Table S1. Comparison of geometrical parameters for B_2H_6, B_4H_{10}, B_5H_{11}, and $B_6H_{12}$from electron diffraction[1-3] and theoretical methods. Bond lengths in Å.

Molecule	Bond	Exp.	MP2/cc-pVDZ	B3LYP/DZVP-DFT	MP2/ccpVTZ
B_2H_6	B-B	1.770	1.784	1.776	1.740
	B-H_t	1.187	1.201	1.191	1.179
	B-H_b	1.334	1.328	1.324	1.301
B_4H_{10}	B1-B2	1.866	1.866	1.871	1.830
	B1-B3	1.737	1.740	1.730	1.712
	B1-H1,2	1.230	1.266	1.261	1.245
	B2-H1,2	1.417	1.428	1.426	1.403
	B1-H1	1.198	1.195	1.185	1.174
	B2-$H2_{endo}$	1.210	1.207	1.195	1.186
	B2-$H2_{exo}$	1.205	1.202	1.191	1.180
B_5H_{11}	B1-B2	1.904	1.901	1.910	1.872
	B1-B3	1.742	1.747	1.746	1.719
	B1-B4	1.755	1.762	1.757	1.734
	B1-B5	1.876	1.881	1.889	1.849
	B2-B3	1.749	1.771	1.791	1.736
	B3-B4	1.800	1.806	1.809	1.771
	B4-B5	1.822	1.835	1.843	1.803
	B1-$H1_{exo}$	1.192	1.196	1.185	1.175
	B1-$H1_{endo}$	1.315	1.258	1.255	1.242
	B2-H2,3	1.377	1.400	1.398	1.367
	B3-H2,3	1.278	1.293	1.289	1.275
	B3-H3,4	1.351	1.367	1.368	1.346
	B4-H3,4	1.314	1.334	1.326	1.309
	B4-H4,5	1.259	1.278	1.268	1.258
	B5-H4,5	1.396	1.415	1.416	1.384
	B2-$H1_{endo}$	1.957	1.993	2.096	1.981
	B5-$H1_{endo}$	1.553	1.474	1.441	1.442
B_6H_{12}	B1-B2	1.897	1.920	1.918	1.891
	B2-B5	1.782	1.811	1.806	1.779
	B2-B6	1.744	1.738	1.737	1.712
	B1-B6	1.748	1.758	1.744	1.723
	B5-B6	1.783	1.814	1.816	1.780
	B5-H5,6	1.305	1.301	1.302	1.282
	B6-H5,6	1.377	1.381	1.367	1.357
	B1-H16	1.371	1.373	1.371	1.342

	B6-H16	1.311	1.308	1.303	1.288
Mean absolute error (MAE)			0.015	0.02	0.023

Table S2. Computed gas phase enthalpy of formation ($\Delta_f H^0$) in kcal mol^{-1}.

Molecule	Avg. exp.	CCSD(T)' //MP2	CCSD(T) //MP2	B3LYP	B3LYP-D3// B3LYP	B3LYP-D3-0// B3LYP	BLYP// B3LYP	BLYP-D3// B3LYP	BLYP-D3-0// B3LYP	ωB97X-D3BJ// B3LYP	ωB97X-D3-0// B3LYP	ωB97X-V//B3LYP
$B_{10}H_{16}$	34.8	29.7	9.4	34.4	-10.7	14.1	65.0	9.9	41.0	-14.1	-1.9	-6.3
B_2H_6	7.9	8.0	3.9	1.8	-3.1	0.3	9.9	3.9	8.0	1.5	3.2	1.7
B_4H_{10}	13.8	13.8	5.5	9.1	-4.4	2.9	23.9	7.2	16.3	-2.4	2.3	0.0
B_5H_{11}	22.2	21.2	11.1	17.9	0.8	9.8	34.9	14.0	25.1	1.1	7.1	4.5
B_5H_9	16.0	14.5	4.6	13.8	-7.9	4.8	29.5	2.9	18.9	-6.5	-0.9	-3.0
B_6H_{10}	19.6	20.4	8.9	20.8	1.5	12.0	38.7	15.1	28.1	-4.1	3.2	0.5
B_6H_{12}	26.5	24.9	12.9	23.1	3.9	13.9	42.5	19.0	31.4	1.0	8.4	5.5
B_8H_{12}	--	21.5	--	--	--	--	--	--	--	--	--	--
B_9H_{15}	--	14.7	--	--	--	--	--	--	--	--	--	--
$B_{10}H_{14}$	5.6	-2.5	-23.5	12.0	-29.2	-8.1	41.8	-8.4	17.7	-47.5	--	-35.9
$B_{20}H_{16}$	--	-33.8	--	--	--	--	--	--	--	--	--	--
B_2Cl_4	-116.9	-117.0	-118.8	-106.0	-116.0	-109.7	-104.8	-116.8	-109.1	-128.2	-122.6	-124.7
B_2F_4	-342.2	-344.0	-346.3	-339.5	-342.5	-340.8	-347.7	-351.3	-349.1	-343.7	-344.0	-346.4
B_2O_3	-199.8	-199.5	-201.2	-200.6	-203.8	-201.3	-215.2	-219.1	-216.1	-201.1	-200.8	-201.8
$B_3N_3H_6$	-123.0	-117.6	-122.8	-129.9	-140.3	-133.5	-129.8	-142.6	-134.2	-136.2	-130.6	-137.0
BCl_3	-96.9	-97.9	-98.7	-89.7	-95.2	-90.8	-89.1	-95.7	-90.4	-104.3	-100.5	-102.2
BF_3	-270.7	-272.7	-273.9	-268.0	-269.3	-268.5	-273.6	-275.2	-274.2	-269.2	-270.2	-271.6
BHO_2	-134.0	-130.6	-130.6	-130.8	-132.4	-131.2	-139.3	-141.2	-139.7	-130.5	-131.0	-131.6
BO_3H_3	-237.2	-238.1	-239.5	-233.7	-237.0	-235.2	-239.4	-243.4	-241.2	-236.8	-237.1	-239.4

The coordinates for the optimized structures of the studied molecules :

8
B2H6, MP2/cc-pVDZ, Energy -33280.67907552641 kcal/mol Converged!
B 0.004061130 2.447633763 -0.891681719
H 0.001705437 1.458062673 -0.006546368
H 1.056158825 2.448300035 -1.469963568
H -1.048696536 2.454839941 -1.469022553
H 0.007819245 3.425052921 0.006849850
B 0.003248251 2.435488718 0.891984259
H 1.054878718 2.428277664 1.471151497
H -1.049975074 2.434834284 1.468438602

8
B2H6, B3LYP/DZVP-DFT, Energy -33403.43947071097 kcal/mol Converged!
B 0.003990208 2.447608455 -0.887983531
H 0.001940877 1.459543815 -0.006536401
H 1.047113061 2.448272675 -1.462393505
H -1.039821111 2.454763097 -1.461179320
H 0.008046271 3.423570179 0.006839866
B 0.003202348 2.435514268 0.888285914
H 1.045830260 2.428361830 1.463570285
H -1.041101918 2.434855681 1.460606693

14
B4H10, MP2/cc-pVDZ, Energy -65836.70477366938 kcal/mol Converged!
B -0.045771339 0.045243638 -0.035410995
B 0.048280613 -0.021413819 1.826809581
B 1.784996697 -0.023284754 -0.388878290
B 0.979327041 1.199808207 0.767609266
H -0.907966324 0.433816090 2.395586590
H -0.499665938 -0.815785622 0.773654795
H 0.707902620 2.343400056 0.554052620
H 2.426021342 -0.925454858 0.092790816
H 0.668739932 -0.925326234 2.331535174
H -0.905002832 0.525092427 -0.712564138
H 0.632401410 -0.819612369 -0.663740746
H 1.075954453 0.954160990 2.005586471
H 2.105874333 0.431091084 -1.454564614
H 2.204254991 0.952854166 0.565165470

14
B4H10, B3LYP/DZVP-DFT, Energy -66065.16301007479 kcal/mol Converged!
B -0.040750532 0.045533711 -0.031409399
B 0.044180158 -0.024067176 1.835943820
B 1.792871866 -0.025996591 -0.395114260
B 0.978510942 1.193448287 0.766968051
H -0.904632419 0.434261765 2.390574135
H -0.504024604 -0.804804093 0.776542274

H 0.723545864 2.333258798 0.566193437
H 2.438158547 -0.919011992 0.067608450
H 0.647204210 -0.918644715 2.349762772
H -0.899148078 0.504231667 -0.707599389
H 0.634157612 -0.808320651 -0.669149142
H 1.064299638 0.957285460 2.002953214
H 2.102068203 0.431496940 -1.450044913
H 2.198905596 0.955917590 0.554402951

16
B5H11, MP2/cc-pVDZ, Energy -81745.93017669841 kcal/mol Converged!
B -0.076102118 0.047294574 0.035657904
B -0.027340541 -0.093267828 1.930489702
B 1.427931521 -0.070927045 0.963357816
B 1.368621625 0.783296660 2.553409034
B -0.260076344 1.619780580 2.671361814
H 1.241044395 0.459119536 -0.201517574
H 1.095714773 2.022493867 2.701853584
H 2.113074589 0.999525091 1.467919279
H -0.933710559 0.746855746 1.693291813
H -0.378764493 -1.076986971 2.512459582
H -0.668932293 1.603702208 3.801371391
H -0.579860703 2.540294669 1.953981414
H -0.628313401 1.063557110 -0.300066803
H -0.238509116 -0.958502092 -0.603993228
H 2.143660906 -1.027980680 0.923571788
H 2.044718759 0.364450575 3.444548484

16
B5H11, B3LYP/DZVP-DFT, Energy -82021.32023509318 kcal/mol Converged!
B -0.061214813 0.018897560 0.011879572
B -0.035554930 -0.075674374 1.919649850
B 1.416069254 -0.059996909 0.949390663
B 1.364369334 0.777783372 2.551064326
B -0.260075779 1.638484593 2.680356531
H 1.244962461 0.462281351 -0.216940872
H 1.106387170 2.005341961 2.735598670
H 2.108031829 0.996576513 1.475040632
H -0.946511437 0.772165030 1.755906950
H -0.400181254 -1.047618367 2.492123384
H -0.669983612 1.600872417 3.797117098
H -0.557346839 2.578788943 2.000022024
H -0.656486002 0.992096665 -0.332374341
H -0.183802655 -0.988103815 -0.614044232
H 2.131544599 -1.003449940 0.918777122
H 2.042949672 0.354261001 3.424128623

14
B5H9, MP2/cc-pVDZ, Energy -81024.01661177716 kcal/mol Converged!

H -0.006483159 0.006044051 -0.063451089
B 0.001243261 -0.000805776 1.128914098
B 1.290669530 0.001312022 2.258157996
B -1.272379696 -0.017023161 2.275834689
B 0.000075164 1.273703540 2.274957252
B 0.018281336 -1.289366219 2.259030010
H 0.957931978 0.942329557 3.176499580
H -0.940444576 0.928944964 3.189479171
H -0.926760052 -0.969435258 3.177796540
H 0.971539230 -0.955967995 3.164597777
H 0.025729908 -2.476545683 2.120984891
H 2.477751592 0.010709105 2.119247374
H -0.009139298 2.462613453 2.152467579
H -2.461387220 -0.024846601 2.154178131

14
B5H9, B3LYP/DZVP-DFT, Energy -81285.89446101974 kcal/mol Converged!
H -0.006160085 0.005759021 -0.040922085
B 0.001330788 -0.000888614 1.142620125
B 1.287251565 0.001279631 2.262155897
B -1.268941283 -0.016991994 2.279736708
B 0.000107774 1.270265076 2.278867621
B 0.018247851 -1.285939478 2.263025031
H 0.972248888 0.956943616 3.166496495
H -0.955112391 0.943417169 3.179651484
H -0.941184195 -0.983952852 3.167811963
H 0.986037688 -0.970280795 3.154391466
H 0.025568132 -2.461976125 2.117998879
H 2.463163853 0.010624935 2.116260365
H -0.009026435 2.448123098 2.149441891
H -2.446904150 -0.024716688 2.151158160

16
B6H10, MP2/cc-pVDZ, Energy -96935.13607267635 kcal/mol Converged!
B -0.030006296 0.064165880 0.072080360
B -0.000595042 0.000612785 1.838897738
B 1.541453108 0.069414080 0.965085046
B 1.411592176 -1.069597397 2.302470246
B -1.045540710 -1.135282355 0.964807080
B -0.090463915 -1.769025858 2.302349711
H 1.173353751 -0.284554681 -0.320465676
H -0.537382792 -1.081323508 -0.320612272
H -0.437256235 0.938735244 -0.633343969
H 2.360026694 0.928452270 0.814986528
H -2.229814515 -1.208873481 0.814416716
H -0.420937784 0.903127855 2.502553599
H 2.216422501 -0.903219562 3.174397883
H -0.735922729 -2.277940861 3.174175124
H 2.040436284 -1.168824972 1.119746687

H -0.419074496 -2.314144437 1.119563197

16
B6H10, B3LYP/DZVP-DFT, Energy -97244.86787255722 kcal/mol Converged!
B -0.027584279 0.058972417 0.067093647
B -0.001943573 0.003514025 1.825750166
B 1.542333438 0.060334588 0.970844548
B 1.404803405 -1.069987233 2.303074740
B -1.039171013 -1.141794121 0.970575831
B -0.085783688 -1.764071571 2.302974518
H 1.172312195 -0.263275245 -0.325694088
H -0.553026464 -1.066805306 -0.325876553
H -0.433180679 0.930012766 -0.625677749
H 2.354478375 0.910872912 0.826268500
H -2.212806354 -1.215936789 0.825687390
H -0.417004540 0.894681722 2.487349343
H 2.203757369 -0.899931177 3.165279652
H -0.730265572 -2.266129814 3.165072006
H 2.056121791 -1.158935308 1.129293828
H -0.436750412 -2.319800867 1.129092220

18
B6H12-arachno, MP2/cc-pVDZ, Energy -97659.33136663596 kcal/mol Converged!
B -0.905126925 0.027146859 -0.318534873
B 0.905126935 -0.027146872 -0.318534851
B -0.118063622 -1.452744750 0.139316597
B 0.118063611 1.452744738 0.139316606
B -1.485207911 -1.043820404 1.165982036
B 1.485207920 1.043820432 1.165982033
H -1.565254879 0.128157836 -1.310853940
H 1.565254909 -0.128157858 -1.310853899
H -0.126456395 -2.402870056 -0.587245458
H 0.126456388 2.402870057 -0.587245418
H -2.393494347 -1.816015104 1.015006440
H 2.393494284 1.816015202 1.015006406
H 1.147235757 -1.021449917 0.485548453
H -1.147235782 1.021449886 0.485548431
H -0.354713859 -1.793525714 1.379436535
H 0.354713809 1.793525649 1.379436574
H 1.457196511 0.325409395 2.132344162
H -1.457196405 -0.325409378 2.132344168

18
B6H12-arachno, B3LYP/DZVP-DFT, Energy -97981.78301626982 kcal/mol Converged!
B -0.902169384 0.033949317 -0.284819440
B 0.902169381 -0.033949313 -0.284819443
B -0.132822091 -1.455983293 0.168318613
B 0.132822091 1.455983297 0.168318611
B -1.542781976 -1.092870881 1.128569472

B 1.542781978 1.092870877 1.128569469
H -1.560583297 0.168785116 -1.260695284
H 1.560583290 -0.168785115 -1.260695290
H -0.110170801 -2.384281168 -0.567110383
H 0.110170800 2.384281171 -0.567110386
H -2.411836512 -1.876822183 0.908307607
H 2.411836524 1.876822163 0.908307609
H 1.120616168 -1.036318723 0.517366141
H -1.120616166 1.036318730 0.517366144
H -0.411799722 -1.824037620 1.387126896
H 0.411799731 1.824037629 1.387126891
H 1.606988602 0.409966131 2.103936386
H -1.606988616 -0.409966134 2.103936386

24
B10H14, MP2/cc-pVDZ, Energy -160635.02955243064 kcal/mol Converged!
B -0.006884363 -0.027081873 0.033598342
B -0.006333898 -0.027332558 1.825862558
B 1.551818844 -0.029157897 0.929266345
B -1.374901377 0.718776594 0.930239006
B 2.256463095 1.565717190 0.929219011
B -1.227945345 2.456208771 0.930491484
B 1.292811665 1.044588208 -0.501812295
B 1.293648316 1.044299449 2.360719006
B -0.633297479 1.536934482 -0.501113939
B -0.632513723 1.536454520 2.361452400
H 1.603410686 2.248805756 -0.031963788
H 1.603901699 2.248619770 1.890853833
H -0.327709788 2.742383005 -0.031077624
H -0.327267967 2.742098019 1.891741182
H 3.397351838 1.924498783 0.928937639
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H 1.832455406 0.962097015 -1.567560340
H 1.833966640 0.961685694 3.426118036
H -1.146959898 1.723813904 -1.566486270
H -1.145584822 1.722855680 3.427192489
H -0.238440520 -0.936607463 2.572464463
H -0.239478683 -0.936141022 -0.713115489
H -2.451834623 0.198914583 0.930462835
H 2.247300022 -1.002012332 0.928951422

26
B10H16_12, MP2/cc-pVDZ, Energy -161324.42685854388 kcal/mol Converged!
B 0.170308586 -1.986322584 -1.278315951
B -0.959831066 -1.917359586 0.005921005
B 0.088975923 -3.273497269 -0.002309534
B 0.243998394 -0.690668124 -0.001545777
B 0.119851857 0.986463090 0.000132040
B -0.915937522 2.013798894 0.903990540

B -0.916017615 2.015158999 -0.901922925
B 0.882771356 2.229475482 -0.902277579
B 0.882887711 2.227968783 0.904387268
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H -0.119744502 -4.451372286 -0.001707697
H 0.028046598 -1.977022506 -2.466277978
H 1.025488298 -3.003115656 0.939244333
H 1.146943635 -1.103595894 0.937211557
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H 1.012182755 -3.001441554 -0.956574284
H -2.150794203 -1.840262893 0.014753401
H 1.732906625 2.196493811 -1.742403396
H 1.209124059 3.187702883 0.001735248
H 1.733169249 2.193958617 1.744334323
H -0.123263962 3.023548250 1.344693751
H -1.732896320 1.779956835 -1.741525714
H -0.123421451 3.025684561 -1.341226447
H -1.732731168 1.777374628 1.743324925
H -1.455099729 2.872534416 0.001712582
B 0.188202961 -1.988155435 1.274048231

36
B20H16, MP2/cc-pVDZ, Energy -316959.0422600347 kcal/mol Converged!
H -0.000000002 2.525159396 2.509783147
H -2.476881525 -1.661701585 1.221343905
B -0.891735330 0.000000031 2.669221481
B -1.561388097 0.894107473 1.252059965
H -0.000000034 -2.525159383 2.509783139
H -2.476881502 1.661701602 1.221343873
B 1.561388107 -0.894107482 1.252059972
B -0.000000007 1.203154327 0.269242875
B 0.000000028 1.432388673 2.020116196
B -0.000000021 -1.432388676 2.020116213
H -0.000000063 1.489517578 -3.706422169
H 0.000000053 -1.489517542 -3.706422183
B -1.561388116 -0.894107465 1.252059989
H 2.476881532 1.661701572 1.221343894
B 0.894107476 1.561388100 -1.252059958
B 0.000000007 -1.203154360 0.269242884
B 1.561388118 0.894107458 1.252059986
H 1.489517558 0.000000015 3.706422159
H 2.476881503 -1.661701603 1.221343909
H -1.489517565 0.000000065 3.706422159
B 0.891735330 -0.000000021 2.669221479
H 2.525159397 0.000000016 -2.509783158
H -1.661701602 -2.476881513 -1.221343925
B 0.000000017 -0.891735326 -2.669221481
B 0.894107482 -1.561388119 -1.252059972
H -2.525159401 -0.000000016 -2.509783130

H 1.661701626 -2.476881502 -1.221343934
B -0.894107473 1.561388098 -1.252059962
B 1.203154322 -0.000000010 -0.269242873
B 1.432388678 0.000000010 -2.020116203
B -1.432388675 -0.000000001 -2.020116193
H -1.661701616 2.476881493 -1.221343872
B -0.000000020 0.891735341 -2.669221483
B -0.894107457 -1.561388120 -1.252059970
H 1.661701588 2.476881510 -1.221343894
B -1.203154315 -0.000000035 -0.269242867

20
B8H12, MP2/cc-pVDZ, Energy -128771.34424709887 kcal/mol Converged!
B 1.594688923 0.841605539 -0.420013658
B 1.511479213 -0.875071186 -0.508801382
B 0.919008157 -0.031642938 0.903704160
B -1.511479213 0.875071186 -0.508801382
B 0.038425188 1.429333757 0.271772872
B -0.038425188 -1.429333757 0.271772872
B -0.919008157 0.031642938 0.903704160
B -1.594688923 -0.841605539 -0.420013658
H 2.539779278 1.539830076 -0.636197294
H 2.398796920 -1.631423684 -0.771858717
H 1.398098742 0.044523481 -1.492586990
H 0.213646846 -1.410042509 -0.996663965
H -2.539779278 -1.539830076 -0.636197294
H 1.446459491 -0.008016400 1.978582272
H -1.398098742 -0.044523481 -1.492586990
H 0.004391062 2.523636426 0.754513703
H -0.213646846 1.410042509 -0.996663965
H -0.004391062 -2.523636426 0.754513703
H -1.446459491 0.008016400 1.978582272
H -2.398796920 1.631423684 -0.771858717

24
B9H15, MP2/cc-pVDZ, Energy -145426.22482286074 kcal/mol Converged!
B 2.979164492 5.312387362 4.078668530
B 3.213153053 5.578253630 2.244078863
B 4.126577964 6.618443997 3.392925785
B 4.863792821 6.078039744 1.887225695
B 4.518846831 4.423010769 1.399973474
B 5.985827163 6.097230413 3.242142124
B 6.221455761 4.904043970 1.872708606
B 5.588465201 3.352844312 2.392854743
B 6.492425166 4.383522315 3.525811271
H 6.806887344 6.928625891 3.503317786
H 4.907768168 6.947865361 1.063127117
H 3.861847076 7.779899123 3.502022795
H 7.497049644 4.016697784 4.059248963

H 7.106421474 5.004783485 1.076015071
H 2.333066071 6.038600207 1.577440149
H 5.944995383 2.246637019 2.114271594
H 4.258396165 4.018076112 0.303663165
H 4.262578347 3.447048562 2.276279763
H 5.527609894 3.459858655 3.740160810
H 5.871572462 5.281011908 4.293766582
H 4.102655907 6.047685134 4.527890574
H 1.945757154 5.761729418 4.494556636
H 3.413332608 4.317015971 4.632428981
H 2.797953852 4.565688858 2.889620923

6
B2Cl4, MP2/cc-pVDZ, Energy -1184910.3514161522 kcal/mol Converged!
Cl 1.500335746 4.721719001 5.005783585
Cl 1.321573851 2.321769599 6.853562557
Cl 4.835845163 4.328839872 7.300380638
Cl 4.886904494 2.459187724 4.911477520
B 2.288487296 3.490643072 5.974060255
B 3.983853451 3.427840733 6.060735445

6
B2Cl4, B3LYP/DZVP-DFT, Energy -1186133.5124191686 kcal/mol Converged!
Cl 1.495497101 4.725302146 5.002833538
Cl 1.314918392 2.318645291 6.856237002
Cl 4.841258775 4.331584084 7.304074268
Cl 4.892906060 2.456642439 4.907825118
B 2.290625385 3.490143967 5.974417635
B 3.981794288 3.427682074 6.060612440

6
B2F4, MP2/cc-pVDZ, Energy -281303.9657274391 kcal/mol Converged!
F 1.650048594 4.416339341 5.245095220
F 1.514518336 2.614798511 6.631931526
F 4.670614656 4.102574638 6.993540784
F 4.709481956 2.698900297 5.200321748
B 2.280164794 3.490329157 5.973901445
B 3.992171664 3.427058057 6.061209277

6
B2F4, B3LYP/DZVP-DFT, Energy -281893.61835768714 kcal/mol Converged!
F 1.649589160 4.413596165 5.247414154
F 1.514497843 2.617661953 6.629719773
F 4.670739121 4.100375942 6.990625418
F 4.709795999 2.701038946 5.203254299
B 2.278781599 3.490377219 5.973799489
B 3.993596279 3.426949775 6.061186867

5

B2O3, MP2/cc-pVDZ, Energy -172471.3879934379 kcal/mol Converged!

O	-0.345140537	0.001131827	0.131052658
B	0.055197425	-0.000163817	1.285229990
O	0.573097946	-0.001858214	2.527031466
B	-0.047276693	0.000222584	3.720878139
O	-0.543556141	0.001884621	4.837190747

5

B2O3, B3LYP/DZVP-DFT, Energy -172854.76920422754 kcal/mol Converged!

O	-0.274529356	0.000933154	0.084624580
B	0.046502999	-0.000147070	1.255663131
O	0.457063148	-0.001535029	2.522192726
B	-0.058509471	0.000250510	3.749736569
O	-0.478205319	0.001715435	4.889165994

12

B3N3H6, MP2/cc-pVDZ, Energy -151809.368655689 kcal/mol Converged!

B	-0.025745150	-0.000025933	-0.014435139
N	0.026850028	0.000035406	1.419889828
B	1.259080438	-0.000005669	2.155851676
N	2.474849539	-0.000508389	1.393050135
B	2.496212348	-0.000916985	-0.042054533
N	1.227730343	-0.000539057	-0.713584354
H	-1.076517800	0.000372423	-0.605921985
H	3.533837253	-0.001552795	-0.656315576
H	-0.845490091	0.000239304	1.936186208
H	1.216639743	-0.000711142	-1.727194101
H	1.272664692	0.000404170	3.361593318
H	3.358124659	-0.000627333	1.890377524

12

B3N3H6, B3LYP/DZVP-DFT, Energy -152199.85114112485 kcal/mol Converged!

B	-0.024597124	-0.000026924	-0.013792282
N	0.027946687	0.000037078	1.419237030
B	1.259065770	-0.000006866	2.154542911
N	2.473744630	-0.000508891	1.392430938
B	2.495071730	-0.000914496	-0.041382174
N	1.227745875	-0.000538905	-0.712312931
H	-1.067681658	0.000369340	-0.600949041
H	3.525107717	-0.001546894	-0.651144292
H	-0.843036198	0.000239114	1.934736792
H	1.216672292	-0.000711844	-1.724353589
H	1.272546483	0.000401060	3.351455449
H	3.355649797	-0.000627771	1.888974190

4

BCl3, MP2/cc-pVDZ, Energy -880917.6275817283 kcal/mol Converged!

B	0.000000026	-0.000000141	0.000001228
Cl	-0.000000043	0.000000047	1.749259699

Cl 1.514900386 0.000000047 -0.874630493
Cl -1.514900371 0.000000047 -0.874630435

4
BCl3, B3LYP/DZVP-DFT, Energy -881811.1128100856 kcal/mol Converged!
B 0.000000058 -0.000000525 0.000000453
Cl -0.000000076 0.000000175 1.755812498
Cl 1.520569472 0.000000175 -0.877906525
Cl -1.520569454 0.000000175 -0.877906427

4
BF3, MP2/cc-pVDZ, Energy -203217.55714661628 kcal/mol Converged!
B 0.000000000 0.000000000 -0.000008632
F -0.000000000 0.000000000 1.327539586
F 1.149683653 0.000000000 -0.663765476
F -1.149683653 0.000000000 -0.663765476

4
BF3, B3LYP/DZVP-DFT, Energy -203633.52025221277 kcal/mol Converged!
B 0.000000000 0.000000000 -0.000007107
F -0.000000000 -0.000000000 1.324801930
F 1.147345704 -0.000000000 -0.662397411
F -1.147345704 -0.000000000 -0.662397411

4
BHO2, MP2/cc-pVDZ, Energy -110157.13781154735 kcal/mol Converged!
O 0.074628024 0.000265049 -0.043758413
B 0.021625843 -0.000015531 1.295805475
O 0.024225248 -0.000124782 2.521768159
H -0.807128116 -0.002430736 -0.439576222

4
BHO2, B3LYP/DZVP-DFT, Energy -110400.56909568513 kcal/mol Converged!
O 0.062152962 0.000231317 -0.028949279
B 0.022614637 -0.000023856 1.303867564
O 0.032456056 -0.000093233 2.523975134
H -0.803872655 -0.002420227 -0.464654419

7
BO3H3, MP2/cc-pVDZ, Energy -158046.82331254 kcal/mol Converged!
O 0.039384575 0.114292271 1.386753596
B 0.422637044 -0.334990137 0.143143273
O -0.259247090 -1.370782356 -0.454691777
O 1.487663058 0.251370694 -0.502745104
H 1.619485810 -0.180501610 -1.355870179
H -0.970525342 -1.662418565 0.129006448
H 0.618000946 0.838391703 1.656129742

7

BO3H3, B3LYP/DZVP-DFT, Energy -158394.382223527 kcal/mol Converged!

O	0.046341951	0.120499270	1.386184283
B	0.422715069	-0.334972345	0.143123534
O	-0.264702100	-1.371044045	-0.447105009
O	1.486268421	0.245384196	-0.509813926
H	1.636730114	-0.173679584	-1.370522051
H	-0.984940678	-1.680070395	0.122787781
H	0.614986223	0.849244903	1.677071387

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2. P. Brain, C. Morrison, S. Parsons and D. Rankin, *J. Chem. Soc., Dalton Trans.* **1996**, 4589–4596.
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