substance: boron compounds with group I elements
property: properties of binary boron-lithium compounds

LiB_{13}

Interstitially doped β-rhombohedral boron (see Landolt-Börnstein III/41C)

Rietveld analysis of LiB_{13} with β-rhombohedral boron structure in [94K, 95K].

LiB_{12} (O), Li_2B_{12} (T_d) and Li_3B_{12}

Ab initio calculation of the stability and electronic properties of boron-lithium compounds with α-rhombohedral boron structure (called intercalation compounds by the authors) [94G].

Compound	Total energy gain [eV/cell]	Lattice constant+) [Å]	Bulk modulus [eV Å^{-3}]*)
LiB_{12} (O)	2.78	5.077	2.60
Li_2B_{12} (T_d)	2.69	5.200	2.28
Li_3B_{12}	5.04	5.222	2.02

*) Unit as given in the original paper

+) Only *a*-value is given in the original paper

Density of states calculation in Fig. 1 [94G].

Li_3B_{14}

Structure: tetragonal, 112 boron atoms and 24 Li atoms per unit cell

Dodecahedral closo B_8 and hexadecahedral closo B_{10} cages are present in the ratio 1 :2

Space group: $I\bar{4}2d$ [88M].

Density of states calculation in [90B].

energy gap

E_g	1.4...1.6 eV	T = 600...900 K	from el. cond.	84M2, 84M1, 88M, 90B

LiB_6

energy gap

E_g	1.4...1.6 eV	T = 600...900 K	from el. cond.	84M2, 84M1, 88M, 90B

Li_5B_4

metallic conduction; crystalline structure: [78W], electronic structure: [79L]

LiB_6

metallic conduction(?); preparation: [75S, 77N], crystalline structure: [77N], CESR (conduction electron spin resonance): [74R]

LiB alloys (0...60 at% B)

metallic conduction; preparation: [75M], electrical conductivity: [75M]

Li_6B_{19}

energy gap

E_g	1.4...1.6 eV	600...900 K	from el. cond.	84M2, 84M1, 88M,

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Fig. 1.

Li_xB_{12} (x = 1...3). Calculated densities of states near E_F for LiB_{12} (O), Li_2B_{12} (T_d) and Li_3B_{12} [94G].