Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Material

Theoretical study of the $Si_{5-n}(BH)_n^{2-}$ and $Na(Si_{5-n}(BH)_n)^-$ (n = 0–5) systems

Edison Osorio,[1,2*] Alina P. Sergeeva,[3] Juan Carlos Santos[1] and William Tiznado[1*]

[1] *Universidad Andres Bello, Facultad Ciencias Exactas, Departamento de Química, Av. República 275, Santiago, Chile*

[2] *Centro de Bioinformática y Simulación Molecular, Universidad de Talca, 2 Norte 685, Talca, Chile*

[3] *Utah State University, Department of Chemistry and Biochemistry, Logan, UT, 84322, USA*

Corresponding authors e-mails:

Edison Osorio : ed.osorio@uandresbello.edu

William Tiznado: wtiznado@unab.cl

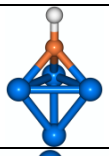
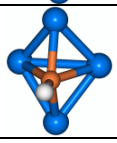
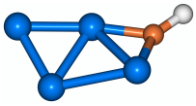
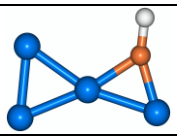
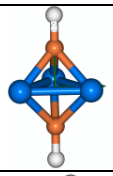
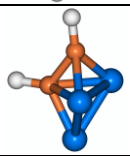
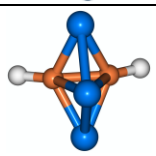
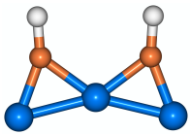
Symmetry	Structure	Cartesians Coordinates			Energy (a.u)	ΔE
B-1 C_{3v}		Si	0.000000000	1.479773000	-0.270422000	-1181.5244144	0.0
		Si	-1.281521000	-0.739887000	-0.270422000		
		Si	1.281521000	-0.739887000	-0.270422000		
		Si	0.000000000	0.000000000	1.611258000		
		B	0.000000000	0.000000000	-1.665649000		
		H	0.000000000	0.000000000	-2.871645000		
B-2 C_{2v}		B	0.000000000	0.000000000	1.176423000	-1181.5179364	4.1
		Si	0.000000000	1.327740000	-0.525906000		
		Si	0.000000000	-1.327740000	-0.525906000		
		Si	-1.814611000	0.000000000	0.230711000		
		Si	1.814611000	0.000000000	0.230711000		
		H	0.000000000	0.000000000	2.383342000		
B-3 C_1		Si	-0.729377000	1.307702000	0.270880000	-1181.4630624	38.5
		Si	0.075948000	-0.968468000	0.071151000		
		Si	1.896533000	0.671002000	-0.282579000		
		Si	-2.144246000	-0.452258000	-0.200340000		
		B	1.978918000	-1.144592000	0.320168000		
		H	2.721401000	-2.088734000	0.371587000		
B-4 C_s		Si	-1.417025000	-1.600198000	0.000000000	-1181.4635495	38.2
		Si	0.000000000	0.271845000	0.000000000		
		Si	-0.109978000	2.611361000	0.000000000		
		Si	0.804051000	-1.970387000	0.000000000		
		B	1.489458000	1.632746000	0.000000000		
		H	2.674040000	1.459574000	0.000000000		

Figure S1-A. Lowest energy isomers for Si_4BH^{2-} and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

Symmetry	Structure	Cartesians Coordinates			Energy (a.u)	ΔE
C-1 D_{3h}		Si	0.000000000	1.464171000	0.000000000	-917.8274267	0.0
		Si	-1.268009000	-0.732086000	0.000000000		
		Si	1.268009000	-0.732086000	0.000000000		
		B	0.000000000	0.000000000	1.417306000		
		B	0.000000000	0.000000000	-1.417306000		
		H	0.000000000	0.000000000	2.619511000		
		H	0.000000000	0.000000000	-2.619511000		
C-2 C_s		Si	-0.300393000	-0.496011000	1.319431000	-917.8268690	0.3
		Si	-0.300393000	-0.496011000	-1.319431000		
		B	-0.300393000	1.222362000	0.000000000		
		Si	1.524217000	0.269868000	0.000000000		
		B	-1.650246000	0.237579000	0.000000000		
		H	-0.325933000	2.433129000	0.000000000		
		H	-2.848896000	0.377315000	0.000000000		
C-3 C_{2v}		B	0.227341000	-1.142260000	0.000000000	-917.8172406	6.4
		B	1.109507000	0.354119000	0.000000000		
		Si	-1.103860000	0.651078000	0.000000000		
		Si	0.227341000	-0.134177000	1.774818000		
		Si	0.227341000	-0.134177000	-1.774818000		
		H	0.235688000	-2.347898000	0.000000000		
		H	2.168557000	0.930471000	0.000000000		
C-4 C_{2v}		Si	0.000000000	2.274843000	0.581609000	-917.7661592	38.4
		Si	0.000000000	0.000000000	0.020660000		
		Si	0.000000000	-2.274843000	0.581609000		
		B	0.000000000	1.628232000	-1.181773000		
		B	0.000000000	-1.628232000	-1.181773000		
		H	0.000000000	-1.712628000	-2.378281000		
		H	0.000000000	1.712628000	-2.378281000		

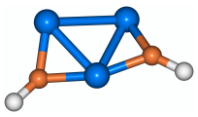
C-5 C_2		Si -1.357085000 -0.946072000 -0.236636000 Si -0.000011000 1.105400000 -0.000010000 Si 1.357100000 -0.946062000 0.236636000 B -1.874963000 0.795731000 0.361404000 B 1.874955000 0.795749000 -0.361387000 H 2.829382000 1.528440000 -0.391543000 H -2.829387000 1.528423000 0.391597000	-917.7609799	41.7

Figure S1-B. Lowest energy isomers for $Si_3B_2H_2^{2-}$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

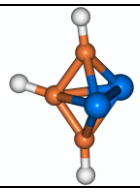
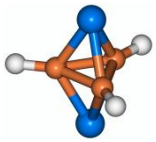
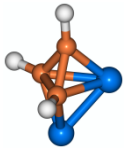
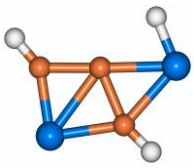
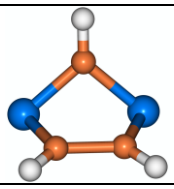
Symmetry	Structure	Cartesians Coordinates	Energy (a.u)	ΔE
D-1 C_s		Si -0.008403000 -0.471933000 1.352608000 Si -0.008403000 -0.471933000 -1.352608000 B -0.008403000 1.334484000 0.000000000 B 1.417680000 0.243574000 0.000000000 B -1.428884000 0.409510000 0.000000000 H 0.363257000 2.512817000 0.000000000 H 2.591431000 0.343315000 0.000000000 H -2.621382000 0.420159000 0.000000000	-653.5495133	0.0
D-2 D_{3h}		B 1.043222142 0.000000000 0.000000000 B -0.521611071 0.903456877 0.000000000 B -0.521611071 -0.903456877 0.000000000 Si 0.000000000 0.000000000 1.737891000 Si 0.000000000 0.000000000 -1.737891000 H -1.124913153 -1.948406735 0.000000000 H 2.249826306 0.000000000 0.000000000 H -1.124913153 1.948406735 0.000000000	-653.5452428	2.7
D-3 C_s		Si -0.342933000 1.234130000 0.000000000 B -0.342933000 -0.809642000 0.884649000 B -0.342933000 -0.809642000 -0.884649000 Si 1.438021000 -0.314407000 0.000000000 B -1.657769000 -0.292160000 0.000000000 H -0.377222000 -1.449768000 -1.911685000 H -0.377222000 -1.449768000 1.911685000 H -2.858607000 -0.419357000 0.000000000	-653.5424039	4.5
D-4 C_s		B 0.425911000 -0.974168000 0.000000000 B 0.000000000 0.780549000 0.000000000 B -1.772016000 1.078698000 0.000000000 H 1.092429000 -1.877469000 0.000000000 H 1.882074000 1.970623000 0.000000000 H -2.371598000 2.042739000 0.000000000 Si -1.794308000 -0.934437000 0.000000000 Si 2.231995000 0.465773000 0.000000000	-653.4894619	37.7
D-5 C_s		Si 0.442078983 -0.296910509 1.588905000 Si 0.442078983 -0.296910509 -1.588905000 B 1.055439367 0.946725267 0.000000000 B -1.507900751 0.174381922 0.903924000 B -1.507900751 0.174381922 -0.903924000 H -2.409908428 0.222693756 1.659840000 H -2.409908428 0.222693756 -1.659840000 H 1.690512616 1.887207783 0.000000000	-653.4836078	41.9

Figure S1-C. Lowest energy isomers for $Si_2B_3H_3^{2-}$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

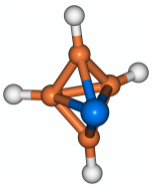
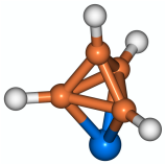
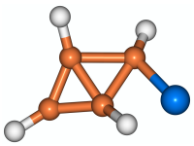
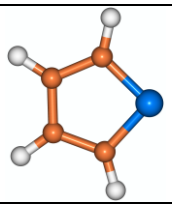
Symmetry	Structure	Cartesians Coordinates			Energy (a.u)	ΔE
E-1 C_{2v}		Si	0.000000000	0.000000000	1.157387000	-390.4411700	0.0
		B	0.000000000	0.888151000	-0.862264000		
		B	0.000000000	-0.888151000	-0.862264000		
		B	-1.333043000	0.000000000	-0.357104000		
		B	1.333043000	0.000000000	-0.357104000		
		H	0.000000000	-1.914633000	-1.515955000		
		H	0.000000000	1.914633000	-1.515955000		
		H	-2.532903000	0.000000000	-0.488916000		
		H	2.532903000	0.000000000	-0.488916000		
E-2 C_{3v}		B	0.000000000	1.053690000	-0.401612000	-390.4326579	5.3
		B	0.912522000	-0.526845000	-0.401612000		
		B	-0.912522000	-0.526845000	-0.401612000		
		B	0.000000000	0.000000000	-1.687328000		
		Si	0.000000000	0.000000000	1.339165000		
		H	-1.960611000	-1.131959000	-0.463771000		
		H	0.000000000	2.263918000	-0.463771000		
		H	1.960611000	-1.131959000	-0.463771000		
		H	0.000000000	0.000000000	-2.896176000		
E-3 C_1		B	0.000000000	1.459969000	-1.194177000	-390.3768755	40.3
		B	0.000000000	-1.459969000	-1.194177000		
		B	0.000000000	0.000000000	0.030288000		
		H	0.000000000	1.289630000	-2.294293000		
		H	0.000000000	-1.289630000	-2.294293000		
		H	0.000000000	0.000000000	1.137076000		
		Si	0.000000000	-2.307817000	0.544351000		
		Si	0.000000000	2.307817000	0.544351000		
E-4 C_{2v}		B	0.000000000	1.465189000	0.012217000	-390.3438059	61.1
		B	0.000000000	-1.465189000	0.012217000		
		B	0.000000000	-0.841885000	-1.552248000		
		H	0.000000000	2.663140000	0.311996000		
		H	0.000000000	-2.663140000	0.311996000		
		H	0.000000000	-1.546606000	-2.576684000		
		B	0.000000000	0.841885000	-1.552248000		
		Si	0.000000000	0.000000000	1.423549000		
		H	0.000000000	1.546606000	-2.576684000		

Figure S1-D. Lowest energy isomers for $SiB_4H_4^{2-}$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

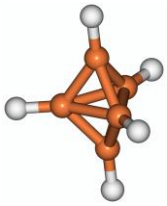
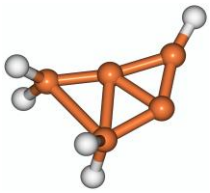
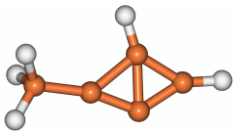
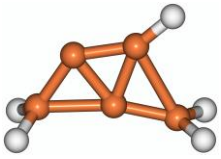
Symmetry	Structure	Cartesians Coordinates				Energy (a.u)	ΔE
F-1 D_{3h}		B	0.002470000	-0.047889000	1.088525000	-126.7456054	0.0
		B	-1.302112000	-0.011472000	0.038020000		
		B	-0.002114000	0.919678000	-0.456858000		
		B	-0.000390000	-0.902859000	-0.521926000		
		B	1.302088000	-0.009265000	0.034541000		
		H	0.001500000	-0.091957000	2.304810000		
		H	-0.002088000	1.994898000	-1.026978000		
		H	-2.510764000	-0.013402000	0.042194000		
		H	2.510742000	-0.008377000	0.030511000		
		H	0.000569000	-1.934054000	-1.168339000		
F-2 C_s		B	-0.890160596	0.876648749	0.000000000	-126.7279262	11.1
		B	0.762634209	1.125657333	0.000000000		
		B	1.486949592	-0.993464307	0.000000000		
		B	-1.702576281	-0.408646804	0.000000000		
		B	-0.048206558	-0.542714462	0.000000000		
		H	2.118679686	-1.232685440	1.017003502		
		H	1.319170621	1.520835973	-1.019074504		
		H	-2.600554119	-1.204208427	0.000000000		
		H	1.319170621	1.520835973	1.019074504		
		H	2.118679686	-1.232685440	-1.017003502		
F-2 C_1		B	-0.818265000	0.803947000	-0.002757000	-126.7251891	12.8
		B	0.622660000	-0.271553000	-0.019531000		
		B	-2.177805000	-0.086244000	0.005212000		
		B	2.310949000	-0.000290000	-0.003564000		
		B	-0.821167000	-0.876082000	-0.003389000		
		H	2.662884000	0.958097000	-0.715764000		
		H	-0.503507000	1.963230000	-0.004461000		
		H	2.646217000	0.289377000	1.162842000		
		H	2.992816000	-0.989857000	-0.334198000		
		H	-3.380272000	-0.069739000	0.011724000		
F-2 C_s		B	0.576570948	-1.138700177	0.000000000	-126.7228686	14.3
		B	0.157970112	0.437846012	0.000000000		
		B	-1.713335512	0.659677783	0.000000000		
		B	-0.941186257	-0.766615811	0.000000000		
		B	1.743726238	0.632666296	0.000000000		
		H	2.422493330	0.762124471	-1.014673500		
		H	-2.167107914	1.191265034	-1.013567501		
		H	-2.167107914	1.191265034	1.013567501		
		H	1.414603227	-1.993733299	0.000000000		
		H	2.422493330	0.762124471	1.014673500		

Figure S1-D. Lowest energy isomers for $B_5H_4^{2-}$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

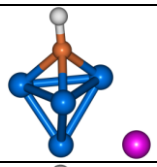
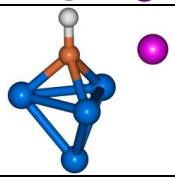
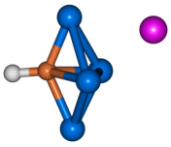
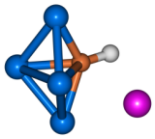
Symmetry	Structure	Cartesians Coordinates	Energy (a.u)	ΔE
2-1 C_s		Na 2.537445928 0.612101578 0.000000000 Si -0.088334815 0.658006838 1.424400670 Si -1.802494878 -0.893843921 0.000000000 Si 0.557840661 -1.485923402 0.000000000 Si -0.088334815 0.658006838 -1.424400670 B -1.476350994 1.232879630 0.000000000 H -2.299497245 2.098890592 0.000000000	-1343.5095472	0.0
2-2 C_s		Na 2.604196711 -0.877774684 0.000000000 Si 0.165151289 -0.288163245 -1.433251943 Si -1.069249971 1.638362396 0.000000000 Si 0.165151289 -0.288163245 1.433251943 Si -1.825485031 -0.857543438 0.000000000 B 0.904806161 1.145710990 0.000000000 H 1.898834946 1.830978096 0.000000000	-1343.5054567	2.6
2-3 C_s		Na 2.326455427 -1.033223439 0.000000000 Si 0.998908506 1.573139520 0.000000000 Si -2.117331657 -0.699515989 0.000000000 Si -0.172902803 -0.276616546 -1.474913866 Si -0.172902803 -0.276616546 1.474913866 B -0.977720098 1.153436986 0.000000000 H -1.742461114 2.075274980 0.000000000	-1343.5009272	5.4
2-4 C_1		Na -2.497400000 -0.799400000 -0.460100000 Si -0.149600000 -0.610200000 1.316900000 Si 1.524500000 -1.379300000 -0.361800000 Si 1.524800000 1.168000000 -0.138700000 Si -0.885200000 1.534200000 0.038900000 B -0.038900000 -0.143200000 -0.975600000 H -0.536300000 -0.467900000 -2.035600000	-1343.4995363	6.3

Figure S2-A. Lowest energy isomers for $NaSi_4BH^-$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

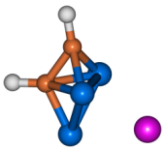
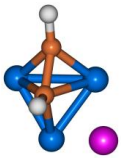
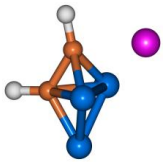
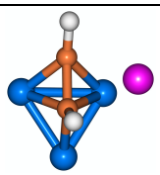
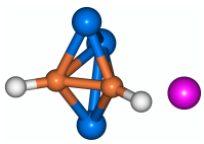
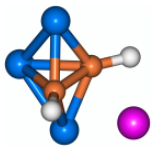
Symmetry	Structure	Cartesians Coordinates	Energy (a.u)	ΔE
3-1 C_s		Si -0.151256000 1.517677000 0.000000000 Si -0.151256000 -0.519957000 1.357917000 B -1.635055000 0.148009000 0.000000000 H -1.867713000 -2.524382000 0.000000000 B -1.254730000 -1.501259000 0.000000000 Na 2.309440000 0.180041000 0.000000000 Si -0.151256000 -0.519957000 -1.357917000 H -2.734454000 0.621489000 0.000000000	-1079.8158840	0.0
3-2 C_1		Na 2.456378000 0.143185000 0.374702000 Si -1.814627000 -0.410839000 0.211859000 Si 0.231645000 -1.393242000 -0.287154000 Si 0.059216000 0.917897000 -1.032448000 B 0.018694000 0.205032000 1.063361000 B -1.000174000 1.429782000 0.592779000 H 0.682820000 0.218913000 2.075573000 H -1.462865000 2.438552000 1.030396000	-1079.8148343	0.7
3-3 C_s		Na -2.421780000 0.585944000 0.000000000 Si 1.333933000 -1.407276000 0.000000000 Si -0.034107000 -0.055150000 1.361471000 H 2.470318000 1.221061000 0.000000000 Si -0.034107000 -0.055150000 -1.361471000 B 1.401794000 0.681825000 0.000000000 B -0.034107000 1.504165000 0.000000000 H -0.389225000 2.649650000 0.000000000	-1079.8125304	2.1
3-4 C_1		Na -2.550753000 -0.185406000 -0.365073000 Si 1.460555000 1.074272000 -0.122375000 B -0.179257000 0.063491000 -0.981538000 B -0.511553000 1.378187000 0.007638000 H -1.239517000 2.333862000 0.023364000 H -0.750069000 -0.232908000 -2.009033000 Si 1.207131000 -1.301331000 -0.319220000 Si -0.274692000 -0.292218000 1.218093000	-1079.8110433	3.0
3-5 C_1		Na 1.875887000 -1.389941000 -0.212889000 Si -0.219995000 -0.142130000 1.240612000 Si 1.105480000 1.343644000 -0.110229000 Si -1.918169000 -0.610149000 -0.290530000 B -0.095613000 -0.097938000 -1.042328000 B -0.899581000 1.198212000 -0.349951000 H -1.525792000 2.207194000 -0.455204000 H 0.324585000 -0.698318000 -1.999559000	-1079.8042932	7.3
3-6 C_s		Si -1.712937000 0.338502000 0.000000000 Si 0.195107000 1.651681000 0.000000000 B 0.195107000 -0.225193000 0.882563000 B 0.195107000 -0.225193000 -0.882563000 H 0.837077000 -0.409819000 1.886817000 H 0.837077000 -0.409819000 -1.886817000 Na 2.517128000 0.047649000 0.000000000 Si -0.718858000 -1.808224000 0.000000000	-1079.8022314	8.6

Figure S2-B. Lowest energy isomers for $NaSi_3B_2H_2^-$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

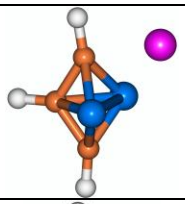
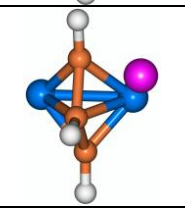
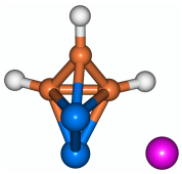
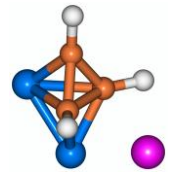
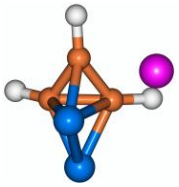
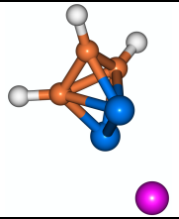
Symmetry	Structure	Cartesians Coordinates			Energy (a.u)	ΔE
4-1 C_s		B	-1.393508000	-1.003310000	0.000000000	-816.1282414	0.0
		H	-2.169273000	-1.918811000	0.000000000		
		B	0.256306000	-1.235194000	0.000000000		
		H	1.017772000	-2.160714000	0.000000000		
		Si	-0.311214000	0.230129000	-1.341594000		
		B	-1.746530000	0.652181000	0.000000000		
		H	-2.705264000	1.357747000	0.000000000		
		Si	-0.311214000	0.230129000	1.341594000		
		Na	2.240031000	0.240132000	0.000000000		
4-2 C_1		Si	1.723962000	-0.650429000	-0.161247000	-816.1267033	1.0
		B	-0.044344000	-0.381159000	0.979473000		
		B	1.036800000	0.900271000	0.978656000		
		H	1.545312000	1.640491000	1.760927000		
		H	-0.659573000	-0.727664000	1.967101000		
		Si	-0.110141000	1.095695000	-0.652693000		
		Na	-2.426245000	-0.269883000	0.184203000		
		B	-0.186978000	-0.989475000	-0.593594000		
		H	-0.817928000	-1.826024000	-1.181770000		
4-3 C_1		Na	2.125435000	-0.604445000	0.216341000	-816.1238335	2.8
		Si	0.286785000	1.413431000	-0.192473000		
		Si	-0.507173000	-0.712368000	-1.024630000		
		B	-1.517042000	-1.007254000	0.664148000		
		B	-0.195413000	-0.133441000	1.154073000		
		B	-1.499653000	0.656764000	0.381039000		
		H	0.474271000	-0.347770000	2.135796000		
		H	-2.422416000	1.413453000	0.434867000		
		H	-2.285675000	-1.812008000	1.092727000		
4-4 C_s		B	1.817082000	-0.200917000	0.000000000	-816.1222985	3.7
		H	3.006946000	-0.116688000	0.000000000		
		Si	-1.303752000	-0.315399000	0.000000000		
		Si	0.501746000	-1.752614000	0.000000000		
		Na	-0.630057000	2.342899000	0.000000000		
		B	0.501746000	0.245777000	0.895158000		
		H	0.524450000	0.921901000	1.895216000		
		B	0.501746000	0.245777000	-0.895158000		
		H	0.524450000	0.921901000	-1.895216000		
4-5 C_1		Na	2.295293000	-0.586476000	-0.245717000	-816.1201618	5.1
		Si	-1.689587000	-0.715495000	-0.282498000		
		Si	-0.027493000	-0.052097000	1.204659000		
		B	0.031428000	0.097398000	-1.079239000		
		B	-0.986088000	1.222522000	-0.269504000		
		B	0.672535000	1.335098000	-0.170843000		
		H	0.429399000	-0.441495000	-2.084098000		
		H	1.497419000	2.204475000	-0.189545000		
		H	-1.725307000	2.159461000	-0.335810000		
4-6 C_s		Na	0.188165000	-2.517749000	0.000000000	-816.1193149	5.6
		B	0.188165000	1.371553000	0.907900000		
		B	-1.133998000	1.857885000	0.000000000		
		H	0.537001000	1.902915000	1.922222000		
		H	-1.928914000	2.745679000	0.000000000		
		Si	1.317147000	-0.024918000	0.000000000		
		Si	-1.133330000	-0.108027000	0.000000000		
		B	0.188165000	1.371553000	-0.907900000		
		H	0.537001000	1.902915000	-1.922222000		

Figure S2-C. Lowest energy isomers for $NaSi_2B_3H_3^-$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

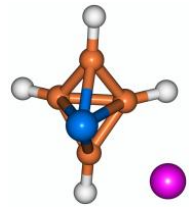
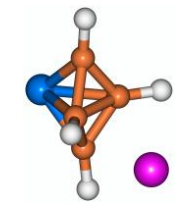
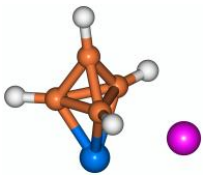
Symmetry	Structure	Cartesians Coordinates			Energy (a.u)	ΔE
5-1 C_1		Na	-2.158939000	-0.045800000	0.289303000	-552.4404155	0.0
		H	-0.266943000	-1.571359000	1.595673000		
		B	1.588106000	0.037586000	0.904804000		
		H	2.397482000	0.249957000	1.752659000		
		B	0.232702000	-0.944958000	0.689569000		
		Si	0.397713000	1.094696000	-0.277108000		
		B	-0.184631000	-0.787596000	-0.924968000		
		B	1.446249000	-0.787895000	-0.549253000		
		H	2.285510000	-1.320352000	-1.219319000		
		H	-0.890651000	-1.248077000	-1.776260000		
5-2 C_s		Na	-1.060404000	2.125360000	0.000000000	-552.4382883	1.3
		B	1.633392000	-0.226550000	0.000000000		
		H	0.333435000	0.920891000	1.895485000		
		H	2.820068000	-0.112142000	0.000000000		
		Si	0.308938000	-1.756505000	0.000000000		
		B	-1.034606000	-0.297911000	0.000000000		
		B	0.308938000	0.227291000	0.901074000		
		B	0.308938000	0.227291000	-0.901074000		
		H	-2.230940000	-0.168129000	0.000000000		
		H	0.333435000	0.920891000	-1.895485000		
5-3 C_s		B	0.242029000	-0.536411000	0.926432000	-552.433126	4.6
		H	-0.354114000	-0.791627000	1.942978000		
		Na	-2.097018000	-0.067006000	0.000000000		
		B	1.680977000	-0.064317000	0.000000000		
		B	1.056101000	-1.625962000	0.000000000		
		H	2.834964000	0.244587000	0.000000000		
		Si	0.242029000	1.331707000	0.000000000		
		B	0.242029000	-0.536411000	-0.926432000		
		H	1.446365000	-2.752655000	0.000000000		
		H	-0.354114000	-0.791627000	-1.942978000		

Figure S2-D. Lowest energy isomers for $NaSiB_4H_4^-$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

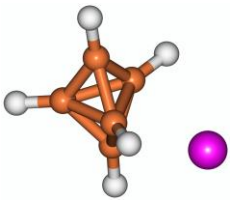
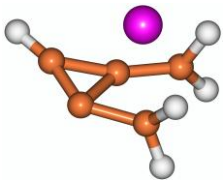
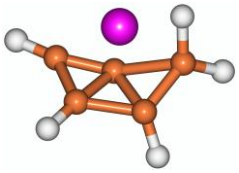
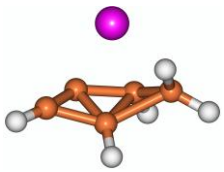
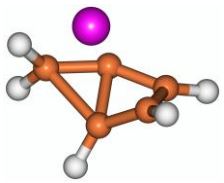
Symmetry	Structure	Cartesians Coordinates			Energy (a.u)	ΔE
6-1 C_s		B	-1.705605000	0.202307000	0.000000000	-288.7520453	0.0
		B	-0.277731000	1.096273000	0.000000000		
		B	-0.277731000	-0.306956000	0.934393000		
		B	-0.277731000	-0.306956000	-0.934393000		
		B	-1.162546000	-1.365535000	0.000000000		
		H	-1.541099000	-2.495709000	0.000000000		
		H	0.296757000	-0.611972000	-1.953072000		
		H	-2.798239000	0.694221000	0.000000000		
		H	0.296757000	-0.611972000	1.953072000		
		H	0.019142000	2.255689000	0.000000000		
		Na	2.021219000	0.379462000	0.000000000		
6-2 C_1		Na	0.483135000	1.536773000	0.035906000	-288.7414074	6.7
		B	-1.862743000	-0.078912000	-0.484757000		
		B	1.230562000	-0.872092000	-0.915676000		
		B	-0.312089000	-0.656865000	-0.575304000		
		B	-1.149163000	-0.349173000	0.828960000		
		B	0.427526000	-0.759399000	1.144754000		
		H	1.198745000	0.129870000	1.532290000		
		H	0.745375000	-1.834437000	1.589746000		
		H	1.795398000	-1.907950000	-1.144296000		
		H	-2.691815000	0.188459000	-1.293632000		
		H	1.967346000	0.101766000	-1.068953000		
6-3 C_1		Na	0.672228000	1.493007000	0.162848000	-288.7313802	13.0
		B	-0.449941000	-0.720347000	-0.647736000		
		B	0.441834000	-1.002805000	0.777473000		
		B	-1.130143000	-0.207243000	0.773767000		
		B	-1.779382000	0.036424000	-0.745496000		
		B	1.456730000	-0.788310000	-0.512338000		
		H	1.768295000	0.238667000	-1.121645000		
		H	-2.781058000	0.468827000	-1.218087000		
		H	-1.723914000	0.005601000	1.789622000		
		H	0.489302000	-2.024303000	1.421333000		
		H	2.157383000	-1.700459000	-0.890904000		
6-4 C_1		Na	-0.803697000	1.483846000	-0.045631000	-288.7277866	15.2
		B	0.933085000	0.067210000	0.867032000		
		B	-1.340753000	-0.950367000	-0.459034000		
		B	-0.464497000	-0.828104000	0.923540000		
		B	0.702321000	-0.868719000	-0.482362000		
		B	1.950706000	0.280020000	-0.218009000		
		H	1.030936000	-1.573912000	-1.386085000		
		H	-0.556087000	-1.730361000	1.725506000		
		H	-1.983442000	-1.934351000	-0.743165000		
		H	-1.445634000	-0.103927000	-1.350976000		
		H	2.890588000	0.520036000	-0.899179000		
6-5 C_1		Na	1.052364000	-1.292764000	-0.118853000	-288.7239064	17.7
		B	1.265794000	1.250655000	-0.002967000		
		B	-0.561831000	0.718631000	0.878767000		
		B	-1.488648000	0.153998000	-0.789551000		
		B	-0.021995000	0.788690000	-0.794960000		
		B	-1.299802000	-0.690793000	0.602162000		
		H	1.506376000	2.411784000	0.208931000		
		H	-2.433454000	0.340593000	-1.514682000		
		H	2.204204000	0.528887000	0.339682000		
		H	-0.662106000	1.570826000	1.723455000		
		H	-1.658605000	-1.737589000	1.082741000		

Figure S2-E. Lowest energy isomers for $NaB_5H_5^-$ and the relative energies in kcal/mol at the CCSD(T)/Def2-TZVPP//B3LYP/Def2-TZVPP level. The zero-point energy correction has been included.

Table S1. Theoretically calculated vertical detachment energies (VDEs) of the local minima of $Na(Si_{5-n}(BH)_n)^-$ (n = 0–5). All energies are given in eV.

Cluster	Final State and Electronic Configuration		VDEs (eV)		
			TD-B3LYP[a]	TD-PW91[b]	ROVGF[c]
2-2 C_S - ^{1}A'	^{2}A'	$5a'^{(2)}2a''^{(2)}6a'^{(2)}7a'^{(2)}3a''^{(2)}8a'^{(1)}$	2.36	2.46	2.40 (0.88)
	^{2}A''	$5a'^{(2)}2a''^{(2)}6a'^{(2)}7a'^{(2)}3a''^{(1)}8a'^{(2)}$	2.57	2.67	2.59 (0.88)
	^{2}A'	$5a'^{(2)}2a''^{(2)}6a'^{(2)}7a'^{(1)}3a''^{(2)}8a'^{(2)}$	2.71	2.75	2.73 (0.87)
	^{2}A'	$5a'^{(2)}2a''^{(2)}6a'^{(1)}7a'^{(2)}3a''^{(2)}8a'^{(2)}$	3.04	3.46	3.46 (0.88)
3-2 C_1 - ^{1}A	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(2)}11a^{(1)}$	2.43	2.49	2.48 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(1)}11a^{(2)}$	2.70	2.75	2.74 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(1)}10a^{(2)}11a^{(2)}$	2.96	3.04	2.84 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(1)}9a'^{(2)}10a^{(2)}11a^{(2)}$	3.12	3.05	2.97 (0.88)
3-3 C_S - ^{1}A'	^{2}A'	$5a'^{(2)}6a'^{(2)}2a''^{(2)}7a'^{(2)}3a''^{(2)}8a'^{(1)}$	2.38	2.46	2.47 (0.88)
	^{2}A''	$5a'^{(2)}6a'^{(2)}2a''^{(2)}7a'^{(2)}3a''^{(2)}8a'^{(1)}$	2.63	2.65	2.67 (0.89)
	^{2}A'	$5a'^{(2)}6a'^{(2)}2a''^{(2)}7a'^{(2)}3a''^{(2)}8a'^{(1)}$	2.96	2.99	2.81 (0.88)
	^{2}A''	$5a'^{(2)}6a'^{(2)}2a''^{(2)}7a'^{(2)}3a''^{(2)}8a'^{(1)}$	3.10	3.09	3.01 (0.88)
3-4 C_1 - ^{1}A	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(2)}11a^{(1)}$	2.35	2.39	2.37 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(1)}11a^{(2)}$	2.63	2.59	2.66 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(1)}10a^{(2)}11a^{(2)}$	2.91	2.85	2.81 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(1)}9a'^{(2)}10a^{(2)}11a^{(2)}$	3.03	3.03	3.08 (0.87)
4-2 C_1 - ^{1}A	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(2)}11a^{(1)}$	2.21	2.27	2.25 (0.89)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(1)}\ 11a^{(2)}$	2.57	2.61	2.62 (0.89)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(1)}10a^{(2)}11a^{(2)}$	2.61	2.70	2.74 (0.88)

	^{2}A	$6a^{(2)}7a^{(2)}8a^{(1)}9a'^{(2)}10a^{(2)}11a^{(2)}$	2.77	2.85	2.49 (0.88)
4-3 C_1 - ^{1}A	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(2)}11a^{(1)}$	2.41	2.50	2.46 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(2)}10a^{(1)}11a^{(2)}$	2.53	2.65	2.54 (0.89)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(2)}9a'^{(1)}10a^{(2)}11a^{(2)}$	2.93	2.96	2.89 (0.88)
	^{2}A	$6a^{(2)}7a^{(2)}8a^{(1)}9a'^{(2)}10a^{(2)}11a^{(2)}$	3.29	3.28	3.29 (0.88)
5-2 C_s- ^{1}A'	^{2}A'	$5a'^{(2)}6a'^{(2)}2a''^{(2)}3a''^{(2)}7a'^{(2)}8a'^{(1)}$	2.16	2.24	2.22 (0.89)
	^{2}A'	$5a'^{(2)}6a'^{(2)}2a''^{(2)}\ 3a''^{(2)}\ 7a'^{(1)}8a'^{(2)}$	2.20	2.38	2.33 (0.90)
	^{2}A''	$5a'^{(2)}6a'^{(2)}2a''^{(2)}3a''^{(1)}7a'^{(2)}8a'^{(2)}$	2.44	3.54	2.08 (0.89)
	^{2}A''	$5a'^{(2)}6a'^{(2)}2a''^{(1)}3a''^{(2)}7a'^{(2)}8a'^{(2)}$	3.50	4.50	3.58 (0.89)

[a] VDEs were calculated at TD-B3LYP/def2-TZVPP// B3LYP/def2-TZVPP
[b] VDEs were calculated at TD-PW91PW91/def2-TZVPP// PW91PW91/def2-TZVPP
[c] VDEs were calculated at ROVGF/def2-TZVPP// B3LYP/def2-TZVPP. Values in parentheses represent the pole strength of the OVGF calculation, which characterizes the validity of the one-electron detachment picture