$Y_3Au_3Sb_4$ Structure: A3B4C3_cI40_220_a_c_b-001

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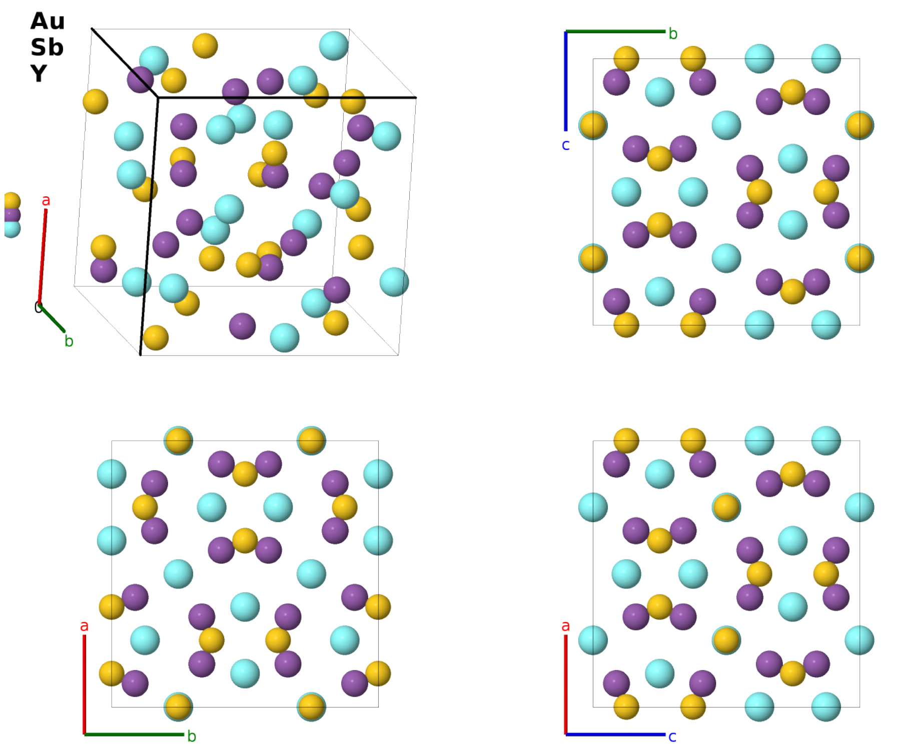
https://aflow.org/prototype-encyclopedia/GET1

https://aflow.org/prototype-encyclopedia/A3B4C3_cI40_220_a_c_b-001



Prototype	$Au_3Sb_4Y_3$
AFLOW prototype label	A3B4C3_cI40_220_a_c_b-001
ICSD	957
CCDC	1591174
Pearson symbol	cI40
Space group number	220
Space group symbol	$I\bar{4}3d$
AFLOW prototype command	`aflow --proto=A3B4C3_cI40_220_a_c_b-001 --params=`a, x_3

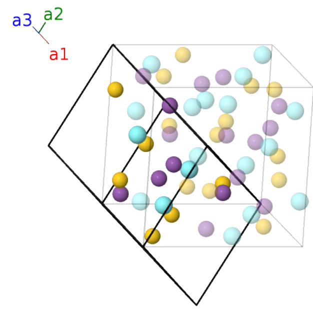
Other compounds with this structure

$Ce_3Pd_3Bi_4$, $Ce_3Pt_3Bi_4$, $Dy_3Au_3Sb_4$, $Dy_3Cu_3Sb_4$, $Er_3Au_3Sb_4$, $Gd_3Au_3Sb_4$, $Hf_3Ni_3Sb_4$, $Ho_3Au_3Sb_4$, $La_3Cu_3Bi_4$, $Lu_3Au_3Sb_4$, $Nd_3Au_3Sb_4$, $Sm_3Au_3Sb_4$, $Sm_3Cu_3Sb_4$, $Tb_3Au_3Sb_4$, $Tb_3Cu_3Sb_4$, $Tm_3Au_3Sb_4$, $U_3Ni_3Sb_4$, U_3NiAs_4

- (Lu, 2008) describe this as a filled Th_3P_4 ($D7_3$) structure, and, like its parent, there can be considerable disorder on the transition metal site. This is seen in the U_3NiAs_4 compound, where 2/3 of the nickel (2b) sites are vacant.

Body-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12a)	Au I
$\mathbf{B_2}$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(12a)	Au I
$\mathbf{B_3}$	=	$\frac{3}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}}$	(12a)	Au I
$\mathbf{B_4}$	=	$\frac{1}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}}$	(12a)	Au I
$\mathbf{B_5}$	=	$\frac{5}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12a)	Au I
$\mathbf{B_6}$	=	$\frac{7}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12a)	Au I
$\mathbf{B_7}$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(12b)	Y I
$\mathbf{B_8}$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(12b)	Y I
$\mathbf{B_9}$	=	$\frac{7}{8}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12b)	Y I
$\mathbf{B_{10}}$	=	$\frac{5}{8}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(12b)	Y I
$\mathbf{B_{11}}$	=	$\frac{1}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(12b)	Y I
$\mathbf{B_{12}}$	=	$\frac{3}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(12b)	Y I
$\mathbf{B_{13}}$	=	$2x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + 2x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{14}}$	=	$\frac{1}{2}\mathbf{a}_1 - \left(2x_3 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + ax_3\,\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{15}}$	=	$-\left(2x_3 - \frac{1}{2}\right)\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} - ax_3\,\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{16}}$	=	$-\left(2x_3 - \frac{1}{2}\right)\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{2}\right)\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{17}}$	=	$\left(2x_3 + \frac{1}{2}\right)\mathbf{a}_1 + \left(2x_3 + \frac{1}{2}\right)\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{18}}$	=	$\frac{1}{2}\mathbf{a}_1 - 2x_3\,\mathbf{a}_3$	=	$-a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{4}\right)\hat{\mathbf{y}} + a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{19}}$	=	$-2x_3\,\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{x}} - a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{y}} - a\left(x_3 - \frac{1}{4}\right)\hat{\mathbf{z}}$	(16c)	Sb I
$\mathbf{B_{20}}$	=	$-2x_3\,\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{4}\right)\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{y}} - a\left(x_3 + \frac{1}{4}\right)\hat{\mathbf{z}}$	(16c)	Sb I

References

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