Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

$Li_7(BH)_5^+$: A New Thermodynamically Favored Star-shaped Molecule

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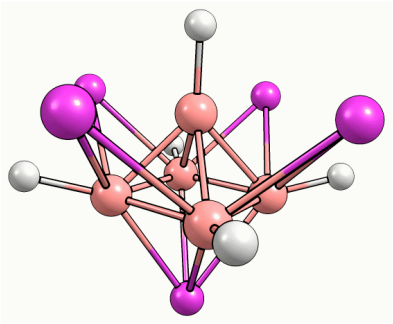
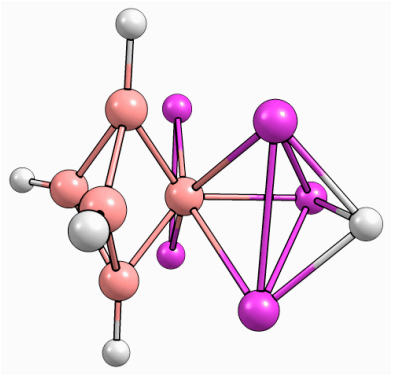
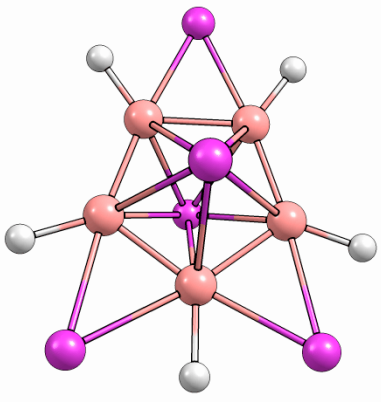
[d.] Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, República 275, Santiago, Chile.

$Li_6(BH)_5^-$: Structure, Cartesian coordinates and relative energies of the singlet state minima conformations

System	Structure			Relative energy
	B -0.911350000 0.801084000 0.474290000 B 0.000080000 -0.000007000 -0.765078000 B -0.801172000 -0.911278000 0.474579000 B 0.911312000 -0.801087000 0.474639000 B 0.801015000 0.911381000 0.474673000 Li 0.146373000 -2.265023000 -0.933459000 Li -0.000472000 0.000202000 2.259218000 Li -2.265230000 -0.146541000 -0.932917000 Li 2.265719000 0.146006000 -0.932316000 Li -0.146235000 2.265473000 -0.933386000 H -1.813975000 1.594099000 0.180768000 H 0.000378000 -0.000356000 -1.972306000 H 1.594353000 1.813773000 0.181243000 H -1.594447000 -1.813854000 0.181815000 H 1.813800000 -1.594481000 0.181545000	PBE0/cc-pvTZ 0.00 CCSD(T) 0.00
	B 0.317995000 0.137616000 0.295044000 B -1.525231000 0.108053000 0.176934000 B -0.625374000 -0.559299000 -1.150216000 B -0.591759000 -1.263459000 0.369003000 B -0.550565000 1.071123000 -0.784043000 Li -0.043989000 -0.368092000 2.392379000 Li 0.052712000 2.155102000 1.118366000 Li 1.518340000 0.653853000 -1.467130000 Li 1.466303000 -1.612790000 -0.359136000 Li 2.432866000 0.453032000 1.024387000 H -0.602833000 -2.331104000 0.923534000 H 2.777693000 -0.459400000 -0.805747000 H -0.532946000 2.167797000 -1.278979000 H -0.496640000 -1.095113000 -2.224541000 H -2.549291000 0.404332000 0.725523000	PBE0/cc-pvTZ 5.97 CCSD(T) 6.41

System	Structure				Relative energy
	B	1.277444000	0.863921000	0.010729000	PBE0/cc-pvTZ 11.14 CCSD(T) 10.89
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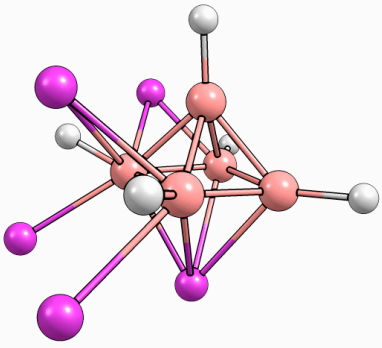
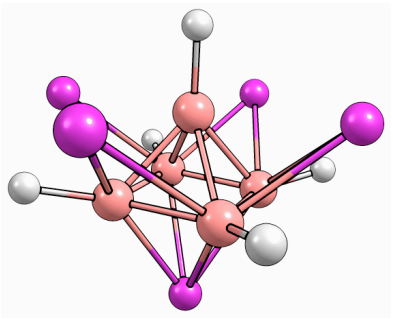
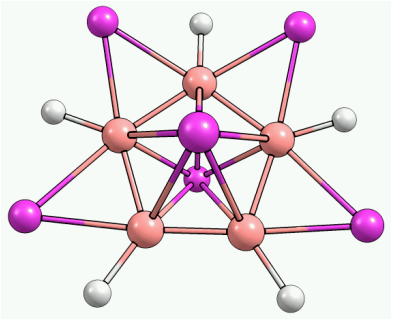
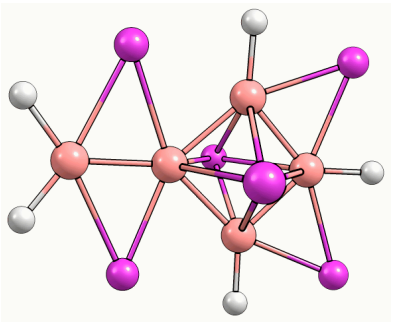
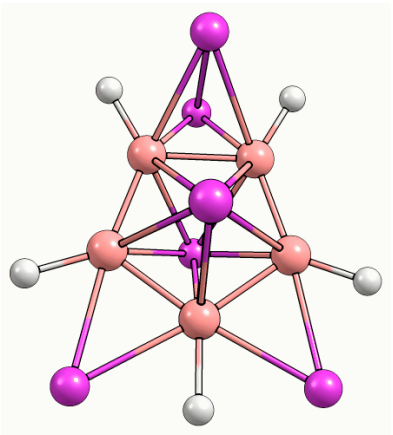
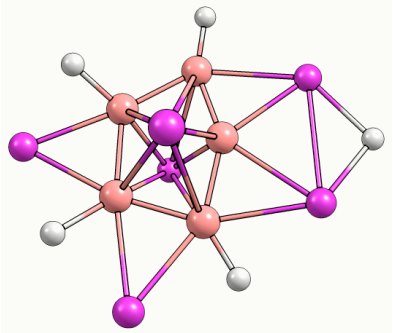
	B	-0.306406000	1.405182000	-0.034210000	
	B	-1.320063000	0.000266000	-0.056722000	
	B	-0.307893000	-1.404900000	-0.025782000	
	Li	-2.254628000	1.809340000	0.102030000	
	Li	3.079081000	-0.001130000	0.047523000	
	Li	-2.257753000	-1.807842000	0.082699000	
	Li	0.155150000	-0.005976000	-1.665002000	
	Li	0.047027000	0.005938000	1.634750000	
	H	-0.694526000	-2.598739000	-0.044987000	
	H	2.295462000	-1.607034000	0.058496000	
	H	2.297285000	1.605410000	0.046370000	
	H	-0.693448000	2.598514000	-0.067807000	
	H	-2.609398000	0.001658000	-0.151453000	
	B	1.078446000	-1.315013000	-0.168646000	PBE0/cc-pvTZ 10.41 CCSD(T) 10.98
	B	1.318948000	0.275600000	-0.681589000	
	B	-0.324868000	0.704238000	-0.210182000	
	B	0.814958000	0.012833000	0.935755000	
	B	-0.481138000	-0.956697000	0.420457000	
	Li	-0.241511000	-0.721881000	-1.824830000	
	Li	-2.513866000	-1.117459000	-0.241850000	
	Li	1.184706000	2.132390000	0.151551000	
	Li	-2.172496000	1.452622000	-1.096321000	
	Li	-1.275116000	0.555555000	1.752932000	
	H	1.769469000	-2.298086000	-0.095356000	
	H	2.242852000	1.013641000	-1.023385000	
	H	-0.803515000	1.800592000	0.187165000	
	H	-1.329503000	-1.430717000	1.189109000	
	H	1.143818000	0.406083000	2.039053000	

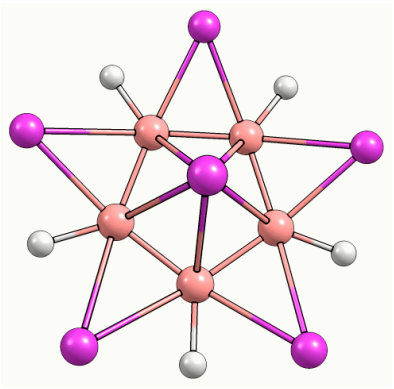
$Li_6(BH)_5^-$: Structure, Cartesian coordinates and relative energies of the triplet state minimum conformation

System	Structure				Relative energy
	B	-0.000072000	1.229981000	0.439381000	PBE0/cc-pvTZ
	B	-0.000193000	-0.000193000	-0.798614000	-4.60
	B	-1.196275000	-0.000103000	0.475333000	
	B	0.000282000	-1.229795000	0.440016000	CCSD(T)
	B	1.196528000	0.000274000	0.474665000	1.75
	Li	-1.758114000	-1.521542000	-0.884386000	
	Li	0.000626000	0.000583000	2.241443000	
	Li	-1.758663000	1.520792000	-0.884620000	
	Li	1.758079000	-1.521402000	-0.884768000	
	Li	1.757750000	1.521453000	-0.885484000	
	H	-0.000329000	2.429440000	0.165593000	
	H	-0.000651000	-0.000603000	-2.009822000	
	H	2.399984000	0.000371000	0.207898000	
	H	-2.399862000	-0.000316000	0.209136000	
	H	0.000476000	-2.429371000	0.166735000	

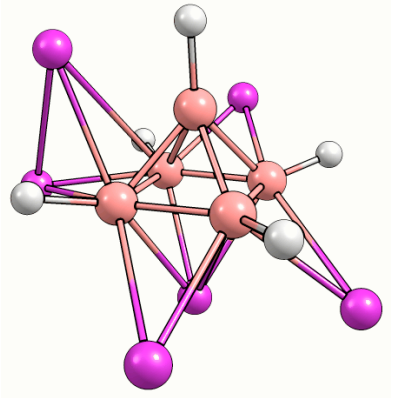
$Li_6(BH)_5$: Structure, Cartesian coordinates and relative energies of the singlet state minima conformations.

System	Structure				Relative energy
	B	0.000065000	1.269288000	0.123501000	PBE0/cc-pvTZ
	B	-1.373121000	0.255229000	0.064621000	0.00
	B	-0.830494000	-1.349997000	-0.038550000	
	B	1.373120000	0.255004000	0.065161000	CCSD(T)
	B	0.830306000	-1.350134000	-0.038220000	0.00
	Li	-1.753065000	2.267163000	-0.170689000	
	Li	0.000382000	-0.042589000	-1.641865000	
	Li	-2.832070000	-1.188131000	-0.060811000	
	Li	1.753566000	2.266888000	-0.169358000	
	Li	2.831874000	-1.188373000	-0.062273000	
	Li	-0.000418000	-0.279998000	1.704186000	
	H	2.581034000	0.661063000	0.124538000	
	H	1.536077000	-2.372960000	-0.130747000	
	H	0.000105000	2.521288000	0.334202000	
	H	-2.581004000	0.661508000	0.123129000	
	H	-1.536395000	-2.372724000	-0.131255000	

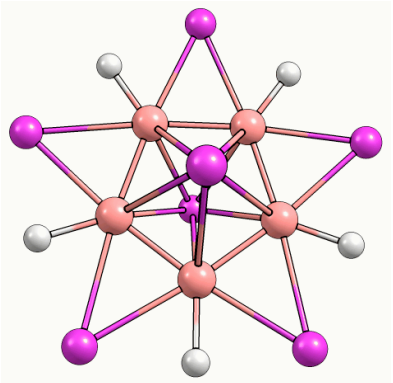
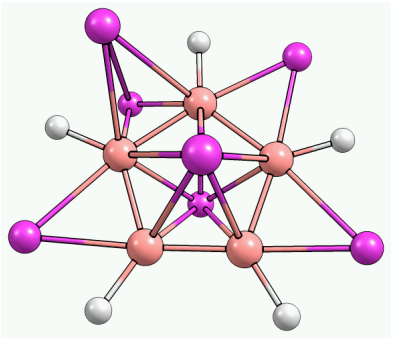
System	Structure				Relative energy
	B	-1.614391000	0.000001000	-0.000250000	PBE0/cc-pvTZ 16.29 CCSD(T) 17.44
	B	-0.449753000	-1.209210000	-0.000284000	
	B	0.827471000	-0.000001000	-0.000267000	
	B	-0.449752000	1.209213000	-0.000204000	
	B	2.437956000	0.000001000	0.000135000	
	Li	-2.310229000	1.945343000	0.001827000	
	Li	-2.310221000	-1.945351000	-0.000330000	
	Li	-0.264478000	-0.000135000	-1.825837000	
	Li	1.530722000	-1.916288000	0.001619000	
	Li	1.530719000	1.916289000	-0.000925000	
	Li	-0.264454000	0.000128000	1.825363000	
	H	-2.879789000	0.000006000	-0.000152000	
	H	-0.469424000	-2.461800000	-0.000683000	
	H	-0.469419000	2.461805000	-0.000590000	
	H	3.162400000	0.997026000	0.000260000	
	H	3.162406000	-0.997020000	0.000370000	
	B	0.440458000	-1.409436000	0.000170000	PBE0/cc-pvTZ 17.05 CCSD(T) 17.82
	B	1.438140000	0.000000000	-0.000142000	
	B	0.440457000	1.409436000	-0.000324000	
	B	-1.131607000	-0.869974000	0.000101000	
	B	-1.131607000	0.869973000	-0.000048000	
	Li	2.408033000	-1.821853000	-0.000248000	
	Li	0.115232000	-0.000373000	-1.652436000	
	Li	0.115478000	0.000373000	1.652340000	
	Li	2.408032000	1.821854000	0.000587000	
	Li	-2.549360000	0.000290000	-1.310961000	
	Li	-2.549151000	-0.000290000	1.311236000	
	H	-2.236239000	-1.521956000	0.000590000	
	H	-2.236240000	1.521954000	-0.000347000	
	H	0.816796000	-2.594037000	0.000440000	
	H	2.714884000	0.000000000	-0.000353000	
	H	0.816795000	2.594037000	-0.000666000	
	B	1.388684000	0.300761000	-0.032668000	PBE0/cc-pvTZ 20.37 CCSD(T) 20.16
	B	0.695606000	-1.251789000	0.042703000	
	B	-0.970715000	-1.524779000	-0.073014000	
	B	-0.860017000	0.001878000	0.054121000	
	B	0.073186000	1.337097000	-0.045217000	
	Li	1.870318000	2.293734000	-0.061838000	
	Li	2.702022000	-1.279806000	-0.091454000	
	Li	0.200472000	0.029365000	1.851719000	
	Li	-2.041668000	1.844591000	0.113396000	
	Li	-2.980774000	-0.549573000	-0.036430000	
	Li	0.188657000	-0.229938000	-1.796100000	
	H	2.616666000	0.557167000	0.179319000	
	H	1.256434000	-2.248510000	0.507278000	
	H	-0.146184000	2.519487000	-0.315744000	
	H	-3.601700000	1.084043000	-0.059234000	
	H	-1.576021000	-2.553145000	0.020879000	

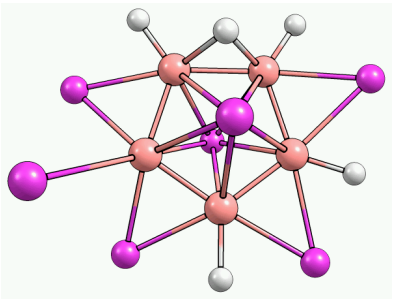
System	Structure				Relative energy
	B	-0.264699000	0.440664000	1.356335000	PBE0/cc-pvTZ
	B	-0.266278000	-1.153569000	-0.837941000	26.08
	B	-0.266278000	-1.153569000	0.837941000	
	B	-0.264699000	0.440664000	-1.356335000	CCSD(T)
	B	-0.263866000	1.426183000	0.000000000	25.03
	Li	0.254520000	2.387013000	-1.735466000	
	Li	0.254520000	2.387013000	1.735466000	
	Li	0.263296000	-0.912583000	2.803525000	
	Li	1.487944000	0.001249000	0.000000000	
	Li	0.263296000	-0.912583000	-2.803525000	
	Li	0.255473000	-2.950258000	0.000000000	
	H	-0.344959000	-2.178997000	1.582887000	
	H	-0.340317000	0.831245000	2.562399000	
	H	-0.337494000	2.694088000	0.000000000	
	H	-0.340317000	0.831245000	-2.562399000	
	H	-0.344959000	-2.178997000	-1.582887000	

$Li_6(BH)_5$: Structure, Cartesian coordinates and relative energies of the triplet state minimum conformations

System	Structure				Relative energy
	B	0.836573000	0.448020000	0.712532000	PBE0/cc-pvTZ
	B	0.313868000	-1.050154000	0.037795000	15.34
	B	0.435657000	0.361575000	-0.982660000	
	B	-1.078177000	-0.272431000	-0.583393000	CCSD(T)
	B	-0.604824000	1.210181000	0.106178000	20.72
	Li	2.161435000	-1.228461000	1.278641000	
	Li	2.215611000	-0.838737000	-1.317672000	
	Li	1.065468000	2.419258000	0.136135000	
	Li	-1.779050000	-2.192387000	0.072627000	
	Li	-0.913488000	-0.260804000	1.724101000	
	Li	-2.914669000	0.565558000	0.130805000	
	H	-0.883543000	2.395011000	-0.061589000	
	H	1.917288000	0.894037000	1.098839000	
	H	0.908548000	-2.100828000	-0.199350000	
	H	-1.983039000	-0.630867000	-1.337011000	
	H	1.019335000	0.563415000	-2.027059000	

$Li_7(BH)_5^+$: Structure, Cartesian coordinates and relative energies of the singlet state minima conformations

System	Structure			Relative energy
	B -1.244878000 -0.707620000 -0.058828000 B 0.287610000 -1.404344000 0.014251000 B 1.422350000 -0.160129000 0.067497000 B -1.056983000 0.967092000 -0.051555000 B 0.591864000 1.305251000 0.027141000 Li -3.038173000 0.344057000 -0.105408000 Li -0.081465000 0.000341000 1.706718000 Li -1.267860000 -2.784682000 -0.012202000 Li 2.660404000 1.508168000 0.101790000 Li 0.083418000 -0.001120000 -1.706396000 Li 2.255758000 -2.065620000 0.087165000 Li -0.609956000 2.997878000 -0.055424000 H 1.113176000 2.453010000 0.060289000 H 2.673141000 -0.301976000 0.137179000 H 0.539710000 -2.639729000 0.021993000 H -2.339759000 -1.329519000 -0.124602000 H -1.985957000 1.817942000 -0.102008000			PBE0/cc-pvTZ 0.00 CCSD(T) 0.00
	B 1.149403000 -1.216470000 -0.018537000 B 1.390929000 0.447629000 0.028250000 B -0.479467000 -1.550104000 -0.041552000 B -1.324004000 -0.076054000 -0.007839000 B -0.153196000 1.196937000 0.035013000 Li -2.504413000 -1.832827000 -0.071879000 Li 3.130416000 -0.744480000 0.012224000 Li -1.784135000 1.529763000 -1.408628000 Li 0.184141000 -0.345013000 1.687631000 Li -1.806446000 1.459490000 1.463217000 Li 0.214069000 -0.253068000 -1.691404000 Li 1.436564000 2.538242000 0.086363000 H -0.459521000 2.433283000 0.067574000 H 2.493212000 1.060328000 0.053134000 H 2.004359000 -2.105843000 -0.035376000 H -0.956695000 -2.687438000 -0.077086000 H -2.584015000 0.166126000 -0.010906000			PBE0/cc-pvTZ 25.36 CCSD(T) 25.98

System	Structure			Relative energy
	B	0.046847000	1.257052000	0.007745000	PBE0/cc-pvTZ 39.86 CCSD(T) 40.18
	B	-1.433858000	0.459338000	0.039830000	
	B	-1.158072000	-1.214049000	-0.063297000	
	B	0.560719000	-1.437308000	-0.089522000	
	B	1.289686000	0.102610000	-0.026480000	
	Li	1.934138000	1.910642000	-0.816547000	
	Li	-0.167730000	-0.154306000	-1.676574000	
	Li	-1.599670000	2.528889000	-0.106284000	
	Li	-0.125579000	-0.126855000	1.704139000	
	Li	-3.156613000	-0.780064000	0.231849000	
	Li	2.542484000	-1.430546000	-0.776074000	
	Li	2.909700000	0.391780000	1.430540000	
	H	-0.341860000	-1.734353000	0.889838000	
	H	-2.584636000	0.983271000	0.062265000	
	H	-1.978387000	-2.124641000	-0.170808000	
	H	0.235656000	2.505963000	0.026030000	
	H	1.114375000	-2.524422000	-0.234249000	

$Li_7(BH)_5^+$: Structure, Cartesian coordinates and relative energies of the triplet state minimum conformation.

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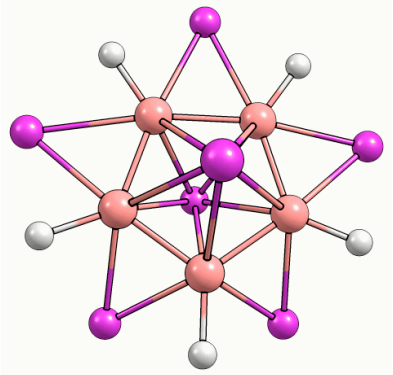	B	-1.349312000	-0.508839000	0.289402000	PBE0/cc-pvTZ 39.68 CCSD(T) 40.27
	B	0.093935000	-1.367708000	0.439495000	
	B	1.404702000	-0.316830000	0.299028000	
	B	-0.949108000	1.070596000	0.056794000	
	B	0.790544000	1.191789000	0.062692000	
	Li	-0.206195000	2.984204000	-0.539002000	
	Li	-0.024885000	0.255732000	1.986632000	
	Li	-2.995262000	0.616682000	-0.281582000	
	Li	2.882022000	1.025729000	-0.264720000	
	Li	1.737796000	-2.273042000	-0.686914000	
	Li	0.019831000	-0.211306000	-1.602962000	
	Li	-1.399910000	-2.492667000	-0.697971000	
	H	-1.742752000	2.037931000	-0.085861000	
	H	1.443353000	2.259733000	-0.076224000	
	H	2.599556000	-0.673573000	0.332628000	
	H	0.180698000	-2.612361000	0.441634000	
	H	-2.483113000	-1.028271000	0.315431000	