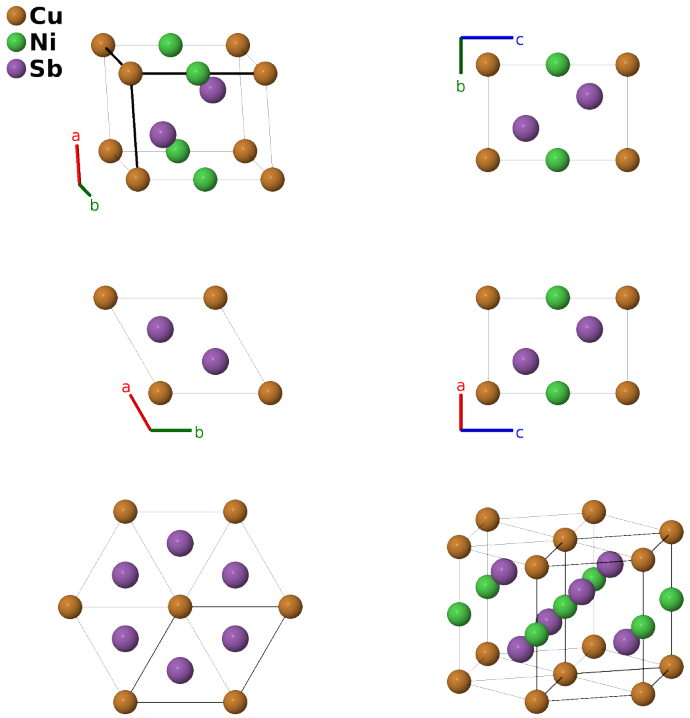
Zlatogorite ($CuNiSb_2$) Structure: ABC2_hP4_164_a_b_d-001

This structure originally had the label `ABC2_hP4_164_a_b_d`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/PUFU

https://aflow.org/p/ABC2_hP4_164_a_b_d-001

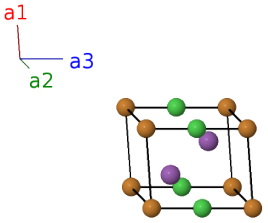


Prototype	$CuNiSb_2$
AFLOW prototype label	ABC2_hP4_164_a_b_d-001
Mineral name	zlatogorite
ICSD	134019
Pearson symbol	hP4
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=ABC2_hP4_164_a_b_d-001 --params=`$a, c/a, z_3$

- Although we use the data from (Kift, 2010), the ICSD entry is from (Skaggs, 2020).

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ni I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	Sb I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	Sb I

References

[1] R. L. Kift, *Intermetallic Compounds by Reductive Annealing*, Ph.D. thesis, University of Hull (2010).

[2] C. M. Skaggs, C.-J. Kang, C. J. Perez, J. Hadermann, T. J. Emge, C. E. Frank, C. Pak, S. H. Lapidus, D. Walker, G. Kotliar, S. M. Kauzlarich, X. Tan, and M. Greenblatt, *Ambient and High Pressure $CuNiSb_2$: Metal-Ordered and Metal-Disordered NiAs-Type Derivative Pnictides*, Inorg. Chem. **59**, 14058–14069 (2020), doi:10.1021/acs.inorgchem.0c01848.