Bogdanovite (Cu_3Au, $L1_2$) Structure: AB3_cP4_221_a_c-001

This structure originally had the label `AB3_cP4_221_a_c`. Calls to that address will be redirected here.

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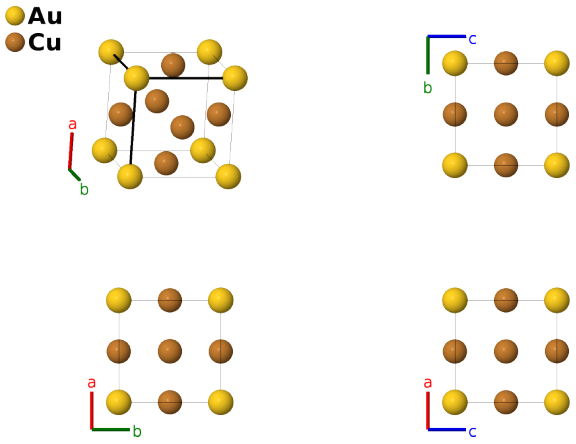
https://aflow.org/p/NK1T

https://aflow.org/p/AB3_cP4_221_a_c-001



Prototype	$AuCu_3$
AFLOW prototype label	AB3_cP4_221_a_c-001
***Strukturbericht* designation**	$L1_2$
Mineral name	bogdanovite
ICSD	42587
Pearson symbol	cP4
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3_cP4_221_a_c-001 --params=`a

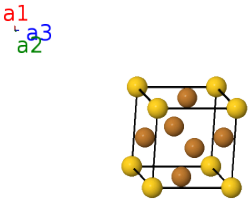
Other compounds with this structure

Al_3Er, Al_3Li (metastable), Al_3Np, Al_3Tm, Al_3U, Br_3Sr, Ca_3Pb, Fe_3Ga, Fe_3Ge, Fe_3Pt, Ga_3Er, Ga_3Ho, Ga_3Lu, Ga_3Tm, Ga_3U, Ge_3U, Hg_3Zr, In_3Dy, In_3Er, In_3Gd, In_3Ho, In_3Lu, In_3Pu, In_3Tb, In_3Th, In_3U, In_3Y, In_3Yb, Ir_3Cr, Ir_3Nb, Ir_3Tl, Ir_3U, Ir_3V, Ir_3Zr, La_3Al, La_3In, Mn_3Ir, Mn_3Pt, Mn_3Rh, Ni_3Al, Ni_3Fe, Ni_3Ga, Ni_3Ge, Ni_3Mn, Ni_3Si, Pb_3Ca, Pb_3Gd, Pb_3Gd, Pb_3La, Pb_3Nd, Pb_3Pr, Pb_3Pu, Pb_3Y, Pd_3Ce, Pd_3Dy, Pd_3Er, Pd_3Fe, Pd_3Ho, Pd_3La, Pd_3Lu, Pd_3Pb, Pd_3Sc, Pd_3Sc, Pd_3Sn, Pd_3Th, Pd_3U, Pr_3Al, Pt_3Co, Pt_3Cr, Pt_3Dy, Pt_3Fe, Pt_3Ga, Pt_3Ho, Pt_3Mg, Pt_3Mn, Pt_3Np, Pt_3Sc, Pt_3Sn, Pt_3Ti, Pt_3V, Pt_3Y, Pt_3Zn, β-Pu_3Ga, Pu_3In, Rh_3Hf, Rh_3Sc, Rh_3Ta, Rh_3Th, Rh_3Ti, Rh_3U, Rh_3U, Rh_3V, Rh_3Zr, Ru_3U, Si_3U, Sn_3Ca, Sn_3Ce, Sn_3Eu, Sn_3Gd, Sn_3Ge, Sn_3La, Sn_3Nd, Sn_3Pm, Sn_3Pr, Sn_3Sm, Sn_3Th, Sn_3U, Ti_3Al, Ti_3In, Ti_3Sn, Tl_3Ca, Tl_3Th, Tl_3U, Tl_3Y, Tl_3Yb, V_3Al, β-U_3Si, Zn_3Mn, Zn_3Th, Zr_3Al

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

Simple Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Au I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(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 $AuCu_3$*, 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.