Er, Pd₃Fe, Pd₃Ho, Pd₃La, Pd₃Lu, Pd₃Pb, Pd₃Sc, Pd₃Sc, Pd₃Sn, Pd₃Th, Pd₃U, Pr₃Al, Pt₃Co, Pt₃Cr, Pt₃Dy, Pt₃Fe, Pt₃Ga, Pt₃Ho, Pt₃Mg, Pt₃Mn, Pt₃Np, Pt₃Sc, Pt₃Sn, Pt₃Ti, Pt₃V, Pt₃Y, Pt₃Zn, β -Pu₃Ga,

Pu₃In, Rh₃Hf, Rh₃Sc, Rh₃Ta, Rh₃Th, Rh₃Ti, Rh₃U, Rh₃V, Rh₃Zr, Ru₃U, Si₃U, Sn₃Ca, Sn₃Ce, Sn₃Eu, Sn₃Gd, Sn₃Ge, Sn₃La, Sn₃Nd, Sn₃Pm, Sn₃Pr, Sn₃Sm, Sn₃Th, Sn₃U, Ti₃Al, Ti₃In, Ti₃Sn, Tl₃Ca, Tl₃Th, Tl₃U, Tl₃Y, Tl₃Yb, V₃Al, β -U₃Si, Zn₃Mn, Zn₃Th, Zr₃Al

- (Owen, 1946) give the lattice constants in kX units, where 1 kX = 1.00202Å. (Wood, 1947)

Simple Cubic primitive vectors



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a) Au I
$\mathbf{B_2}$	=	$\frac{1}{2} \mathbf{a_2} + \frac{1}{2} \mathbf{a_3}$	=	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c) Cu I
$\mathbf{B_3}$	=	$\frac{1}{2} \mathbf{a_1} + \frac{1}{2} \mathbf{a_3}$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	(3c) Cu I
$\mathbf{B_4}$	=	$\frac{1}{2} \mathbf{a_1} + \frac{1}{2} \mathbf{a_2}$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	(3c) Cu I

References

[1] E. A. Owen and Y. H. Liu, *The Thermal Expansion of the Gold-Copper Alloy AuCu₃*, Phil. Mag. **38**, 354–360 (1947), doi:10.1080/14786444708521607.

[2] E. A. Wood, *The Conversion Factor for kX Units to Angström Units*, J. Appl. Phys. **18**, 929–930 (1947), doi:10.1063/1.1697570.

Found in

[1] P. Villars and L. Calvert, *Pearson’s Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.

First cited in

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