$LaLi_3Sb_2$ Structure: AB3C2_hP6_164_a_bd_d-001

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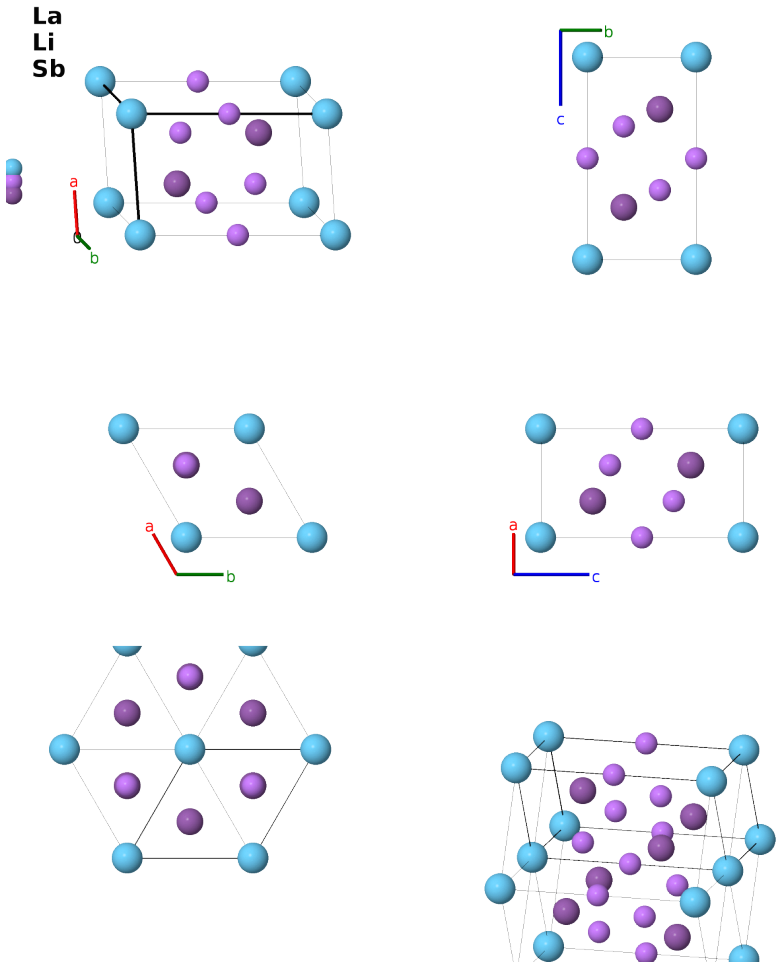
https://aflow.org/prototype-encyclopedia/J1XS

https://aflow.org/prototype-encyclopedia/AB3C2_hP6_164_a_bd_d-001



Prototype	$LaLi_3Sb_2$
AFLOW prototype label	AB3C2_hP6_164_a_bd_d-001
ICSD	49625
CCDC	1614794
Pearson symbol	hP6
Space group number	164
Space group symbol	$P\bar{3}m1$

AFLOW prototype command `aflow --proto=AB3C2_hP6_164_a_bd_d-001 --params=`$a, c/a, z_3, z_4$

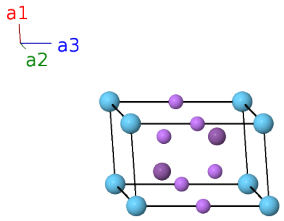
Other compounds with this structure

$CeLi_3Bi_2$, $CeLi_3Sb_2$, $DyLi_3Sb_2$, $GdLi_3Bi_2$, $HoLi_3Sb_2$, $LaLi_3As_2$, $LaLi_3Bi_2$, $LaLi_3P_2$, $NdLi_3As_2$, $NdLi_3Bi_2$, $NdLi_3Sb_2$, $PrLi_3Bi_2$, $PrLi_3Sb_2$, $SmLi_3Bi_2$, $SmLi_3Sb_2$, $TbLi_3Bi_2$, YLi_3Bi_2, YLi_3Sb_2

- (Grund, 1984) refer to this as a "filled" $LiAl_2Si_2$ structure. That compound is isostructural with Ce_2O_2S. Removing the (1b) atom reduces this structure to the Ce_2O_2S prototype.
- The quaternary form of this structure, with the (1b) site containing a different species, is $TbLiCu_2P_2$.

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)	La I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Li 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)	Li II
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	Li II
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2d)	Sb I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2d)	Sb I

References

[1] I. Grund, H.-U. Schuster, and P. Müller, *Ternäre Verbindungen von Lithium mit Yttrium, Lanthan bzw. Neodym und 5b-Elementen im "aufgefüllten" $CaAl_2Si_2$-Typ*, Z. Anorganische und Allgemeine Chemie **515**, 151–158 (1984), doi:10.1107/S2053229615016393.

Found in

[1] J. Prakash, M. C. Schäfer, and S. Bobev, *Synthesis and structure determination of seven ternary bismuthides: crystal chemistry of the $RELi_3Bi_2$ family (RE = La-Nd, Sm, Gd, and Tb)*, Acta Crystallogr. Sect. C **71**, 894–899 (2015), doi:10.1107/S2053229615016393.

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