

Li[BH ₄]	<i>hP</i> 12	(186) <i>P</i> 6 ₃ <i>mc</i> – cb ³
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LiBH₄ ht [1]

Structural features: BH₄ tetrahedra in h stacking; Li in "tetrahedral" voids.

Soulié J.P. et al. (2002) [1]

BH₄Li

$a = 0.42763$, $c = 0.69484$ nm, $c/a = 1.625$, $V = 0.1100$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
H1	6 <i>c</i>	. <i>m</i> .	0.828	0.172	0.124		single atom B
Li2	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0		non-coplanar hexagon H ₆
H3	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.37		single atom B
B4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.553		tetrahedron H ₄

Experimental: powder, diffractometer, X-rays, synchrotron, R_B = 0.055, T = 408 K

Remarks: Phase stable at T > 381 K.

References: [1] Soulié J.P., Renaudin G., Cerny R., Yvon K. (2002), J. Alloys Compd. 346, 200-205.