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New global minima of 6-vertex dicarboranes: classical but unexpected

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Supporting Information Available.

1. Theoretical methods.

The global isomeric search of $C_2B_4R_6$ (R=H/F) used our locally developed "skeleton-ligand cluster-growth" method.[1] In order to get the isomers as many as possible, we performed a "grid-based comprehensive isomeric strategy"[1b-1h,2] at the B3LYP[3]/6-31G(d) level to construct the C_2B_4-skeleton. Subsequently, we added one H/F-atom to the optimized C_2B_4-skeleton and optimize hydrogenated/fluorinated structures at the B3LYP/6-31G(d) level. Such steps are repeated until all H/F have been added. Up to 4081 $C_2B_4H_6$ and 2520 $C_2B_4F_6$ isomers were eventually obtained as local minima at the B3LYP/6-31G(d) level. For the low-lying isomers of the parent $C_2B_4R_6$ (R=H/F) within 50 kcal/mol (to guarantee the global minimum), the geometries and energetics were refined at the composite CBS-QB3[4] level. Finally, the obtained structures for both R=H and R=F were subject to the substitution by the other seven groups at the CBS-QB3 level. All the presented structures are minima with no imaginary frequency. All these calculations were performed by using the commercial Gaussian 09[5] packages.

References

1 (a) Y. H. Ding, Skeleton-ligand Cluster-growth Isomeric Search Algorithm, Jilin University, Changchun, China, 2014; (b) X. X. Bo, H. F. Zheng, J. F. Xin and Y. H. Ding, *Chem. Commun*., 2019, **55**, 2597; (c) H. F. Zheng, S. Yu, T. D. Hu, J. Xu and Y. H. Ding, *Phys. Chem. Chem. Phys.*, 2018, **20**, 26266; (d) J. Xu, X. Zhang, S. Yu, Y. H. Ding and K. H. Bowen, *J. Phys. Chem. Lett.*, 2017, **8**, 2263; (e) Y. Y. Xue, J. J. Sui, J. Xu and Y. H. Ding, *ACS Omega*, 2017, **2**, 5407; (f) J. J. Sui, J. Xu and Y. H. Ding, *Dalton Trans.*, 2016, **45**, 56; (g) Z. H. Cui, Y. H. Ding, J. L. Cabellos, E. Osorio, R. Islas, A. Restrepo and G. Merino, *Phys. Chem. Chem. Phys*., 2015, **17**, 8769; (i) X. Y. Zhang and Y. H. Ding, *RSC Adv*., 2015, **5**, 27134.

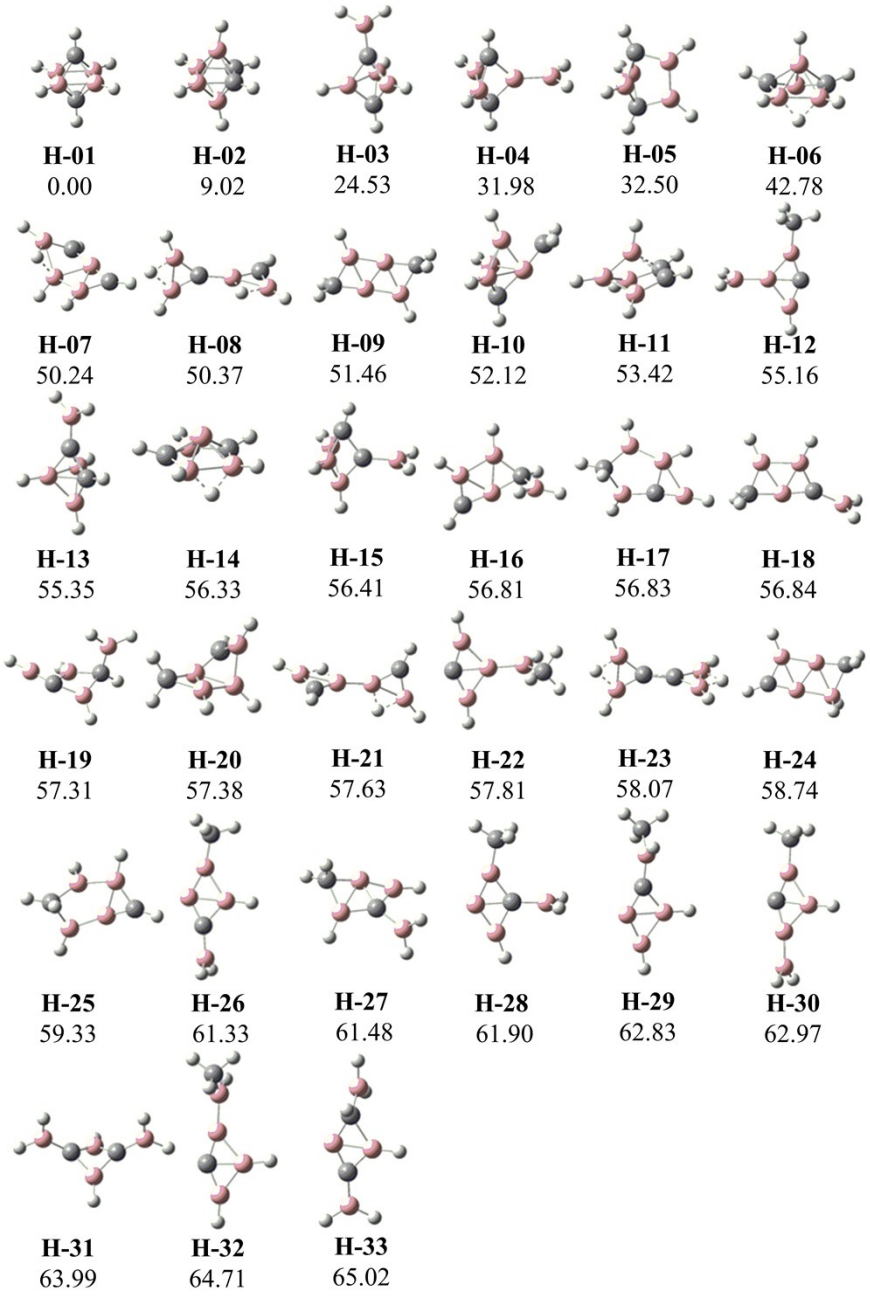
2 (a) C. B. Shao, Y. H. Ding, Jilin University, Changchun, China, **2010**; (b) Z. H. Cui, M. Contreras, Y. H. Ding and G. Merino, *J. Am. Chem. Soc.,* 2011, **133**, 13228; (c) S. M. Gao and Y. H. Ding, *RSC Advances*, 2012, **2**, 11764; (d) X. Y. Tang, Z. H. Cui, C. B. Shao and Y. H. Ding, *Int. J. Quantum. Chem*., 2012, **112**, 1299; (e) C. Guo, Z. H. Cui and Y. H. Ding, *Struct. Chem*., 2013, **24**, 263; (f) C. Guo, Z. H. Cui and Y. H. Ding, *Int. J. Quantum. Chem.*, 2013, **113**, 2213; (g) C. Guo, C. Wang and Y. H. Ding, *Struct. Chem.*, 2014, **25**, 1023.

3 (a) C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 1988, **37**, 785; (b) P. J. Stephens, F. J. Devlin, C. F. Chabalowski and M. J. Frisch, *J. Phys. Chem*., 1994, **98**, 11623; (c) A. D. Becke, *J. Chem. Phys*., 1993, **98**, 5648.

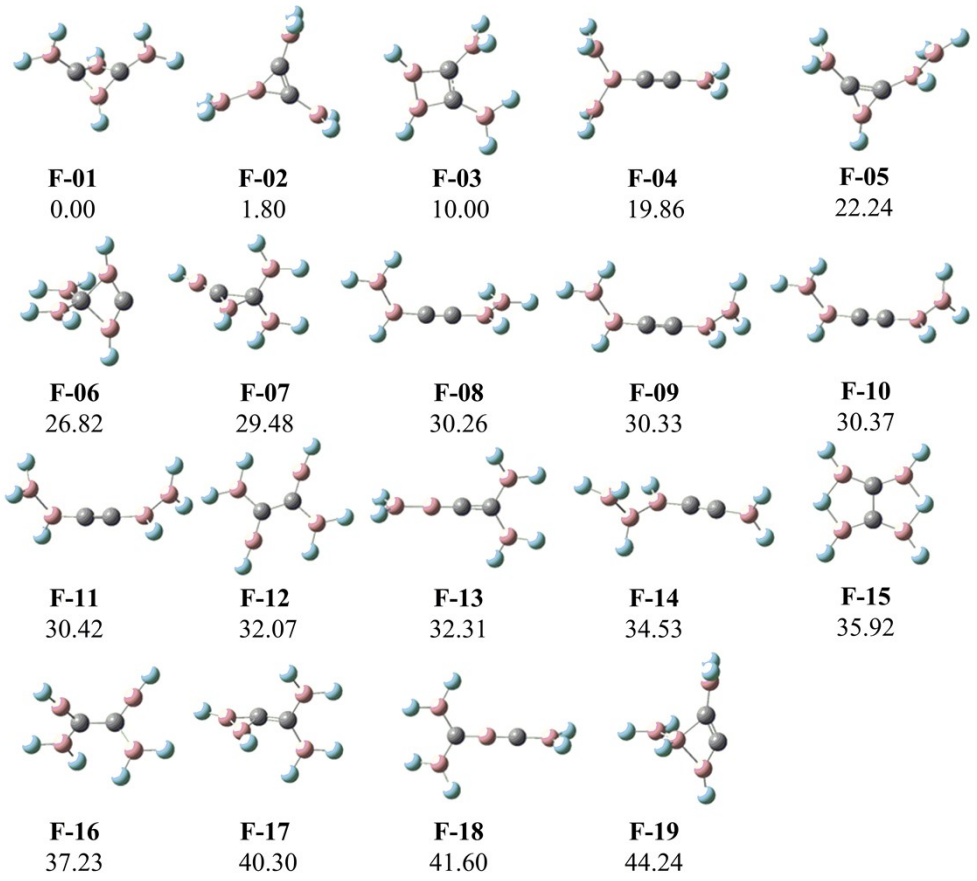
4 (a) J. A. Montgomery, M. J. Frisch, J. W. Ochterski and G. A. Petersson, *J. Chem. Phys.*, 2000, **112**, 6532; (b) J. A. Montgomery, M. J. Frisch, J. W. Ochterski and G. A. Petersson, *J. Chem. Phys.*, 1999, **110**, 2822.

5 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision D.01; Gaussian, Inc., Wallingford CT, **2009**.

2. Fig. S1 The structures and relative energies of all the low-lying $C_2B_4H_6$ at the level of CBS-QB3.



3. Fig. S2 The structures and relative energies of all the low-lying $C_2B_4F_6$ at the level of CBS-QB3.



4. Table S1 The Cartesian coordinates and total energies of all the low-lying $C_2B_4H_6$ at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##

01-C2H6B4
lf=374.3 te_zpe=-179.198275 te_gfe=-179.225449 te_ms_zpe=-178.819889 te_ms_gfe=-178.847085

5 0.890358 -0.820301 0.000779
5 -0.890267 0.820315 -0.000172
5 -0.820059 -0.890476 0.000202
6 -0.000226 0.000548 1.081600
5 0.820123 0.890432 -0.000752
6 0.000174 -0.000577 -1.081583
1 -1.755278 1.614490 -0.000947
1 -0.000165 0.001344 2.160196
1 1.755286 -1.614562 0.001174
1 -1.616445 -1.753456 0.000047
1 -0.000027 -0.001215 -2.160179
1 1.616168 1.753722 -0.000669

02-C2H6B4
lf=388.0 te_zpe=-179.184427 te_gfe=-179.211585 te_ms_zpe=-178.805513 te_ms_gfe=-178.832692

5 -0.002398 -0.848958 0.900924
5 -1.218189 0.002670 0.005936
5 1.218201 -0.001746 0.007891
5 0.001034 0.856169 0.894140
6 0.001628 0.768084 -0.732513
6 -0.000497 -0.774602 -0.725698
1 -2.377222 0.002789 -0.189448
1 -0.004739 -1.773384 1.629565
1 -0.001426 -1.437608 -1.575490
1 0.001842 1.787303 1.614206
1 2.377486 -0.004364 -0.185992
1 0.004032 1.423696 -1.588032

03-C2H6B4
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5 0.490265 0.937418 -0.513728
5 0.433664 -0.002315 1.058699

5 0.490152 -0.935303 -0.517544
 5 -2.204948 0.000106 -0.013491
 6 -0.680051 -0.000176 -0.019352
 6 1.599869 0.000209 -0.000575
 1 0.483195 -1.957733 -1.106757
 1 0.420534 -0.004886 2.238479
 1 -2.813199 -1.026037 -0.007901
 1 2.675207 -0.000037 0.032762
 1 0.482439 1.962451 -1.098393
 1 -2.812747 1.026519 -0.008307

04-C2H6B4
lf=173.5 te_zpe=-179.163611 te_gfe=-179.192206 te_ms_zpe=-178.768925 te_ms_gfe=-178.797552

 5 -2.256444 -0.000038 -0.000026
 5 1.015050 0.000181 -0.930165
 5 -0.612377 -0.000148 -0.000052
 6 0.483187 -1.122431 -0.000127
 5 1.014961 -0.000014 0.930202
 6 0.483032 1.122451 0.000120
 1 1.598482 0.000240 -1.957134
 1 0.483291 -2.198281 -0.000221
 1 -2.882940 -0.000179 1.016804
 1 0.482831 2.198302 0.000238
 1 1.598253 -0.000213 1.957252
 1 -2.883182 0.000105 -1.016695

05-C2H6B4
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 5 -0.000414 -0.699300 0.901254
 5 0.857283 1.126954 -0.000367
 5 -0.856394 1.127365 -0.000261
 6 -1.244612 -0.337185 -0.000009
 6 1.244396 -0.337876 -0.000041
 1 1.640930 2.023393 -0.000409
 1 -0.000461 -1.346312 1.893260
 1 -1.639284 2.024467 -0.000980
 1 2.225990 -0.788155 0.000324
 1 -2.226765 -0.786218 0.000137
 1 -0.000749 -1.348625 -1.892007

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 5 -0.000034 -1.155113 -0.505590
 5 0.886383 0.979320 -0.157287
 5 -0.886335 0.979343 -0.157198
 5 -0.000048 -0.074664 0.936102

6 1.268494 -0.550513 -0.162330
6 -1.268532 -0.550462 -0.162237
1 -1.622155 1.885258 0.034169
1 1.622317 1.885071 0.034431
1 0.000268 -0.251173 2.101844
1 -2.229740 -0.922058 0.151758
1 2.229578 -0.922206 0.151945
1 0.000123 1.286532 -1.106884

07-C2H6B4
lf=211.7 te_zpe=-179.136331 te_gfe=-179.164602 te_ms_zpe=-178.739813 te_ms_gfe=-178.768115

5 0.473634 -0.647951 0.005816
5 -0.498256 0.791607 0.406317
5 1.292103 0.855809 -0.063222
5 -1.903694 0.119317 -0.453366
6 -1.023285 -0.862863 0.165574
6 1.877014 -0.481159 -0.120857
1 1.634025 1.981593 -0.208278
1 -0.742295 1.535045 1.300391
1 -3.041498 0.311756 -0.690234
1 2.808281 -0.976612 -0.323758
1 -1.181203 1.202315 -0.698440
1 -1.418624 -1.583873 0.874293

08-C2H6B4
lf=66.2 te_zpe=-179.143532 te_gfe=-179.173909 te_ms_zpe=-178.739606 te_ms_gfe=-178.770024

5 0.681109 -0.000053 0.009688
5 -2.002988 0.846223 -0.012198
5 2.293741 0.005871 -0.633731
6 -0.832608 0.000237 -0.019181
5 -2.002872 -0.845938 -0.025179
6 1.922693 -0.006900 0.745935
1 -3.023195 0.000060 -0.020367
1 3.115500 0.013643 -1.483093
1 -2.458039 1.934415 -0.002230
1 2.319323 -0.016104 1.742958
1 -2.457692 -1.934249 -0.032038
1 1.118643 0.011701 -1.258652

09-C2H6B4
lf=148.7 te_zpe=-179.137421 te_gfe=-179.166173 te_ms_zpe=-178.737875 te_ms_gfe=-178.766661

5 0.529706 0.600159 0.000257
5 1.089170 -0.982897 -0.000109
5 -0.529706 -0.600149 -0.000260
6 2.016128 0.343995 0.000035
5 -1.089169 0.982900 -0.000205
6 -2.016127 -0.344003 0.000131

1 1.416504 -2.119056 0.000059
1 2.606333 0.499270 0.901885
1 -1.416520 2.119052 -0.000030
1 -2.606443 -0.499491 -0.901606
1 2.606098 0.499717 -0.901889
1 -2.605982 -0.499501 0.902171

10-C2H6B4
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5 -0.275092 -0.629763 -0.004321
5 0.791715 0.388266 -0.975930
5 -0.594410 0.953880 0.005539
5 0.791430 0.376818 0.980471
6 1.342705 -0.639883 -0.003579
6 -1.730446 -0.470831 -0.002594
1 -1.101182 2.016430 0.011136
1 1.210960 0.843921 -1.982158
1 1.210539 0.819737 1.992435
1 -2.318494 -0.508586 -0.914025
1 -2.317732 -0.520394 0.908762
1 2.074136 -1.432834 -0.007901

11-C2H6B4
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5 -0.388782 1.047760 -0.498541
5 -1.522662 -0.000065 0.164599
5 -0.388697 -1.047696 -0.498655
5 -0.155091 -0.000085 1.047103
6 1.062767 0.697499 -0.152109
6 1.062821 -0.697451 -0.152098
1 -2.697275 -0.000044 0.187391
1 1.892349 -1.333862 0.140046
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1 -0.871424 2.033264 -0.948631
1 1.892249 1.334009 0.139958
1 0.178083 -0.000146 2.182954

12-C2H6B4
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5 0.778047 0.233944 -0.000021
5 1.449854 1.682155 0.000006
5 1.599997 -1.244720 -0.000012
6 -2.322151 0.237722 -0.000039
5 -0.864304 -0.263682 -0.000186
6 0.184911 -1.223398 0.000050
1 1.712686 2.237808 -1.023258
1 2.649916 -1.763789 0.000123

1 -2.508555 0.872080 -0.873105
1 -3.051505 -0.575697 -0.002430
1 1.712322 2.237829 1.023354
1 -2.509391 0.867348 0.876321

13-C2H6B4
lf=135.3 te_zpe=-179.125131 te_gfe=-179.153767 te_ms_zpe=-178.731679 te_ms_gfe=-178.760350

5 1.746760 0.076935 0.000049
5 0.460294 -0.598270 -0.895291
5 -2.182970 0.067166 -0.000148
5 0.459834 -0.593274 0.898497
6 0.501641 0.901542 -0.002453
6 -0.678719 -0.081633 -0.000153
1 0.491425 -1.051415 1.983582
1 0.307004 1.968103 -0.005316
1 -2.696274 1.143280 -0.002322
1 -2.862619 -0.909962 0.002077
1 0.492425 -1.062217 -1.977892
1 2.910918 0.229975 -0.000030

14-C2H6B4
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5 1.090677 0.919113 -0.115647
5 1.113300 -0.891722 -0.115834
5 -0.012249 -0.000294 0.751973
6 -0.453162 1.246904 -0.075791
5 -1.388761 -0.017183 -0.226687
6 -0.421743 -1.257800 -0.075998
1 2.043241 -1.561449 0.168755
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1 -0.788767 -2.240198 0.183103
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1 1.392149 0.017928 -1.080780
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5 -0.992390 0.004606 0.923915
5 -0.993001 0.005206 -0.923525
5 2.018344 -0.049821 -0.000185
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5 0.083306 1.201884 -0.064024
5 -1.451776 0.485427 0.492298
5 1.929065 -0.532172 0.590099
6 1.136595 0.134385 -0.539862
6 -1.643911 -0.826266 -0.180766
1 -2.124403 1.136315 1.221020
1 0.138887 2.372145 -0.231565
1 3.039801 -0.912238 0.382240
1 -2.396864 -1.587371 -0.277176
1 1.455898 -0.677602 1.674476
1 1.646364 0.274359 -1.489806

17-C2H6B4
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5 0.764730 0.957976 0.037711
5 -0.889547 1.125147 -0.232944
5 2.117898 -0.286260 0.109221
5 -0.629182 -1.131932 -0.235397
6 -1.673808 -0.095267 0.355570
6 0.808141 -0.613561 -0.115961
1 1.646334 1.754075 0.152884
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1 -0.924078 -2.128887 -0.817166
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1 3.252685 -0.131029 0.341557
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18-C2H6B4
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5 0.158469 1.136761 0.150600
5 -1.546073 0.718282 -0.102081
5 2.529446 -0.362677 -0.063633
6 1.073739 -0.061558 -0.008837
6 -1.780656 -0.834481 0.032282
1 -2.268291 1.579470 -0.478359
1 0.439474 2.273195 0.331989
1 3.119963 -0.670408 0.927385
1 -2.312518 -1.359326 -0.757905
1 3.125695 -0.292307 -1.094916
1 -2.117094 -1.157131 1.020516

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 5 -0.391186 -0.327758 0.753766
 5 1.777943 -0.750416 -0.533960
 5 -2.046306 -0.508152 -0.200173
 6 1.106717 0.156997 0.499267
 5 0.153334 1.200234 -0.226878
 6 -1.087420 0.403650 -0.495429
 1 1.174363 -1.215648 -1.448533
 1 -2.903823 -1.265519 0.031220
 1 2.944087 -0.985862 -0.425592
 1 1.735136 0.494907 1.321235
 1 -0.797077 -0.843743 1.747349
 1 0.262605 2.382441 -0.212483

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 5 0.320431 -0.559768 -0.430797
 6 1.698805 -0.493108 0.164306
 1 -1.999036 0.364737 1.784577
 1 -1.752168 -1.583678 -0.741626
 1 -1.052720 1.696814 -1.306694
 1 2.599249 -0.270264 -0.405273
 1 1.906472 -1.120523 1.027506
 1 1.360985 1.988268 0.271602

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 5 0.830668 0.012240 -0.025006
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 6 2.060057 0.586685 0.471256
 5 -2.448611 0.467695 -0.409338
 6 -2.060114 -0.586826 0.470969
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 1 -2.423984 -1.356214 1.124447
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 1 1.269359 -0.949618 -0.826425

22-C2H6B4
lf=58.1 te_zpe=-179.134384 te_gfe=-179.165915 te_ms_zpe=-178.727752 te_ms_gfe=-178.759331

 5 -0.366862 -0.000155 0.197335
 5 1.192878 -0.001119 0.623919
 5 -1.397556 1.319941 -0.064905
 6 2.414920 -0.000016 -0.363392
 5 -1.398245 -1.319610 -0.065574
 6 -1.896912 0.000318 -0.194189
 1 1.427658 -0.001784 1.800202
 1 -1.479962 2.488179 -0.085742
 1 3.046112 0.874504 -0.156607
 1 2.172624 -0.003971 -1.427886
 1 -1.481007 -2.487809 -0.086973
 1 3.055460 -0.866219 -0.151387

23-C2H6B4
lf=111.9 te_zpe=-179.132274 te_gfe=-179.161884 te_ms_zpe=-178.727344 te_ms_gfe=-178.756991

 5 -1.875249 0.601758 -0.596059
 5 1.875359 -0.596094 -0.601641
 5 -1.875093 -0.601833 0.596109
 5 1.874973 0.596269 0.601767
 6 0.705267 -0.000115 -0.000199
 6 -0.705270 -0.000023 -0.000191
 1 -2.332533 -1.374015 1.361235
 1 2.333813 -1.361002 -1.373440
 1 2.332329 1.361535 1.373860
 1 -2.333539 1.373682 -1.360938
 1 2.880686 0.000244 0.000441
 1 -2.880688 -0.000118 0.000302

24-C2H6B4
lf=152.9 te_zpe=-179.127710 te_gfe=-179.156513 te_ms_zpe=-178.726265 te_ms_gfe=-178.755104

 5 0.401639 0.643817 0.000071
 5 1.118555 -1.017551 0.000190
 5 -0.609984 -0.690994 0.000102
 6 1.865740 0.515084 -0.000190
 5 -1.296302 0.948267 0.000267
 6 -1.993090 -0.363967 -0.000260
 1 1.281083 -1.600140 -1.036474
 1 2.414582 0.769714 -0.902986
 1 -1.693493 2.065838 0.000109
 1 -3.003076 -0.730885 -0.000500
 1 1.280336 -1.599487 1.037374
 1 2.415123 0.770560 0.902024

25-C2H6B4
lf=167.9 te_zpe=-179.126016 te_gfe=-179.154858 te_ms_zpe=-178.725329 te_ms_gfe=-178.754208

 5 1.095886 -1.043382 0.176302
 5 0.491531 0.860485 0.416745
 5 -0.559554 -0.687014 0.251239
 6 1.685249 0.276259 -0.417862
 5 -1.201950 0.849693 -0.075957
 6 -1.883438 -0.467629 -0.177656
 1 0.668229 1.373686 1.481653
 1 2.727730 0.540104 -0.262387
 1 -1.589159 1.970897 -0.137064
 1 -2.852542 -0.862719 -0.419640
 1 1.667844 -2.010356 0.557908
 1 1.437462 0.237698 -1.489006

26-C2H6B4
lf=60.8 te_zpe=-179.129711 te_gfe=-179.160858 te_ms_zpe=-178.722143 te_ms_gfe=-178.753339

 5 0.161078 -0.873151 -0.012237
 5 2.884908 -0.017874 0.011708
 5 -1.220576 -0.190626 -0.024902
 6 1.404645 -0.167129 -0.001254
 5 0.227756 0.810163 -0.010634
 6 -2.745602 0.013489 0.002000
 1 3.473445 0.052947 1.046793
 1 -3.291391 -0.792261 -0.497248
 1 3.491024 0.058021 -1.012793
 1 -3.071937 0.974557 -0.404232
 1 0.241860 1.993638 -0.011579
 1 -3.063090 -0.007618 1.054907

27-C2H6B4
lf=126.7 te_zpe=-179.122021 te_gfe=-179.151429 te_ms_zpe=-178.721909 te_ms_gfe=-178.751356

 5 -0.654807 0.844479 -0.057482
 5 -0.760623 -0.968200 -0.237931
 5 0.787190 1.316893 -0.226907
 6 -1.925902 -0.014366 0.181625
 5 2.013414 -0.631105 0.180021
 6 0.569542 -0.193577 0.086683
 1 -0.736341 -1.968312 -0.877700
 1 1.763975 1.971000 -0.286076
 1 -2.825700 0.077491 -0.419790
 1 -2.157140 -0.058966 1.247474
 1 2.572486 -1.072736 -0.775412
 1 2.595009 -0.511156 1.213148

28-C2H6B4
lf=62.9 te_zpe=-179.124233 te_gfe=-179.155303 te_ms_zpe=-178.721243 te_ms_gfe=-178.752359

 5 0.427108 -1.434019 -0.000119

5 1.847420 -0.833587 0.000207
5 -0.804120 -0.493798 -0.000508
6 0.637574 0.143661 -0.000091
5 0.971397 1.611248 -0.000048
6 -2.240529 0.077397 0.000016
1 3.012488 -0.687595 0.000518
1 -2.404164 0.720666 -0.872507
1 1.106087 2.191276 -1.032681
1 -3.005491 -0.701332 -0.005115
1 1.105823 2.191247 1.032635
1 -2.406035 0.710169 0.879938

29-C2H6B4
lf=62.2 te_zpe=-179.127037 te_gfe=-179.158237 te_ms_zpe=-178.719750 te_ms_gfe=-178.750996

5 2.654845 -0.139399 -0.284658
5 1.253582 0.828337 0.074008
5 1.323509 -0.857012 -0.021404
6 0.106061 -0.173856 0.277651
5 -1.355319 -0.086707 0.608089
6 -2.489633 0.031089 -0.467705
1 1.207176 2.008818 0.143145
1 -3.082560 0.934529 -0.276998
1 3.787733 0.039783 -0.530431
1 -3.192050 -0.802765 -0.339652
1 -1.652169 -0.095143 1.768488
1 -2.149773 0.045286 -1.504397

30-C2H6B4
lf=14.2 te_zpe=-179.128856 te_gfe=-179.161674 te_ms_zpe=-178.719534 te_ms_gfe=-178.752406

5 -3.077152 -0.116724 0.000525
5 -0.189205 0.920852 -0.000264
5 -1.472982 -0.198883 -0.000107
6 2.745447 -0.090002 -0.000075
5 1.202488 -0.104796 -0.001620
6 -0.107828 -0.627380 -0.000712
1 -0.178483 2.096212 -0.000161
1 3.119807 0.415576 0.896478
1 -3.696140 -0.048717 -1.017997
1 3.180521 -1.091937 -0.033626
1 -3.694898 -0.049830 1.019911
1 3.127734 0.480744 -0.852553

31-C2H6B4
lf=105.8 te_zpe=-179.126150 te_gfe=-179.156422 te_ms_zpe=-178.717907 te_ms_gfe=-178.748224

5 0.000463 -0.681900 -0.976112
5 2.268284 0.681809 -0.000032
5 -2.268283 0.681809 -0.000457

6 1.014856 -0.130706 0.000603
5 -0.000463 -0.681176 0.976599
6 -1.014856 -0.130706 -0.000527
1 2.236907 1.872097 -0.000898
1 -2.236907 1.872097 -0.000422
1 3.318736 0.114957 0.000240
1 0.001055 -1.204932 -2.036200
1 -3.318735 0.114957 -0.000244
1 -0.001056 -1.203417 2.037076

32-C2H6B4
lf=59.8 te_zpe=-179.125960 te_gfe=-179.157618 te_ms_zpe=-178.716766 te_ms_gfe=-178.748474

5 -1.408937 0.883403 0.030726
5 1.509899 -0.076196 0.608836
5 -2.690004 -0.170728 -0.244838
6 2.666581 0.016633 -0.446268
5 -0.075954 -0.204180 0.271391
6 -1.389047 -0.675571 0.003654
1 3.322096 0.869017 -0.229670
1 2.362929 0.060376 -1.493586
1 -3.832555 -0.295884 -0.474439
1 1.820021 -0.028228 1.766588
1 -1.320168 2.054945 0.072278
1 3.307453 -0.868091 -0.316061

33-C2H6B4
lf=99.7 te_zpe=-179.121236 te_gfe=-179.151944 te_ms_zpe=-178.716272 te_ms_gfe=-178.747028

5 -0.057444 0.839779 -0.303605
5 2.365347 -0.010239 0.648201
5 -2.665557 -0.044749 0.281542
6 1.339110 -0.129757 -0.494381
5 0.037795 -0.816923 -0.229434
6 -1.184833 -0.163517 -0.016229
1 1.993338 0.146123 1.770714
1 -3.372990 -1.003454 0.228289
1 3.534370 -0.073107 0.425256
1 1.730212 -0.174900 -1.511491
1 -3.142992 1.010789 0.564869
1 -0.068308 2.014851 -0.397492

5. Table S2 The Cartesian coordinates and total energies of all the low-lying $C_2B_4F_6$ at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"

"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2B4F6
lf=33.5 te_zpe=-775.184939 te_gfe=-775.225911 te_ms_zpe=-774.172282 te_ms_gfe=-774.213342

 5 2.107171 0.561446 -0.000023
 6 0.962830 -0.467388 -0.000039
 5 0.000034 -0.992003 1.036192
 5 -0.000036 -0.992006 -1.036197
 5 -2.107172 0.561449 0.000026
 6 -0.962830 -0.467386 0.000033
 9 0.000079 -1.477077 2.262488
 9 -0.000080 -1.477086 -2.262490
 9 -1.871930 1.863429 -0.000010
 9 3.369315 0.164444 -0.000032
 9 -3.369313 0.164442 0.000057
 9 1.871930 1.863428 -0.000008

02-C2B4F6
lf=28.6 te_zpe=-775.183285 te_gfe=-775.226378 te_ms_zpe=-774.169407 te_ms_gfe=-774.212594

 5 1.277952 1.918329 -0.000209
 6 0.373661 0.678998 -0.000116
 5 -0.940824 -0.000031 -0.000131
 5 -2.603085 -0.000067 0.000029
 6 0.373686 -0.679010 -0.000161
 5 1.278059 -1.918285 0.000063
 9 1.663990 2.478399 -1.133317
 9 1.664621 -2.478407 -1.132831
 9 -3.303315 -0.000177 -1.127537
 9 1.664142 2.478562 1.132760
 9 -3.302723 0.000006 1.128001
 9 1.663886 -2.478345 1.133247

03-C2B4F6
lf=10.3 te_zpe=-775.168490 te_gfe=-775.210808 te_ms_zpe=-774.156331 te_ms_gfe=-774.198739

 5 1.039708 -1.627314 -0.043602
 5 1.551290 1.253519 0.087431
 6 0.754479 -0.094637 -0.001602
 5 0.024431 1.969747 -0.080311
 6 -0.508839 0.478339 0.007614
 5 -1.899908 -0.214975 0.045089
 9 2.831877 1.486773 0.298856
 9 0.057791 -2.496868 0.172209
 9 2.238649 -2.117786 -0.293749
 9 -2.569172 -0.339620 1.178841

9 -2.480605 -0.642255 -1.063981
9 -0.639812 3.086745 -0.300965

04-C2B4F6
lf=33.2 te_zpe=-775.157971 te_gfe=-775.201908 te_ms_zpe=-774.140622 te_ms_gfe=-774.184659

5 -1.801945 -1.479224 -0.000509
5 -1.801941 1.479262 -0.000122
5 -0.977324 0.000023 -0.000302
6 1.732726 -0.000151 0.000093
5 3.246956 -0.000025 0.000395
6 0.509434 -0.000135 -0.000075
9 -2.150229 -2.076988 1.129651
9 -2.149867 2.077627 -1.130043
9 3.923630 0.000235 -1.134423
9 3.923151 -0.000121 1.135495
9 -2.149918 -2.077335 -1.130546
9 -2.150289 2.076753 1.130154

05-C2B4F6
lf=18.6 te_zpe=-775.153671 te_gfe=-775.197265 te_ms_zpe=-774.136828 te_ms_gfe=-774.180516

5 -2.462259 -0.352513 -0.366100
5 -1.261317 0.112575 0.775507
5 0.991843 1.713944 -0.157668
6 0.096981 0.640146 0.323922
6 1.398816 0.321136 -0.017602
5 2.311091 -0.914039 -0.083520
9 2.315622 -1.704712 -1.143976
9 1.212609 2.973270 -0.468352
9 -1.549666 0.073972 2.077172
9 -2.298646 -0.137691 -1.664479
9 3.141244 -1.205223 0.903265
9 -3.584671 -0.951563 -0.001299

06-C2B4F6
lf=34.1 te_zpe=-775.139690 te_gfe=-775.180068 te_ms_zpe=-774.129535 te_ms_gfe=-774.170006

5 1.358097 0.718215 -0.001513
6 -0.000020 -0.033561 0.000351
5 -0.000068 -1.238429 1.245641
5 -1.358136 0.718194 -0.001714
5 0.000133 -1.244593 -1.239939
6 -0.000198 -1.890962 0.004403
9 -0.000109 -1.154086 2.543977
9 1.434121 2.039612 -0.004006
9 2.508057 0.052496 -0.000750
9 -1.434146 2.039591 -0.004053
9 0.000305 -1.165624 -2.538576
9 -2.508098 0.052478 -0.001138

07-C2B4F6
lf=32.6 te_zpe=-775.141040 te_gfe=-775.182423 te_ms_zpe=-774.125297 te_ms_gfe=-774.166772

 5 0.988577 -1.340576 -0.322582
 6 0.319358 0.000034 0.048688
 5 -0.485910 -0.002582 1.396382
 5 0.985368 1.342897 -0.320110
 5 -2.456290 -0.001040 -0.494886
 6 -1.277213 -0.002188 0.193658
 9 2.291550 1.450296 -0.525688
 9 2.294984 -1.444482 -0.528536
 9 -3.589449 -0.000445 -1.086090
 9 0.283189 -2.462634 -0.435341
 9 0.277273 2.463420 -0.431215
 9 -0.381058 -0.003996 2.701525

08-C2B4F6
lf=13.9 te_zpe=-775.141568 te_gfe=-775.186714 te_ms_zpe=-774.124054 te_ms_gfe=-774.169302

 5 2.068015 0.581486 -0.487022
 5 3.125707 -0.494121 0.339020
 6 0.589038 0.647983 -0.161147
 5 -3.125803 -0.493920 -0.339168
 6 -0.589035 0.647920 0.161268
 5 -2.068000 0.581297 0.487214
 9 4.417160 -0.546406 0.054560
 9 -2.556845 1.374813 1.437310
 9 2.691355 -1.309512 1.288015
 9 -2.691486 -1.308701 -1.288704
 9 2.557064 1.375309 -1.436732
 9 -4.417203 -0.546517 -0.054553

09-C2B4F6
lf=13.8 te_zpe=-775.141331 te_gfe=-775.186654 te_ms_zpe=-774.123933 te_ms_gfe=-774.169357

 5 -2.049461 -0.759098 -0.151338
 5 -3.132513 0.571222 -0.029818
 6 -0.576877 -0.623914 0.186173
 5 2.064586 -0.209713 0.769327
 6 0.591286 -0.445879 0.493994
 5 3.129360 0.257109 -0.486748
 9 -2.719336 1.779141 0.322262
 9 3.332660 1.530663 -0.792704
 9 -4.423751 0.434548 -0.285676
 9 2.523892 -0.373686 2.010799
 9 3.782970 -0.638500 -1.213175
 9 -2.512692 -1.940927 -0.551296

10-C2B4F6
lf=11.9 te_zpe=-775.141319 te_gfe=-775.186601 te_ms_zpe=-774.123877 te_ms_gfe=-774.169261

 5 2.065802 -0.276081 0.739304
 5 3.125929 0.333235 -0.459611
 6 0.594344 -0.494187 0.441037
 5 -2.043829 -0.752013 -0.238014
 6 -0.572565 -0.646811 0.115149
 5 -3.136727 0.545604 0.043774
 9 3.070321 1.594113 -0.864337
 9 -4.420581 0.444587 -0.261535
 9 4.036052 -0.435723 -1.040023
 9 -2.738904 1.691807 0.574278
 9 -2.497285 -1.879444 -0.780764
 9 2.529669 -0.571755 1.954117

11-C2B4F6
lf=8.7 te_zpe=-775.141196 te_gfe=-775.187424 te_ms_zpe=-774.123792 te_ms_gfe=-774.170121

 5 -2.046159 -0.578751 -0.578405
 5 -3.123727 0.488273 0.214831
 6 -0.579560 -0.638515 -0.190825
 5 2.046003 -0.577564 0.580207
 6 0.579365 -0.638102 0.192886
 5 3.123902 0.486516 -0.216523
 9 -3.309312 1.731101 -0.207398
 9 2.487566 -1.369619 1.558264
 9 -3.805270 0.119495 1.290010
 9 3.799680 0.116724 -1.294969
 9 3.315464 1.728213 0.206399
 9 -2.488008 -1.373989 -1.553742

12-C2B4F6
lf=46.3 te_zpe=-775.139427 te_gfe=-775.179718 te_ms_zpe=-774.121168 te_ms_gfe=-774.161552

 5 -1.825909 0.775983 0.000138
 5 1.103604 1.579408 -0.000594
 5 -1.103459 -1.579197 -0.000120
 5 1.825941 -0.776035 -0.000314
 6 -0.707871 -0.237135 0.000120
 6 0.708118 0.237324 -0.000263
 9 1.511395 -2.089264 0.001113
 9 -1.511780 2.089283 0.000527
 9 -1.592312 -2.758444 -0.000874
 9 1.592336 2.758701 -0.000516
 9 3.130325 -0.488201 0.000040
 9 -3.130226 0.487711 0.000301

13-C2B4F6
lf=18.6 te_zpe=-775.138758 te_gfe=-775.182325 te_ms_zpe=-774.120789 te_ms_gfe=-774.164452

5 1.771551 1.373092 -0.042472
5 1.770861 -1.373342 0.042439
6 -0.321206 0.000404 0.000164
6 1.004212 0.000069 0.000033
5 -1.697359 0.000691 0.000309
5 -3.338468 0.000331 0.000020
9 3.055751 1.419748 -0.352411
9 -4.029129 -0.011410 -1.133023
9 3.055010 -1.420678 0.352490
9 1.160494 -2.515514 -0.206784
9 -4.029534 0.011515 1.132821
9 1.161745 2.515594 0.206610

14-C2B4F6
lf=13.4 te_zpe=-775.134664 te_gfe=-775.179650 te_ms_zpe=-774.117248 te_ms_gfe=-774.162335

5 -2.830770 0.781329 -0.002855
6 2.040224 -0.206594 -0.156975
5 -1.744085 -0.417079 0.567207
5 3.449785 0.334475 0.018016
5 -0.523465 -1.125375 -0.407999
6 0.919029 -0.654094 -0.311347
9 -1.847960 -0.810369 1.843550
9 4.296377 -0.237819 0.854009
9 -0.839891 -2.066949 -1.301334
9 -4.041503 0.474978 -0.450365
9 3.859727 1.389972 -0.661104
9 -2.483733 2.061008 -0.069412

15-C2B4F6
lf=73.1 te_zpe=-775.135598 te_gfe=-775.172350 te_ms_zpe=-774.115025 te_ms_gfe=-774.151858

5 -1.355829 1.266304 -0.000476
5 1.355330 1.266810 0.000655
6 -0.000108 0.764295 0.000242
5 1.355755 -1.266504 -0.000140
5 -1.355255 -1.267010 0.000401
6 0.000108 -0.764363 0.000266
9 -2.280418 0.000073 0.000008
9 2.280416 0.000119 -0.000806
9 -2.107430 2.335748 -0.000633
9 2.107154 2.336040 0.000665
9 2.107622 -2.335709 -0.000298
9 -2.107346 -2.336003 0.000481

16-C2B4F6
lf=15.1 te_zpe=-775.130241 te_gfe=-775.172465 te_ms_zpe=-774.112939 te_ms_gfe=-774.155258

5 1.513735 1.214352 -0.756154

5 1.580739 -0.759731 0.682737
6 0.755786 0.306590 -0.017830
5 -1.580712 -0.759699 -0.682778
6 -0.755761 0.306586 0.017845
5 -1.513705 1.214313 0.756217
9 1.037145 -1.728271 1.414943
9 -2.232243 2.038519 1.416356
9 2.232143 2.038676 -1.416288
9 -2.922988 -0.767300 -0.595053
9 2.923014 -0.767318 0.595030
9 -1.037121 -1.728220 -1.415009

17-C2B4F6
lf=33.5 te_zpe=-775.123484 te_gfe=-775.165076 te_ms_zpe=-774.108059 te_ms_gfe=-774.149745

5 1.153061 1.370526 -0.165282
5 1.158699 -1.365937 -0.171567
6 0.415286 0.001072 -0.301479
5 -1.589933 -0.007857 0.910685
6 -0.909430 -0.000909 -0.617686
5 -2.319685 0.001275 -0.497142
9 0.489307 -2.482363 0.069870
9 -1.221060 -0.014177 2.154847
9 0.479131 2.483144 0.080930
9 2.465898 1.463741 -0.280325
9 2.471839 -1.453407 -0.287542
9 -3.467986 0.004060 -1.167612

18-C2B4F6
lf=17.7 te_zpe=-775.128480 te_gfe=-775.172099 te_ms_zpe=-774.105977 te_ms_gfe=-774.149694

5 3.282281 -0.000271 0.000037
6 1.789939 0.000114 -0.000173
5 0.405535 0.000271 -0.000155
5 -1.785080 -1.355800 -0.059753
5 -1.785497 1.355680 0.059387
6 -1.018506 0.000077 -0.000637
9 -3.042497 -1.417141 -0.467143
9 3.956644 0.026459 -1.143319
9 -1.203176 -2.498406 0.271482
9 -1.204186 2.498572 -0.271905
9 3.956308 -0.026090 1.143621
9 -3.042513 1.416543 0.468073

19-C2B4F6
lf=33.5 te_zpe=-775.113509 te_gfe=-775.154539 te_ms_zpe=-774.101777 te_ms_gfe=-774.142902

5 -1.113772 1.297127 0.059372
5 -1.478206 -1.389047 -0.413674
5 -0.575875 -0.194887 0.636349

6 0.853832 -0.639830 -0.171568
5 2.303179 -0.136154 -0.195986
6 -0.030012 -1.511809 -0.514981
9 -1.594239 2.244499 0.852535
9 -2.632039 -1.829534 -0.781507
9 -1.106883 1.578150 -1.247342
9 -0.586705 -0.539019 1.972584
9 3.176356 -0.547596 0.699690
9 2.674671 0.762903 -1.086071

6. Table S3 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=SiH_3) (ΔE< 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2H18B4Si6
lf=25.0 te_zpe=-1923.447364 te_gfe=-1923.502035 te_ms_zpe=-1920.350185 te_ms_gfe=-1920.405050

5 0.861493 0.861019 -0.028229
5 -0.861512 -0.861030 0.028232
5 -0.861521 0.861013 -0.028181
6 -0.000049 -0.035952 -1.101084
5 0.861502 -0.861020 0.028180
6 0.000019 0.035943 1.101084
14 -2.284296 -2.268106 0.058798
1 -3.515589 -1.779276 0.726122
1 -2.637288 -2.655274 -1.329893
1 -1.830163 -3.485591 0.774106
14 -0.000149 -0.088596 -2.979690
1 1.207405 0.601487 -3.482248
1 0.001706 -1.494551 -3.435014
1 -1.209654 0.598223 -3.482020
14 2.284406 -2.267979 0.058643
1 3.514923 -1.779698 0.727799
1 1.829736 -3.486341 0.772117
1 2.638903 -2.653535 -1.330110
14 2.284320 2.268053 -0.058776
1 1.829781 3.486101 -0.772866
1 2.638326 2.654170 1.329948
1 3.515100 1.779616 -0.727334
14 -2.284321 2.268077 -0.058666
1 -2.637897 2.654590 1.330057
1 -1.829927 3.485908 -0.773221
1 -3.515322 1.779527 -0.726732
14 0.000052 0.088558 2.979691

 1 1.208399 -0.600227 3.482115
 1 0.000427 1.494504 3.435045
 1 -1.208663 -0.599581 3.482125

02-C2H18B4Si6
lf=18.8 te_zpe=-1923.432466 te_gfe=-1923.487219 te_ms_zpe=-1920.334043 te_ms_gfe=-1920.388991

 5 -0.015085 0.861755 0.961453
 5 1.219141 -0.032757 0.116185
 5 -1.228596 0.036554 0.015380
 5 -0.067605 -0.851084 0.968131
 6 0.006759 -0.789803 -0.676949
 6 0.045310 0.779996 -0.686538
14 -0.028476 2.412789 2.231028
 1 -1.175596 3.318726 1.970017
 1 -0.132906 1.935504 3.631671
 1 1.213807 3.218395 2.115829
14 -3.205248 0.077968 -0.306539
 1 -3.519576 0.226988 -1.750505
 1 -3.837985 -1.175486 0.170857
 1 -3.826587 1.215474 0.414025
14 -0.161804 -2.386375 2.253434
 1 -1.302098 -3.284438 1.938480
 1 1.076029 -3.205400 2.213552
 1 -0.338699 -1.894117 3.641437
14 0.041647 -2.012718 -2.104607
 1 0.772974 -1.407862 -3.238961
 1 0.733438 -3.234799 -1.646942
 1 -1.339173 -2.337647 -2.518450
14 3.215217 -0.084326 -0.049452
 1 3.634389 -0.544749 -1.398175
 1 3.795074 1.262956 0.171593
 1 3.798925 -1.010577 0.950111
14 0.145284 1.991369 -2.120155
 1 -0.856334 1.627564 -3.145024
 1 -0.139584 3.338305 -1.585110
 1 1.499536 1.955763 -2.711164

03-C2H18B4Si6
lf=24.0 te_zpe=-1923.410446 te_gfe=-1923.464204 te_ms_zpe=-1920.294087 te_ms_gfe=-1920.348041

 5 0.007515 -0.645589 0.897259
 5 -0.007530 -0.645871 -0.897175
 5 -0.863757 1.121241 0.006633
 5 0.863845 1.121188 -0.006824
 6 1.280891 -0.337991 -0.010454
 6 -1.280890 -0.337914 0.010403
14 2.980898 -1.113317 -0.022477
 1 3.658194 -0.771677 -1.292962
 1 3.765254 -0.582913 1.114088
 1 2.890855 -2.586688 0.095628

14 -0.005860 -1.644801 -2.655945
 1 1.030478 -2.705589 -2.668599
 1 -1.321687 -2.259712 -2.950412
 1 0.309195 -0.665806 -3.726243
14 -2.980965 -1.113086 0.022611
 1 -3.658192 -0.771109 1.293045
 1 -3.765295 -0.582837 -1.114046
 1 -2.891087 -2.586488 -0.095184
14 -2.075094 2.735550 -0.026083
 1 -3.486719 2.433103 0.324511
 1 -1.587953 3.783934 0.906480
 1 -2.066844 3.316679 -1.395144
14 2.075333 2.735387 0.025774
 1 2.067454 3.316345 1.394912
 1 3.486846 2.432823 -0.325164
 1 1.588107 3.783943 -0.906549
14 0.005681 -1.644290 2.656160
 1 -1.029310 -2.706411 2.667932
 1 1.322029 -2.257521 2.951810
 1 -0.311572 -0.665681 3.726160

04-C2H18B4Si6
lf=31.5 te_zpe=-1923.417059 te_gfe=-1923.472737 te_ms_zpe=-1920.292743 te_ms_gfe=-1920.348620

 5 -2.061021 -0.000024 -0.000142
 5 1.185622 0.907704 -0.210730
 5 -0.423685 -0.000002 -0.000110
 6 0.661894 -0.258977 -1.116630
 5 1.185598 -0.907668 0.210863
 6 0.661668 0.259001 1.116651
14 -3.109013 -1.702283 0.286166
 1 -2.358034 -2.778200 0.979518
 1 -4.378181 -1.473049 1.021006
 1 -3.453563 -2.189883 -1.077944
14 -3.109131 1.702160 -0.286457
 1 -4.378186 1.472816 -1.021461
 1 -3.453902 2.189659 1.077632
 1 -2.358190 2.778193 -0.979671
14 2.228464 2.583780 -0.593675
 1 3.672572 2.306786 -0.383964
 1 2.044536 3.042018 -1.991936
 1 1.833999 3.686706 0.316270
14 0.663642 -0.675956 -2.928250
 1 2.056552 -0.742979 -3.424677
 1 0.009237 -1.985613 -3.146032
 1 -0.071538 0.361454 -3.686154
14 2.228479 -2.583683 0.593967
 1 3.672586 -2.306623 0.384339
 1 2.044483 -3.041870 1.992237
 1 1.834131 -3.686668 -0.315956
14 0.663078 0.675972 2.928273
 1 2.055903 0.743122 3.424921

 1 0.008515 1.985567 3.145959
 1 -0.072128 -0.361509 3.686054

05-C2H18B4Si6
lf=7.8 te_zpe=-1923.415359 te_gfe=-1923.471030 te_ms_zpe=-1920.291713 te_ms_gfe=-1920.347582

 5 -0.714718 1.028071 -0.323997
 5 -0.679033 -0.807519 -0.705506
 5 -0.605992 -0.226906 1.024579
 5 2.023525 0.025006 -0.057942
 6 0.496434 0.024451 -0.047606
 6 -1.812446 -0.006537 0.008756
14 3.095714 1.748313 -0.074631
 1 2.369424 2.909807 0.498166
 1 4.384213 1.600870 0.647652
 1 3.412217 2.057308 -1.495594
14 3.070494 -1.712406 -0.016931
 1 3.606799 -1.867784 1.362666
 1 2.262802 -2.917332 -0.333232
 1 4.231596 -1.666909 -0.941762
14 -0.795379 2.944414 -0.925032
 1 0.308697 3.271723 -1.858190
 1 -2.081360 3.232086 -1.605973
 1 -0.688659 3.829463 0.261180
14 -3.669310 -0.048928 0.078968
 1 -4.130667 -1.395117 0.485052
 1 -4.155704 0.946732 1.059876
 1 -4.220289 0.272366 -1.256006
14 -0.718429 -2.316164 -2.033219
 1 -0.773258 -3.604919 -1.299423
 1 -1.918502 -2.226474 -2.900768
 1 0.483040 -2.319250 -2.901346
14 -0.539104 -0.626735 2.992846
 1 -1.871046 -0.997366 3.527781
 1 0.403260 -1.739358 3.266825
 1 -0.061213 0.574498 3.722519

06-C2H18B4Si6
lf=15.9 te_zpe=-1923.406973 te_gfe=-1923.462616 te_ms_zpe=-1920.289563 te_ms_gfe=-1920.345399

 5 -0.495977 0.619929 0.000076
 5 -1.140558 -0.917932 -0.000048
 5 0.495983 -0.619929 -0.000027
 6 -2.006001 0.469207 0.000043
 5 1.140566 0.917929 0.000076
 6 2.006007 -0.469210 0.000010
14 1.829269 2.801576 -0.000282
 1 0.747097 3.811408 0.000504
 1 2.674715 3.005141 1.202219
 1 2.672976 3.005179 -1.204001
14 2.953162 -0.855204 -1.582637

 1 4.250036 -0.137076 -1.607201
 1 3.227171 -2.309857 -1.662929
 1 2.152154 -0.448231 -2.760599
14 2.953065 -0.855192 1.582730
 1 3.224555 -2.310224 1.664565
 1 4.251199 -0.139290 1.606014
 1 2.153205 -0.445522 2.760540
14 -1.829284 -2.801571 -0.000090
 1 -2.675326 -3.004792 1.202050
 1 -2.672401 -3.005494 -1.204169
 1 -0.747127 -3.811420 0.001498
14 -2.953069 0.854962 1.582815
 1 -3.223654 2.310119 1.665390
 1 -4.251657 0.139860 1.605509
 1 -2.153653 0.444165 2.760535
14 -2.953148 0.855431 -1.582552
 1 -4.249564 0.136502 -1.607708
 1 -3.228065 2.309955 -1.662099
 1 -2.151698 0.449592 -2.760602

07-C2H18B4Si6
lf=40.9 te_zpe=-1923.386597 te_gfe=-1923.437366 te_ms_zpe=-1920.286930 te_ms_gfe=-1920.337887

 5 0.011009 -0.954421 -1.439182
 5 0.888458 0.661789 -0.096940
 5 -0.874998 0.666620 -0.101564
 5 0.001409 -0.815522 0.344959
 6 1.301807 -0.695866 -0.831525
 6 -1.284641 -0.697165 -0.840752
14 -2.165950 1.701995 1.078799
 1 -1.484846 2.785332 1.827325
 1 -3.262047 2.313374 0.285281
 1 -2.781897 0.780063 2.064872
14 -2.935064 -1.553883 -0.917082
 1 -3.655829 -1.079784 -2.119774
 1 -2.754659 -3.020647 -1.013792
 1 -3.726309 -1.233599 0.288246
14 0.000751 -2.015327 1.952153
 1 0.263992 -3.420052 1.544579
 1 1.053074 -1.617975 2.918946
 1 -1.305783 -1.984968 2.653992
14 2.947693 -1.567809 -0.888460
 1 2.784973 -2.917175 -1.475430
 1 3.879172 -0.785754 -1.731608
 1 3.505775 -1.692126 0.473891
14 2.180190 1.765206 1.012942
 1 2.943877 2.725838 0.177133
 1 1.482399 2.535466 2.069989
 1 3.163599 0.862502 1.662039
14 -0.042567 2.265401 -1.382687
 1 0.035083 3.503986 -0.583615
 1 1.105959 2.188821 -2.312482

1 -1.269661 2.284396 -2.211606

08-C2H18B4Si6
lf=30.3 te_zpe=-1923.399214 te_gfe=-1923.450891 te_ms_zpe=-1920.281414 te_ms_gfe=-1920.333281

5 -0.082790 0.700232 -0.026819
5 -0.828018 -0.939416 -0.009621
5 0.864229 -0.682449 0.015224
6 -1.534099 0.683353 0.002173
5 1.629978 0.892315 -0.027124
6 2.278741 -0.455390 0.013229
14 3.964935 -1.211589 0.045240
1 4.102399 -2.136678 -1.102086
1 5.009171 -0.167725 -0.035481
1 4.125843 -1.972396 1.305024
14 2.383119 2.759064 -0.076551
1 3.864218 2.758756 -0.042735
1 1.933569 3.445275 -1.313147
1 1.878932 3.534995 1.083443
14 -1.159704 -2.121530 1.620105
1 -2.531924 -2.690538 1.580987
1 -0.206093 -3.257658 1.650280
1 -1.022286 -1.392662 2.908904
14 -2.310323 1.302549 1.615601
1 -2.891484 2.641409 1.361751
1 -3.385219 0.378085 2.035150
1 -1.303376 1.413025 2.692292
14 -2.518602 1.268798 -1.495448
1 -3.911866 0.783106 -1.383369
1 -2.528649 2.748604 -1.530268
1 -1.913747 0.754359 -2.741775
14 -1.083049 -2.062381 -1.702619
1 -0.605852 -3.443755 -1.441129
1 -2.519993 -2.145788 -2.074676
1 -0.347777 -1.560341 -2.892461

09-C2H18B4Si6
lf=17.3 te_zpe=-1923.390193 te_gfe=-1923.444343 te_ms_zpe=-1920.278615 te_ms_gfe=-1920.332961

5 0.077119 -0.000024 -0.832481
5 -0.882036 -0.985102 0.269295
5 0.539285 0.000029 0.725817
5 -0.882007 0.985173 0.269199
6 -1.515842 -0.000006 -0.740030
6 1.554047 -0.000073 -0.878731
14 2.481626 1.607389 -1.178710
1 3.019784 1.599084 -2.560729
1 1.566104 2.760122 -1.013747
1 3.619451 1.755676 -0.242049
14 1.537354 0.000122 2.454020
1 2.399758 1.201730 2.564080

 1 0.599071 0.000229 3.602532
 1 2.399689 -1.201521 2.564249
14 -1.616677 2.648965 1.113015
 1 -2.321869 3.483534 0.107293
 1 -2.598322 2.259154 2.157347
 1 -0.565744 3.475890 1.750426
14 -1.616787 -2.648753 1.113319
 1 -2.322474 -3.483196 0.107842
 1 -0.565822 -3.475882 1.750414
 1 -2.598018 -2.258713 2.157954
14 -2.936576 -0.000098 -1.950808
 1 -2.877246 -1.206237 -2.805225
 1 -4.198334 -0.000971 -1.178242
 1 -2.878295 1.206798 -2.804225
14 2.481512 -1.607623 -1.178583
 1 3.019801 -1.599398 -2.560551
 1 3.619233 -1.755992 -0.241810
 1 1.565869 -2.760270 -1.013680

10-C2H18B4Si6
lf=32.6 te_zpe=-1923.395498 te_gfe=-1923.449758 te_ms_zpe=-1920.276909 te_ms_gfe=-1920.331365

 5 -0.688375 0.788179 -0.431714
 5 -1.752592 -0.004432 0.599400
 5 0.924822 0.727636 0.153083
 6 -1.282316 -1.016408 -0.381511
 5 0.171127 -0.747324 -0.305131
 6 1.622641 -0.715625 0.095432
14 -3.047513 0.272547 2.093215
 1 -4.110009 -0.763073 2.140156
 1 -2.288886 0.209834 3.369079
 1 -3.694872 1.603563 2.008486
14 -2.213066 -2.253592 -1.424882
 1 -2.277374 -3.540876 -0.693501
 1 -3.588994 -1.773717 -1.680384
 1 -1.527282 -2.469585 -2.719794
14 -1.259530 2.242730 -1.703153
 1 -0.123307 2.953830 -2.344440
 1 -2.069963 1.630640 -2.790012
 1 -2.103080 3.266390 -1.037500
14 1.727180 2.484132 0.717932
 1 2.156411 2.359200 2.134048
 1 2.927927 2.776347 -0.104099
 1 0.777649 3.612650 0.601155
14 2.962647 -0.738914 -1.234247
 1 4.229073 -0.214058 -0.676896
 1 3.172571 -2.132138 -1.688789
 1 2.551098 0.093091 -2.386863
14 2.111042 -1.669063 1.646523
 1 0.998455 -1.628569 2.621461
 1 2.405746 -3.076472 1.293643
 1 3.317333 -1.064909 2.257111

11-C2H18B4Si6
lf=8.2 te_zpe=-1923.391461 te_gfe=-1923.446465 te_ms_zpe=-1920.273131 te_ms_gfe=-1920.328331

 5 0.996236 1.045976 -0.229337
 5 0.181744 -0.713296 -0.402841
 5 -0.699550 0.816114 -0.486430
 6 1.434369 -0.245546 0.481318
 5 -1.541611 -0.517720 0.030790
 6 -2.075871 0.879216 -0.159629
14 -3.642572 1.837143 -0.013274
 1 -4.352782 1.813212 -1.313425
 1 -4.523967 1.246559 1.019368
 1 -3.350653 3.243306 0.346285
14 -2.500998 -2.211757 0.532768
 1 -2.716168 -2.177540 2.001188
 1 -3.820642 -2.286700 -0.137638
 1 -1.735689 -3.437567 0.205465
14 0.424044 -1.774445 -2.136441
 1 1.117048 -0.950640 -3.164485
 1 1.245170 -2.994768 -1.924387
 1 -0.880480 -2.191101 -2.710873
14 3.181830 -0.909592 0.194852
 1 4.154620 -0.146504 1.011654
 1 3.248116 -2.336239 0.581723
 1 3.545182 -0.777469 -1.234335
14 1.155336 -0.095553 2.353364
 1 -0.270863 0.140550 2.660129
 1 1.589304 -1.371566 2.968181
 1 1.967017 1.002493 2.927164
14 1.922436 2.768325 -0.729378
 1 1.340350 3.849090 0.105193
 1 3.387449 2.733147 -0.504421
 1 1.660840 3.086668 -2.154301

12-C2H18B4Si6
lf=30.5 te_zpe=-1923.379106 te_gfe=-1923.431457 te_ms_zpe=-1920.271139 te_ms_gfe=-1920.323683

 5 0.403626 -1.017311 -0.589118
 5 1.419423 -0.028293 0.282770
 5 0.434184 1.034312 -0.544265
 5 -0.174621 -0.033192 0.859268
 6 -1.106527 -0.692260 -0.518479
 6 -1.080475 0.732540 -0.513190
14 1.361400 -2.653686 -1.281140
 1 2.791792 -2.688831 -0.907777
 1 0.706902 -3.884040 -0.768572
 1 1.268087 -2.654205 -2.762516
14 3.313223 -0.048827 0.906273
 1 4.278766 0.044634 -0.216481
 1 3.568567 1.091371 1.821507

 1 3.603576 -1.299601 1.651188
14 1.400996 2.708078 -1.123263
 1 0.571705 3.909574 -0.844086
 1 2.714168 2.884454 -0.464614
 1 1.621940 2.627099 -2.588574
14 -2.500643 1.972919 -0.468282
 1 -2.677227 2.497023 -1.841163
 1 -3.751386 1.318442 -0.028078
 1 -2.151135 3.080434 0.444825
14 -2.570900 -1.879442 -0.475926
 1 -3.607346 -1.405918 0.466091
 1 -3.141236 -1.944005 -1.840728
 1 -2.089075 -3.215586 -0.072355
14 -0.853476 -0.099120 2.751566
 1 -1.281232 -1.479385 3.099536
 1 0.198910 0.307669 3.712693
 1 -2.025217 0.792687 2.956655

13-C2H18B4Si6
lf=32.8 te_zpe=-1923.384348 te_gfe=-1923.436043 te_ms_zpe=-1920.271118 te_ms_gfe=-1920.323006

 5 -0.658168 1.015342 -0.232054
 5 0.300544 -0.432999 0.335306
 5 -1.563175 -0.420426 -0.017904
 5 1.708525 0.183574 -0.605567
 6 0.827555 1.213645 -0.071822
 6 -2.069665 0.933440 -0.350803
14 3.660974 0.025391 -1.101746
 1 3.811679 -0.660058 -2.404513
 1 4.245684 1.382325 -1.198331
 1 4.377652 -0.750773 -0.062954
14 0.697408 -1.307643 2.137128
 1 0.736994 -2.788097 2.048819
 1 2.013329 -0.859965 2.663920
 1 -0.341053 -0.934523 3.129695
14 -2.638171 -2.103973 0.211706
 1 -3.870133 -1.798784 0.980023
 1 -3.049921 -2.632444 -1.113927
 1 -1.914604 -3.189060 0.920005
14 -3.624398 1.825012 -0.752963
 1 -3.926451 2.821098 0.303060
 1 -3.488914 2.544435 -2.042327
 1 -4.767670 0.888403 -0.855860
14 1.468151 2.622418 0.998308
 1 1.214518 3.899376 0.296717
 1 0.757833 2.620915 2.296796
 1 2.919946 2.468707 1.238233
14 0.930273 -1.840447 -1.235198
 1 2.179579 -2.590361 -0.985019
 1 0.897784 -1.353641 -2.637013
 1 -0.201531 -2.768125 -1.041800

7. Table S4 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=PH_2) ($\Delta E<$ 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2H12B4P6
lf=38.7 te_zpe=-2231.037452 te_gfe=-2231.087714 te_ms_zpe=-2227.920198 te_ms_gfe=-2227.970629

 5 0.861979 -0.860768 -0.010592
 5 -0.856023 0.857755 -0.055955
 5 -0.855990 -0.857806 0.055803
 6 0.003647 0.034637 1.099730
 5 0.861938 0.860800 0.010775
 6 0.003846 -0.034635 -1.099718
15 2.205258 2.242510 0.109768
 1 3.211492 1.563904 -0.623076
 1 1.753445 2.991227 -1.005854
15 -2.223421 2.206969 -0.231980
 1 -3.114062 1.674161 0.734184
 1 -1.653767 3.149287 0.661210
15 -2.223376 -2.207067 0.231576
 1 -3.114060 -1.674037 -0.734425
 1 -1.653757 -3.149178 -0.661853
15 2.205337 -2.242453 -0.109392
 1 3.211515 -1.563799 0.623483
 1 1.753444 -2.991109 1.006237
15 0.078165 0.007472 2.936856
 1 0.165656 1.410208 3.117129
 1 -1.321041 -0.032028 3.156294
15 0.078683 -0.007388 -2.936826
 1 0.167484 -1.410046 -3.117071
 1 -1.320513 0.030841 -3.156537

02-C2H12B4P6
lf=11.2 te_zpe=-2231.052709 te_gfe=-2231.102642 te_ms_zpe=-2227.910457 te_ms_gfe=-2227.960556

 5 -0.607126 -0.182387 1.042749
 5 -0.670345 1.043561 -0.356909
 5 -0.636671 -0.809216 -0.713981
 5 2.046739 0.015895 0.013191
 6 0.507202 0.023311 -0.034915
 6 -1.770789 0.010067 -0.002654
15 -0.579280 -0.694898 2.889123
 1 0.450156 0.179655 3.312363
 1 -1.650398 0.121216 3.326725

15 -3.588633 0.041013 0.130533
 1 -3.864261 0.457152 -1.197720
 1 -3.828766 -1.327912 -0.153745
15 -0.728772 2.898193 -0.827973
 1 0.297432 2.890871 -1.802298
 1 -1.802736 2.826264 -1.748210
15 -0.705438 -2.364640 -1.826145
 1 -1.739322 -1.924991 -2.688297
 1 0.362191 -2.038446 -2.695495
15 2.981922 -1.649092 -0.148103
 1 4.061628 -1.442792 0.739038
 1 2.193684 -2.449676 0.709191
15 3.024450 1.655311 -0.147684
 1 2.268243 2.469480 0.726052
 1 4.106982 1.411352 0.726320

03-C2H12B4P6
lf=42.7 te_zpe=-2231.024236 te_gfe=-2231.074547 te_ms_zpe=-2227.905889 te_ms_gfe=-2227.956370

 5 0.108266 0.845458 0.977176
 5 1.214885 -0.127649 0.071272
 5 -1.214913 0.127784 0.071150
 5 -0.108379 -0.845241 0.977329
 6 -0.052105 -0.784351 -0.670369
 6 0.052122 0.784143 -0.670620
15 -3.114570 0.213513 -0.270486
 1 -3.521511 0.011304 1.071906
 1 -3.224059 1.625637 -0.199584
15 -0.114443 -1.890926 -2.140719
 1 0.311870 -3.048541 -1.444488
 1 -1.489547 -2.221458 -2.050083
15 0.114790 1.890203 -2.141333
 1 -0.313163 3.047743 -1.445989
 1 1.489520 2.221964 -2.049602
15 0.171646 2.398100 2.126083
 1 -0.126186 1.705984 3.326909
 1 1.572735 2.389536 2.350092
15 3.114599 -0.213374 -0.270068
 1 3.521303 -0.012425 1.072583
 1 3.223900 -1.625573 -0.200429
15 -0.171736 -2.397520 2.126721
 1 0.124500 -1.704772 3.327576
 1 -1.573042 -2.389850 2.349423

04-C2H12B4P6
lf=41.6 te_zpe=-2231.029025 te_gfe=-2231.076316 te_ms_zpe=-2227.891206 te_ms_gfe=-2227.938659

 5 -0.027198 -0.735876 -0.901175
 5 0.035161 -0.591724 0.945833
 5 0.846068 1.170367 -0.098550
 5 -0.868232 1.158539 -0.059756

 6 -1.244800 -0.322759 0.022249
 6 1.244847 -0.305005 -0.039391
15 2.017316 2.675852 0.005335
 1 3.067669 2.267056 -0.850756
 1 1.375685 3.531986 -0.918949
15 -2.061816 2.630366 -0.299924
 1 -3.109524 2.282142 0.585643
 1 -1.437320 3.575083 0.546554
15 -2.927405 -1.049260 -0.009005
 1 -2.659974 -2.257364 0.684907
 1 -3.444429 -0.391822 1.136129
15 0.078177 -1.277176 2.732660
 1 -0.959780 -2.230952 2.617701
 1 1.149084 -2.190622 2.595111
15 2.936715 -1.005515 0.061468
 1 2.673727 -2.291169 -0.478455
 1 3.429866 -0.484690 -1.162072
15 -0.036193 -1.988762 -2.350067
 1 -1.114851 -1.432098 -3.076870
 1 0.998655 -1.400074 -3.114840

05-C2H12B4P6
lf=26.2 te_zpe=-2231.032376 te_gfe=-2231.082276 te_ms_zpe=-2227.888216 te_ms_gfe=-2227.938283

 5 -2.071015 -0.020463 0.076538
 5 1.210490 0.915159 0.219675
 5 -0.413020 -0.005506 0.011847
 6 0.664818 0.250249 -1.103569
 5 1.215503 -0.909642 -0.231425
 6 0.696421 -0.250779 1.103232
15 0.663981 -0.592513 2.894663
 1 0.343629 -1.972933 2.822082
 1 2.052379 -0.836788 3.059782
15 2.007101 -2.614158 -0.592194
 1 2.917513 -2.205168 -1.596106
 1 2.949461 -2.613632 0.464896
15 0.599063 0.588284 -2.896003
 1 0.207303 1.949643 -2.820256
 1 1.972016 0.905202 -3.067971
15 -3.020670 -1.589264 -0.432423
 1 -2.229749 -2.594931 0.166066
 1 -4.080504 -1.605828 0.502583
15 -3.011254 1.624882 0.250861
 1 -4.096842 1.262766 1.080218
 1 -2.234399 2.277422 1.233312
15 1.993808 2.627427 0.560711
 1 2.949138 2.221273 1.523476
 1 2.892394 2.648543 -0.533465

06-C2H12B4P6
lf=37.8 te_zpe=-2231.013766 te_gfe=-2231.060484 te_ms_zpe=-2227.864077 te_ms_gfe=-2227.910952

 5 -1.464577 -1.311240 -0.025757
 5 -1.466111 1.312128 0.056871
 6 -0.760606 0.000110 0.039922
 5 1.476915 1.321487 0.039367
 5 1.478253 -1.319082 0.067869
 6 0.784554 0.000852 0.054072
15 -3.301447 1.855565 -0.047656
 1 -3.877884 1.006984 0.928293
 1 -3.244790 3.004062 0.779881
15 -3.297643 -1.865314 0.057034
 1 -3.884582 -0.965260 -0.865562
 1 -3.242939 -2.965795 -0.833469
15 3.291638 -1.924111 -0.083064
 1 3.933850 -1.097078 0.868400
 1 3.217073 -3.067294 0.750472
15 3.286732 1.926853 -0.145544
 1 3.225407 3.076083 0.680769
 1 3.945529 1.107757 0.801067
15 0.001289 -2.621314 -0.007762
 1 -0.024098 -3.548577 1.050927
15 -0.002537 2.620811 -0.043272
 1 -0.019619 3.419163 -1.202718
 1 0.026137 -3.500414 -1.106709
 1 0.009351 3.620764 0.946887

07-C2H12B4P6
lf=23.6 te_zpe=-2231.002152 te_gfe=-2231.050808 te_ms_zpe=-2227.862036 te_ms_gfe=-2227.910857

 5 1.912983 -0.062961 0.066100
 5 0.630451 -0.985523 -0.571929
 5 -2.018698 0.041136 -0.075003
 5 0.563618 -0.208866 1.093281
 6 0.732411 0.784877 -0.370712
 6 -0.492707 -0.066451 -0.034028
15 0.683197 2.494413 -1.031298
 1 1.935762 2.456646 -1.689757
 1 -0.064825 2.213675 -2.200618
15 -2.996756 1.666033 -0.333474
 1 -2.409342 2.171514 -1.515282
 1 -4.164363 1.148047 -0.938484
15 -3.017900 -1.566522 0.225339
 1 -2.334231 -2.103076 1.341575
 1 -4.128732 -1.049291 0.930325
15 0.431655 -0.019452 2.993730
 1 -0.572156 -0.995920 3.210340
 1 1.510759 -0.858117 3.360380
15 3.817491 0.109479 0.197568
 1 4.135530 -1.215641 -0.192149
 1 4.041167 0.662297 -1.091076
15 0.667284 -2.311851 -1.948683
 1 1.745805 -3.086929 -1.459906

1 -0.349931 -3.154198 -1.436902

08-C2H12B4P6
lf=26.8 te_zpe=-2231.023711 te_gfe=-2231.074834 te_ms_zpe=-2227.861027 te_ms_gfe=-2227.912323

5 -0.026322 -0.891311 1.009154
5 -2.266656 0.459782 -0.049547
5 2.266644 0.459800 0.049520
6 -0.997515 -0.355358 -0.025877
5 0.026320 -0.891385 -1.009151
6 0.997513 -0.355351 0.025837
15 2.265517 2.353775 0.334327
1 3.387630 2.712301 -0.448364
1 1.280077 2.734601 -0.606134
15 3.929875 -0.468027 -0.206884
1 4.742406 0.267853 0.687428
1 3.727833 -1.587889 0.633745
15 0.066523 -1.543402 -2.811915
1 1.106410 -2.490746 -2.649842
1 -0.987065 -2.482730 -2.695731
15 -0.066478 -1.543179 2.811972
1 -1.106374 -2.490533 2.650018
1 0.987102 -2.482521 2.695831
15 -2.265568 2.353730 -0.334517
1 -3.387688 2.712303 0.448140
1 -1.280135 2.734665 0.605906
15 -3.929855 -0.468049 0.207030
1 -4.742464 0.267763 -0.687265
1 -3.727861 -1.587962 -0.633542

09-C2H12B4P6
lf=26.0 te_zpe=-2231.000708 te_gfe=-2231.051495 te_ms_zpe=-2227.860351 te_ms_gfe=-2227.911308

5 -0.803287 -0.279415 1.185657
5 -1.254172 -0.854929 -0.357077
5 -1.229773 0.948933 0.106382
5 1.787055 -0.074404 0.191660
6 0.249770 -0.031185 0.105309
6 -0.594678 0.286027 -1.136249
15 -0.809809 -0.637006 3.073049
1 -2.104451 -1.211624 3.129821
1 -0.140537 -1.887660 3.027317
15 -1.894339 -2.581440 -0.876192
1 -2.889552 -2.745308 0.116298
1 -2.787104 -2.157669 -1.892549
15 -0.054777 0.661147 -2.840101
1 -1.199320 0.127262 -3.481959
1 -0.528700 1.995882 -2.903991
15 2.700866 -1.685465 -0.287076
1 3.708245 -1.695129 0.704132
1 1.843749 -2.629353 0.321268

15 2.739978 1.569438 0.416061
 1 1.927176 2.177548 1.398197
 1 3.774568 1.140665 1.277600
15 -1.786188 2.757957 0.393919
 1 -2.679605 2.859613 -0.702074
 1 -2.790119 2.526308 1.363581

10-C2H12B4P6
lf=29.5 te_zpe=-2230.995030 te_gfe=-2231.042986 te_ms_zpe=-2227.857036 te_ms_gfe=-2227.905155

 5 -0.539893 0.843767 -0.101639
 5 0.012146 -0.797079 0.340931
 5 -1.747073 -0.359462 -0.009822
 5 1.909372 0.149319 -0.833336
 6 0.963803 0.817431 0.122433
 6 -1.939689 1.092724 -0.192903
15 0.297348 -1.683681 2.064342
 1 -0.358372 -2.904581 1.760038
 1 1.592257 -2.210967 1.806155
15 -2.873859 -1.889917 -0.340445
 1 -2.646550 -2.614680 0.853165
 1 -4.101576 -1.323933 0.080518
15 -3.192677 2.268421 -0.689864
 1 -4.247696 1.852108 0.162054
 1 -2.817534 3.366184 0.124577
15 1.496644 1.910509 1.530200
 1 2.901983 1.810217 1.357994
 1 1.413240 3.151908 0.846076
15 3.816118 0.212147 -0.999042
 1 3.878344 0.022740 -2.400385
 1 3.994885 1.615750 -1.012662
15 0.876749 -1.437440 -1.317443
 1 0.156477 -1.477106 -2.522309
 1 1.612251 -2.631877 -1.329293

11-C2H12B4P6
lf=15.4 te_zpe=-2231.004995 te_gfe=-2231.055097 te_ms_zpe=-2227.852264 te_ms_gfe=-2227.902527

 5 -0.420095 0.176860 0.171266
 5 2.125943 1.129998 -0.293856
 5 -2.745563 0.367126 0.103929
 6 1.094201 0.076974 -0.038273
 5 2.038129 -1.058098 0.213178
 6 -1.650192 -0.611910 -0.164342
15 2.226352 3.048382 -0.342253
 1 1.469925 3.342144 0.819420
 1 3.492868 3.204919 0.272515
15 2.009915 -2.777913 1.064238
 1 3.254056 -2.694811 1.737575
 1 1.213739 -2.456558 2.189881
15 -1.769483 -2.194393 -1.058877

 1 -0.796721 -2.947108 -0.353350
 1 -2.866399 -2.767662 -0.364382
15 -4.650630 0.426908 -0.101662
 1 -4.778719 1.777481 -0.508387
 1 -4.756238 -0.129236 -1.400532
15 3.497075 -0.180005 -0.736396
 1 4.849642 -0.123437 -0.330344
15 -1.532720 1.595283 0.989232
 1 -1.586480 1.683632 2.394764
 1 3.630846 -0.505495 -2.095559
 1 -1.490291 2.972395 0.667270

12-C2H12B4P6
lf=16.9 te_zpe=-2231.003575 te_gfe=-2231.053205 te_ms_zpe=-2227.851784 te_ms_gfe=-2227.901574

 5 1.781328 0.869230 -0.657118
 5 -1.594935 1.079469 0.524928
 5 1.594863 -1.079436 0.525131
 5 -1.781245 -0.869214 -0.657326
 6 -0.726091 0.074295 -0.166027
 6 0.726106 -0.074264 -0.165934
15 3.186227 -0.438143 -0.377160
 1 3.664875 -1.161465 -1.485237
15 1.844938 2.619570 -1.439484
 1 0.902385 3.273654 -0.609690
 1 2.993476 3.106839 -0.768273
15 1.353426 -2.534293 1.752762
 1 2.446044 -2.268471 2.615239
 1 0.364625 -1.954835 2.584833
15 -1.353652 2.534315 1.752602
 1 -2.446304 2.268417 2.615013
 1 -0.364866 1.954900 2.584721
15 -1.844733 -2.619579 -1.439648
 1 -0.902207 -3.273603 -0.609774
 1 -2.993293 -3.106885 -0.768502
15 -3.186210 0.438109 -0.377473
 1 -4.399675 0.145844 0.283274
 1 -3.664798 1.161406 -1.485590
 1 4.399652 -0.145915 0.283676

13-C2H12B4P6
lf=43.0 te_zpe=-2230.983249 te_gfe=-2231.031434 te_ms_zpe=-2227.851314 te_ms_gfe=-2227.899665

 5 0.436851 -1.079618 -0.579181
 5 1.476680 -0.069429 0.256009
 5 0.539537 1.086083 -0.508097
 5 -0.014179 -0.056303 0.937477
 6 -1.050569 -0.641459 -0.480538
 6 -0.980674 0.766142 -0.480104
15 1.016184 -2.792617 -1.241039
 1 0.525749 -2.656456 -2.564906

 1 2.359204 -2.488800 -1.556715
15 -0.726107 -0.277618 2.720949
 1 0.091177 0.702203 3.335570
 1 -1.867813 0.557876 2.622402
15 -2.572238 -1.660019 -0.291182
 1 -3.263450 -1.114814 -1.402868
 1 -2.107928 -2.797917 -0.989886
15 -2.377584 1.938308 -0.282518
 1 -1.880470 2.942654 -1.144232
 1 -3.233709 1.359123 -1.252030
15 1.254686 2.817082 -0.979884
 1 2.593523 2.464498 -1.260254
 1 0.830534 2.821515 -2.333730
15 3.320262 -0.030330 0.776964
 1 3.332713 -1.194458 1.586669
 1 3.885426 -0.669253 -0.356577

14-C2H12B4P6
lf=23.4 te_zpe=-2230.996604 te_gfe=-2231.045498 te_ms_zpe=-2227.849694 te_ms_gfe=-2227.898751

 5 -0.524127 -0.681000 -0.579329
 5 -0.119473 0.987087 -0.224331
 5 -1.774846 0.377616 0.030989
 5 1.803080 -0.557986 0.586804
 6 0.922477 -0.188648 -0.648772
 6 -1.900266 -1.020906 -0.496446
15 -3.087960 1.426755 0.974699
 1 -2.874471 2.681455 0.354242
 1 -4.211410 1.083905 0.181852
15 -3.098072 -2.336415 -0.555238
 1 -4.241985 -1.595582 -0.943056
 1 -2.823799 -2.852547 -1.844745
15 0.256905 2.830331 -0.369331
 1 -0.466618 3.351538 0.723249
 1 1.546846 2.870809 0.204298
15 1.622690 -0.041597 -2.387110
 1 2.667372 0.882273 -2.120759
 1 2.490043 -1.163591 -2.332218
15 1.052064 -0.743745 2.352763
 1 0.008213 -1.669695 2.126450
 1 1.975426 -1.653365 2.915983
15 3.699899 -0.819209 0.453620
 1 4.099240 0.341475 -0.248176
 1 4.091807 -0.389744 1.742502

15-C2H12B4P6
lf=22.1 te_zpe=-2231.000077 te_gfe=-2231.049765 te_ms_zpe=-2227.847107 te_ms_gfe=-2227.896961

 5 0.265582 -0.581497 0.023489
 5 -0.203815 1.066431 -0.188823
 5 1.522024 0.651516 -0.011316

 5 -2.536683 -0.524153 0.132374
 6 -1.087413 -0.140883 0.042453
 6 1.747483 -0.942705 -0.029179
15 2.507337 -1.699297 1.499416
 1 2.398609 -3.056847 1.099713
 1 3.868262 -1.610254 1.102787
15 2.282008 -1.478978 -1.745476
 1 3.681212 -1.489745 -1.505391
 1 2.145778 -2.877183 -1.546235
15 2.803823 1.929513 0.514895
 1 3.917780 1.500693 -0.240632
 1 2.445763 3.046144 -0.268755
15 -0.726431 2.910836 -0.385994
 1 0.083450 3.239964 -1.500645
 1 -1.909784 2.704652 -1.133946
15 -3.472377 -0.321164 1.800701
 1 -4.286143 -1.477107 1.763601
 1 -2.489302 -0.836493 2.675736
15 -3.535565 -0.821759 -1.485336
 1 -2.586530 -1.585791 -2.201701
 1 -4.346967 -1.905264 -1.075874

16-C2H12B4P6
lf=23.7 te_zpe=-2230.996784 te_gfe=-2231.046903 te_ms_zpe=-2227.846280 te_ms_gfe=-2227.896568

 5 -0.252932 -0.711649 -0.875802
 5 1.374662 1.079468 -0.005640
 5 -2.721792 0.063069 -0.014645
 6 1.014851 -0.436139 0.056450
 5 -0.241127 -0.627448 1.037610
 6 -1.412083 -0.354162 0.076669
15 -0.300126 -1.498737 2.746450
 1 0.775012 -0.820993 3.369863
 1 -1.332116 -0.722047 3.325432
15 -4.449475 0.694090 -0.360076
 1 -5.091663 -0.143809 0.585634
 1 -4.358674 1.827127 0.486161
15 -0.324330 -1.455101 -2.644203
 1 0.751610 -2.369560 -2.558906
 1 -1.352863 -2.404582 -2.443819
15 0.120431 2.549316 0.206569
 1 -0.485931 2.230186 1.444011
 1 1.023118 3.506741 0.730417
15 3.185947 1.676695 -0.288718
 1 3.557896 0.908207 -1.416284
 1 2.922416 2.880249 -0.984125
15 2.357748 -1.746201 0.085621
 1 3.022591 -1.406618 -1.121151
 1 3.305015 -1.061253 0.891808

17-C2H12B4P6

lf=7.4 te_zpe=-2230.996946 te_gfe=-2231.048496 te_ms_zpe=-2227.843423 te_ms_gfe=-2227.895142

 5 0.210325 0.304242 0.696782
 5 -2.288789 0.084143 -0.658996
 5 2.777194 -0.371009 -0.362193
 6 -1.255252 -0.571752 0.324263
 5 0.020679 -1.033014 -0.278823
 6 1.281360 -0.436438 -0.100509
15 0.210642 1.894122 1.751598
 1 -0.600002 1.425997 2.813515
 1 1.448976 1.689367 2.404180
15 3.741673 1.271450 -0.173680
 1 4.759769 1.099569 -1.138407
 1 2.926430 2.149235 -0.925998
15 3.703641 -1.963499 -0.883184
 1 4.980349 -1.736940 -0.319045
 1 3.232271 -2.867102 0.097344
15 -2.069680 1.857426 -1.371902
 1 -0.680675 1.873973 -1.627709
 1 -2.484732 1.627500 -2.702686
15 -4.018165 -0.718248 -0.934423
 1 -4.182164 -0.447791 -2.311852
 1 -3.635538 -2.072372 -1.069957
15 -1.832454 -1.557030 1.825412
 1 -3.003012 -0.805619 2.105113
 1 -2.550215 -2.571809 1.141805

18-C2H12B4P6
lf=32.6 te_zpe=-2230.984802 te_gfe=-2231.032686 te_ms_zpe=-2227.842725 te_ms_gfe=-2227.890773

 5 -1.180522 -0.584917 0.084931
 5 0.427053 -1.055900 -0.188950
 5 -2.159121 0.947104 -0.199867
 5 0.719233 1.167639 -0.187937
 6 1.498475 -0.076903 0.444930
 6 -0.787508 0.930283 -0.255679
15 -2.540487 -1.923841 0.266710
 1 -1.889761 -2.730257 1.230650
 1 -3.458741 -1.332843 1.165797
15 -3.978286 1.408619 0.024309
 1 -4.016315 2.327333 -1.053637
 1 -4.536006 0.329603 -0.706080
15 0.818337 -2.257136 -1.637422
 1 1.956731 -2.914152 -1.114988
 1 -0.118431 -3.272675 -1.336365
15 3.275540 -0.287768 -0.106593
 1 3.861793 0.712537 0.711925
 1 3.638388 -1.333874 0.781078
15 1.162465 0.006896 2.311703
 1 1.937621 -1.127625 2.670084
 1 2.200864 0.915013 2.651658
15 1.530543 2.671825 -1.052298

1 0.583955 3.651906 -0.675726
1 2.519192 3.006187 -0.096948

8. Table S5 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=CH_3) (ΔE< 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C8H18B4
lf=27.9 te_zpe=-415.037855 te_gfe=-415.083998 te_ms_zpe=-414.245782 te_ms_gfe=-414.292070

5 -0.840125 0.873907 -0.033326
5 0.840026 -0.873961 0.033217
5 -0.870652 -0.838934 0.096509
6 -0.039872 -0.077168 -1.088440
5 0.870652 0.838817 -0.096580
6 0.039772 0.077256 1.088299
6 0.102170 0.197054 2.585984
1 -0.822916 0.616869 2.988999
1 0.255808 -0.778143 3.055013
1 0.924674 0.846690 2.896337
6 -1.941400 1.997820 -0.067182
1 -1.793993 2.685934 -0.905898
1 -2.954413 1.592866 -0.158082
1 -1.919769 2.605266 0.843479
6 2.014487 1.914940 -0.197083
1 2.972142 1.482649 -0.504523
1 1.773294 2.707372 -0.912689
1 2.181594 2.404510 0.768195
6 -0.102030 -0.197171 -2.586155
1 0.816444 -0.632937 -2.987375
1 -0.934891 -0.833116 -2.897229
1 -0.238448 0.780037 -3.056318
6 1.941535 -1.997628 0.067504
1 2.955844 -1.591817 0.137795
1 1.806060 -2.672680 0.918763
1 1.906592 -2.619061 -0.833234
6 -2.014698 -1.914907 0.196881
1 -2.975332 -1.480667 0.492027
1 -2.172923 -2.413710 -0.765151
1 -1.779056 -2.700382 0.921939

02-C8H18B4
lf=67.8 te_zpe=-415.027844 te_gfe=-415.071172 te_ms_zpe=-414.235610 te_ms_gfe=-414.279078

 5 -0.004258 0.856419 0.960849
 5 1.219241 0.006058 0.069186
 5 -1.219267 -0.006011 0.069062
 5 0.004132 -0.856045 0.961175
 6 0.003889 -0.776433 -0.677732
 6 -0.003833 0.776172 -0.678038
 6 -0.010756 2.090486 1.940919
 1 -0.893743 2.724148 1.806011
 1 -0.011716 1.765136 2.985778
 1 0.868018 2.730726 1.809648
 6 0.010544 -2.089749 1.941703
 1 0.893567 -2.723433 1.807133
 1 0.011371 -1.764020 2.986444
 1 -0.868193 -2.730064 1.810558
 6 -2.772255 -0.013552 -0.178231
 1 -3.254951 0.862761 0.265458
 1 -3.028788 -0.015212 -1.243797
 1 -3.246683 -0.893959 0.266253
 6 0.008939 -1.714023 -1.849580
 1 0.891423 -1.569787 -2.478965
 1 0.018892 -2.748956 -1.499882
 1 -0.879080 -1.585248 -2.474540
 6 -0.008710 1.713320 -1.850243
 1 -0.016847 2.748399 -1.500933
 1 0.878537 1.583051 -2.475987
 1 -0.891991 1.570091 -2.478738
 6 2.772262 0.013475 -0.177927
 1 3.246627 0.894163 0.266067
 1 3.254916 -0.862558 0.266361
 1 3.028922 0.014481 -1.243463

03-C8H18B4
lf=49.2 te_zpe=-415.011930 te_gfe=-415.057302 te_ms_zpe=-414.201969 te_ms_gfe=-414.247487

 5 -0.000002 -0.672947 -0.912805
 5 -0.000004 -0.673161 0.916114
 5 0.860584 1.174521 0.007302
 5 -0.860573 1.174530 0.007283
 6 -1.243736 -0.301855 0.000396
 6 1.243733 -0.301868 0.000397
 6 -0.000008 -1.540521 -2.222080
 1 -0.000002 -2.602400 -1.940456
 1 -0.888861 -1.381443 -2.838890
 1 0.888835 -1.381437 -2.838902
 6 -2.621476 -0.920739 -0.004034
 1 -3.272133 -0.449881 0.738799
 1 -3.107072 -0.793204 -0.976852
 1 -2.601635 -1.994182 0.208811

6 -0.000016 -1.506287 2.246904
1 0.889522 -2.131657 2.364756
1 -0.000172 -0.802201 3.089679
1 -0.889441 -2.131847 2.364601
6 2.621466 -0.920767 -0.004028
1 3.107011 -0.793357 -0.976888
1 3.272169 -0.449827 0.738712
1 2.601623 -1.994184 0.208947
6 1.876222 2.383153 -0.005408
1 1.946313 2.759924 -1.036339
1 1.527815 3.231729 0.592611
1 2.894400 2.130847 0.307618
6 -1.876189 2.383181 -0.005413
1 -1.946164 2.760065 -1.036310
1 -2.894403 2.130875 0.307494
1 -1.527813 3.231686 0.592726

04-C8H18B4
lf=55.3 te_zpe=-415.015743 te_gfe=-415.060550 te_ms_zpe=-414.201097 te_ms_gfe=-414.246049

5 -2.122850 -0.000040 -0.000051
5 1.177465 0.675833 -0.643192
5 -0.456142 -0.000029 -0.000036
6 0.635504 -0.777119 -0.816209
5 1.177460 -0.675785 0.643245
6 0.635403 0.777132 0.816221
6 0.654066 1.811196 1.902082
1 0.152519 1.457228 2.807454
1 1.679009 2.074682 2.180961
1 0.155660 2.734003 1.591348
6 1.929779 1.674983 -1.594643
1 2.549063 2.394747 -1.051509
1 2.559919 1.167391 -2.330807
1 1.193947 2.259089 -2.161659
6 0.654316 -1.811182 -1.902067
1 1.679298 -2.074743 -2.180733
1 0.155779 -2.733953 -1.591438
1 0.152983 -1.457176 -2.807542
6 1.929752 -1.674909 1.594739
1 1.193904 -2.259149 2.161596
1 2.549202 -2.394560 1.051642
1 2.559725 -1.167302 2.331036
6 -2.932685 -1.038527 0.870089
1 -3.918436 -0.674556 1.180737
1 -3.125634 -1.900986 0.211220
1 -2.406610 -1.434663 1.742922
6 -2.932686 1.038444 -0.870192
1 -3.918434 0.674468 -1.180843
1 -3.125642 1.900901 -0.211323
1 -2.406610 1.434583 -1.743022

05-C8H18B4
lf=32.9 te_zpe=-415.012559 te_gfe=-415.061526 te_ms_zpe=-414.184075 te_ms_gfe=-414.233201

 5 0.006967 -0.901340 1.009298
 5 -2.221048 0.543628 0.015857
 5 2.221059 0.543607 -0.015977
 6 -0.974099 -0.330063 0.009548
 5 -0.006967 -0.901515 -1.009221
 6 0.974099 -0.330070 -0.009570
 6 3.632954 -0.166597 0.008377
 1 4.360447 0.350240 -0.627369
 1 4.024957 -0.087750 1.033031
 1 3.622305 -1.227295 -0.251675
 6 2.133084 2.117722 -0.054495
 1 2.107489 2.417381 -1.113050
 1 1.229229 2.527297 0.403055
 1 3.009743 2.607888 0.380084
 6 0.034283 -1.562164 2.430293
 1 0.798554 -2.341927 2.503630
 1 0.289627 -0.809058 3.186337
 1 -0.924876 -1.998911 2.720004
 6 -0.034336 -1.562704 -2.430045
 1 -0.797045 -2.344113 -2.502264
 1 -0.292194 -0.810422 -3.186047
 1 0.925403 -1.997561 -2.720663
 6 -2.133008 2.117752 0.054044
 1 -1.229520 2.527155 -0.404397
 1 -3.010000 2.607922 -0.379844
 1 -2.106363 2.417611 1.112515
 6 -3.632967 -0.166535 -0.008180
 1 -4.360080 0.350098 0.628176
 1 -4.025524 -0.087178 -1.032579
 1 -3.622272 -1.227335 0.251441

06-C8H18B4
lf=43.8 te_zpe=-414.989337 te_gfe=-415.034007 te_ms_zpe=-414.178285 te_ms_gfe=-414.223102

 5 1.879630 -0.004580 0.010752
 5 0.585471 -0.737024 -0.835320
 5 -2.058109 0.044741 -0.020832
 5 0.567418 -0.527326 0.974948
 6 0.669753 0.883311 -0.101818
 6 -0.532804 -0.063978 -0.008472
 6 -2.820080 1.427980 -0.100451
 1 -3.867597 1.326682 -0.399052
 1 -2.826437 1.871270 0.906746
 1 -2.343492 2.168190 -0.748776
 6 -2.907394 -1.283235 0.074108
 1 -3.401464 -1.449454 -0.894402
 1 -2.337449 -2.184979 0.310281
 1 -3.725236 -1.185049 0.798444
 6 0.600676 -1.553763 -2.178962

1 1.603502 -1.800857 -2.534851
1 0.051719 -2.493899 -2.053139
1 0.087376 -1.002648 -2.974666
6 0.549801 -1.016498 2.469228
1 -0.016847 -1.950438 2.554780
1 1.543547 -1.191012 2.887961
1 0.039511 -0.287818 3.108922
6 3.439196 0.148988 0.008224
1 3.886363 -0.255479 0.922520
1 3.895424 -0.394443 -0.826309
1 3.760202 1.193278 -0.073361
6 0.545635 2.372383 -0.273455
1 0.048417 2.605734 -1.219360
1 -0.062432 2.804445 0.525912
1 1.524145 2.856297 -0.269801

07-C8H18B4
lf=25.6 te_zpe=-414.986916 te_gfe=-415.032497 te_ms_zpe=-414.174932 te_ms_gfe=-414.220661

5 0.701156 1.074950 -0.600720
5 1.174577 -0.555519 -0.755551
5 1.177861 0.347987 0.867250
5 -1.862545 0.103907 -0.054964
6 -0.319227 0.091556 -0.049814
6 0.554680 -1.014985 0.564671
6 1.793563 -1.319042 -1.987021
1 2.041784 -0.674113 -2.833067
1 2.712442 -1.834611 -1.684495
1 1.109723 -2.096598 -2.346638
6 0.179980 -2.281118 1.266409
1 1.086836 -2.816984 1.558851
1 -0.396000 -2.096605 2.178366
1 -0.401306 -2.953272 0.627634
6 1.803728 0.996141 2.159861
1 2.705541 0.448675 2.457279
1 2.079300 2.046686 2.042708
1 1.108833 0.924553 3.004551
6 0.733700 2.446442 -1.364927
1 -0.262786 2.857036 -1.556375
1 1.290783 3.203905 -0.803168
1 1.233065 2.351559 -2.335229
6 -2.630261 0.862420 1.089752
1 -3.628099 0.455920 1.281050
1 -2.083123 0.936720 2.033126
1 -2.783244 1.895490 0.741479
6 -2.645479 -0.616608 -1.214186
1 -2.964826 -1.598182 -0.831140
1 -3.568014 -0.092882 -1.485965
1 -2.060250 -0.802758 -2.117508

08-C8H18B4

lf=28.4 te_zpe=-414.991525 te_gfe=-415.039705 te_ms_zpe=-414.169653 te_ms_gfe=-414.217986

 5 -0.263093 -0.539782 -0.953626
 5 1.583934 1.012213 -0.001029
 5 -2.707717 0.301319 -0.000242
 6 1.012022 -0.443591 0.000269
 5 -0.263079 -0.537694 0.954427
 6 -1.390698 -0.085719 -0.000106
 6 -4.155373 0.776665 -0.000447
 1 -4.684331 0.400272 -0.882720
 1 -4.684798 0.399926 0.881394
 1 -4.231129 1.868292 -0.000275
 6 -0.350212 -1.232140 -2.364887
 1 -1.365887 -1.326288 -2.756337
 1 0.244832 -0.666112 -3.093003
 1 0.096871 -2.233231 -2.335439
 6 0.762105 2.365272 -0.002627
 1 1.065603 2.964372 -0.872497
 1 -0.324308 2.288057 -0.003243
 1 1.064464 2.965679 0.866750
 6 3.167034 1.175439 -0.000734
 1 3.498115 2.217872 -0.001476
 1 3.614927 0.682118 0.870940
 1 3.615294 0.680787 -0.871472
 6 2.041934 -1.586051 0.001492
 1 2.693119 -1.553191 -0.877467
 1 2.693011 -1.551462 0.880461
 1 1.557581 -2.568188 0.002434
 6 -0.350119 -1.226903 2.367225
 1 -1.365912 -1.321866 2.758170
 1 0.098851 -2.227217 2.340633

9. Table S6 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=SH) (ΔE< 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2H6B4S6
lf=9.8 te_zpe=-2568.680398 te_gfe=-2568.727436 te_ms_zpe=-2565.515196 te_ms_gfe=-2565.562369

 5 -0.584846 -0.055662 1.091322
 5 -0.645472 0.990124 -0.493397
 5 -0.637140 -0.907503 -0.623505

 5 2.050092 -0.014193 -0.019991
 6 0.505180 -0.005593 -0.027169
 6 -1.738733 0.009795 0.012158
16 2.897088 1.591864 -0.019161
 1 4.172044 1.166744 -0.006754
16 2.866519 -1.636973 0.012448
 1 4.149547 -1.237184 0.030059
16 -0.539290 -0.158618 2.884273
 1 -1.873041 -0.101217 3.067811
16 -0.595933 2.598423 -1.304039
 1 -1.926729 2.777003 -1.395540
16 -0.646786 -2.398576 -1.629580
 1 -1.983385 -2.472063 -1.780602
16 -3.503219 0.065920 0.055290
 1 -3.704350 -1.214988 0.415249

02-C2H6B4S6
lf=17.4 te_zpe=-2568.674003 te_gfe=-2568.722096 te_ms_zpe=-2565.494825 te_ms_gfe=-2565.543058

 5 0.057603 -1.011657 1.053806
 5 -2.136524 0.502032 0.107790
 5 2.136525 0.501994 -0.107992
 6 -0.923806 -0.448562 0.046736
 5 -0.057602 -1.012027 -1.053472
 6 0.923804 -0.448574 -0.046601
16 -0.061569 -1.722773 -2.701314
 1 -1.397373 -1.816086 -2.832948
16 -1.872644 2.268184 0.413552
 1 -3.152140 2.678062 0.362692
16 -3.742411 -0.318867 -0.134734
 1 -4.549795 0.746663 0.007685
16 0.061565 -1.721839 2.701890
 1 1.397369 -1.815108 2.833563
16 1.872644 2.268067 -0.414214
 1 3.152143 2.677954 -0.363482
16 3.742414 -0.318837 0.134755
 1 4.549793 0.746661 -0.007930

03-C2H6B4S6
lf=39.8 te_zpe=-2568.641087 te_gfe=-2568.685582 te_ms_zpe=-2565.478367 te_ms_gfe=-2565.522994

 5 -0.028068 -0.707198 -0.946327
 5 0.026979 -0.657485 0.956914
 5 0.852164 1.226866 -0.063286
 5 -0.851595 1.223339 0.006004
 6 -1.208808 -0.278860 0.056245
 6 1.207533 -0.278822 -0.068337
16 2.078592 2.543393 -0.101234
 1 1.232367 3.587650 -0.050950
16 -1.949873 2.644743 0.023216
 1 -3.131024 2.007626 0.147856

16 -2.877467 -0.919194 0.069252
 1 -2.606270 -2.141174 0.562132
16 0.086619 -1.595110 2.479942
 1 1.432009 -1.694463 2.523684
16 2.870967 -0.933548 -0.060471
 1 2.564416 -2.209221 -0.360716
16 -0.086962 -1.727004 -2.415208
 1 -1.431270 -1.844406 -2.443940

04-C2H6B4S6
lf=14.5 te_zpe=-2568.660226 te_gfe=-2568.708964 te_ms_zpe=-2565.478136 te_ms_gfe=-2565.527012

 5 1.710645 -0.893455 -0.271125
 5 0.774717 1.774037 0.297469
 6 0.695770 0.264221 -0.048598
 5 -0.775086 1.773448 -0.297859
 6 -0.695198 0.263808 0.048760
 5 -1.709341 -0.894417 0.271739
16 -2.003695 2.651840 -1.270164
 1 -1.384135 3.844590 -1.313548
16 2.002769 2.653545 1.269468
 1 1.382462 3.845922 1.312404
16 2.457432 -1.011220 -1.916359
 1 3.266911 -2.063903 -1.704992
16 2.052388 -1.953330 1.157557
 1 2.961460 -2.773666 0.600328
16 -2.457405 -1.010873 1.916485
 1 -3.267583 -2.062990 1.704985
16 -2.051840 -1.953878 -1.157067
 1 -2.961614 -2.773536 -0.599986

05-C2H6B4S6
lf=14.5 te_zpe=-2568.665266 te_gfe=-2568.716121 te_ms_zpe=-2565.475187 te_ms_gfe=-2565.526186

 5 1.265858 -1.907430 0.000082
 6 0.345106 -0.681764 0.000009
 5 -0.972383 -0.000191 -0.000060
 5 -2.629656 -0.000416 -0.000176
 6 0.344924 0.681736 0.000007
 5 1.265351 1.907646 0.000083
16 1.742155 -2.564618 -1.622149
 1 2.487299 -3.604544 -1.208969
16 1.741322 2.565077 -1.622145
 1 2.486218 3.605178 -1.208960
16 1.740784 2.565270 1.622391
 1 2.485885 3.605272 1.209328
16 1.741500 -2.564908 1.622388
 1 2.486869 -3.604718 1.209321
16 -3.459429 -0.000377 1.609698
 1 -4.743337 -0.000418 1.203899
16 -3.459195 -0.000337 -1.610171

1 -4.743161 -0.000337 -1.204559

06-C2H6B4S6
lf=11.5 te_zpe=-2568.660109 te_gfe=-2568.710837 te_ms_zpe=-2565.471049 te_ms_gfe=-2565.521920

5 -2.409240 -0.400986 -0.241917
5 -1.178982 0.028808 0.839829
5 0.925549 1.831364 -0.096322
6 0.107727 0.673098 0.347101
6 1.393773 0.437507 -0.064248
5 2.395019 -0.708410 -0.262168
16 1.051595 3.591870 -0.379443
1 2.328061 3.608483 -0.805931
16 3.512141 -1.059804 1.123021
1 4.219925 -2.060785 0.570806
16 2.360674 -1.550442 -1.868531
1 3.361134 -2.425734 -1.665977
16 -1.357430 -0.192977 2.620533
1 -2.592075 -0.727438 2.636453
16 -3.292427 0.946346 -1.058255
1 -4.181003 0.237126 -1.781270
16 -2.717956 -2.168224 -0.466935
1 -3.712309 -2.117472 -1.374541

07-C2H6B4S6
lf=37.4 te_zpe=-2568.640895 te_gfe=-2568.686012 te_ms_zpe=-2565.465881 te_ms_gfe=-2565.511137

5 -1.408662 1.321255 -0.010695
5 -1.408649 -1.321262 0.010606
6 -0.755748 -0.000001 -0.000071
5 1.408649 -1.321261 0.010591
5 1.408660 1.321255 -0.010683
6 0.755745 -0.000001 -0.000071
16 -3.150329 -1.848861 -0.110717
1 -2.986786 -3.142607 0.212469
16 -3.150345 1.848849 0.110608
1 -2.986739 3.142695 -0.212142
16 3.150346 1.848843 0.110596
1 2.986741 3.142690 -0.212151
16 3.150331 -1.848856 -0.110705
1 2.986785 -3.142604 0.212471
16 0.000001 2.677470 -0.196484
16 -0.000001 -2.677431 0.196746
1 -0.000004 3.174684 1.055719
1 -0.000008 -3.175001 -1.055313

08-C2H6B4S6
lf=11.9 te_zpe=-2568.630824 te_gfe=-2568.677941 te_ms_zpe=-2565.462751 te_ms_gfe=-2565.510007

5 -2.108418 -0.000115 -0.000169

 5 1.212925 -0.719287 0.629659
 5 -0.432137 -0.000061 -0.000104
 6 0.674525 0.702230 0.867002
 5 1.212973 0.719398 -0.629497
 6 0.674760 -0.702186 -0.866966
16 0.631155 -1.914414 -2.151233
 1 1.776489 -1.556939 -2.759323
16 -2.926824 1.372894 -0.842990
 1 -4.213309 1.029351 -0.641739
16 0.630474 1.914489 2.151229
 1 1.775493 1.556902 2.759845
16 2.077083 1.937786 -1.629003
 1 2.179304 2.869422 -0.660189
16 2.076978 -1.937611 1.629294
 1 2.179397 -2.869245 0.660498
16 -2.926774 -1.373134 0.842687
 1 -4.213271 -1.029595 0.641511

09-C2H6B4S6
lf=15.6 te_zpe=-2568.606473 te_gfe=-2568.653063 te_ms_zpe=-2565.462561 te_ms_gfe=-2565.509294

 5 -0.788762 -0.905986 -0.233791
 5 0.706871 0.988505 0.090422
 5 -0.958477 0.786074 -0.120195
 6 -0.216115 -0.025585 1.088850
 5 0.891982 -0.751418 0.258215
 6 0.242184 -0.017319 -1.067142
16 1.863038 2.385971 0.263302
 1 2.953757 1.641748 0.530217
16 -2.315977 1.975013 -0.355026
 1 -3.307624 1.078934 -0.508551
16 -1.933183 -2.298709 -0.513362
 1 -1.105218 -3.261535 -0.067034
16 -0.662777 0.020830 2.794359
 1 0.293754 -0.818981 3.227749
16 2.282436 -1.883327 0.603637
 1 2.581277 -2.101354 -0.690576
16 0.624229 -0.066596 -2.781978
 1 1.445326 1.001822 -2.770222

10-C2H6B4S6
lf=7.9 te_zpe=-2568.624485 te_gfe=-2568.671790 te_ms_zpe=-2565.459955 te_ms_gfe=-2565.507397

 5 1.891186 -0.049488 -0.003427
 5 0.609317 -0.689004 -0.919779
 5 -2.003327 0.080763 0.003809
 5 0.604453 -0.613938 0.973172
 6 0.716731 0.912304 -0.044574
 6 -0.466885 -0.042725 0.006304
16 -2.778500 1.722765 0.008233
 1 -4.066588 1.341115 0.001794

16 -2.898688 -1.502781 0.005073
 1 -4.155443 -1.028436 0.017904
16 0.461941 -1.354519 2.602639
 1 1.778588 -1.479261 2.853983
16 0.562400 2.649922 -0.134378
 1 1.881712 2.913351 -0.172075
16 3.705821 0.183165 0.008184
 1 4.025733 -1.117031 -0.102570
16 0.433586 -1.560325 -2.482369
 1 1.743820 -1.700503 -2.756397

11-C2H6B4S6
lf=8.7 te_zpe=-2568.652872 te_gfe=-2568.704507 te_ms_zpe=-2565.459764 te_ms_gfe=-2565.511544

 6 -0.590358 0.224688 -0.605122
 6 0.594246 -0.085680 -0.644699
 5 2.054451 -0.429166 -0.642587
 5 -2.046136 0.572489 -0.534776
 5 -3.138773 -0.361690 0.373503
 5 3.112249 0.245922 0.497940
16 -4.029311 0.476928 1.702233
 1 -4.746590 -0.554071 2.190163
16 -3.299235 -2.100693 -0.085258
 1 -4.257176 -2.481391 0.782057
16 -2.700636 1.999162 -1.423166
 1 -1.561412 2.428954 -1.999369
16 2.630120 -1.573646 -1.914159
 1 3.929680 -1.615421 -1.568110
16 3.531175 1.990461 0.288876
 1 4.394035 2.147079 1.311696
16 3.730452 -0.849168 1.796110
 1 4.508147 0.014304 2.477900

12-C2H6B4S6
lf=7.9 te_zpe=-2568.652822 te_gfe=-2568.704345 te_ms_zpe=-2565.459679 te_ms_gfe=-2565.511347

 5 2.061393 -0.563909 0.506456
 5 3.105009 0.555273 -0.224161
 6 0.607620 -0.622509 0.141516
 5 -2.020771 -0.628571 -0.571491
 6 -0.570822 -0.636214 -0.193536
 5 -3.152893 0.321319 0.269694
16 -4.064555 1.553272 -0.685680
 1 -4.813167 2.100618 0.291864
16 -3.329675 -0.002122 2.037302
 1 -4.316651 0.865308 2.334191
16 -2.625846 -1.641796 -1.935581
 1 -1.465114 -2.221515 -2.297675
16 2.640434 -1.727796 1.758807
 1 3.936371 -1.366601 1.779357
16 4.294824 -0.095472 -1.420116

 1 4.919324 1.045003 -1.773043
16 2.936548 2.281245 0.278113
 1 3.927098 2.831670 -0.450599

13-C2H6B4S6
lf=11.9 te_zpe=-2568.651478 te_gfe=-2568.702858 te_ms_zpe=-2565.459612 te_ms_gfe=-2565.511138

 5 -2.546419 0.921568 0.127333
 6 2.024721 -0.306524 -0.213105
 5 -1.752675 -0.520647 0.492147
 5 3.446341 0.163766 -0.022081
 5 -0.555674 -1.135220 -0.518187
 6 0.878274 -0.693770 -0.376326
16 3.923085 1.683514 -0.893903
 1 5.201251 1.757443 -0.483638
16 4.498395 -0.850773 1.055650
 1 5.630364 -0.130787 0.967444
16 -0.924893 -2.299172 -1.847773
 1 -2.247466 -2.433439 -1.637385
16 -2.161047 -1.466667 1.955332
 1 -3.136626 -0.698348 2.481095
16 -4.192817 0.774562 -0.613976
 1 -4.481085 2.075490 -0.812730
16 -1.687499 2.466922 0.501995
 1 -2.625864 3.349912 0.108534

14-C2H6B4S6
lf=10.5 te_zpe=-2568.651154 te_gfe=-2568.702746 te_ms_zpe=-2565.459081 te_ms_gfe=-2565.510819

 5 -2.551664 0.937295 0.139754
 5 -0.570631 -1.137208 -0.542579
 5 -1.769861 -0.525459 0.467194
 6 2.001995 -0.298053 -0.212990
 5 3.421979 0.173751 -0.014240
 6 0.855632 -0.684797 -0.380470
16 -4.209438 0.834232 -0.577803
 1 -4.459685 2.143476 -0.774131
16 -1.646224 2.461938 0.495357
 1 -2.564760 3.367741 0.107516
16 -2.257885 -1.398015 1.950764
 1 -1.457963 -2.481504 1.879702
16 -1.025386 -2.341543 -1.807587
 1 0.190719 -2.538599 -2.352210
16 3.926597 1.647786 -0.945947
 1 5.196965 1.732550 -0.514122
16 4.444586 -0.796820 1.130809
 1 5.583856 -0.089695 1.033871

15-C2H6B4S6
lf=23.3 te_zpe=-2568.631492 te_gfe=-2568.678925 te_ms_zpe=-2565.457231 te_ms_gfe=-2565.504805

 5 0.376451 1.135917 -0.354665
 5 -1.472462 -0.760819 -0.712226
 5 2.784834 -0.113988 0.056870
 6 -0.917531 0.383515 0.208638
 5 0.263618 -0.173939 1.140148
 6 1.469422 0.245086 0.275609
16 0.089899 -0.836618 2.810919
 1 1.400259 -0.958149 3.087946
16 -2.185104 1.388049 1.097132
 1 -2.782811 1.920058 0.015408
16 -3.267073 -1.071551 -0.693315
 1 -3.291708 -2.076848 -1.587367
16 -0.312945 -1.729880 -1.755704
 1 -1.214641 -2.533169 -2.343745
16 0.409236 2.705408 -1.246973
 1 1.744588 2.837771 -1.329473
16 4.392733 -0.679375 -0.329283
 1 5.042840 0.186349 0.476720

16-C2H6B4S6
lf=18.9 te_zpe=-2568.626111 te_gfe=-2568.673606 te_ms_zpe=-2565.455674 te_ms_gfe=-2565.503310

 5 -1.262905 -1.248790 -0.296963
 5 -0.938311 1.456103 -0.286205
 6 -0.301908 0.011313 -0.263860
 5 1.022088 -0.100223 0.635811
 6 1.018035 -0.152966 -0.907567
 5 2.334807 -0.315312 -0.636884
16 -1.391706 -2.123134 -1.878916
 1 -2.252888 -3.091435 -1.520814
16 -2.125516 -1.703364 1.231913
 1 -2.884449 -2.708772 0.762142
16 -2.610062 1.703386 0.391999
 1 -2.709057 3.024621 0.168286
16 0.085376 2.785109 -0.993915
 1 -0.750122 3.813290 -0.769762
16 1.397518 -0.055796 2.370945
 1 2.736597 -0.198226 2.279557
16 4.120554 -0.429641 -0.529362
 1 4.166141 -1.773413 -0.452257

17-C2H6B4S6
lf=16.7 te_zpe=-2568.630222 te_gfe=-2568.677800 te_ms_zpe=-2565.455158 te_ms_gfe=-2565.502876

 5 -0.118033 0.099057 0.664285
 5 2.271826 -0.408092 -0.626380
 5 -2.811470 0.068021 -0.280240
 6 1.220518 0.698908 -0.253957
 5 -0.131717 0.786131 -0.873528
 6 -1.307558 0.316604 -0.283828

16 3.983247 -0.168283 -0.078813
 1 4.491067 -1.316672 -0.562540
16 1.664776 -1.845115 -1.569545
 1 2.800348 -2.561717 -1.601355
16 0.128459 -0.528035 2.327326
 1 -1.163187 -0.803666 2.589947
16 -3.448258 -1.266809 0.785110
 1 -4.766651 -1.094806 0.592770
16 -3.823865 1.135098 -1.348020
 1 -5.035492 0.606240 -1.103501
16 1.861450 2.269018 0.481441
 1 2.290182 2.817982 -0.669283

18-C2H6B4S6
lf=18.3 te_zpe=-2568.631206 te_gfe=-2568.677401 te_ms_zpe=-2565.454773 te_ms_gfe=-2565.501105

 5 -1.746307 1.062712 -0.021155
 5 1.747398 -1.056170 0.029860
 5 -1.740868 -1.068534 -0.025010
 5 1.742508 1.063508 0.036364
 6 0.719964 0.003950 0.081517
 6 -0.723986 -0.000518 -0.078185
16 -1.828390 -2.823199 0.453894
 1 -3.108654 -3.043509 0.110225
16 -3.313519 -0.010673 -0.535087
16 -2.025977 2.803969 0.405785
 1 -0.748910 3.080549 0.731103
16 1.854973 2.809951 -0.486379
 1 3.076138 3.079045 0.005689
16 3.298983 0.009325 0.587726
16 1.865880 -2.797337 -0.484375
 1 3.137733 -3.014675 -0.109024
 1 -4.075478 -0.014771 0.591382
 1 4.098442 0.012625 -0.514703

19-C2H6B4S6
lf=74.5 te_zpe=-2568.598100 te_gfe=-2568.642295 te_ms_zpe=-2565.453051 te_ms_gfe=-2565.497384

 5 0.776152 0.136639 1.025395
 5 -0.911780 0.610739 0.550739
 5 0.978808 -0.405155 -0.646407
 5 0.417819 1.208916 -0.278957
 6 -0.522158 -0.122277 -0.888720
 6 -0.277660 -0.888052 0.488159
16 -2.528659 1.093885 1.243329
 1 -2.430935 2.400933 0.943584
16 0.838172 2.846367 -0.961529
 1 1.839806 2.440265 -1.763245
16 2.247264 -1.330972 -1.558911
 1 3.206506 -1.197845 -0.624494
16 1.797413 0.138802 2.536365

 1 2.282760 1.381109 2.362835
16 -0.855505 -2.492171 0.930904
 1 -1.744043 -2.588495 -0.080359
16 -1.621579 -0.521586 -2.190741
 1 -2.693876 0.121112 -1.679465

20-C2H6B4S6
lf=16.7 te_zpe=-2568.618188 te_gfe=-2568.664317 te_ms_zpe=-2565.451924 te_ms_gfe=-2565.498194

 5 -1.406005 0.193572 0.550321
 6 0.000009 0.000004 -0.128500
 5 0.228012 1.255603 -1.331536
 5 1.405922 -0.193575 0.550525
 5 -0.227816 -1.255585 -1.331580
 6 0.000140 0.000011 -1.913813
16 -2.800977 0.589294 -0.565746
 1 -3.757534 0.690981 0.374006
16 -1.621068 -0.031002 2.346195
 1 -2.940345 0.214409 2.411238
16 1.620737 0.031039 2.346425
 1 2.939977 -0.214516 2.411675
16 2.801044 -0.589350 -0.565335
 1 3.757471 -0.691003 0.374552
16 0.559278 2.995014 -1.171814
 1 0.608189 3.235409 -2.495488
16 -0.559102 -2.994998 -1.171921
 1 -0.607808 -3.235383 -2.495604

21-C2H6B4S6
lf=14.7 te_zpe=-2568.643548 te_gfe=-2568.695145 te_ms_zpe=-2565.450834 te_ms_gfe=-2565.502581

 5 1.760414 1.443197 0.275762
 5 1.760354 -1.443162 -0.275793
 5 0.917684 0.000073 -0.000217
 6 -1.798482 0.000107 -0.000078
 5 -3.303053 0.000142 -0.000018
 6 -0.572361 0.000088 -0.000132
16 -4.115499 -0.340342 1.589790
 1 -5.392088 -0.247316 1.179495
16 -4.115610 0.340515 -1.589793
 1 -5.392170 0.247411 -1.179426
16 2.547814 -1.651820 -1.889924
 1 3.048911 -2.892576 -1.735203
16 1.815327 -2.619625 1.096797
 1 2.649992 -3.538893 0.573883
16 1.815936 2.619775 -1.096705
 1 2.650771 3.538760 -0.573565
16 2.547869 1.651381 1.889957
 1 3.049258 2.892049 1.735478

22-C2H6B4S6
lf=23.4 te_zpe=-2568.614038 te_gfe=-2568.660189 te_ms_zpe=-2565.449851 te_ms_gfe=-2565.496141

 5 0.890546 -0.657079 -0.934403
 5 1.211874 -0.577249 0.783134
 5 1.205685 0.916606 -0.377598
 5 -1.821921 -0.225647 -0.242308
 6 -0.273730 -0.123408 -0.156361
 6 0.469000 0.723274 0.955690
16 1.937453 -1.796458 1.892025
 1 2.266108 -2.706925 0.956513
16 1.136658 -1.805010 -2.322898
 1 2.452596 -1.575106 -2.473954
16 -2.573900 -1.666781 0.548197
 1 -3.861106 -1.403978 0.260960
16 -0.153342 1.696967 2.271135
 1 -0.502815 2.776781 1.544440
16 -2.657416 1.108210 -1.136563
 1 -3.926470 0.693125 -0.978174
16 1.884933 2.344487 -1.252335
 1 1.778961 3.231083 -0.242874

23-C2H6B4S6
lf=9.6 te_zpe=-2568.625708 te_gfe=-2568.674325 te_ms_zpe=-2565.448685 te_ms_gfe=-2565.497444

 5 0.978124 -1.327926 -0.373941
 6 0.274731 0.011490 0.039031
 5 -0.233453 0.023357 1.522379
 5 0.678384 1.419347 -0.509220
 5 -2.501084 -0.208248 -0.077158
 6 -1.249366 -0.117318 0.476283
16 2.349675 1.722137 -1.179023
 1 2.217141 3.038249 -1.414821
16 -0.599439 2.730136 -0.432834
 1 0.133594 3.738624 -0.935761
16 0.298351 0.117168 3.210285
 1 -0.920349 0.020099 3.775219
16 -0.095856 -2.711690 -0.871884
 1 0.856760 -3.619015 -1.148171
16 2.794494 -1.452567 -0.263258
 1 2.940396 -2.707123 -0.720482
16 -4.097401 -0.421300 -0.748508
 1 -4.386764 0.889346 -0.894611

24-C2H6B4S6
lf=13.4 te_zpe=-2568.616561 te_gfe=-2568.664404 te_ms_zpe=-2565.438327 te_ms_gfe=-2565.486311

 5 0.509778 -0.172146 -0.333802
 5 -2.115696 -1.000577 -0.125357
 5 2.629528 -0.473450 -0.010766
 6 -0.994896 -0.049061 -0.190012

 5 -1.854664 1.111097 0.117274
 6 1.751959 0.601426 -0.489878
16 4.279608 -0.730519 0.709793
 1 4.594936 0.572858 0.826292
16 1.978766 2.321576 -0.779877
 1 3.322536 2.350298 -0.723666
16 -2.335903 -2.799646 0.011252
 1 -3.675642 -2.840012 -0.077660
16 -1.657583 2.817353 0.690464
 1 -2.946986 3.188055 0.607968
16 1.444334 -1.980720 -0.275494
16 -3.633998 0.267797 -0.161242
 1 -4.127114 0.183200 1.099143
 1 1.241595 -2.426659 0.992183

10. Table S7 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=Cl) ($\Delta E<$ 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2B4Cl6
lf=23.7 te_zpe=-2937.217894 te_gfe=-2937.264238 te_ms_zpe=-2933.999997 te_ms_gfe=-2934.046452

 5 0.000056 -0.964031 -1.025496
 5 2.202887 0.473893 0.000055
 5 -2.202887 0.473895 -0.000132
 6 0.971955 -0.432907 0.000075
 5 -0.000059 -0.963901 1.025597
 6 -0.971956 -0.432906 -0.000041
17 -2.068860 2.222935 -0.000149
17 -3.785209 -0.291881 -0.000107
17 0.000155 -1.634292 -2.636001
17 2.068864 2.222934 -0.000119
17 3.785209 -0.291883 0.000170
17 -0.000157 -1.633954 2.636189

02-C2B4Cl6
lf=5.8 te_zpe=-2937.202640 te_gfe=-2937.247559 te_ms_zpe=-2933.998777 te_ms_gfe=-2934.043800

 5 0.665457 1.105307 -0.149693
 5 0.609979 -0.410409 1.004969
 5 0.625674 -0.670711 -0.861609
 5 -2.023116 0.028106 -0.012213
 6 -0.492034 0.042420 -0.015921

 6 1.747196 -0.004880 0.002697
17 -2.894960 -1.502662 -0.010264
17 -2.950427 1.523715 -0.002668
17 0.632939 -1.748451 -2.227532
17 0.736111 2.828060 -0.383754
17 3.467569 -0.049679 0.022922
17 0.601653 -1.079613 2.611419

03-C2B4Cl6
lf=20.1 te_zpe=-2937.208300 te_gfe=-2937.256628 te_ms_zpe=-2933.980737 te_ms_gfe=-2934.029179

 5 -1.261094 -1.931920 -0.000215
 6 -0.396600 -0.678641 -0.000072
 5 0.922624 0.000045 0.000033
 5 2.569861 0.000108 0.000098
 6 -0.396651 0.678632 0.000036
 5 -1.261240 1.931845 0.000113
17 -1.735247 -2.667206 1.522209
17 -1.735123 -2.666938 -1.522807
17 3.467927 0.000202 -1.516325
17 3.467789 -0.000037 1.516605
17 -1.735398 2.666855 1.522669
17 -1.735316 2.667105 -1.522347

04-C2B4Cl6
lf=12.6 te_zpe=-2937.198672 te_gfe=-2937.246094 te_ms_zpe=-2933.980106 te_ms_gfe=-2934.027638

 5 -1.713526 -0.885652 0.198429
 5 -0.766650 1.781617 -0.309867
 6 -0.695840 0.265428 0.027944
 5 0.766081 1.781943 0.309533
 6 0.695805 0.265688 -0.028118
 5 1.713913 -0.885044 -0.198433
17 -1.927867 2.684647 -1.255074
17 -2.703616 -0.966149 1.642098
17 -1.910722 -2.077031 -1.076857
17 2.704048 -0.965380 -1.642078
17 1.911490 -2.076205 1.076998
17 1.926732 2.685353 1.255073

05-C2B4Cl6
lf=45.4 te_zpe=-2937.191125 te_gfe=-2937.233076 te_ms_zpe=-2933.976705 te_ms_gfe=-2934.018760

 5 -1.400763 -1.307270 -0.000021
 5 1.400705 -1.307306 0.000050
 5 -1.400795 1.307236 0.000066
 5 1.400741 1.307271 -0.000019
 6 0.745551 -0.000006 0.000089
 6 -0.745548 -0.000007 0.000093
17 -3.019485 1.953477 0.000011

17 -3.019484 -1.953460 -0.000014
17 0.000024 2.661547 -0.000065
17 3.019485 1.953428 -0.000043
17 0.000018 -2.661545 0.000018
17 3.019474 -1.953422 0.000006

06-C2B4Cl6
lf=15.7 te_zpe=-2937.194791 te_gfe=-2937.243596 te_ms_zpe=-2933.968000 te_ms_gfe=-2934.016920

 5 -2.411320 -0.487493 -0.227469
 5 -1.214251 0.152175 0.775408
 5 0.922781 1.817527 -0.282837
 6 0.087483 0.725161 0.251713
 6 1.391781 0.442828 -0.092426
 5 2.408906 -0.691663 -0.136473
17 1.149471 3.465641 -0.762936
17 3.481861 -0.963021 1.226758
17 2.545042 -1.689863 -1.576178
17 -1.533713 0.207578 2.515808
17 -3.618470 0.553930 -0.965450
17 -2.459846 -2.219010 -0.532053

07-C2B4Cl6
lf=16.0 te_zpe=-2937.167890 te_gfe=-2937.213808 te_ms_zpe=-2933.959156 te_ms_gfe=-2934.005185

 5 1.014326 1.429465 -0.353231
 5 1.176346 -1.298956 -0.243745
 6 0.334207 0.022871 -0.296405
 5 -0.987787 -0.036950 0.632039
 6 -1.030051 -0.085081 -0.881636
 5 -2.354311 -0.171454 -0.644498
17 2.747426 1.662864 -0.159171
17 0.039045 2.875539 -0.637537
17 -1.404808 -0.034461 2.307325
17 -4.051926 -0.283850 -0.532873
17 0.873477 -2.601433 -1.391099
17 2.381033 -1.573792 1.008379

08-C2B4Cl6
lf=9.3 te_zpe=-2937.163750 te_gfe=-2937.209496 te_ms_zpe=-2933.957360 te_ms_gfe=-2934.003219

 5 -1.376141 0.046879 0.560296
 6 -0.000042 0.000478 -0.174646
 5 0.129274 1.264462 -1.385025
 5 1.371516 -0.050639 0.568097
 5 -0.121034 -1.255138 -1.393637
 6 0.004261 0.006730 -1.987546
17 -1.604885 -0.733731 2.123322
17 -2.796152 0.785945 -0.186001
17 1.587368 0.708746 2.143379

17 2.799205 -0.773484 -0.179535
17 0.345476 2.959447 -1.315618
17 -0.333564 -2.951104 -1.337047

09-C2B4Cl6
lf=25.3 te_zpe=-2937.186439 te_gfe=-2937.235478 te_ms_zpe=-2933.955601 te_ms_gfe=-2934.004761

 5 -1.754005 1.456530 -0.000120
 5 -1.754116 -1.456487 -0.000025
 5 -0.912474 -0.000011 -0.000064
 6 1.798272 -0.000069 0.000035
 5 3.293868 -0.000056 0.000114
 6 0.572012 -0.000071 -0.000018
17 4.169142 -0.000073 -1.524893
17 4.168981 0.000011 1.525214
17 -2.210887 -2.209333 1.520757
17 -2.210902 -2.209415 -1.520760
17 -2.210769 2.209483 1.520610
17 -2.210746 2.209384 -1.520906

10-C2B4Cl6
lf=21.2 te_zpe=-2937.170336 te_gfe=-2937.216226 te_ms_zpe=-2933.955302 te_ms_gfe=-2934.001302

 5 -0.402266 0.997816 -0.430204
 5 1.728968 -0.000016 0.838717
 5 -2.866272 -0.000058 0.182996
 6 0.854991 0.000049 -0.438849
 5 -0.402237 -0.997758 -0.430311
 6 -1.516419 -0.000003 -0.128686
17 -0.457261 -2.705807 -0.839051
17 -4.482507 -0.000065 0.591524
17 -0.457343 2.705908 -0.838760
17 1.770887 0.000146 -2.007287
17 0.948158 -0.000137 2.437516
17 3.482630 -0.000056 0.808953

11-C2B4Cl6
lf=12.9 te_zpe=-2937.168250 te_gfe=-2937.215504 te_ms_zpe=-2933.951873 te_ms_gfe=-2933.999240

 5 0.839257 -1.378287 -0.328087
 6 0.256383 0.024617 0.011876
 5 -0.307051 0.145286 1.482307
 5 0.856253 1.338721 -0.550780
 5 -2.548493 -0.033931 -0.093602
 6 -1.282657 0.060628 0.422316
17 -0.137037 2.799356 -0.690278
17 2.533740 1.484777 -1.077750
17 2.532699 -1.787157 -0.071922
17 -0.209911 -2.664699 -0.941896
17 0.101808 0.256976 3.152096

17 -4.117899 -0.140454 -0.673447

12-C2B4Cl6
lf=14.3 te_zpe=-2937.181984 te_gfe=-2937.231988 te_ms_zpe=-2933.951035 te_ms_gfe=-2934.001159

 5 2.033288 -0.599796 0.558972
 5 3.136199 0.430460 -0.199455
 6 0.585054 -0.640092 0.179731
 5 -2.033308 -0.599842 -0.558945
 6 -0.585055 -0.640135 -0.179777
 5 -3.136178 0.430468 0.199467
17 -3.411805 2.048544 -0.428960
17 -4.029933 -0.112650 1.611258
17 -2.623943 -1.660133 -1.845102
17 2.623878 -1.660124 1.845118
17 4.029946 -0.112725 -1.611225
17 3.411856 2.048553 0.428916

13-C2B4Cl6
lf=14.1 te_zpe=-2937.179083 te_gfe=-2937.228687 te_ms_zpe=-2933.948822 te_ms_gfe=-2933.998547

 5 -2.665265 0.860430 0.066098
 6 2.081495 -0.275139 -0.206197
 5 -1.726176 -0.467263 0.496061
 5 3.495331 0.209244 -0.051796
 5 -0.491908 -1.122452 -0.447988
 6 0.936390 -0.678095 -0.340467
17 4.068797 1.557063 -1.020649
17 4.566899 -0.573931 1.097882
17 -2.065193 -1.247060 2.047111
17 -0.931170 -2.375518 -1.617873
17 -4.149851 0.648912 -0.850441
17 -2.146376 2.479921 0.518565

14-C2B4Cl6
lf=8.9 te_zpe=-2937.160274 te_gfe=-2937.206508 te_ms_zpe=-2933.945121 te_ms_gfe=-2933.991464

 5 0.141916 0.702660 -0.042834
 5 -2.294342 -0.646936 -0.293162
 5 2.790012 -0.300683 0.159068
 6 -1.238565 -0.072974 0.695930
 5 0.092961 -0.705630 0.905768
 6 1.288160 -0.206402 0.375759
17 3.624864 0.802816 -0.930386
17 3.740945 -1.525454 1.000651
17 0.004549 2.172317 -0.960787
17 -1.861649 0.901614 2.075595
17 -4.011684 -0.400892 -0.089944
17 -1.729397 -1.572213 -1.687737

15-C2B4Cl6
lf=23.1 te_zpe=-2937.142022 te_gfe=-2937.185933 te_ms_zpe=-2933.938300 te_ms_gfe=-2933.982317

 5 1.899784 -0.001284 0.000126
 5 0.605118 -0.645944 -0.931247
 5 -2.000399 0.059109 -0.000183
 5 0.604968 -0.645489 0.931587
 6 0.710947 0.915229 -0.000194
 6 -0.480450 -0.053032 -0.000073
17 -2.851815 1.596727 -0.000401
17 -2.935195 -1.433723 0.000079
17 0.569799 2.626831 -0.000616
17 0.584027 -1.442093 2.481349
17 3.641042 0.154079 0.000226
17 0.584475 -1.443300 -2.480626

16-C2B4Cl6
lf=21.2 te_zpe=-2937.152106 te_gfe=-2937.198470 te_ms_zpe=-2933.937656 te_ms_gfe=-2933.984135

 5 -1.063067 1.155091 0.459860
 5 -1.487271 -1.202384 -1.038439
 5 -0.542437 -0.441681 0.333206
 6 0.899403 -0.616032 -0.582999
 5 2.355792 -0.232756 -0.361659
 6 -0.058872 -1.193227 -1.213234
17 -1.718886 1.807799 1.955475
17 -1.008079 2.244329 -0.945770
17 -0.630245 -1.598950 1.768096
17 -3.051097 -1.604548 -1.538840
17 3.346642 -1.214977 0.689960
17 2.981766 1.217182 -1.116419

17-C2B4Cl6
lf=63.8 te_zpe=-2937.121884 te_gfe=-2937.163526 te_ms_zpe=-2933.937503 te_ms_gfe=-2933.979246

 5 0.862108 -0.861750 -0.000205
 5 -0.862037 0.861744 0.000443
 5 -0.861513 -0.862290 0.001257
 6 0.001018 0.000615 1.085179
 5 0.861591 0.862237 -0.001438
 6 -0.001014 -0.000631 -1.085149
17 0.002767 0.001693 2.802780
17 -2.098780 2.095629 0.000755
17 -2.097276 -2.097158 0.002904
17 2.098798 -2.095694 -0.000686
17 2.097224 2.097237 -0.003031
17 -0.002779 -0.001685 -2.802748

18-C2B4Cl6

lf=39.1 te_zpe=-2937.140653 te_gfe=-2937.183281 te_ms_zpe=-2933.937239 te_ms_gfe=-2933.979970

 5 -0.000026 -0.700294 -0.944172
 5 0.000027 -0.700036 0.944264
 5 0.854070 1.241919 -0.000410
 5 -0.854071 1.241918 -0.000054
 6 -1.201163 -0.263173 0.000040
 6 1.201164 -0.263171 -0.000066
17 -2.011810 2.550095 -0.000328
17 2.011807 2.550098 -0.000085
17 2.809231 -0.954745 -0.000008
17 -2.809231 -0.954747 0.000180
17 0.000084 -1.661477 2.383470
17 -0.000081 -1.662134 -2.383110

19-C2B4Cl6
lf=12.5 te_zpe=-2937.161197 te_gfe=-2937.209889 te_ms_zpe=-2933.932528 te_ms_gfe=-2933.981337

 5 -1.793695 1.425058 -0.000163
 5 -1.681441 -1.322560 0.000080
 6 0.348404 0.060394 0.000014
 6 -0.974899 0.082033 -0.000025
 5 1.724376 0.000436 0.000057
 5 3.338536 -0.056100 0.000100
17 -3.552203 1.341767 -0.000251
17 -1.012010 2.988234 -0.000257
17 -2.065550 -2.108481 1.518979
17 -2.065433 -2.108762 -1.518706
17 4.224670 -0.088638 -1.525202
17 4.224649 -0.088164 1.525419

20-C2B4Cl6
lf=27.5 te_zpe=-2937.138111 te_gfe=-2937.182234 te_ms_zpe=-2933.930615 te_ms_gfe=-2933.974844

 5 2.106241 -0.000022 -0.000144
 5 -1.226082 -0.953864 0.000020
 5 0.443813 -0.000021 -0.000076
 6 -0.674598 0.000075 -1.102589
 5 -1.226049 0.953877 0.000158
 6 -0.674411 -0.000081 1.102660
17 2.988942 -1.519161 -0.000299
17 2.988917 1.519135 -0.000084
17 -0.696995 -0.000205 2.825864
17 -2.068047 -2.476834 -0.000027
17 -2.067962 2.476876 0.000321
17 -0.697535 0.000202 -2.825788

21-C2B4Cl6
lf=22.2 te_zpe=-2937.132396 te_gfe=-2937.176892 te_ms_zpe=-2933.928822 te_ms_gfe=-2933.973425

 5 0.878733 -0.000034 1.137486
 5 1.216346 0.951190 -0.258569
 5 1.216345 -0.951174 -0.258629
 5 -1.814801 -0.000010 0.303436
 6 -0.274938 -0.000005 0.186124
 6 0.496317 0.000036 -1.194090
17 1.153632 -0.000089 2.865737
17 1.906208 -2.552075 -0.376070
17 1.906208 2.552098 -0.375918
17 -0.152072 0.000088 -2.785817
17 -2.666148 1.525078 0.378115
17 -2.666146 -1.525103 0.378021

22-C2B4Cl6
lf=80.9 te_zpe=-2937.112849 te_gfe=-2937.154278 te_ms_zpe=-2933.928362 te_ms_gfe=-2933.969891

 5 -0.002697 0.986651 0.853946
 5 -1.224222 0.085372 -0.002862
 5 1.224108 0.087134 0.002790
 5 0.001300 0.987445 -0.853068
 6 0.002167 -0.652128 -0.782436
 6 -0.001232 -0.652733 0.781947
17 0.003676 2.087477 -2.216826
17 0.005749 -1.991087 -1.847424
17 2.951541 -0.178065 0.006497
17 -0.002820 -1.992564 1.845826
17 -0.006746 2.085642 2.218530
17 -2.951286 -0.182218 -0.006666

23-C2B4Cl6
lf=6.7 te_zpe=-2937.156623 te_gfe=-2937.206090 te_ms_zpe=-2933.923411 te_ms_gfe=-2933.972996

 5 3.309369 -0.123833 0.000253
 6 1.852046 -0.068419 0.000183
 5 0.468508 0.004455 0.000026
 5 -1.761597 -1.282821 -0.000114
 5 -1.700329 1.409564 -0.000137
 6 -0.956574 0.044123 -0.000081
17 -3.465121 1.452043 0.000363
17 -0.838836 2.943448 -0.000666
17 -2.218864 -2.036368 -1.518130
17 -2.218488 -2.036719 1.517839
17 4.166119 -0.158018 1.546611
17 4.166215 -0.157977 -1.546061

24-C2B4Cl6
lf=14.3 te_zpe=-2937.146513 te_gfe=-2937.193613 te_ms_zpe=-2933.920518 te_ms_gfe=-2933.967734

 5 -0.276052 -0.000020 0.413214
 5 2.142410 -1.095516 0.048291

 5 -2.664527 -0.000092 -0.498469
 6 1.175284 -0.000005 0.200449
 5 2.142356 1.095536 0.048273
 6 -1.672113 -0.000183 0.626693
17 2.315645 -2.802117 0.016450
17 3.796793 -0.000024 -0.204853
17 2.315646 2.802121 0.016364
17 -2.046021 0.000037 -2.184897
17 -4.415522 -0.000066 -0.272838
17 -2.186538 0.000143 2.334516

11. Table S8 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=NH_2) (ΔE< 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2H12B4N6
lf=30.3 te_zpe=-511.572391 te_gfe=-511.614080 te_ms_zpe=-510.711356 te_ms_gfe=-510.753175

 5 -0.074425 -1.099057 1.088782
 5 -1.958846 0.600776 -0.146502
 5 1.959079 0.601071 0.142316
 6 -0.898363 -0.545733 -0.053305
 5 0.074066 -1.106670 -1.081174
 6 0.898229 -0.545697 0.057020
 7 1.564023 1.922287 0.505687
 1 2.216395 2.676309 0.652676
 1 0.637921 2.111911 0.853403
 7 3.316397 0.309972 -0.166254
 1 4.070796 0.971784 -0.081162
 1 3.611793 -0.614945 -0.426539
 7 0.141577 -1.632863 -2.376350
 1 1.011419 -1.823951 -2.845117
 1 -0.676254 -1.807293 -2.936599
 7 -0.142198 -1.616094 2.387625
 1 -1.012150 -1.803535 2.857661
 1 0.675542 -1.787024 2.949086
 7 -1.562917 1.920038 -0.515794
 1 -0.635942 2.107984 -0.862103
 1 -2.214880 2.673438 -0.667688
 7 -3.316803 0.311333 0.160887
 1 -3.612815 -0.612245 0.425197
 1 -4.070935 0.972836 0.071176

02-C2H12B4N6
lf=42.6 te_zpe=-511.563203 te_gfe=-511.604375 te_ms_zpe=-510.698257 te_ms_gfe=-510.739552

5 1.466173 -1.327799 -0.267176
5 1.185243 1.516494 0.249298
6 0.717892 0.039753 -0.022196
5 -0.449253 1.887157 -0.008742
6 -0.638341 0.325693 0.070818
5 -1.886722 -0.622612 0.129509
7 2.422116 1.997875 0.703073
1 3.205141 1.389345 0.892957
1 2.582169 2.956975 0.966205
7 -1.366724 2.884874 -0.366093
1 -2.344005 2.694571 -0.532760
1 -1.120187 3.856454 -0.464241
7 -2.028260 -1.550854 1.208514
1 -1.447583 -1.460303 2.026803
1 -2.882414 -2.057614 1.387283
7 0.862679 -2.570712 0.047098
1 1.305552 -3.464309 -0.095732
1 -0.078401 -2.622930 0.407046
7 2.793780 -1.255693 -0.784382
1 3.328866 -2.059478 -1.072780
1 3.160216 -0.384560 -1.130677
7 -2.881205 -0.527057 -0.881710
1 -3.669005 -1.152215 -0.951229
1 -2.711556 -0.003856 -1.724555

03-C2H12B4N6
lf=40.2 te_zpe=-511.547543 te_gfe=-511.588278 te_ms_zpe=-510.696322 te_ms_gfe=-510.737182

5 -0.601482 -0.081668 1.112627
5 -0.604613 1.007095 -0.498195
5 -0.599941 -0.931112 -0.599619
5 2.070048 0.019131 -0.005110
6 0.515723 0.031522 -0.006771
6 -1.716282 -0.016699 0.007529
7 -0.597133 -0.175012 2.515614
1 0.249603 -0.221920 3.057499
1 -1.438651 -0.314995 3.050272
7 -3.152434 -0.093417 0.050155
1 -3.545743 0.707531 0.534563
1 -3.546522 -0.090868 -0.885599
7 -0.634983 2.263855 -1.130373
1 0.196913 2.727103 -1.457933
1 -1.490190 2.711811 -1.417061
7 -0.565272 -2.106393 -1.373551
1 0.290221 -2.484454 -1.745714
1 -1.394533 -2.601354 -1.657492
7 2.773542 -1.221380 -0.065677
1 2.289194 -2.098454 0.020231
1 3.775824 -1.306103 -0.009389

7 2.799272 1.245100 0.029271
1 2.333553 2.123084 0.181432
1 3.802670 1.303178 0.098057

04-C2H12B4N6
lf=9.5 te_zpe=-511.562275 te_gfe=-511.607326 te_ms_zpe=-510.694799 te_ms_gfe=-510.739984

5 1.283958 1.888813 -0.010800
6 0.278130 0.687371 -0.003612
5 -1.031119 -0.017060 0.007926
5 -2.715004 -0.049296 0.022707
6 0.303033 -0.678278 0.000783
5 1.348716 -1.840730 -0.012042
7 0.810981 3.166328 0.372759
1 1.382643 3.990224 0.464512
1 -0.150011 3.296307 0.640755
7 2.637581 -1.616202 0.549142
1 2.838418 -0.764864 1.048250
1 3.319810 -2.343100 0.697226
7 0.992006 -3.071715 -0.611871
1 1.616450 -3.851141 -0.740676
1 0.076686 -3.205005 -1.007502
7 2.636854 1.653696 -0.375435
1 2.932722 0.748075 -0.702645
1 3.325228 2.379050 -0.498619
7 -3.452946 0.767438 -0.879554
1 -4.457102 0.745549 -0.972778
1 -3.003117 1.401263 -1.516876
7 -3.406048 -0.890984 0.938494
1 -4.408584 -0.907472 1.048486
1 -2.921873 -1.511991 1.563129

05-C2H12B4N6
lf=23.9 te_zpe=-511.555486 te_gfe=-511.598887 te_ms_zpe=-510.686376 te_ms_gfe=-510.729910

5 -2.303386 -0.127170 -0.314898
5 -1.178960 0.539287 0.794185
5 1.387038 1.678478 -0.231937
6 0.237546 0.882274 0.293065
6 1.390463 0.215615 -0.056295
5 1.847708 -1.279576 -0.089211
7 1.954070 2.904023 -0.609668
1 1.456399 3.776978 -0.556350
1 2.882036 2.982893 -0.991072
7 3.214875 -1.588966 0.134772
1 3.587806 -2.522963 0.183751
1 3.888302 -0.867131 0.324828
7 0.881809 -2.288802 -0.340965
1 -0.077213 -2.063438 -0.558456
1 1.110920 -3.261776 -0.466702
7 -1.496489 0.711738 2.151851

1 -0.837331 1.059975 2.832704
1 -2.403609 0.503288 2.537565
7 -2.909463 0.646559 -1.337376
1 -3.518064 0.267618 -2.047772
1 -2.668010 1.610117 -1.493086
7 -2.567517 -1.531576 -0.239244
1 -2.275996 -2.082650 0.550851
1 -3.216289 -2.016163 -0.843170

06-C2H12B4N6
lf=22.3 te_zpe=-511.555147 te_gfe=-511.599849 te_ms_zpe=-510.684667 te_ms_gfe=-510.729504

5 -2.071471 -0.558699 -0.534250
5 -3.149180 0.478475 0.305519
6 -0.587477 -0.622411 -0.169182
5 2.071472 -0.558595 0.534356
6 0.587479 -0.622413 0.169299
5 3.149155 0.478492 -0.305555
7 2.670475 1.694094 -0.854951
1 1.692594 1.929237 -0.829119
1 3.232243 2.351247 -1.374440
7 4.527965 0.131458 -0.409561
1 5.207550 0.675970 -0.919883
1 4.866184 -0.782357 -0.160329
7 2.539082 -1.360673 1.587928
1 1.947155 -1.976635 2.125253
1 3.490179 -1.316042 1.918557
7 -2.539011 -1.360778 -1.587852
1 -1.947047 -1.976733 -2.125143
1 -3.490088 -1.316151 -1.918542
7 -4.528024 0.131537 0.409376
1 -4.866282 -0.782253 0.160102
1 -5.207626 0.676099 0.919621
7 -2.670475 1.694052 0.854954
1 -3.232255 2.351249 1.374375
1 -1.692574 1.929120 0.829237

07-C2H12B4N6
lf=18.1 te_zpe=-511.553438 te_gfe=-511.598209 te_ms_zpe=-510.684074 te_ms_gfe=-510.728979

5 -3.286410 -0.259607 0.094380
6 2.217226 0.246869 -0.078883
5 -1.590320 -0.487917 0.164174
5 3.717126 -0.094722 0.012836
5 -0.480209 0.769791 -0.221837
6 1.035824 0.539469 -0.158819
7 -3.861570 0.937096 0.631608
1 -4.857831 1.091581 0.698908
1 -3.335826 1.529711 1.253120
7 -4.133086 -1.207034 -0.546682
1 -3.762589 -1.998622 -1.044528

1 -5.126465 -1.083800 -0.680618
7 -1.054452 -1.730057 0.522477
1 -1.608868 -2.530716 0.790186
1 -0.056677 -1.896182 0.563632
7 -0.971267 2.027846 -0.596237
1 -0.387574 2.813004 -0.844484
1 -1.964566 2.200734 -0.661381
7 4.371793 -0.621465 -1.129513
1 3.886962 -0.761962 -1.998580
1 5.349062 -0.860984 -1.157856
7 4.397094 0.122445 1.238177
1 5.375881 -0.065124 1.379702
1 3.929687 0.504799 2.041534

08-C2H12B4N6
lf=18.4 te_zpe=-511.551547 te_gfe=-511.596849 te_ms_zpe=-510.682547 te_ms_gfe=-510.727986

5 2.308072 -1.155961 -0.009234
5 0.694178 1.334582 -0.427224
5 1.970381 0.491619 0.328560
6 -1.860690 0.365880 -0.077700
5 -3.269611 -0.222128 0.131665
6 -0.748088 0.832325 -0.254947
7 3.658610 -1.615074 -0.079948
1 3.922167 -2.560474 -0.316932
1 4.436242 -0.977327 -0.085277
7 0.907139 2.461679 -1.238490
1 0.165316 2.936670 -1.731951
1 1.824319 2.836865 -1.421503
7 2.779073 1.153049 1.269092
1 3.513618 0.686549 1.783491
1 2.639459 2.108696 1.565142
7 -4.047667 0.228112 1.227447
1 -4.970679 -0.112638 1.439950
1 -3.697984 0.907420 1.880385
7 -3.741493 -1.203261 -0.777631
1 -3.199963 -1.489177 -1.574607
1 -4.653326 -1.626507 -0.724916
7 1.235416 -2.068854 -0.183290
1 0.275766 -1.769058 -0.122134
1 1.345096 -3.060366 -0.334856

09-C2H12B4N6
lf=18.6 te_zpe=-511.541658 te_gfe=-511.587057 te_ms_zpe=-510.671616 te_ms_gfe=-510.717155

5 -1.818235 1.504071 0.098097
5 -1.818622 -1.503934 -0.098106
5 -0.992296 -0.000041 0.000017
6 1.738350 -0.000223 0.000005
5 3.276607 -0.000120 0.000003
6 0.512558 -0.000248 0.000002

7 -3.172459 -1.522749 -0.545072
1 -3.702771 -2.364831 -0.714308
1 -3.610926 -0.690921 -0.904641
7 -1.173674 2.699503 -0.308953
1 -0.205000 2.698684 -0.582267
1 -1.599337 3.614246 -0.314517
7 -3.172053 1.523257 0.545107
1 -3.702140 2.365482 0.714331
1 -3.610730 0.691553 0.904707
7 -1.174365 -2.699544 0.308902
1 -0.205687 -2.698979 0.582202
1 -1.600266 -3.614177 0.314455
7 3.961712 -0.027335 1.241371
1 3.474431 -0.019567 2.120283
1 4.964605 -0.030175 1.326304
7 3.961707 0.027172 -1.241365
1 3.474424 0.019358 -2.120276
1 4.964599 0.030147 -1.326301

10-C2H12B4N6
lf=56.6 te_zpe=-511.527129 te_gfe=-511.567775 te_ms_zpe=-510.671282 te_ms_gfe=-510.712059

5 1.392135 0.182557 0.678042
6 0.000008 -0.000127 -0.067420
5 0.241104 -1.235305 -1.214306
5 -1.392103 -0.181206 0.678470
5 -0.241103 1.232619 -1.216943
6 -0.000016 -0.002043 -1.869190
7 1.503487 -0.123296 2.072144
1 0.786940 -0.655028 2.538982
1 2.390998 -0.139544 2.550258
7 2.517429 0.647804 -0.047769
1 2.450542 0.776650 -1.045519
1 3.453618 0.691433 0.319035
7 0.519629 -2.597673 -1.121215
1 0.638799 -3.186786 -1.928206
1 0.594822 -3.073768 -0.238644
7 -2.517474 -0.647804 -0.046357
1 -2.450613 -0.778703 -1.043843
1 -3.453679 -0.690449 0.320522
7 -1.503469 0.127838 2.071857
1 -0.786882 0.660549 2.537511
1 -2.390986 0.145233 2.549919
7 -0.519626 2.595182 -1.126734
1 -0.638755 3.182595 -1.934969
1 -0.594753 3.073155 -0.245172

11-C2H12B4N6
lf=46.2 te_zpe=-511.530951 te_gfe=-511.571240 te_ms_zpe=-510.670800 te_ms_gfe=-510.711212

5 1.382633 -1.276516 -0.000745

5 -1.382638 -1.276511 0.000739
6 -0.000001 -0.775802 0.000002
5 -1.382634 1.276516 0.000730
5 1.382637 1.276513 -0.000735
6 0.000000 0.775804 0.000002
7 2.061981 -2.539022 0.062205
1 1.536898 -3.392948 -0.034698
1 3.026123 -2.656749 -0.206399
7 -2.061986 -2.539017 -0.062210
1 -1.536906 -3.392945 0.034680
1 -3.026133 -2.656747 0.206370
7 -2.061982 2.539021 -0.062193
1 -3.026146 2.656743 0.206326
1 -1.536912 3.392953 0.034716
7 2.061989 2.539017 0.062187
1 1.536924 3.392950 -0.034733
1 3.026151 2.656731 -0.206348
7 2.354635 -0.000003 -0.017686
1 2.981067 -0.000011 0.787513
7 -2.354635 0.000003 0.017705
1 -2.981083 -0.000002 -0.787481
1 2.958214 0.000002 -0.840235
1 -2.958198 0.000008 0.840266

12-C2H12B4N6
lf=39.7 te_zpe=-511.532091 te_gfe=-511.573864 te_ms_zpe=-510.667235 te_ms_gfe=-510.709139

5 -0.790090 1.452302 -0.392121
6 -0.317445 0.018615 0.094479
5 0.333812 -0.083197 1.485616
5 -1.103700 -1.273012 -0.360735
5 2.437170 -0.191681 -0.369898
6 1.252404 -0.148052 0.319627
7 -2.540516 -1.281807 -0.303642
1 -3.073123 -2.127088 -0.440661
1 -3.022172 -0.606065 0.267141
7 -0.402349 -2.407668 -0.832716
1 -0.823930 -3.291310 -1.065853
1 0.605247 -2.403076 -0.834536
7 0.172353 -0.116751 2.865212
1 -0.725304 -0.019877 3.311843
1 0.944506 -0.220864 3.503809
7 0.078404 2.567398 -0.236479
1 1.020750 2.435384 0.092618
1 -0.125437 3.494301 -0.570700
7 -2.094948 1.631899 -0.941520
1 -2.623630 0.835683 -1.261302
1 -2.404953 2.511250 -1.323512
7 3.643478 -0.230982 -1.030565
1 4.164296 0.598210 -1.272561
1 4.073083 -1.086590 -1.347265

13-C2H12B4N6
lf=37.2 te_zpe=-511.518638 te_gfe=-511.560005 te_ms_zpe=-510.657095 te_ms_gfe=-510.698583

 5 1.802909 -0.982610 0.239250
 5 -1.802913 -0.982593 -0.239311
 5 1.802966 0.982607 -0.238945
 5 -1.802968 0.982600 0.238976
 6 -0.729131 0.000010 -0.000071
 6 0.729129 0.000008 0.000059
 7 3.046660 -0.000011 0.000273
 1 3.648573 0.198333 0.798838
 7 2.042298 -2.355664 0.549701
 1 1.277470 -2.928088 0.871314
 1 2.939759 -2.694763 0.857887
 7 2.042448 2.355670 -0.549294
 1 2.939960 2.694733 -0.857373
 1 1.277686 2.928123 -0.871017
 7 -2.042301 -2.355643 -0.549789
 1 -2.939753 -2.694723 -0.858023
 1 -1.277466 -2.928052 -0.871412
 7 -2.042439 2.355640 0.549432
 1 -2.939959 2.694701 0.857491
 1 -1.277679 2.928060 0.871214
 7 -3.046662 -0.000003 -0.000294
 1 -3.648566 0.198377 -0.798856
 1 -3.648725 -0.198389 0.798148
 1 3.648713 -0.198363 -0.798184

14-C2H12B4N6
lf=45.1 te_zpe=-511.524556 te_gfe=-511.564719 te_ms_zpe=-510.657059 te_ms_gfe=-510.697341

 5 -0.095802 -1.262106 -0.487668
 5 -0.342589 1.168755 -0.309787
 5 -1.562842 -0.915115 0.285124
 5 2.147084 0.133781 0.278804
 6 0.643047 0.023833 -0.148396
 6 -1.766854 0.566168 -0.105928
 7 0.389209 -2.412359 -1.164390
 1 -0.190071 -3.208896 -1.374753
 1 1.238744 -2.386445 -1.708747
 7 -0.055815 2.562211 -0.505435
 1 0.862427 2.852768 -0.803105
 1 -0.758481 3.260279 -0.688841
 7 -2.942812 1.204236 -0.161786
 1 -3.031427 2.131671 -0.551255
 1 -3.810741 0.736211 0.057081
 7 2.687104 1.399636 0.675244
 1 3.607094 1.507250 1.073794
 1 2.061778 2.155029 0.905485
 7 2.985867 -1.021181 0.249404
 1 2.584312 -1.933039 0.104041

1 3.928963 -1.042079 0.603766
7 -2.384571 -1.648485 1.172498
1 -3.027210 -1.214001 1.819027
1 -2.204673 -2.613734 1.398349

15-C2H12B4N6
lf=21.3 te_zpe=-511.526308 te_gfe=-511.570669 te_ms_zpe=-510.655229 te_ms_gfe=-510.699726

5 -1.787826 1.403916 0.039975
5 -1.787630 -1.403980 -0.039982
6 0.311508 0.000115 0.000036
6 -1.021032 0.000019 0.000045
5 1.682347 0.000091 0.000028
5 3.344234 0.000055 0.000017
7 4.054794 -0.175458 -1.220340
1 5.060436 -0.150408 -1.286047
1 3.600016 -0.341972 -2.100745
7 -1.104351 2.563334 -0.380750
1 -0.125406 2.505593 -0.616394
1 -1.474204 3.498185 -0.336057
7 -3.142517 1.439849 0.477738
1 -3.575362 0.631528 0.893838
1 -3.642906 2.298600 0.644917
7 -3.142285 -1.440088 -0.477842
1 -3.575210 -0.631815 -0.893952
1 -3.642545 -2.298902 -0.645079
7 -1.104024 -2.563315 0.380760
1 -0.125107 -2.505444 0.616488
1 -1.473745 -3.498216 0.336019
7 4.054817 0.175550 1.220364
1 5.060458 0.150459 1.286057
1 3.600056 0.342067 2.100777

16-C2H12B4N6
lf=33.1 te_zpe=-511.520210 te_gfe=-511.561317 te_ms_zpe=-510.650109 te_ms_gfe=-510.691341

5 -1.184051 -1.501687 0.134166
5 -1.300751 1.250164 -0.224023
6 -0.477360 -0.104087 -0.136364
5 1.979343 0.905704 0.348166
6 0.878128 -0.069595 -0.259615
5 2.267525 -0.625945 -0.110249
7 -0.463768 -2.540141 0.769537
1 -0.829158 -3.456914 0.967475
1 0.488005 -2.395602 1.064797
7 -2.549625 -1.690691 -0.246729
1 -3.012424 -1.027815 -0.846924
1 -2.999252 -2.592991 -0.228068
7 -2.639943 1.298028 0.250914
1 -3.187030 2.142929 0.299137
1 -3.041567 0.518793 0.747200

7 -0.685532 2.424045 -0.758819
1 0.160364 2.325920 -1.298805
1 -1.205576 3.259141 -0.979079
7 2.016201 2.176472 0.898910
1 2.736976 2.495696 1.527222
1 1.243764 2.818444 0.766746
7 3.113855 -1.574818 -0.693907
1 2.774820 -2.313230 -1.292273
1 4.117832 -1.523723 -0.631205

17-C2H12B4N6
lf=39.7 te_zpe=-511.509852 te_gfe=-511.551884 te_ms_zpe=-510.648810 te_ms_gfe=-510.690973

5 0.252369 -0.575639 0.998149
5 -1.577783 1.022351 -0.003700
5 2.691527 0.286715 -0.000222
6 -0.986528 -0.466801 0.000884
5 0.253051 -0.582731 -0.994658
6 1.384276 -0.154414 0.000607
7 0.326026 -1.141724 -2.279982
1 -0.477654 -1.536490 -2.741962
1 1.196079 -1.306338 -2.759822
7 3.982485 0.758195 -0.001506
1 4.787318 0.150387 0.000826
1 4.210769 1.740607 -0.005067
7 0.324715 -1.124993 2.287679
1 -0.479242 -1.515001 2.753180
1 1.194498 -1.284961 2.769576
7 -0.755108 2.183120 -0.009273
1 0.248946 2.112420 -0.009444
1 -1.114635 3.123114 -0.011061
7 -2.995427 1.178387 -0.002320
1 -3.462261 2.070134 -0.004761
1 -3.618053 0.389738 0.002144
7 -1.991607 -1.566059 0.003912
1 -2.601292 -1.488450 0.814642
1 -2.604377 -1.489826 -0.804612

18-C2H12B4N6
lf=28.5 te_zpe=-511.515361 te_gfe=-511.559716 te_ms_zpe=-510.647878 te_ms_gfe=-510.692376

5 1.438607 1.291792 -0.674681
5 1.541474 -0.846886 0.774835
6 0.762480 0.267006 -0.009780
5 -1.540749 -0.847353 -0.775007
6 -0.762456 0.266530 0.010322
5 -1.439196 1.290843 0.675328
7 2.136875 2.275017 -1.330331
1 2.394998 2.212414 -2.304178
1 2.397653 3.149219 -0.898139
7 2.918210 -1.133202 0.508329

1 3.481962 -1.733576 1.087195
1 3.439826 -0.659352 -0.208594
7 0.848915 -1.567725 1.785853
1 1.208965 -2.383923 2.251862
1 -0.137732 -1.412085 1.916779
7 -0.847605 -1.567427 -1.786170
1 -1.207163 -2.383578 -2.252640
1 0.139007 -1.411286 -1.916767
7 -2.917420 -1.134420 -0.508975
1 -3.480747 -1.734810 -1.088238
1 -3.439427 -0.661163 0.208054
7 -2.139025 2.273127 1.330723
1 -2.397080 2.210338 2.304575
1 -2.400734 3.147016 0.898462

19-C2H12B4N6
lf=30.4 te_zpe=-511.506749 te_gfe=-511.548744 te_ms_zpe=-510.645751 te_ms_gfe=-510.687874

5 0.191328 0.302274 0.729785
5 -2.306910 0.194805 -0.610119
5 2.809541 -0.152914 -0.345207
6 -1.248183 -0.629157 0.249151
5 0.071441 -0.987625 -0.340670
6 1.294990 -0.336154 -0.081731
7 -0.002351 1.363309 1.639324
1 -0.848234 1.392168 2.189699
1 0.783984 1.807752 2.087942
7 3.358371 1.163674 -0.389965
1 4.311584 1.358655 -0.651206
1 2.759120 1.970256 -0.430622
7 3.648337 -1.288820 -0.506784
1 4.645729 -1.243961 -0.636964
1 3.286570 -2.222300 -0.418534
7 -2.136495 1.578662 -0.836746
1 -1.408016 2.099861 -0.375349
1 -2.742889 2.133597 -1.418659
7 -3.460633 -0.501940 -1.078688
1 -4.172327 -0.064654 -1.643048
1 -3.464285 -1.506075 -1.152383
7 -1.842531 -1.321130 1.374617
1 -2.832531 -1.485234 1.244339
1 -1.379433 -2.187179 1.619010

20-C2H12B4N6
lf=65.0 te_zpe=-511.488270 te_gfe=-511.527463 te_ms_zpe=-510.636062 te_ms_gfe=-510.675372

5 -0.064000 -0.719958 -0.958006
5 0.064002 -0.719948 0.958009
5 0.857089 1.246923 0.007146
5 -0.857100 1.246918 -0.007151
6 -1.191492 -0.277870 0.060309

6 1.191491 -0.277862 -0.060311
7 1.845441 2.246265 0.066716
1 2.825240 2.026021 0.171304
1 1.643303 3.229471 0.145075
7 -1.845458 2.246251 -0.066727
1 -2.825257 2.026001 -0.171307
1 -1.643328 3.229460 -0.145086
7 -2.555896 -0.782148 0.069392
1 -2.578080 -1.791255 0.185207
1 -3.078213 -0.391581 0.848709
7 0.138702 -1.526706 2.099487
1 -0.671040 -1.816368 2.624984
1 1.017769 -1.785737 2.519562
7 2.555896 -0.782134 -0.069387
1 2.578087 -1.791238 -0.185222
1 3.078224 -0.391546 -0.848685
7 -0.138683 -1.526722 -2.099481
1 -1.017741 -1.785771 -2.519563
1 0.671069 -1.816380 -2.624965

21-C2H12B4N6
lf=14.0 te_zpe=-511.509692 te_gfe=-511.554306 te_ms_zpe=-510.636007 te_ms_gfe=-510.680758

5 -3.286038 -0.041196 0.062013
6 -1.773044 -0.025098 0.036151
5 -0.405162 -0.033278 0.015894
5 1.761303 1.399618 -0.216204
5 1.831308 -1.349517 0.146922
6 1.030975 0.002461 -0.019135
7 1.345519 -2.531012 -0.462938
1 0.477808 -2.536682 -0.972564
1 1.798610 -3.428781 -0.407070
7 3.056329 -1.353250 0.883107
1 3.319802 -0.558121 1.442025
1 3.513609 -2.205989 1.167176
7 3.171062 1.422097 -0.406609
1 3.701073 0.570025 -0.490605
1 3.695421 2.258306 -0.608648
7 1.001819 2.595064 -0.190538
1 0.001030 2.572711 -0.073759
1 1.382638 3.515509 -0.336052
7 -3.986933 0.508616 1.183428
1 -4.925769 0.213482 1.402183
1 -3.488894 0.860618 1.983815
7 -4.018019 -0.601973 -1.033256
1 -4.972254 -0.331143 -1.212861
1 -3.546152 -0.949052 -1.851215

22-C2H12B4N6
lf=57.9 te_zpe=-511.489115 te_gfe=-511.529469 te_ms_zpe=-510.635611 te_ms_gfe=-510.676090

5 1.865298 0.033167 -0.026476
5 0.650351 -0.970455 -0.649106
5 -1.997330 0.079150 0.004715
5 0.635213 -0.320545 1.167769
6 0.612630 0.880243 -0.349652
6 -0.454509 -0.067402 0.074369
7 0.401175 2.115626 -0.863764
1 1.186469 2.578250 -1.297162
1 -0.514101 2.344025 -1.225727
7 -2.587532 1.387087 0.008285
1 -3.585787 1.526761 0.048945
1 -2.075526 2.165796 0.390840
7 -2.813777 -1.080144 -0.103982
1 -3.820253 -1.069372 -0.068407
1 -2.417509 -2.004360 -0.083800
7 0.546334 -0.558538 2.548597
1 -0.327605 -0.625664 3.046020
1 1.357564 -0.671762 3.133783
7 3.293854 0.354895 -0.207983
1 3.711510 0.894004 0.541245
1 3.891083 -0.443602 -0.379615
7 0.461121 -2.053393 -1.532777
1 1.219674 -2.486806 -2.032572
1 -0.450123 -2.349628 -1.844993

23-C2H12B4N6
lf=57.1 te_zpe=-511.486665 te_gfe=-511.526194 te_ms_zpe=-510.634163 te_ms_gfe=-510.673811

5 0.038209 -0.679398 0.962451
5 0.843457 1.278235 -0.057213
5 -0.026411 -0.798363 -0.923541
6 -1.188416 -0.296709 0.023609
5 -0.869496 1.242652 -0.064015
6 1.195203 -0.238438 -0.045069
7 -1.874318 2.223723 -0.104675
1 -2.858385 1.996083 -0.082882
1 -1.693672 3.212741 -0.158447
7 1.809254 2.301669 -0.030559
1 2.792863 2.111518 0.094715
1 1.583989 3.282519 -0.002038
7 -0.032842 -1.702857 -1.990953
1 0.809373 -2.026398 -2.440322
1 -0.872984 -2.150629 -2.321788
7 0.111816 -1.430460 2.138659
1 0.989956 -1.658454 2.577680
1 -0.698292 -1.816180 2.596859
7 -2.522044 -0.898152 0.101054
1 -3.028867 -0.522679 0.899247
1 -3.070272 -0.637740 -0.715293
7 2.560487 -0.735556 0.016840
1 2.592952 -1.746842 -0.075793
1 3.117358 -0.357263 -0.744140

12. Table S9 The Cartesian coordinates and total energies of $C_2B_4R_6$ (R=OH) ($\Delta E <$ 50kcal/mol) at the level of CBS-QB3.

"level"----"CBS-QB3"
"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"te_zpe"----"total energy with zero-point energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_gfe"----"total energy with Gibbs free energy (a.u.) at RB3LYP/6-311G(2d,d,p)"
"te_ms_zpe"----"total energy with zero-point energy (a.u.) at CBS-QB3"
"te_ms_gfe"----"total energy with Gibbs free energy (a.u.) at CBS-QB3"

##
01-C2H6B4O6
lf=18.5 te_zpe=-630.935968 te_gfe=-630.977757 te_ms_zpe=-630.001970 te_ms_gfe=-630.043863

5 0.111973 -1.061348 -1.070537
5 -1.997207 -0.214536 0.576003
5 1.997215 0.210510 0.577645
6 -0.921229 -0.085580 -0.532990
5 -0.111879 1.069132 -1.062803
6 0.921291 0.089484 -0.532283
8 -0.174965 2.328683 -1.560974
1 -1.080728 2.610403 -1.721378
8 -1.691784 -0.899199 1.724160
1 -2.384018 -0.911064 2.391336
8 -3.221928 0.363097 0.339088
1 -3.887612 0.199288 1.013738
8 0.175114 -2.317228 -1.577887
1 1.080886 -2.597752 -1.740312
8 1.691353 0.885841 1.731204
1 2.383506 0.892640 2.398535
8 3.222134 -0.364897 0.336388
1 3.887699 -0.206104 1.012350

02-C2H6B4O6
lf=17.3 te_zpe=-630.927840 te_gfe=-630.971869 te_ms_zpe=-629.990123 te_ms_gfe=-630.034264

5 1.288198 -1.902874 0.000068
6 0.345354 -0.680005 0.000017
5 -0.969515 -0.000005 -0.000064
5 -2.640170 -0.000022 -0.000150
6 0.345349 0.680004 0.000013
5 1.288184 1.902879 0.000074
8 1.668644 -2.415841 -1.211298
1 2.231781 -3.193905 -1.167018
8 1.668650 -2.415746 1.211472
1 2.231662 -3.193903 1.167252
8 1.668598 2.415885 -1.211285
1 2.231714 3.193962 -1.166996
8 1.668641 2.415732 1.211485
1 2.231625 3.193910 1.167275

8 -3.298828 -0.000009 1.205762
1 -4.260247 -0.000015 1.145318
8 -3.298717 -0.000012 -1.206122
1 -4.260141 -0.000020 -1.145766

03-C2H6B4O6
lf=15.8 te_zpe=-630.923357 te_gfe=-630.965311 te_ms_zpe=-629.988150 te_ms_gfe=-630.030210

5 1.651845 -0.997490 -0.058713
5 0.825828 1.781187 0.207487
6 0.693272 0.234960 0.005938
5 -0.824340 1.781812 -0.207500
6 -0.692949 0.235482 -0.005895
5 -1.652611 -0.996116 0.058743
8 1.876556 2.472183 0.727413
1 1.682057 3.405169 0.850620
8 -1.874564 2.473561 -0.727436
1 -1.679386 3.406400 -0.850681
8 -2.609427 -1.015134 1.038011
1 -3.160702 -1.802816 1.057965
8 -1.496506 -1.984140 -0.880317
1 -2.124747 -2.710081 -0.817973
8 1.494491 -1.985634 0.880015
1 2.121933 -2.712254 0.817552
8 2.608925 -1.017173 -1.037708
1 3.159512 -1.805337 -1.057653

04-C2H6B4O6
lf=14.9 te_zpe=-630.913537 te_gfe=-630.956901 te_ms_zpe=-629.973636 te_ms_gfe=-630.017109

5 -2.428860 -0.133814 -0.395557
5 -1.170028 0.165792 0.737084
5 1.201952 1.750196 -0.050515
6 0.196499 0.725625 0.336223
6 1.465783 0.312212 -0.020757
5 2.161860 -1.067642 -0.138522
8 1.497864 3.059434 -0.253460
1 2.414163 3.191206 -0.514163
8 3.493379 -1.152392 0.174009
1 3.867712 -2.037313 0.134654
8 1.403681 -2.134559 -0.547672
1 1.876416 -2.967980 -0.629757
8 -1.429264 -0.077860 2.055385
1 -2.331084 -0.400714 2.169060
8 -2.292469 0.119512 -1.729896
1 -3.059361 -0.085243 -2.276745
8 -3.580180 -0.647917 0.164153
1 -4.310248 -0.829385 -0.438442

05-C2H6B4O6

lf=14.2 te_zpe=-630.895323 te_gfe=-630.935250 te_ms_zpe=-629.969579 te_ms_gfe=-630.009608

 5 -0.553250 -0.319371 1.064070
 5 -0.622162 1.083062 -0.246739
 5 -0.576162 -0.756703 -0.822084
 5 2.068126 0.013828 -0.013802
 6 0.525911 0.014423 -0.019272
 6 -1.699839 -0.017728 0.012743
 8 2.733068 1.215806 -0.039859
 1 3.692082 1.149867 -0.030914
 8 2.718869 -1.197007 0.021524
 1 3.678498 -1.141658 0.027877
 8 -0.476879 -0.704017 2.367646
 1 -1.338141 -0.778634 2.789232
 8 -0.625195 2.408275 -0.549881
 1 -1.516976 2.762195 -0.624927
 8 -0.531729 -1.672110 -1.828431
 1 -1.403181 -1.912406 -2.156798
 8 -3.095319 0.034479 0.019603
 1 -3.433998 -0.847026 0.202661

06-C2H6B4O6
lf=27.0 te_zpe=-630.908951 te_gfe=-630.952271 te_ms_zpe=-629.967190 te_ms_gfe=-630.010622

 5 -2.078388 -0.558966 -0.457431
 5 -3.182686 0.478939 0.351934
 6 -0.590811 -0.617401 -0.153421
 5 2.078452 -0.559375 0.456976
 6 0.590789 -0.617340 0.153298
 5 3.182545 0.479670 -0.351204
 8 -2.804247 1.345594 1.334527
 1 -3.509669 1.877569 1.719526
 8 -4.483952 0.350153 -0.088164
 1 -5.143198 0.910464 0.336393
 8 -2.576454 -1.375682 -1.429119
 1 -3.527769 -1.244065 -1.522807
 8 4.483879 0.350446 0.088567
 1 5.142981 0.911521 -0.335203
 8 2.577034 -1.378597 1.426287
 1 3.528451 -1.247446 1.519595
 8 2.803817 1.347900 -1.332293
 1 3.509110 1.880560 -1.716580

07-C2H6B4O6
lf=13.0 te_zpe=-630.906151 te_gfe=-630.952366 te_ms_zpe=-629.964440 te_ms_gfe=-630.010770

 6 -0.584479 -0.579987 -0.177113
 6 0.584600 -0.580004 0.177144
 5 2.057574 -0.551709 0.588292
 5 -2.057422 -0.551775 -0.588384
 5 -3.177636 0.468507 0.207284

5 3.177513 0.468995 -0.207215
8 -2.497726 -1.352447 -1.601797
1 -1.796101 -1.889005 -1.988643
8 -3.667873 0.067700 1.423111
1 -4.293671 0.673019 1.837231
8 -3.528348 1.648528 -0.393694
1 -4.151379 2.195251 0.098722
8 2.498070 -1.352573 1.601471
1 1.796530 -1.889269 1.988278
8 3.670416 0.066979 -1.421556
1 4.295882 0.672662 -1.835650
8 3.525389 1.650537 0.392437
1 4.148438 2.197406 -0.099792

08-C2H6B4O6
lf=25.5 te_zpe=-630.904036 te_gfe=-630.948665 te_ms_zpe=-629.963182 te_ms_gfe=-630.007930

5 -1.812226 1.483357 0.000007
5 -1.812289 -1.483336 0.000029
5 -0.978144 -0.000008 -0.000023
6 1.738511 -0.000029 -0.000041
5 3.263633 -0.000027 -0.000043
6 0.515045 -0.000027 -0.000036
8 3.897650 -0.000035 -1.213616
1 4.857739 -0.000034 -1.171211
8 3.897653 -0.000020 1.213529
1 4.857742 -0.000017 1.171121
8 -2.139237 -2.042347 1.207833
1 -2.612595 -2.880695 1.160965
8 -2.139244 -2.042438 -1.207731
1 -2.612635 -2.880764 -1.160797
8 -2.139125 2.042414 1.207802
1 -2.612417 2.880799 1.160923
8 -2.139143 2.042463 -1.207761
1 -2.612463 2.880829 -1.160841

09-C2H6B4O6
lf=74.9 te_zpe=-630.895401 te_gfe=-630.933815 te_ms_zpe=-629.961244 te_ms_gfe=-629.999765

5 -1.367481 -1.269963 0.001282
5 1.367523 -1.269941 -0.001310
6 -0.000011 -0.766123 -0.000033
5 1.367484 1.269966 -0.001222
5 -1.367526 1.269936 0.001200
6 0.000014 0.766130 -0.000042
8 2.049441 -2.455035 0.076188
1 2.879809 -2.480173 -0.405726
8 -2.049654 -2.454911 -0.076356
1 -2.879311 -2.480385 0.406772
8 -2.049420 2.455039 -0.076298
1 -2.879993 2.480072 0.405265

 8 2.049641 2.454923 0.076431
 1 2.879413 2.480339 -0.406503
 8 -2.275092 0.000087 0.078906
 8 2.275102 -0.000082 -0.078793
 1 3.103130 -0.000057 0.415259
 1 -3.103203 -0.000013 -0.415004

10-C2H6B4O6
lf=17.8 te_zpe=-630.901914 te_gfe=-630.946407 te_ms_zpe=-629.960978 te_ms_gfe=-630.005586

 5 2.804133 -0.764280 -0.033452
 6 -2.049071 0.161540 -0.105036
 5 1.786701 0.561674 0.395280
 5 -3.448240 -0.396984 0.165457
 5 0.484813 1.138660 -0.540879
 6 -0.937576 0.609127 -0.320706
 8 -3.791284 -1.572494 -0.445027
 1 -4.677482 -1.889970 -0.250237
 8 -4.265397 0.315866 0.999202
 1 -5.133323 -0.069136 1.149420
 8 0.724241 2.051722 -1.530229
 1 -0.072149 2.290031 -2.018596
 8 2.060143 1.168292 1.586392
 1 2.813224 0.753499 2.027683
 8 2.630684 -1.464913 -1.194040
 1 3.247830 -2.189916 -1.345973
 8 3.794457 -1.051829 0.882132
 1 4.381996 -1.787012 0.672674

11-C2H6B4O6
lf=9.3 te_zpe=-630.889390 te_gfe=-630.931383 te_ms_zpe=-629.960507 te_ms_gfe=-630.002610

 5 -1.367942 0.104653 0.704822
 6 0.000122 0.000060 -0.057325
 5 0.065633 1.249230 -1.213808
 5 1.369876 -0.112193 0.700737
 5 -0.068534 -1.236381 -1.226832
 6 -0.001636 0.009957 -1.886916
 8 -2.518629 -0.254296 0.042919
 1 -3.329314 -0.137397 0.545274
 8 -1.368715 0.585342 1.989422
 1 -2.230276 0.608268 2.415110
 8 1.374027 -0.609290 1.979069
 1 2.236421 -0.635850 2.402856
 8 2.518654 0.257022 0.041180
 1 3.330574 0.134863 0.540279
 8 0.106304 2.587806 -1.085435
 1 0.138285 3.045184 -1.931142
 8 -0.110081 -2.576272 -1.113123
 1 -0.144259 -3.024211 -1.963781

12-C2H6B4O6
lf=25.2 te_zpe=-630.891533 te_gfe=-630.933933 te_ms_zpe=-629.954848 te_ms_gfe=-629.997359

 5 -0.400699 1.523443 0.214723
 6 -0.310606 -0.030056 0.155595
 5 0.202557 -0.820341 1.376565
 5 -1.281016 -0.804890 -0.786914
 5 2.311046 -0.423211 -0.425849
 6 1.192703 -0.679873 0.317575
 8 -2.248252 -0.099110 -1.467979
 1 -2.859756 -0.640578 -1.974926
 8 -1.145667 -2.169252 -0.912252
 1 -1.760832 -2.581494 -1.524095
 8 -0.139481 -1.275462 2.600629
 1 0.569491 -1.782473 3.009602
 8 3.377481 -0.211666 -1.175412
 1 3.822572 0.629441 -1.019572
 8 0.710429 2.272818 -0.122691
 1 0.588411 3.222347 -0.033955
 8 -1.580321 2.104398 0.609966
 1 -1.605419 3.063516 0.553228

13-C2H6B4O6
lf=22.0 te_zpe=-630.883703 te_gfe=-630.925656 te_ms_zpe=-629.952950 te_ms_gfe=-629.995015

 5 1.027395 1.416370 -0.242609
 5 1.282563 -1.271580 -0.106444
 6 0.364819 -0.001183 -0.145392
 5 -0.926786 -0.040562 0.734307
 6 -1.001514 -0.140254 -0.784526
 5 -2.331588 -0.225716 -0.665218
 8 2.395318 1.517895 -0.272760
 1 2.735709 2.416737 -0.273249
 8 0.201918 2.517302 -0.294502
 1 0.656384 3.359984 -0.373955
 8 -1.342480 -0.010387 2.020343
 1 -2.298816 -0.080353 2.119010
 8 0.999157 -2.321083 -0.944733
 1 1.567637 -3.088543 -0.836187
 8 2.313227 -1.297244 0.799820
 1 2.870250 -2.079243 0.759381
 8 -3.667127 -0.340818 -0.503654
 1 -4.169006 0.402156 -0.851775

14-C2H6B4O6
lf=16.5 te_zpe=-630.885068 te_gfe=-630.928965 te_ms_zpe=-629.944009 te_ms_gfe=-629.988021

 5 -1.812521 1.393947 -0.000104
 5 -1.742715 -1.334879 0.000111
 6 0.342166 0.036596 -0.000262

6 -0.982284 0.050528 -0.000087
5 1.713173 -0.011808 -0.000454
5 3.363562 -0.042078 -0.000033
8 4.013735 -0.054028 -1.210593
1 4.974844 -0.067287 -1.158858
8 4.013126 -0.053843 1.210858
1 4.974260 -0.067119 1.159609
8 -1.167985 2.594591 -0.000268
1 -1.737957 3.368526 -0.000275
8 -3.177549 1.248536 0.000042
1 -3.684226 2.065621 0.000023
8 -2.046213 -1.891186 -1.210419
1 -2.503831 -2.736548 -1.172051
8 -2.045908 -1.891003 1.210802
1 -2.503531 -2.736374 1.172677

15-C2H6B4O6
lf=23.5 te_zpe=-630.880727 te_gfe=-630.923671 te_ms_zpe=-629.941957 te_ms_gfe=-629.985019

5 -1.476228 1.260713 0.745953
5 -1.598470 -0.796178 -0.637462
6 -0.756872 0.301156 0.033651
5 1.598282 -0.796010 0.637656
6 0.756582 0.301220 -0.033495
5 1.475804 1.260595 -0.746181
8 -2.164425 2.134870 1.454711
1 -2.485091 2.902859 0.967836
8 -2.980234 -0.752735 -0.475439
1 -3.461379 -1.462124 -0.907430
8 -0.983964 -1.773623 -1.388361
1 -1.581007 -2.435337 -1.746286
8 0.983909 -1.773332 1.388828
1 1.581021 -2.434955 1.746806
8 2.980025 -0.752545 0.475450
1 3.461256 -1.461834 0.907510
8 2.165121 2.133619 -1.455251
1 2.486554 2.901494 -0.968703

16-C2H6B4O6
lf=23.9 te_zpe=-630.873013 te_gfe=-630.913947 te_ms_zpe=-629.937948 te_ms_gfe=-629.978989

5 1.720526 0.973387 0.044644
5 -1.819305 -1.076114 0.020479
5 1.869859 -1.027233 -0.004020
5 -1.720236 0.930250 -0.000928
6 -0.717054 -0.132690 0.054045
6 0.737983 -0.118193 0.031254
8 2.339783 -2.296424 -0.108757
1 3.234656 -2.410869 0.222848
8 3.023827 0.148702 0.128640
8 1.895508 2.320701 -0.012432

1 1.046421 2.771030 -0.083582
8 -1.821557 2.293900 -0.027629
1 -2.682418 2.623256 -0.301172
8 -3.030529 0.083724 -0.066337
8 -2.268031 -2.354379 0.036334
1 -3.136213 -2.472697 -0.359068
1 3.616427 0.281447 -0.624557
1 -3.570688 0.141877 0.734315

17-C2H6B4O6
lf=43.4 te_zpe=-630.866245 te_gfe=-630.906823 te_ms_zpe=-629.932580 te_ms_gfe=-629.973265

5 -0.147863 -0.636392 -0.199184
5 2.301895 0.605726 -0.201978
5 -2.750717 0.253572 0.119932
6 1.260935 -0.143804 0.687503
5 -0.050906 0.464473 1.083531
6 -1.261840 0.178238 0.454523
8 3.580006 0.097926 -0.158278
1 4.231250 0.518300 -0.725710
8 1.910898 1.659755 -0.979552
1 2.588608 2.034750 -1.547839
8 -0.087463 -1.544659 -1.209021
1 -0.974575 -1.712040 -1.552064
8 -3.169826 -0.550618 -0.928742
1 -4.106814 -0.503984 -1.137789
8 -3.602150 1.062432 0.824444
1 -4.521656 1.032085 0.545463
8 1.787442 -1.180902 1.498965
1 2.675320 -1.364077 1.171759

18-C2H6B4O6
lf=33.6 te_zpe=-630.865970 te_gfe=-630.907106 te_ms_zpe=-629.931121 te_ms_gfe=-629.972367

5 0.285447 -0.543468 1.022873
5 -1.606956 0.919035 -0.032703
5 2.681708 0.336124 -0.009346
6 -0.949628 -0.497452 0.014590
5 0.287264 -0.612919 -0.985107
6 1.417211 -0.210144 0.007312
8 0.297940 -1.117469 -2.248822
1 1.184926 -1.212525 -2.607264
8 -1.899547 -1.575370 0.049669
1 -2.777713 -1.181854 0.051354
8 -2.988962 0.917518 -0.025630
1 -3.416292 1.777151 -0.053263
8 -0.867390 2.077249 -0.076411
1 -1.386388 2.885267 -0.101251
8 0.292640 -0.958805 2.318693
1 1.178549 -1.029628 2.685333
8 3.857546 0.926111 -0.027239

1 4.636298 0.359432 -0.006995

19-C2H6B4O6
lf=10.1 te_zpe=-630.872099 te_gfe=-630.917234 te_ms_zpe=-629.929365 te_ms_gfe=-629.974619

5 3.308621 -0.000183 -0.000003
6 1.801520 -0.000156 -0.000015
5 0.428799 -0.000139 -0.000016
5 -1.795649 -1.343566 -0.125185
5 -1.795452 1.343619 0.125114
6 -0.998077 -0.000032 -0.000030
8 -1.405422 2.420371 -0.621465
1 -1.939654 3.212688 -0.513433
8 -2.849578 1.355627 1.002786
1 -3.296514 2.201107 1.102780
8 -2.849992 -1.355304 -1.002601
1 -3.297119 -2.200689 -1.102543
8 -1.405737 -2.420407 0.621327
1 -1.940149 -3.212612 0.513365
8 3.949507 -0.036972 1.218638
1 4.907360 -0.084656 1.166329
8 3.949529 0.036914 -1.218623
1 4.907370 0.084814 -1.166284

20-C2H6B4O6
lf=35.0 te_zpe=-630.870219 te_gfe=-630.910165 te_ms_zpe=-629.929006 te_ms_gfe=-629.969051

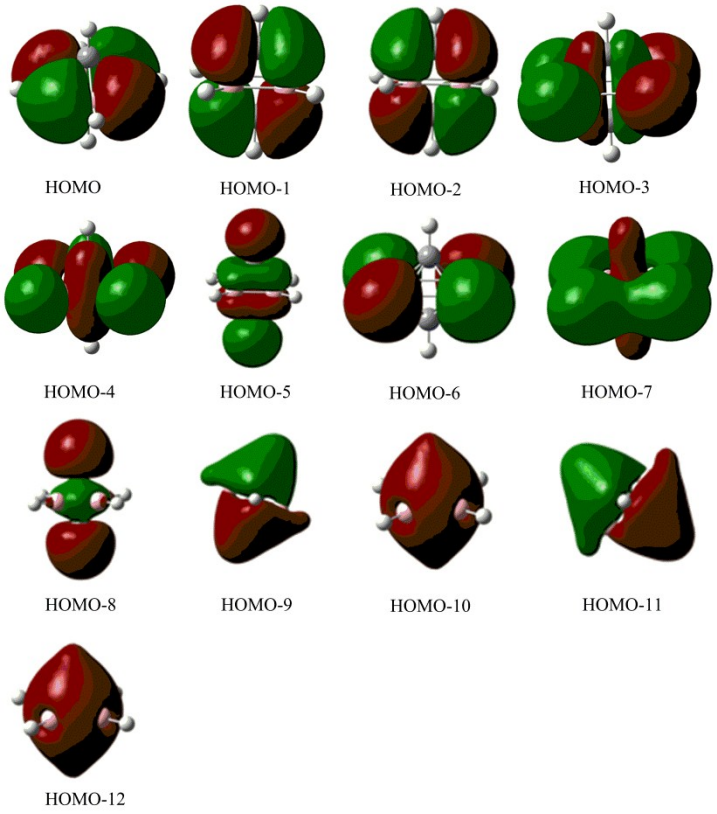
5 0.267191 -1.275668 0.597348
5 0.149696 1.200681 0.340120
5 1.699753 -0.736911 -0.111436
5 -2.082218 -0.127075 -0.328083
6 -0.612294 -0.109848 0.165194
6 1.614749 0.800796 0.039896
8 -0.325459 2.469558 0.525196
1 -1.290576 2.461808 0.555442
8 -0.154359 -2.379004 1.296641
1 0.554559 -3.001561 1.474057
8 -2.856972 0.965563 0.032877
1 -3.779350 0.936080 -0.238927
8 2.609506 1.631648 -0.231386
1 3.354704 1.123763 -0.592045
8 -2.559106 -1.152320 -1.100639
1 -3.467469 -1.055038 -1.400984
8 2.743664 -1.248916 -0.852921
1 2.783099 -2.208104 -0.875975

21-C2H6B4O6
lf=23.5 te_zpe=-630.861522 te_gfe=-630.903537 te_ms_zpe=-629.928896 te_ms_gfe=-629.971025

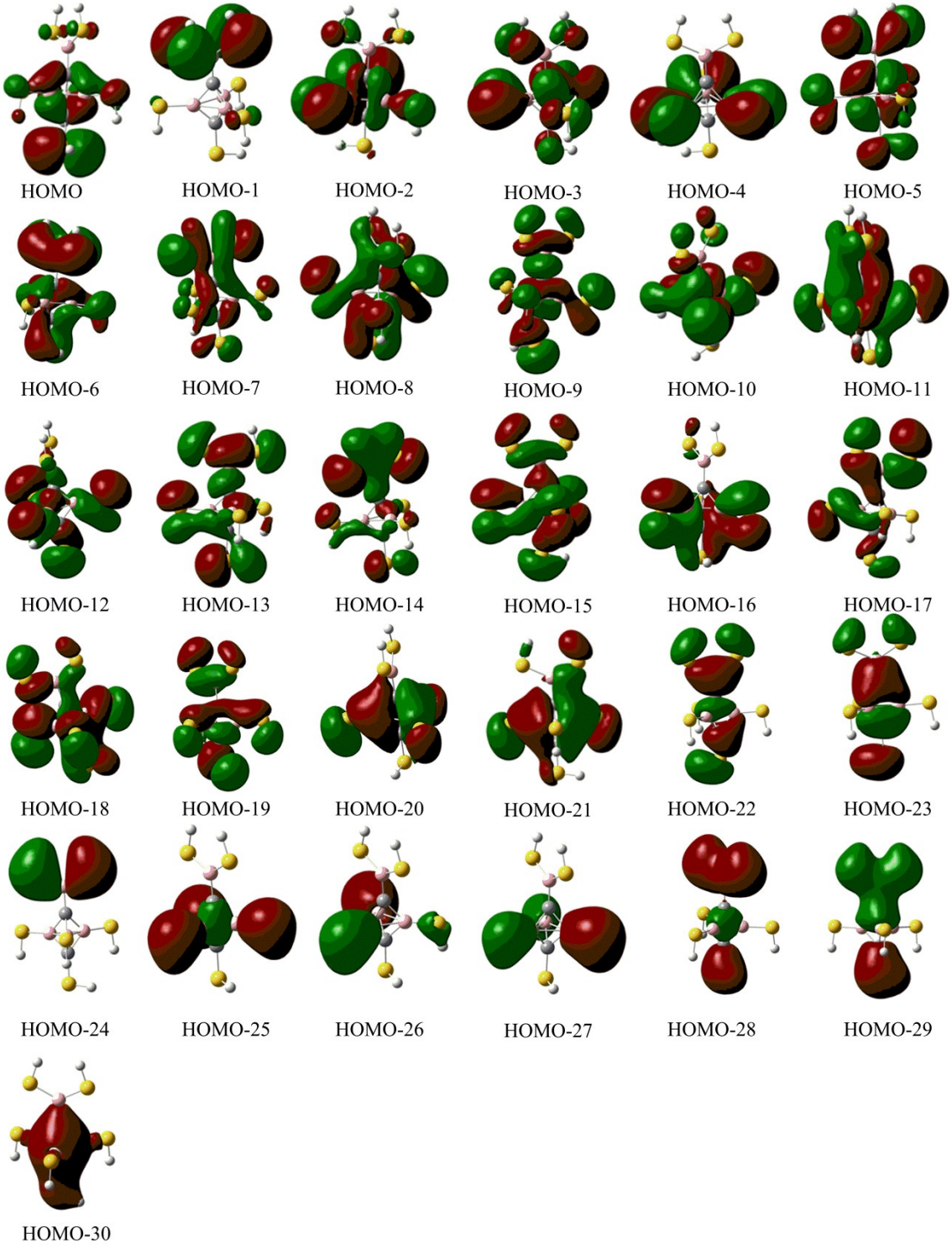
5 -1.185958 1.276078 -0.011944

5 -1.426280 -1.448457 -0.407629
5 -0.557649 -0.175744 0.599274
6 0.895181 -0.610487 -0.153210
5 2.358968 -0.124605 -0.172055
6 0.023603 -1.512867 -0.458917
8 -2.619641 -1.934794 -0.724208
1 -2.596887 -2.750501 -1.238107
8 -1.749034 2.134199 0.912162
1 -2.125514 2.944882 0.551820
8 -0.590387 -0.515980 1.989774
1 -1.102550 0.138197 2.472417
8 -1.159746 1.563991 -1.358036
1 -1.550636 2.409061 -1.603749
8 2.760671 0.602477 -1.258815
1 3.663791 0.929600 -1.219292
8 3.136326 -0.413828 0.912221
1 4.028189 -0.055990 0.886663

13. Molecular orbitals of the global minimum $C_2B_4H_6$ at the level of CBS-QB3.



14. Molecular orbitals of the global minimum $C_2B_4(SH)_6$ at the level of CBS-QB3.



15. Molecular orbitals of the global minimum $C_2B_4F_6$ at the level of CBS-QB3.