$Li_3Zn_2SbO_6$ Structure: A3B6CD2_mC24_12_ag_ij_c_h-001

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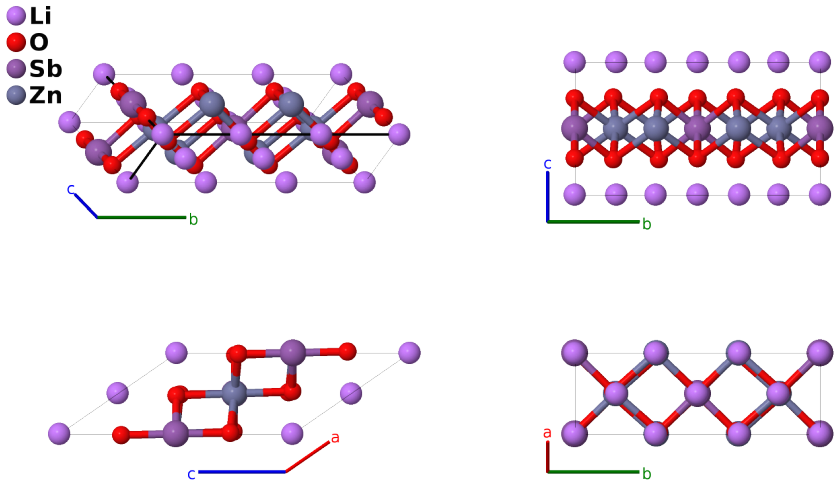
https://aflow.org/p/72ZM

https://aflow.org/p/A3B6CD2_mC24_12_ag_ij_c_h-001



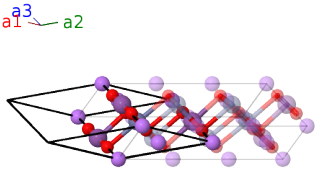
Prototype	$Li_3O_6SbZn_2$
AFLOW prototype label	A3B6CD2_mC24_12_ag_ij_c_h-001
ICSD	69189
Pearson symbol	mC24
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=A3B6CD2_mC24_12_ag_ij_c_h-001 --params=`$a, b/a, c/a, \beta, y_3, y_4, x_5, z_5, x_6, y_6, z_6$

Other compounds with this structure

$Li_3Bi_2SbO_6$, $Li_3Cu_2SbO_6$, $Li_3Co_2SbO_6$, Li_4ZnTeO_6, $Na_2Co_2TeO_6$, $Na_3Co_2SbO_6$

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Li I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2c)	Sb I
$\mathbf{B_3}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$by_3\,\hat{\mathbf{y}}$	(4g)	Li II
$\mathbf{B_4}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-by_3\,\hat{\mathbf{y}}$	(4g)	Li II
$\mathbf{B_5}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Zn I
$\mathbf{B_6}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(4h)	Zn I
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4i)	O I
$\mathbf{B_9}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + (x_6 + y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{10}}$	=	$-(x_6 + y_6)\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{11}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - (x_6 + y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II
$\mathbf{B_{12}}$	=	$(x_6 + y_6)\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(8j)	O II

References

[1] C. Greaves and S. M. A. Katib, *The structural chemistry of $Li_3Zn_2MO_6$ (M=Sb, Bi) and related phases*, Mater. Res. Bull. **25**, 1175–1182 (1990), doi:10.1016/0025-5408(90)90148-U.