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Boron avoids cycloalkane-like structures in the $Li_nB_nH_{2n}$ series

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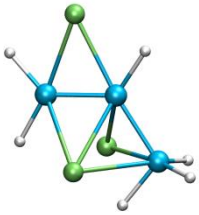
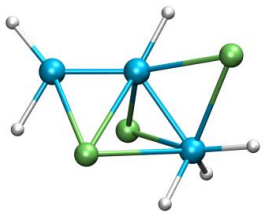
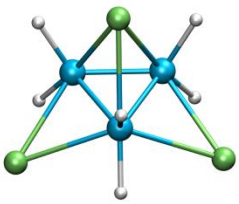
Table S1. Structures, cartesian coordinates and relative energies of the lowest energy isomers (GEGA and CK searches) of $Li_3B_3H_6$ calculated at the CCSD(T)/Def2-TZVP//PBE0/Def2-TZVP level of theory (values in parentheses correspond to the relative energies at the PBE0/Def2-TZVP level).

Structure	Coordinates (Å)				ΔE(kcal/mol)
	B	1.195366000	-0.641189000	0.052617000	0.00 (0.00)
	B	0.187674000	0.613077000	-0.050101000	
	Li	-0.454714000	-0.936450000	-1.362609000	
	H	0.538881000	1.797171000	-0.057859000	
	H	0.754715000	-1.799006000	0.020357000	
	H	2.424649000	-0.681039000	0.138343000	
	B	-1.559333000	0.369110000	-0.051299000	
	Li	2.183530000	1.098553000	-0.025207000	
	Li	-0.649740000	-0.715804000	1.426605000	
	H	-1.802750000	-0.890296000	-0.151050000	
	H	-2.241622000	0.918031000	-0.889361000	
	H	-2.029633000	0.611250000	1.067120000	
	B	1.232510000	-0.543132000	0.039092000	7.52 (7.84)
	Li	-0.341479000	-1.119528000	-1.411673000	
	Li	1.631180000	1.567068000	0.141895000	
	H	2.381824000	-0.076118000	0.167987000	
	H	1.385689000	-1.327666000	-0.927056000	
	H	0.110848000	1.674968000	-0.762282000	
	B	-1.677498000	0.229350000	0.029554000	
	Li	-0.429170000	-0.573618000	1.525461000	
	H	-1.993143000	-0.843051000	0.615750000	
	H	1.116875000	-1.333986000	1.002314000	
	H	-2.668095000	0.832434000	-0.292723000	
	B	-0.138130000	0.604112000	-0.182853000	
	B	0.000002000	0.621508000	0.574617000	11.16 (8.81)
	B	0.850113000	-0.528846000	-0.487548000	
	B	-0.850119000	-0.528825000	-0.487565000	
	H	-0.000020000	0.485128000	1.803790000	
	H	0.000026000	1.832551000	0.283475000	
	H	1.492429000	-1.441503000	0.052461000	
	H	1.471581000	-0.084984000	-1.452570000	
	H	-1.471545000	-0.084936000	-1.452606000	
	H	-1.492469000	-1.441480000	0.052389000	
	Li	1.965086000	1.188565000	-0.130987000	

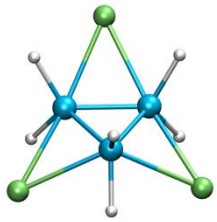
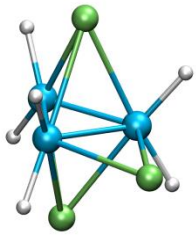
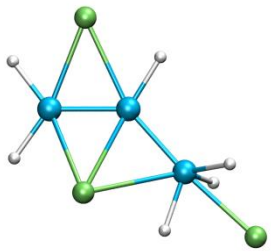
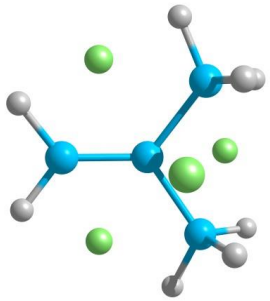
	Li	-0.000041000	-1.405163000	1.167154000	
	Li	-1.965038000	1.188611000	-0.130986000	
	B	0.491078000	0.863053000	-0.184883000	11.98 (9.72)
	B	0.490720000	-0.863066000	-0.185296000	
	B	-0.832773000	0.000141000	0.555278000	
	H	1.286450000	1.483501000	0.547361000	
	H	0.304687000	1.510016000	-1.228593000	
	H	1.286027000	-1.484327000	0.546368000	
	H	0.303717000	-1.509425000	-1.229269000	
	H	-1.903767000	0.000355000	-0.142953000	
	H	-1.117181000	0.000179000	1.735081000	
	Li	2.345772000	-0.000421000	0.245350000	
	Li	-1.323919000	-1.876821000	-0.314626000	
	Li	-1.323540000	1.876928000	-0.315221000	
	B	-0.313325000	0.015774000	-0.876822000	13.03 (9.91)
	B	1.225527000	-0.014167000	-0.062758000	
	B	-0.250024000	-0.002650000	0.912558000	
	Li	-2.231973000	0.011709000	-0.001476000	
	Li	0.325635000	-1.812751000	0.011389000	
	H	1.951109000	0.971770000	-0.072246000	
	H	1.930846000	-1.013993000	-0.099213000	
	H	-0.571776000	-1.015777000	1.539748000	
	H	-0.526979000	0.997386000	1.577814000	
	H	-0.711294000	1.027298000	-1.464438000	
	Li	0.361853000	1.806813000	0.030642000	
	H	-0.749338000	-0.978786000	-1.468216000	
	B	-1.647247000	0.547208000	0.195936000	20.27 (19.70)
	B	-0.395406000	-0.451735000	0.001522000	
	B	1.308773000	-0.180188000	0.010847000	
	Li	-2.244891000	-1.321338000	-0.197804000	
	Li	0.004384000	1.525016000	-0.464190000	
	Li	3.264685000	-0.087203000	0.128547000	
	H	-1.571458000	1.769963000	0.325770000	
	H	1.843415000	-0.525818000	1.091628000	
	H	1.758251000	1.024215000	-0.100517000	
	H	-0.555431000	-1.677051000	-0.122442000	
	H	1.966175000	-0.774229000	-0.881168000	
	H	-2.844086000	0.257067000	0.245549000	

Table S2. Structures, cartesian coordinates and relative energies of the lowest energy isomers (GEGA and CK searches) of $Li_4B_4H_8$ calculated at the CCSD(T)/Def2-TZVP//PBE0/Def2-TZVP level of theory (values in parentheses correspond to the relative energies at the PBE0/Def2-TZVP level).

Structure	Coordinates (Å)				ΔE (kcal/mol)
	H	2.594996000	-0.360777000	-0.041332000	0.00 (0.00)
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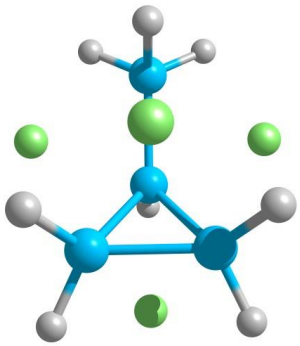
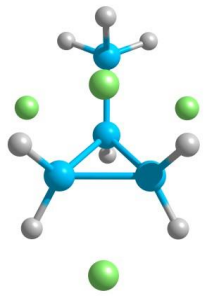
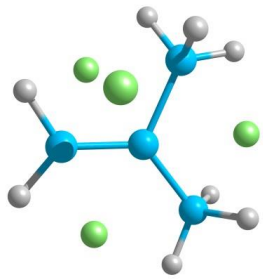
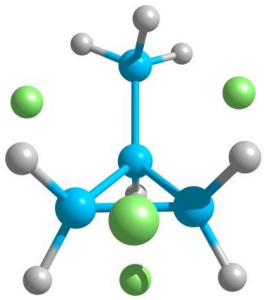
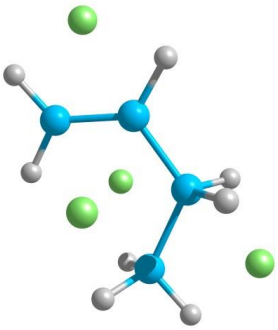
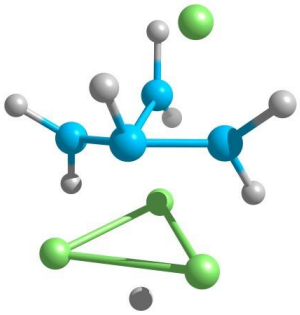
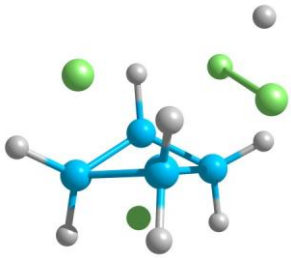
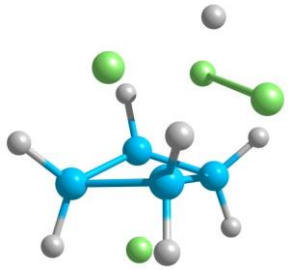
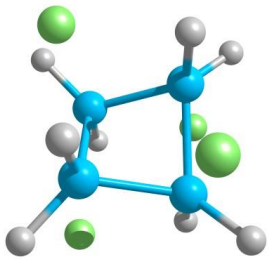
	Li	1.835653000	1.138529000	-0.594930000	
	B	-0.001472000	1.771068000	0.096407000	
	H	-0.988569000	2.506172000	0.188444000	
	Li	-1.838027000	1.135548000	-0.595253000	
	B	-0.000122000	0.177862000	-0.161273000	
	B	1.461763000	-0.862331000	0.096002000	
	H	1.530402000	-1.914228000	-0.574428000	
	H	-1.480975000	-1.304062000	1.262519000	
	Li	0.000274000	-0.381054000	1.789545000	
	B	-1.460215000	-0.864797000	0.096097000	
	H	-2.594379000	-0.365908000	-0.043355000	
	H	1.481874000	-1.303028000	1.261858000	
	H	-1.525826000	-1.917753000	-0.572961000	
	Li	0.001580000	-1.545515000	-1.367764000	
	H	2.447924000	-0.989754000	-0.473588000	(0.94)
	H	2.000814000	0.003223000	1.160820000	
	Li	0.294630000	0.003153000	1.691957000	
	B	1.798367000	-0.002310000	-0.079031000	
	H	-0.676641000	-1.548553000	1.356063000	
	Li	-1.913771000	-0.003066000	-1.283459000	
	B	-1.076083000	0.893179000	0.385124000	
	B	-1.074478000	-0.891948000	0.384384000	
	H	-2.085719000	1.424333000	-0.069818000	
	H	-0.684477000	1.548465000	1.360015000	
	Li	0.813293000	1.926624000	-0.462035000	
	B	0.082468000	0.002504000	-0.576290000	
	H	-0.021888000	0.005471000	-1.818533000	
	H	-2.084305000	-1.425231000	-0.067551000	
	H	2.454476000	0.976825000	-0.482931000	
	Li	0.805332000	-1.927345000	-0.458266000	
	H	-2.596309000	-0.982739000	-0.097812000	(3.39)
	H	-2.596126000	0.983255000	-0.095493000	
	Li	-0.111242000	-0.001711000	1.585412000	
	B	-1.887204000	-0.000131000	0.209245000	
	H	1.885457000	-1.475230000	-0.621361000	
	Li	-1.023242000	-1.859229000	-0.621635000	
	B	1.035825000	-0.903695000	0.069317000	
	B	1.035866000	0.903523000	0.072100000	
	H	1.885231000	1.476895000	-0.617372000	
	H	0.912069000	-1.515252000	1.146350000	
	Li	-1.023649000	1.859613000	-0.622022000	
	B	-0.274991000	0.000780000	-0.586529000	
	H	-0.410142000	0.003724000	-1.809274000	
	H	0.912775000	1.511854000	1.150964000	
	H	-1.901943000	-0.001653000	1.463210000	
	Li	2.945303000	0.000247000	-0.121713000	

	H	0.523413000	-2.492535000	-0.254200000	(4.29)
	H	1.959131000	-1.339293000	-0.795042000	
	Li	-1.124295000	-1.912018000	-0.123929000	
	B	0.978907000	-1.360347000	-0.021805000	
	H	1.529543000	-1.555675000	1.084478000	
	Li	1.408383000	0.131644000	1.573287000	
	B	-1.875512000	-0.109519000	0.042305000	
	B	-0.096808000	0.113040000	-0.034417000	
	H	-2.631888000	0.864834000	0.127770000	
	H	-2.278172000	-0.748320000	-0.951338000	
	Li	1.596538000	0.249568000	-1.433355000	
	B	0.743543000	1.508383000	0.028403000	
	H	-2.162696000	-0.828697000	1.014464000	
	H	0.360349000	2.676468000	0.113197000	
	H	1.991652000	1.525826000	-0.009162000	
	Li	-1.227952000	1.910675000	-0.150202000	
	H	-1.807978000	1.413567000	0.770890000	(6.44)
	H	-0.810183000	1.614835000	-0.975518000	
	Li	-1.391349000	-0.191731000	1.774778000	
	B	-0.962580000	0.893660000	0.032718000	
	H	-1.843201000	-1.514498000	0.444951000	
	Li	-2.041752000	0.203221000	-1.675404000	
	B	-0.982420000	-0.863785000	-0.162490000	
	B	1.964126000	0.013014000	-0.135710000	
	H	-0.830604000	-1.357407000	-1.297616000	
	H	2.639146000	-1.028206000	-0.162627000	
	Li	0.996524000	-1.810481000	-0.416366000	
	B	0.364231000	-0.070281000	0.642245000	
	H	1.777914000	0.333222000	-1.333897000	
	H	0.412222000	-0.202404000	1.881434000	
	H	2.696655000	0.886800000	0.339546000	
	Li	1.052992000	1.796006000	-0.200001000	
	H	3.024825000	-0.920144000	-0.000593000	(7.01)
	H	-1.142176000	1.449048000	-0.983300000	
	Li	0.018868000	-0.721687000	1.370605000	
	B	1.808413000	-0.714712000	-0.000480000	
	H	-1.592890000	-1.513445000	0.985124000	
	Li	-2.697537000	1.180293000	-0.000517000	
	B	-0.754377000	0.773788000	-0.000083000	
	B	-1.750470000	-0.771301000	0.000437000	
	H	-2.982299000	-0.574398000	-0.000474000	
	H	1.225842000	-1.799341000	-0.000836000	
	Li	3.040113000	0.860502000	0.000393000	
	B	0.998191000	0.680846000	-0.000206000	
	H	-1.142270000	1.449035000	0.983092000	
	H	-1.591836000	-1.515533000	-0.982487000	
	H	1.551946000	1.791311000	0.000123000	
	Li	0.018579000	-0.722322000	-1.370144000	

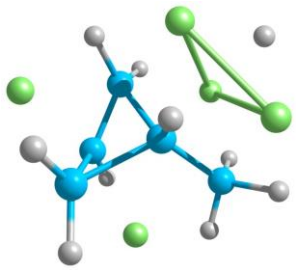
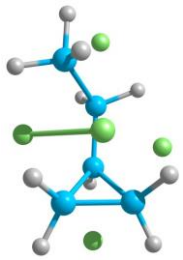
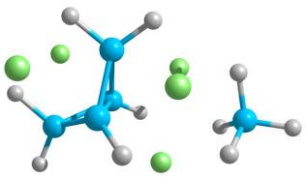
	H	1.813357000	-1.422131000	0.574859000	(8.96)
	H	0.694284000	-0.430751000	-1.751187000	
	Li	-0.964037000	0.396903000	1.302932000	
	B	0.809708000	-0.727985000	0.687529000	
	H	-1.724310000	-1.203743000	0.672326000	
	Li	-2.343476000	-0.037439000	-0.674209000	
	B	-0.737707000	-1.350571000	-0.098371000	
	B	0.909500000	1.043006000	0.182949000	
	H	-2.304553000	1.456544000	0.324425000	
	H	0.487765000	-0.647925000	1.855633000	
	Li	-0.856661000	2.126000000	-0.463023000	
	B	0.052803000	-0.040858000	-0.773479000	
	H	0.414429000	1.815551000	1.015143000	
	H	-0.804044000	-2.425516000	-0.633432000	
	H	1.981267000	1.510305000	-0.195240000	
	Li	2.254268000	-0.242229000	-0.784254000	
	H	-1.929507000	1.207161000	0.076844000	(9.45)
	H	2.282768000	-1.337979000	-0.396905000	
	Li	-1.946748000	0.008307000	-1.369498000	
	B	1.699650000	-0.285986000	-0.142344000	
	H	2.473031000	0.517885000	0.359447000	
	Li	1.294115000	1.829639000	-0.339710000	
	B	0.235955000	0.081544000	-0.782821000	
	B	-0.706844000	1.091170000	0.165848000	
	H	-2.886658000	-1.131069000	-0.434845000	
	H	-0.418168000	-1.388495000	1.214847000	
	Li	-2.097781000	-0.540642000	1.007275000	
	B	0.144439000	-0.298192000	0.972617000	
	H	-0.269835000	2.146779000	0.617103000	
	H	0.697948000	0.104704000	1.955705000	
	H	-0.291241000	-0.824574000	-1.442932000	
	Li	0.575633000	-2.043001000	-0.303322000	
	H	-1.851493000	1.803646000	-0.279554000	(9.95)
	H	-2.636153000	-0.002899000	0.183888000	
	Li	1.875558000	0.273721000	-1.308679000	
	B	-1.632864000	0.604337000	-0.168101000	
	H	-0.926270000	-0.688875000	1.674331000	
	Li	-1.538824000	-1.522351000	-0.213311000	
	B	0.646513000	-1.206600000	-0.144233000	
	B	-0.270489000	0.005897000	-0.855717000	
	H	2.276491000	1.464176000	0.024065000	
	H	0.281990000	-2.360038000	0.034349000	
	Li	1.973499000	0.107362000	1.171805000	
	B	-0.208533000	-0.044245000	0.951194000	
	H	1.890078000	-1.227084000	-0.265686000	
	H	0.295143000	0.962834000	-1.389402000	
	H	0.375603000	0.803207000	1.647682000	
	Li	0.230259000	1.957297000	0.168390000	

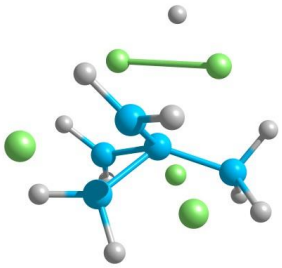
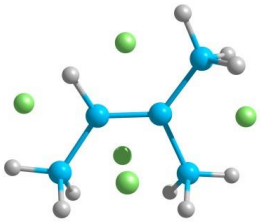


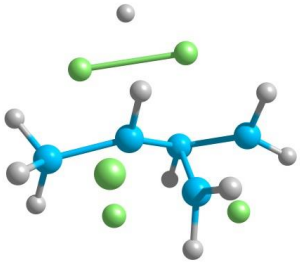
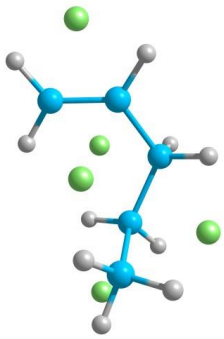
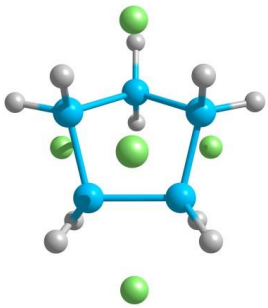
H	-0.898899000	0.790901000	1.605297000
H	-0.796874000	-0.895984000	-1.603764000
Li	-1.156235000	1.028321000	-1.565437000
B	-0.884865000	0.779634000	0.348199000
H	-1.799744000	1.584672000	0.039732000
Li	-1.022815000	-1.158389000	1.567420000
B	0.779965000	0.886315000	-0.343344000
B	-0.780941000	-0.884116000	-0.346680000
H	-1.584771000	-1.799231000	-0.036934000
H	0.793280000	0.905051000	-1.600200000
Li	1.027056000	1.149441000	1.571789000
B	0.885142000	-0.781746000	0.341773000
H	1.584922000	1.799798000	-0.030201000
H	0.902049000	-0.799903000	1.598569000
H	1.798701000	-1.585628000	0.027243000
Li	1.153602000	-1.019409000	-1.573602000

41.77
(21.11)

Table S3. Structures, cartesian coordinates and relative energies of the lowest energy isomers of $Li_5B_5H_{10}$ calculated at the CCSD(T)/Def2-TZVP//PBE0/Def2-TZVP level of theory (values in parentheses correspond to the relative energies at the PBE0/Def2-TZVP level).

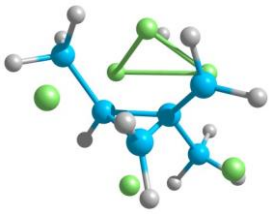
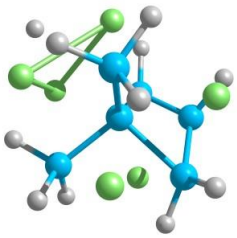
Structure	Coordinates (Å)				ΔE (kcal/mol)
	B	-1.237182000	-0.288981000	-0.755551000	0.00 (0.00)
	B	-0.528331000	1.220012000	-0.751852000	
	H	-0.955324000	-1.056700000	-1.661624000	
	H	0.036099000	1.734774000	-1.715218000	
	H	2.550611000	-1.262959000	0.583074000	
	Li	-0.370381000	-2.187602000	-0.306970000	
	B	1.618818000	-1.103176000	-0.229046000	
	H	1.366759000	-2.279754000	-0.515823000	
	Li	2.162886000	0.235636000	1.377658000	
	H	2.178193000	-0.706109000	-1.267887000	
	Li	1.695119000	1.008346000	-1.022784000	
	H	0.220326000	0.287433000	1.483331000	
	H	2.335806000	1.882610000	0.674323000	
	H	-1.628080000	-1.998792000	1.100259000	
	B	-1.591557000	-0.825224000	0.744151000	
	H	-2.050445000	-0.101381000	1.628469000	
	Li	0.591058000	2.142145000	0.884305000	
	H	-1.044354000	2.147648000	-0.054426000	
	Li	-2.554489000	1.029422000	0.159600000	
	B	0.221818000	-0.068753000	0.286317000	
	B	1.696101000	0.414364000	0.808587000	(1.20)
	B	0.664919000	0.370987000	-0.641007000	
	H	1.103384000	0.889421000	-1.685933000	
	H	1.138036000	0.718386000	1.878934000	
	H	2.838797000	0.870376000	0.816095000	
	Li	0.363433000	2.110833000	0.486040000	
	B	1.461636000	-1.089727000	-0.030025000	
	H	2.451499000	-1.572737000	-0.572898000	
	Li	2.729337000	0.245005000	-0.987605000	
	H	0.767446000	-2.017936000	0.400583000	
	Li	-0.059488000	-0.656894000	1.401442000	
	H	-3.308220000	-0.489910000	0.405029000	
	H	-2.053709000	-1.795139000	-0.287308000	
	H	-1.829665000	-1.028323000	1.519080000	
	B	-2.083969000	-0.726572000	0.345222000	
	H	-1.637501000	0.897618000	-1.489429000	
	Li	-0.459884000	-1.438227000	-1.109948000	
	H	-1.380788000	1.663596000	0.300545000	
	Li	-3.037274000	1.076318000	-0.351362000	
	B	-1.078217000	0.601656000	-0.402857000	
	B	-1.867149000	1.047089000	0.000015000	(1.88)
	B	-0.539224000	-1.181340000	0.000052000	
	H	0.221657000	0.819718000	-1.678320000	
	H	-2.209571000	2.204625000	0.000076000	
	H	0.380804000	-2.018767000	-0.000021000	
	Li	-2.285122000	-0.676812000	-1.362048000	
	B	-0.560394000	0.341695000	-0.850342000	
	H	-2.952697000	0.300880000	0.000057000	
	Li	-2.285038000	-0.676956000	1.362041000	

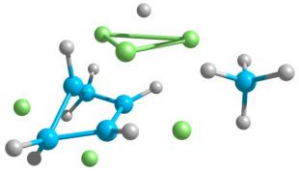
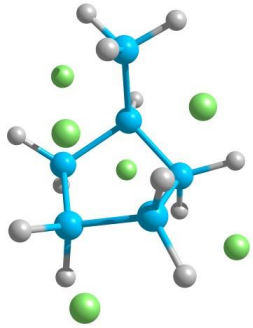
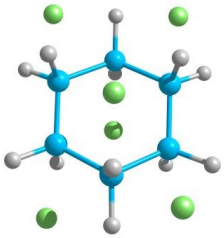
	H	-1.633756000	-1.854841000	0.000026000	
	Li	1.187649000	-0.779982000	-1.327269000	
	H	4.200847000	0.113367000	-0.000166000	
	H	2.611960000	-1.069994000	0.002250000	
	H	0.221576000	0.819884000	1.678324000	
	B	-0.560386000	0.341725000	0.850354000	
	H	2.583210000	0.680610000	1.010108000	
	Li	1.187683000	-0.778877000	1.327700000	
	H	2.582920000	0.676682000	-1.012116000	
	Li	1.071304000	1.595767000	-0.000712000	
	B	2.999878000	0.106516000	0.000049000	
	B	-0.897057000	-0.885254000	0.563095000	(2.28)
	B	-1.098587000	0.009615000	-1.010663000	
	H	-2.160367000	0.609400000	-1.100793000	
	H	-1.770579000	-0.541307000	1.382136000	
	H	-0.833483000	-0.457593000	-2.116401000	
	Li	-0.376065000	1.070199000	1.954177000	
	B	-0.331165000	1.614780000	-0.289566000	
	H	-1.216715000	2.127941000	0.385787000	
	Li	-2.934082000	-0.658224000	-0.053861000	
	H	0.184150000	2.478517000	-1.006104000	
	Li	0.113735000	-1.758968000	-1.100608000	
	H	-0.714018000	-2.106822000	0.642952000	
	H	1.862450000	-1.613911000	-1.119908000	
	H	0.760576000	0.426723000	3.126586000	
	B	1.891721000	-0.588570000	-0.416748000	
	H	2.710798000	0.117046000	-1.036131000	
	Li	1.732276000	1.554224000	-0.734055000	
	H	2.520078000	-0.943707000	0.591178000	
	Li	1.196914000	-0.732609000	1.877116000	
	B	0.326844000	0.145400000	0.038360000	
	B	0.667479000	-0.108023000	0.027924000	1.67 (3.02)
	B	-0.878428000	-0.678882000	-0.094989000	
	H	-1.062806000	-1.894761000	-0.455646000	
	B	-2.360075000	0.341379000	-0.171642000	
	H	-3.461894000	-0.241420000	-0.200033000	
	H	-2.487996000	1.159380000	0.757488000	
	H	-2.428293000	1.066220000	-1.180835000	
	B	0.775935000	1.693102000	0.174658000	
	H	1.871972000	2.242496000	0.389806000	
	H	0.406202000	2.291411000	-0.856773000	
	H	0.079278000	2.228259000	1.050122000	
	B	2.175024000	-1.062252000	-0.167675000	
	H	2.972753000	-0.879287000	0.775892000	
	H	2.113676000	-2.289940000	-0.313409000	
	H	2.766999000	-0.644739000	-1.171899000	
	Li	0.492069000	-2.183735000	0.376641000	
	Li	2.754311000	0.797485000	0.078481000	
	Li	-2.649005000	-1.690488000	0.346215000	
	Li	-0.846905000	0.775901000	1.443624000	
	Li	-0.640325000	0.979423000	-1.456993000	

	B	0.776895000	-0.950271000	0.578232000	(4.76)
	B	0.780362000	0.301966000	-0.704969000	
	H	-0.838118000	3.273808000	-0.173880000	
	H	0.909603000	-2.085807000	0.055489000	
	H	2.044520000	1.176725000	1.270433000	
	Li	-0.595768000	-1.398975000	-1.172218000	
	B	-0.629453000	0.128550000	0.165920000	
	H	0.996498000	-1.018503000	1.765274000	
	Li	-1.755111000	1.841674000	-0.566318000	
	H	0.904765000	-0.310934000	-1.795062000	
	Li	0.556805000	2.282112000	0.256782000	
	H	-3.071898000	0.465700000	-0.528567000	
	H	-2.836761000	-0.944536000	0.801299000	
	H	-0.667099000	0.865900000	1.162491000	
	B	2.075133000	0.480248000	0.276546000	
	H	3.237859000	0.175259000	-0.004804000	
	Li	-1.268398000	-0.959883000	1.752728000	
	H	-2.391847000	-1.286594000	-1.091883000	
	Li	2.431490000	-1.093247000	-0.959641000	
	B	-2.281852000	-0.425704000	-0.194687000	
	B	2.136305000	-1.012576000	0.140184000	(9.89)
	B	-2.121440000	-0.608760000	-0.867488000	
	H	3.233425000	-1.569374000	0.029996000	
	H	-1.462872000	-1.341749000	-1.607493000	
	H	-2.581577000	0.267384000	-1.624579000	
	Li	3.629864000	-0.013866000	-0.730724000	
	B	-1.256729000	0.121136000	0.567476000	
	H	1.327388000	-1.829354000	0.584267000	
	Li	0.145276000	-0.888341000	-0.827953000	
	H	-2.141725000	0.779802000	1.187844000	
	Li	-2.852593000	-0.990561000	1.110629000	
	H	0.378197000	1.851729000	1.244601000	
	H	2.498410000	1.328743000	-0.712330000	
	H	-0.142892000	2.125603000	-0.620533000	
	B	0.147479000	1.224638000	0.191128000	
	H	-0.969357000	-0.779791000	1.396880000	
	Li	0.868802000	0.058297000	1.715231000	
	H	-3.131534000	-1.302441000	-0.605994000	
	Li	-1.821540000	1.613723000	-0.699060000	
	B	1.711007000	0.501901000	-0.226706000	
	B	1.110129000	-0.932049000	-0.029968000	15.23 (16.06)
	B	-0.605494000	-1.347280000	-0.345473000	
	H	1.981217000	1.416925000	-0.823043000	
	H	-0.934004000	-0.000144000	1.824467000	
	H	1.981380000	-1.418284000	-0.822061000	
	Li	0.481603000	0.000448000	-1.779016000	
	B	-1.339161000	0.000146000	0.627680000	
	H	-0.908361000	-2.520613000	-0.043800000	
	Li	-0.246515000	-1.783601000	1.521606000	
	H	1.511587000	1.374993000	1.079321000	
	Li	-2.276713000	0.000778000	-1.074602000	
	H	-2.593856000	0.000284000	0.737279000	
	H	-0.947581000	1.276566000	-1.559182000	
	H	-0.948019000	-1.275229000	-1.559779000	
	B	1.110465000	0.931343000	-0.029974000	
	H	1.509801000	-1.375279000	1.080004000	

	Li	-0.244982000	1.782960000	1.522270000	
	H	-0.906966000	2.521070000	-0.042534000	
	Li	2.919959000	-0.000425000	0.057146000	
	B	-0.604989000	1.347687000	-0.344843000	

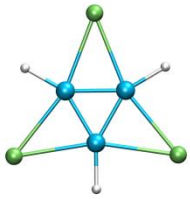
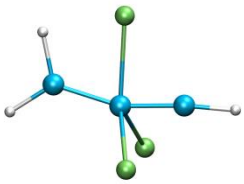
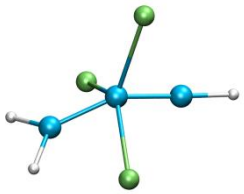
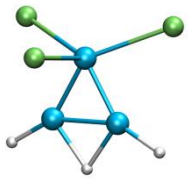
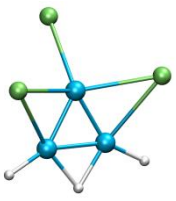
Table S4. Structures, cartesian coordinates and relative energies of the lowest energy isomers of $Li_6B_6H_{12}$ calculated at the CCSD(T)/Def2-TZVP//PBE0/Def2-TZVP level of theory (values in parentheses correspond to the relative energies at the PBE0/Def2-TZVP level).

Structure	Coordinates (Å)				ΔE (kcal/mol)
	Li	-1.024301000	0.857925000	1.481154000	0.00 (0.00)
	H	-2.677155000	0.075647000	1.049742000	
	Li	-0.969712000	2.110576000	-0.519791000	
	Li	2.275635000	-1.260046000	0.377401000	
	B	0.631207000	-0.645689000	1.517284000	
	H	-0.296126000	-0.754670000	2.304758000	
	H	1.659822000	-1.050034000	2.068066000	
	H	-0.647210000	-2.278102000	0.509752000	
	B	0.030169000	-1.495533000	-0.138316000	
	H	0.800179000	-2.176633000	-0.849064000	
	B	2.151641000	0.651280000	-0.712706000	
	H	3.198448000	0.038284000	-0.401666000	
	H	2.157154000	0.667407000	-1.958428000	
	H	2.413139000	1.827690000	-0.426531000	
	B	-2.489492000	0.364134000	-0.152907000	
	H	-2.800962000	1.551589000	-0.277323000	
	B	-0.858307000	-0.027564000	-0.741930000	
	H	-0.825370000	0.273519000	-1.960766000	
	H	-3.382574000	-0.260492000	-0.736787000	
	H	-0.373011000	2.662491000	1.095751000	
	Li	0.772740000	-0.481249000	-2.006796000	
	Li	1.269285000	1.917295000	1.055246000	
	Li	-2.224117000	-1.662878000	-0.270204000	
	B	0.629796000	0.149060000	0.074867000	
	Li	0.650170000	-2.038329000	0.739463000	(4.41)
	H	0.662329000	2.542011000	0.266798000	
	Li	1.807275000	1.314932000	-0.838237000	
	Li	-2.150226000	1.087917000	0.395205000	
	B	-0.202020000	1.871237000	-0.343482000	
	H	0.041135000	2.120974000	-1.539546000	
	H	-0.668101000	-1.530468000	2.005832000	
	H	-0.692483000	-2.363365000	-0.569514000	
	B	-0.036473000	0.079865000	0.054184000	
	H	-1.228635000	2.518325000	-0.111646000	
	B	1.800317000	-0.276899000	0.593734000	
	H	1.838998000	-0.911286000	1.638664000	
	H	2.519693000	0.728353000	0.754093000	
	H	1.688501000	-0.122613000	-1.877320000	
	B	1.329865000	-0.778741000	-0.897820000	
	H	-0.670977000	-1.313514000	-2.270395000	
	B	-0.165106000	-1.395810000	-1.154835000	
	H	-2.163952000	-0.403047000	1.470307000	
	H	-2.806600000	0.279553000	-1.034217000	
	H	-0.727328000	0.367689000	2.532334000	
	Li	-1.156739000	0.482265000	-1.883429000	
	Li	-2.138386000	-1.200209000	-0.240500000	
	Li	0.674137000	1.220234000	1.714069000	
	B	-0.896837000	-0.402260000	1.563197000	

	Li	-3.293749000	0.405330000	0.152275000	(8.02)
	H	-1.270229000	2.379228000	-1.024059000	
	Li	-0.273607000	2.264236000	0.611935000	
	Li	-1.642102000	-0.985603000	-1.612634000	
	B	-1.457724000	1.174975000	-0.855712000	
	H	-2.511955000	0.857783000	-1.455772000	
	H	-2.342849000	-1.973614000	1.519587000	
	H	-0.950011000	0.836679000	1.750814000	
	B	-1.224655000	0.293849000	0.666793000	
	H	4.686888000	-0.853735000	0.418725000	
	B	3.731903000	-0.422669000	-0.168231000	
	H	3.421258000	-1.157493000	-1.104318000	
	H	3.962681000	0.698081000	-0.627188000	
	H	2.779969000	-0.354439000	0.645814000	
	B	-0.073847000	0.207529000	-0.715113000	
	H	1.027749000	0.728763000	-0.918528000	
	B	-1.984204000	-1.312918000	0.579441000	
	H	0.500137000	-1.794937000	0.791670000	
	H	1.363760000	1.949749000	1.367068000	
	H	-2.903794000	-1.307048000	-0.300916000	
	Li	2.507540000	1.451811000	0.139992000	
	Li	1.641848000	-1.213435000	-0.702261000	
	Li	0.768928000	0.164780000	1.640028000	
	B	-0.369507000	-1.194840000	0.142643000	
	Li	0.415286000	1.913994000	-0.881840000	28.36 (29.02)
	H	-1.043875000	0.865584000	-1.631075000	
	Li	-2.237522000	1.961429000	0.828591000	
	Li	2.548822000	-1.092897000	0.341295000	
	B	2.051719000	0.624874000	-0.985514000	
	H	-0.365330000	2.415348000	0.839825000	
	H	1.503002000	0.413346000	-2.096933000	
	H	1.960483000	0.430193000	1.420956000	
	B	1.073656000	0.262779000	0.502605000	
	H	-0.999004000	0.898624000	1.923230000	
	B	-0.426733000	1.125386000	0.817655000	
	H	-2.685114000	0.824121000	-0.563450000	
	H	0.271302000	-1.917196000	1.732989000	
	H	1.186462000	-2.324054000	0.033758000	
	B	-1.436752000	0.453341000	-0.502000000	
	H	-1.314097000	-1.994797000	-1.304636000	
	B	-1.193594000	-1.345939000	-0.204286000	
	H	-2.158516000	-1.769396000	0.457244000	
	H	2.364743000	1.818355000	-1.063939000	
	H	3.113998000	-0.011486000	-1.056217000	
	Li	0.335570000	-0.784930000	-1.446388000	
	Li	-2.916538000	-1.036319000	-1.078256000	
	Li	0.454829000	-0.253875000	2.347596000	
	B	0.404626000	-1.474610000	0.566590000	
	Li	-0.067842000	-0.109692000	1.435699000	34.05 (33.86)
	H	1.357333000	-2.603969000	0.177577000	
	Li	-2.619948000	1.793960000	-0.785605000	
	Li	-2.814297000	-1.715944000	0.473480000	
	B	0.843367000	-1.534540000	-0.209770000	
	H	1.067445000	-1.570475000	-1.469716000	
	H	2.996152000	-0.033745000	0.014975000	
	H	1.873853000	-0.144079000	1.643944000	

	B	1.748283000	-0.048874000	0.409393000	
	H	1.420906000	2.517698000	0.565847000	
	B	0.866504000	1.528937000	0.042564000	
	H	1.068494000	1.754621000	-1.211624000	
	H	-1.377404000	2.620134000	0.090648000	
	H	-1.035798000	1.455959000	1.627292000	
	B	-0.882871000	1.499751000	0.387576000	
	H	-3.001392000	0.064943000	0.031352000	
	B	-1.759797000	0.037129000	-0.297432000	
	H	-1.866557000	0.172838000	-1.563285000	
	H	-1.468836000	-2.517284000	-0.442340000	
	H	-1.109479000	-1.721155000	1.308450000	
	Li	0.105698000	0.110404000	-1.251061000	
	Li	2.769675000	-1.763653000	-0.505694000	
	Li	2.791323000	1.758778000	-0.277370000	
	B	-0.899196000	-1.525811000	0.059377000	

Table S5. Structures, cartesian coordinates and relative energies of the lowest energy isomers of $Li_3B_3H_3^+$ calculated at the CCSD(T)/Def2-TZVP//PBE0/Def2-TZVP level of theory (values in parentheses correspond to the relative energies at the PBE0/Def2-TZVP level).

Structure	Coordinates (Å)				ΔE (kcal/mol)
	B	0.706334000	0.576669000	-0.001189000	0.00 (0.00)
	B	-0.852664000	0.322751000	-0.001120000	
	B	0.146830000	-0.900587000	-0.001189000	
	H	1.644032000	1.342513000	-0.000815000	
	H	-1.984827000	0.751408000	-0.000754000	
	H	0.341562000	-2.095427000	-0.000841000	
	Li	2.323555000	-0.878633000	0.002291000	
	Li	-1.924823000	-1.569842000	0.002146000	
	Li	-0.399822000	2.450922000	0.002197000	
	B	1.570304000	-0.290822000	0.001856000	25.34 (29.67)
	B	-0.028536000	-0.106112000	0.001115000	
	B	-1.369562000	0.514343000	-0.003931000	
	H	2.277241000	0.716164000	-0.001036000	
	H	2.234683000	-1.284914000	0.004415000	
	H	-2.487716000	0.907845000	-0.007451000	
	Li	-0.836298000	-1.068412000	1.762752000	
	Li	0.705038000	1.845529000	-0.006356000	
	Li	-0.830487000	-1.085828000	-1.753439000	
	B	1.361309000	-0.003823000	-0.619824000	25.87 (29.56)
	B	0.110528000	0.000207000	0.163518000	
	B	-1.481905000	0.001584000	0.222166000	
	Li	1.480096000	0.007274000	1.813605000	
	Li	-0.406812000	-1.893206000	-0.560914000	
	Li	-0.402534000	1.890648000	-0.571793000	
	H	2.382226000	-0.006749000	-1.218054000	
	H	-2.172052000	1.002603000	0.170705000	
	H	-2.172083000	-0.999841000	0.175353000	
	B	-0.000117000	-0.549283000	-0.101537000	28.78 (28.61)
	B	0.820123000	0.814362000	-0.075492000	
	B	-0.820130000	0.814541000	-0.075553000	
	Li	0.000426000	-0.801765000	1.953758000	
	Li	1.861306000	-1.271510000	-0.719505000	
	Li	-1.861583000	-1.271569000	-0.718858000	
	H	-1.869545000	1.387385000	-0.080346000	
	H	0.000187000	1.861800000	-0.122708000	
	H	1.869537000	1.387248000	-0.080221000	
	B	0.809016000	-0.858022000	-0.200877000	29.79 (28.99)
	Li	1.987190000	0.630021000	0.895615000	
	Li	-0.000743000	2.363044000	-0.942710000	
	H	0.000482000	-1.898247000	-0.313770000	
	H	1.873667000	-1.403497000	-0.287977000	
	B	-0.000113000	0.484445000	0.070573000	
	B	-0.808588000	-0.858396000	-0.200980000	
	Li	-1.987375000	0.628948000	0.895878000	
	H	-1.872940000	-1.404431000	-0.288179000	

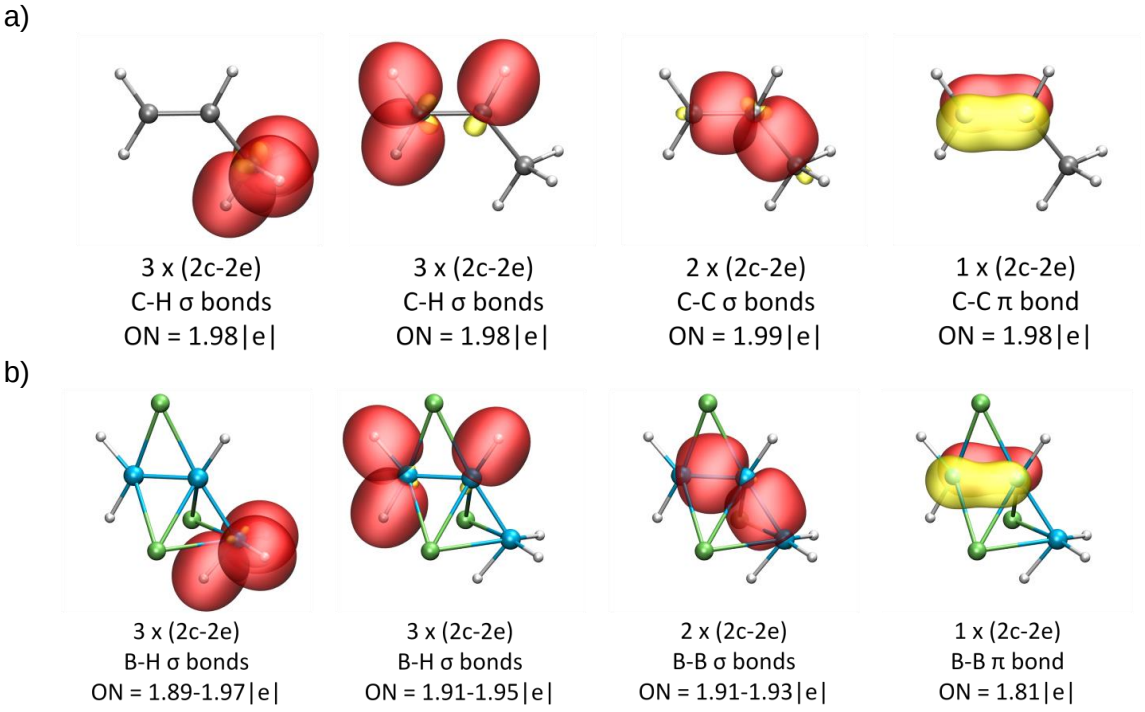


Figure S1. Results of the AdNDP analysis at the PBE0/Def2-TZVP level of theory of systems a) I.1 and b) I'.1. ON stands for occupation number.

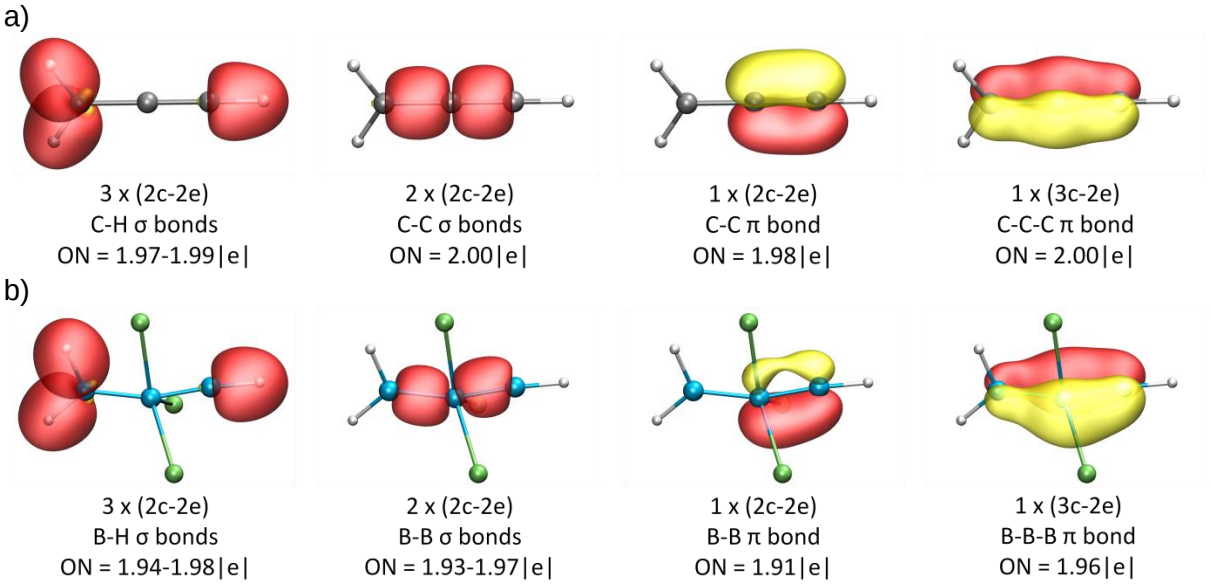


Figure S2. Results of the AdNDP analysis at the PBE0/Def2-TZVP level of theory of systems a) II.2 and b) II'.2. ON stands for occupation number.

Table S6. Natural population analysis (NPA) charges of the boron analogues of cyclopropane and cyclopropenyl cation.

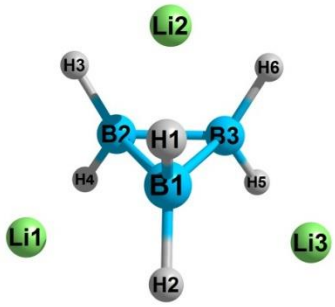
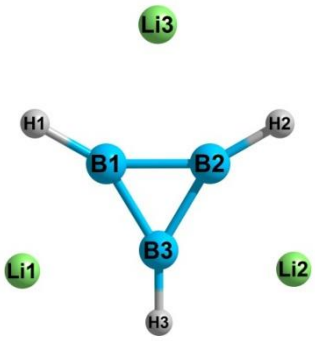
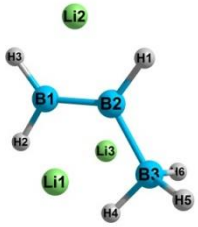
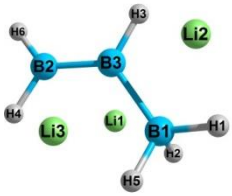
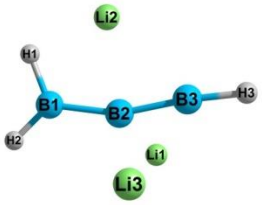
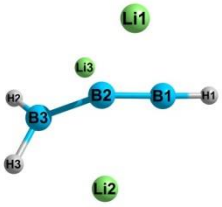
	NPA Charge	
Atom		
Li1	0.872	0.954
Li2	0.809	0.954
Li3	0.872	0.954
B1	-1.004	-0.638
B2	-0.755	-0.638
B3	-0.755	-0.638
H1	0.008	0.017
H2	-0.012	0.017
H3	-0.012	0.017
H4	-0.005	
H5	-0.005	
H6	-0.012	

Table S7. Natural population analysis (NPA) charges of the lowest energy isomers of $Li_3B_3H_6$ and $Li_3B_3H_3^+$(see Tables 1 and 2 in the supporting information).

	NPA Charge			
	$Li_3B_3H_6$		$Li_3B_3H_3^+$	
Atom				
Li1	0.789	0.850	0.944	0.940
Li2	0.826	0.859	0.898	0.909
Li3	0.787	0.733	0.944	0.909
B1	-0.875	-0.800	-0.014	-0.103
B2	-0.665	-0.502	-1.411	-1.445
B3	-0.788	-0.943	-0.266	-0.121
H1	-0.036	-0.030	-0.081	-0.021
H2	-0.009	-0.040	-0.007	-0.034
H3	-0.032	-0.023	-0.007	-0.034
H4	-0.072	-0.079		
H5	0.054	-0.025		
H6	0.021	0.000		