Zr_2CuSb_3 Structure: AB3C2_tP6_115_a_bg_g-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/NQAB

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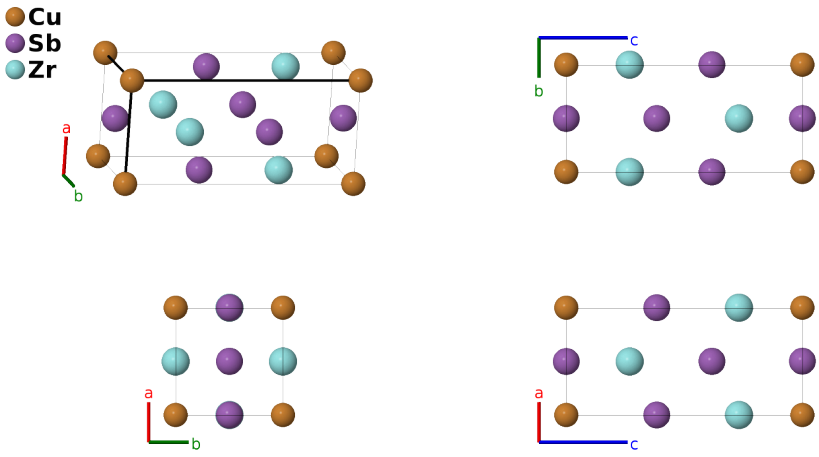
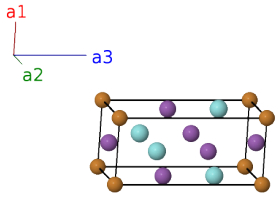


Prototype	$CuSb_3Zr_2$
AFLOW prototype label	AB3C2_tP6_115_a_bg_g-001
ICSD	93242
Pearson symbol	tP6
Space group number	115
Space group symbol	$P\bar{4}m2$
AFLOW prototype command	`aflow --proto=AB3C2_tP6_115_a_bg_g-001 --params=`$a, c/a, z_3, z_4$

Other compounds with this structure
Hf_2CuSb_3, Hf_2GaSb_3, Ti_2CuSb_3, Zr_2PdSb_3

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)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1b)	Sb I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2g)	Sb II
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_3\,\hat{\mathbf{z}}$	(2g)	Sb II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2g)	Zr I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(2g)	Zr I

References

[1] N. Koblyuk, G. Melnyk, L. Romaka, O. I. Bodak, and D. Fruchart, *Crystal structure of Zr_2CuSb_3 and related compounds*, J. Alloys Compd. **317-318**, 284–286 (2001), doi:10.1016/S0925-8388(00)01349-9.