Cu_2Sb ($C38$) Structure: A2B_tP6_129_ac_c-001

This structure previously used the label(s) `A2B_tP6_129_ac_c`. Calls to these addresses will be redirected here.

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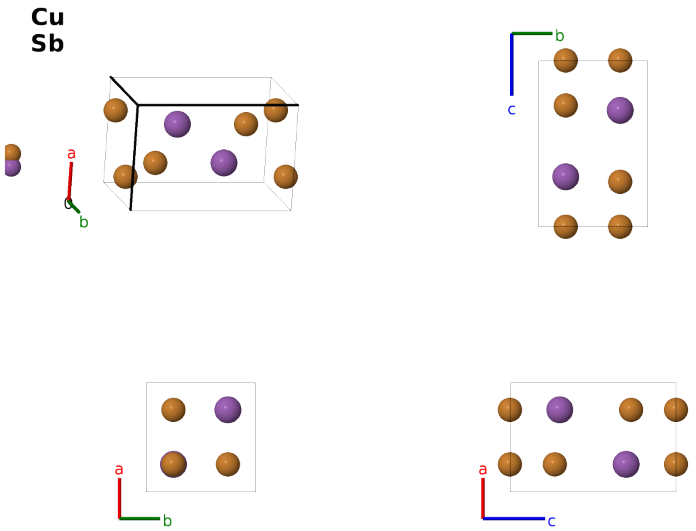
https://aflow.org/prototype-encyclopedia/YG4M

https://aflow.org/prototype-encyclopedia/A2B_tP6_129_ac_c-001



Prototype	Cu_2Sb
AFLOW prototype label	A2B_tP6_129_ac_c-001
***Strukturbericht* designation**	$C38$
ICSD	42323
CCDC	1612021
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=A2B_tP6_129_ac_c-001 --params=`$a, c/a, z_2, z_3$

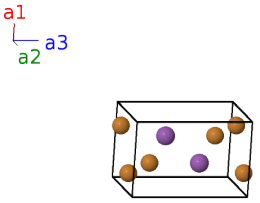
Other compounds with this structure

Cr_2As, Cu_2As, Cu_2Sb, Cu_2Te, Fe_2As, Fe_2Se, Fe_2Te, Mn_2As, Mn_2Sb, Nd_2S, Ni_2Se, Ni_2Te, O_2Eu, O_2Gd, Si_2Al, As_2Th, As_2U, Bi_2Th, Bi_2U, Pu_2U, S_2Ce, S_2Yb, Sb_2Hf, Sb_2Th, Sb_2U, Se_2Ce, Se_2Ho, Te_2Ce, Te_2La, Te_2U

- Cu_2Sb ($C38$), UP_2, and $LaSe_{1.85}$ have similar AFLOW prototype labels, A2B_tP6_129_ac_c for the first two and AB2_tP6_129_c_ac for the third. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We consider all of these to be binary forms of Matlockite ($E0_1$)/PrOI.
- We somewhat arbitrarily assign
  - Structures with c/a < 2 to the Cu_2Sb prototype,
  - Structures with $2 <$ c/a < 3 to the UP_2 prototype, and
  - Structures with c/a ≈ 4 to the $LaSe_{1.85}$ prototype.
- The ICSD distinction between Cu_2Sb and UP_2 is not the same as ours, and they often assign binary compounds to the ternary prototypes.

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
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	Cu I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	Sb I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	Sb I

References

[1] W. B. Pearson, *The Cu_2Sb and related structures*, Zeitschrift für Kristallographie **171**, 23–39 (1985), doi:10.1524/zkri.1985.171.14.23.

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