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ELECTRONIC SUPPLEMENTARY INFORMATION

Study of the influence of intermolecular interaction on classical and reverse substituent effects in *para*-substituted phenylboranes*

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Abstract

Using two families of $XC_6H_4BH_2\cdots SiH_4$ and $XC_6H_4BH_2\cdots SiMeH_3$ dimers where X represents 18 different substituents featuring a wide range of electronic properties, from significantly electron-withdrawing to significantly electron-donating, correlations between the cSAR(X) and cSAR(BH_2) values, determined using Mulliken, Hirshfeld, Merz-Kolmann, NBO, QTAIM, and Voronoi atomic charges, and various parameters are investigated. It is shown that the cSAR values obtained by means of Hirshfeld's atomic charges match the quality obtained by the Voronoi method, while Mulliken's atomic charges should definitely not be used for this purpose. For the first time, we notice that the quality of the correlation between cSAR values and parameters characterizing the strength of an intermolecular interaction depends to a large extent on the locality of the correlated parameter. Therefore, quite good linear correlations occur for the local distance H$\cdots$B and the angle SiHB, while the correlations are poor for non-local interaction and binding energy. Moreover, cSAR values are strongly correlated with the parameters characterizing an intermolecular interaction if only this interaction has got a dominant influence on both the dimer structure and its overall binding effect. Thus relationships involving cSAR not always can be used to predict values of other properties, as the local or non-local character of the latter must be taken into account. Another important issue discussed in the article is the influence of the intermolecular interaction on the reverse substituent effect. It is shown that an intermolecular interaction can have a considerable influence on the electronic properties of the BH_2 group, especially if X is a highly electron-withdrawing substituent. Most importantly, in contrast to the BH_2 group itself, an intermolecular interaction reduces slightly the influence of the substituent effect. Although the influence on reverse substituent effect is small, the X substituents gain more electron charge. It has been shown that the presence of the BH_2 group leads to both a significant reduction in the aromaticity of the benzene ring in $XC_6H_4BH_2$ compared to XC_6H_5, as well as to its greater diversity in the former of these molecules. On the other hand, the influence of intermolecular interaction with either SiH_4 or $SiMeH_3$ on the aromaticity of the benzene ring in $XC_6H_4BH_2$ is negligible.

*This article is dedicated to the memory of Prof. Andrzej J. Sadlej (1941 – 2010), our friend and teacher.

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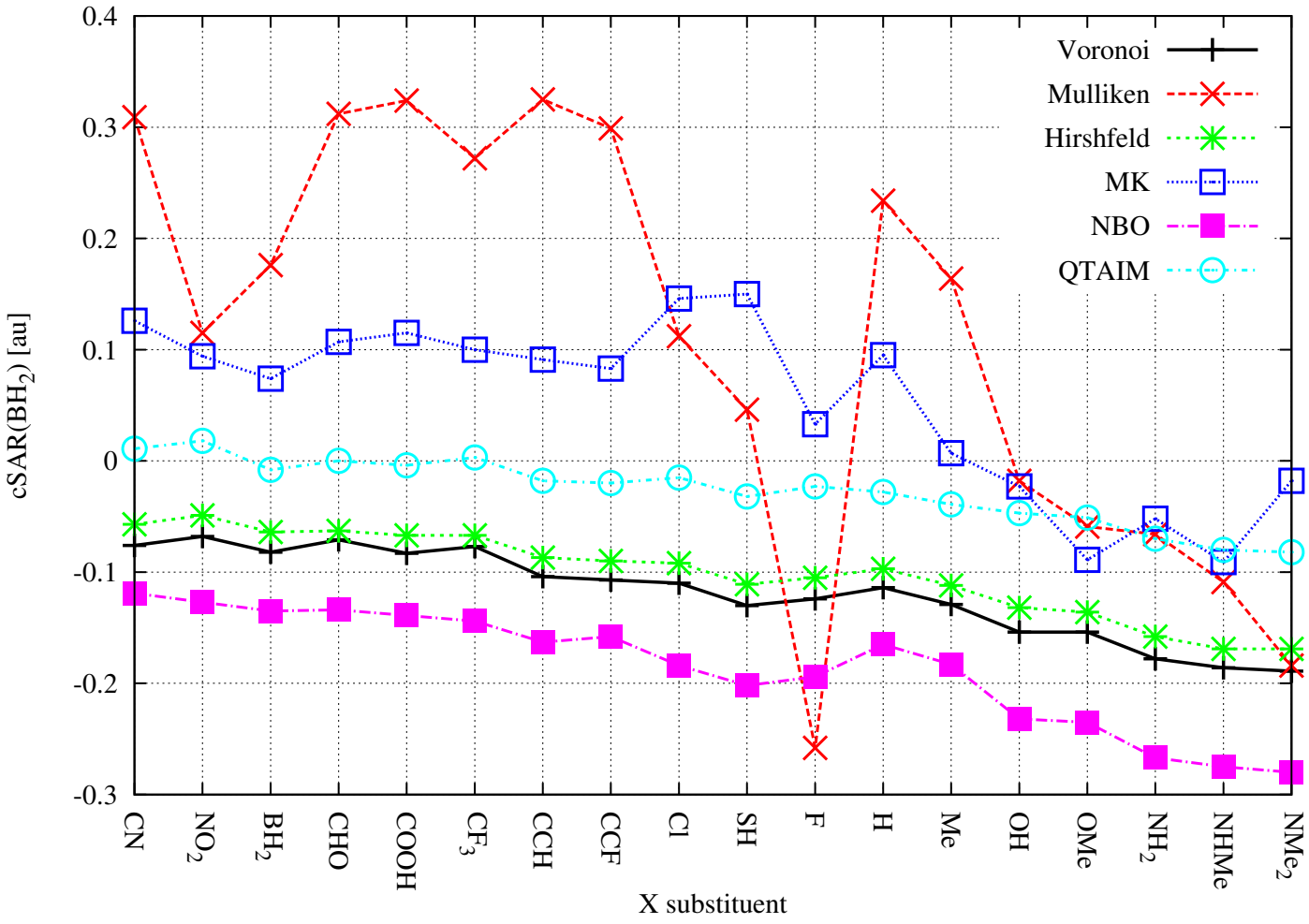

Figure S1: Relationships between cSAR(BH_2) values.

Table S1: HOMA values determined for the XC_6H_5 and $XC_6H_4BH_2$ monomers and the $XC_6H_4BH_2\cdots SiH_4$ and $XC_6H_4BH_2\cdots SiMeH_3$ dimers.

X	XC_6H_5	$XC_6H_4BH_2$	Δ^a	$\cdots SiH_4$	$\Delta_{mon}{}^b$	$\cdots SiMeH_3$	$\Delta_{mon}{}^b$
CN	0.996	0.978	-0.018	0.980	0.002	0.982	0.003
NO_2	0.997	0.981	-0.016	0.983	0.002	0.985	0.003
BH_2	0.980	0.963	-0.017	0.965	0.001	0.966	0.003
CHO	0.997	0.977	-0.020	0.979	0.001	0.980	0.003
COOH	0.998	0.980	-0.017	0.981	0.001	0.983	0.003
CF_3	0.998	0.983	-0.016	0.983	0.001	0.985	0.003
CCH	0.994	0.971	-0.023	0.972	0.001	0.974	0.004
CCF	0.994	0.971	-0.023	0.972	0.001	0.975	0.003
Cl	0.999	0.981	-0.018	0.981	0.000	0.983	0.000
SH	0.998	0.973	-0.025	0.973	0.000	0.975	0.002
F	0.995	0.975	-0.021	0.975	0.001	0.977	0.002
H	1.000	0.980	-0.020	0.981	0.001	0.983	0.003
Me	0.999	0.976	-0.022	0.977	0.000	0.978	0.002
OH	0.999	0.968	-0.031	0.969	0.000	0.969	0.002
OMe	0.994	0.962	-0.032	0.962	0.000	0.964	0.002
NH_2	0.994	0.947	-0.048	0.945	-0.001	0.948	0.001
NHMe	0.986	0.928	-0.058	0.927	-0.001	0.930	0.002
NMe_2	0.975	0.917	-0.058	0.915	-0.002	0.918	0.001
range	0.025	0.066	0.041^a	0.068	0.002^b	0.067	0.001^b

[a] The change relative to monomer XC_6H_5. [b] The change relative to monomer $XC_6H_4BH_2$.

*** Geometries of $XC_6H_4BH_2$ ***

- $NCC_6H_4BH_2$

  E_{tot} = -349.904075 au

  6 0.000000 0.000000 -1.789284
  6 0.000000 1.200920 -1.067005
  6 0.000000 1.211425 0.314878
  6 0.000000 0.000000 1.004900
  6 0.000000 -1.211425 0.314878
  6 0.000000 -1.200920 -1.067005
  1 0.000000 2.140288 -1.604864
  1 0.000000 2.141614 0.865454
  6 0.000000 0.000000 2.439041
  1 0.000000 -2.141614 0.865454
  1 0.000000 -2.140288 -1.604864
  5 0.000000 0.000000 -3.334101
  1 0.000000 1.033254 -3.932019
  1 0.000000 -1.033254 -3.932019
  7 0.000000 0.000000 3.587277

- $O_2NC_6H_4BH_2$

  E_{tot} = -462.1776088 au

  6 0.000000 -2.153724 0.000000
  6 1.201596 -1.432918 0.000000
  6 1.214130 -0.049624 0.000000
  6 0.000000 0.612965 0.000000
  6 -1.214130 -0.049624 0.000000
  6 -1.201597 -1.432918 0.000000
  1 2.140876 -1.970523 0.000000
  1 2.133374 0.515783 0.000000
  7 0.000000 2.090640 0.000000
  1 -2.133374 0.515783 0.000000
  1 -2.140876 -1.970523 0.000000
  5 0.000000 -3.700476 0.000000
  1 1.033227 -4.297836 0.000000
  1 -1.033227 -4.297837 0.000000
  8 -1.075119 2.650507 0.000000
  8 1.075119 2.650507 0.000000

- $H_2BC_6H_4BH_2$

  E_{tot} = -283.1034774 au

  6 0.000000 0.000000 1.413205
  6 0.000000 1.202214 0.691475
  6 0.000000 1.202214 -0.691475
  6 0.000000 0.000000 -1.413205
  6 0.000000 -1.202214 -0.691475
  6 0.000000 -1.202214 0.691475
  1 0.000000 2.140563 1.232412
  1 0.000000 2.140563 -1.232412
  5 0.000000 0.000000 -2.958140
  1 0.000000 -2.140563 -1.232412
  1 0.000000 -2.140563 1.232412
  5 0.000000 0.000000 2.958140
  1 0.000000 1.032804 3.558389
  1 0.000000 -1.032804 3.558389
  1 0.000000 1.032804 -3.558389
  1 0.000000 -1.032804 -3.558389

- $HCOC_6H_4BH_2$

  E_{tot} = -370.9939785 au

  6 0.311673 1.824263 0.000000
  6 1.426487 0.976518 0.000000
  6 1.274778 -0.399397 0.000000
  6 0.000000 -0.954444 0.000000
  6 -1.125104 -0.133211 0.000000
  6 -0.964772 1.238017 0.000000
  1 2.418976 1.409047 0.000000
  1 2.142319 -1.048912 0.000000
  6 -0.146915 -2.431502 0.000000
  1 -2.105763 -0.589828 0.000000
  1 -1.836675 1.880014 0.000000
  5 0.483038 3.359070 0.000000
  1 1.576578 3.839288 0.000000
  1 -0.476590 4.069768 0.000000
  8 -1.199894 -3.010420 0.000000
  1 0.808233 -2.992836 0.000000

- $HOOCC_6H_4BH_2$

  E_{tot} = -446.2566024 au

  6 -0.101774 2.201559 0.000000
  6 -1.275853 1.435154 0.000000
  6 -1.231144 0.053960 0.000000
  6 0.000000 -0.594308 0.000000
  6 1.181958 0.140537 0.000000
  6 1.123993 1.522669 0.000000
  1 -2.234258 1.938757 0.000000
  1 -2.134546 -0.539827 0.000000
  6 0.001803 -2.084283 0.000000
  1 2.133098 -0.371487 0.000000
  1 2.043229 2.094720 0.000000
  5 -0.157289 3.744189 0.000000
  1 -1.211013 4.306492 0.000000
  1 0.853380 4.380830 0.000000
  8 1.237815 -2.609790 0.000000
  8 -0.986833 -2.767045 0.000000
  1 1.134798 -3.567486 0.000000

- $F_3CC_6H_4BH_2$

  E_{tot} = -594.7458075 au

  6 0.340920 2.472226 0.000000
  6 -0.942986 1.907556 0.000000
  6 -1.125229 0.538591 0.000000

6 -0.014339 -0.297293 0.000000
6 1.268319 0.227000 0.000000
6 1.436706 1.602105 0.000000
1 -1.806623 2.560236 0.000000
1 -2.120461 0.115019 0.000000
6 -0.242587 -1.786763 0.000000
1 2.123861 -0.432474 0.000000
1 2.437846 2.014030 0.000000
5 0.539707 4.002549 0.000000
1 -0.407378 4.730035 0.000000
1 1.641566 4.463042 0.000000
9 0.897954 -2.481201 0.000000
9 -0.942986 -2.172909 1.075946
9 -0.942986 -2.172909 -1.075946

- $HCCC_6H_4BH_2$

  E_{tot} = -333.8088965 au

  6 0.000000 0.000000 -1.819374
  6 0.000000 1.199408 -1.092559
  6 0.000000 1.207838 0.288521
  6 0.000000 0.000000 0.990868
  6 0.000000 -1.207838 0.288521
  6 0.000000 -1.199408 -1.092559
  1 0.000000 2.139814 -1.629453
  1 0.000000 2.139293 0.837519
  6 0.000000 0.000000 2.420277
  1 0.000000 -2.139293 0.837519
  1 0.000000 -2.139814 -1.629453
  5 0.000000 0.000000 -3.358182
  1 0.000000 1.032801 -3.959379
  1 0.000000 -1.032801 -3.959379
  6 0.000000 0.000000 3.618348
  1 0.000000 0.000000 4.681281

- $FCCC_6H_4BH_2$

  E_{tot} = -433.0302364 au

  6 0.000000 0.000000 -2.397926
  6 0.000000 1.198923 -1.670323
  6 0.000000 1.207161 -0.289246
  6 0.000000 0.000000 0.413969
  6 0.000000 -1.207161 -0.289246
  6 0.000000 -1.198923 -1.670323
  1 0.000000 2.139653 -2.206710
  1 0.000000 2.139296 0.258716
  6 0.000000 0.000000 1.844858
  1 0.000000 -2.139296 0.258716
  1 0.000000 -2.139653 -2.206710
  5 0.000000 0.000000 -3.936095
  1 0.000000 1.032790 -4.537455
  1 0.000000 -1.032790 -4.537455
  6 0.000000 0.000000 3.036959
  9 0.000000 0.000000 4.308783

- $ClC_6H_4BH_2$

  E_{tot} = -717.2833419 au

  6 0.000000 0.000000 -1.897395
  6 0.000000 1.198486 -1.169761
  6 0.000000 1.210458 0.212993
  6 0.000000 0.000000 0.890211
  6 0.000000 -1.210458 0.212993
  6 0.000000 -1.198486 -1.169761
  1 0.000000 2.140070 -1.704508
  1 0.000000 2.138757 0.766036
  17 0.000000 0.000000 2.626301
  1 0.000000 -2.138757 0.766036
  1 0.000000 -2.140070 -1.704508
  5 0.000000 0.000000 -3.434847
  1 0.000000 1.032818 -4.035804
  1 0.000000 -1.032818 -4.035804

- $HSC_6H_4BH_2$

  E_{tot} = -655.875162 au

  6 0.002484 1.918220 0.000000
  6 -1.194941 1.186946 0.000000
  6 -1.205519 -0.193353 0.000000
  6 0.000000 -0.895239 0.000000
  6 1.206333 -0.196649 0.000000
  6 1.197749 1.184299 0.000000
  1 -2.137097 1.721151 0.000000
  1 -2.144288 -0.732037 0.000000
  16 -0.082359 -2.655084 0.000000
  1 2.146172 -0.732939 0.000000
  1 2.141222 1.716357 0.000000
  5 0.005185 3.451548 0.000000
  1 -1.026320 4.056032 0.000000
  1 1.039208 4.051912 0.000000
  1 1.236278 -2.882212 0.000000

- $FC_6H_4BH_2$

  E_{tot} = -356.9194079 au

  6 0.000000 0.000000 -1.454389
  6 0.000000 1.200173 -0.726869
  6 0.000000 1.213936 0.655483
  6 0.000000 0.000000 1.318254
  6 0.000000 -1.213936 0.655483
  6 0.000000 -1.200173 -0.726869
  1 0.000000 2.140252 -1.264102
  1 0.000000 2.133800 1.222702
  9 0.000000 0.000000 2.653651
  1 0.000000 -2.133800 1.222702
  1 0.000000 -2.140252 -1.264102
  5 0.000000 0.000000 -2.988983

1 0.000000 1.032692 -3.590849
1 0.000000 -1.032692 -3.590849

- $C_6H_5BH_2$

  E_{tot} = -257.6707321 au

  6 0.000000 0.000000 -1.008379
  6 0.000000 1.200739 -0.283257
  6 0.000000 1.204993 1.101004
  6 0.000000 0.000000 1.791350
  6 0.000000 -1.204993 1.101004
  6 0.000000 -1.200739 -0.283257
  1 0.000000 2.139726 -0.823232
  1 0.000000 2.140287 1.644834
  1 0.000000 0.000000 2.873838
  1 0.000000 -2.140287 1.644834
  1 0.000000 -2.139726 -0.823232
  5 0.000000 0.000000 -2.546075
  1 0.000000 1.032519 -3.148729
  1 0.000000 -1.032519 -3.148729

- $MeC_6H_4BH_2$

  E_{tot} = -296.9900951 au

  6 -0.785952 1.196870 -0.001936
  6 -1.517197 0.000000 0.002966
  6 -0.785952 -1.196870 -0.001936
  6 0.596423 -1.198396 -0.009911
  6 1.308003 0.000000 -0.011298
  6 0.596423 1.198396 -0.009911
  5 -3.051429 0.000000 0.009545
  6 2.809970 0.000000 0.012373
  1 -1.320808 -2.138945 -0.002280
  1 1.136991 -2.137198 -0.017598
  1 1.136991 2.137198 -0.017598
  1 -1.320809 2.138945 -0.002281
  1 -3.655055 -1.032462 0.012416
  1 -3.655056 1.032462 0.012414
  1 3.215472 0.883831 -0.478521
  1 3.173638 -0.000011 1.042188
  1 3.215472 -0.883821 -0.478540

- $HOC_6H_4BH_2$

  E_{tot} = HF=-332.9041636 au

  6 -0.014325 1.474831 0.000000
  6 -1.207901 0.731790 0.000000
  6 -1.212935 -0.646481 0.000000
  6 0.000000 -1.330581 0.000000
  6 1.204794 -0.631119 0.000000
  6 1.186730 0.749329 0.000000
  1 -2.152676 1.261444 0.000000
  1 -2.133592 -1.213167 0.000000
  8 -0.050089 -2.680102 0.000000
  1 2.144362 -1.171785 0.000000
  1 2.125911 1.288807 0.000000
  5 -0.021782 3.003666 0.000000
  1 -1.056877 3.603148 0.000000
  1 1.008339 3.612081 0.000000
  1 0.835976 -3.044661 0.000000

- $MeOC_6H_4BH_2$

  E_{tot} = -372.2025927 au

  6 0.476758 1.870081 0.000000
  6 1.534489 0.940523 0.000000
  6 1.310779 -0.415857 0.000000
  6 0.000000 -0.901508 0.000000
  6 -1.074449 -0.013077 0.000000
  6 -0.822434 1.348037 0.000000
  1 2.553683 1.307266 0.000000
  1 2.124731 -1.127600 0.000000
  8 -0.126720 -2.240945 0.000000
  1 -2.093360 -0.370241 0.000000
  1 -1.661447 2.033321 0.000000
  5 0.729630 3.377438 0.000000
  1 1.847456 3.803819 0.000000
  1 -0.189795 4.143136 0.000000
  6 -1.420763 -2.802704 0.000000
  1 -1.281075 -3.879688 0.000000
  1 -1.980430 -2.511308 0.891986
  1 -1.980430 -2.511308 -0.891986

- $H_2NC_6H_4BH_2$

  E_{tot} = -313.039277 au

  6 0.757746 1.195622 -0.000485
  6 1.497682 0.000000 0.002274
  6 0.757746 -1.195622 -0.000485
  6 -0.618869 -1.206769 -0.005026
  6 -1.330531 0.000000 -0.006229
  6 -0.618869 1.206769 -0.005026
  5 3.021489 0.000000 0.007792
  7 -2.703850 0.000000 -0.050767
  1 1.290866 -2.138802 0.001819
  1 -1.161095 -2.144595 -0.010675
  1 -1.161095 2.144595 -0.010675
  1 1.290866 2.138802 0.001819
  1 3.627316 -1.032597 0.010133
  1 3.627316 1.032597 0.010133
  1 -3.182052 -0.845457 0.201859
  1 -3.182052 0.845457 0.201859

- $HMeNC_6H_4BH_2$

  E_{tot} = -352.3445789 au

  6 -1.048023 -1.200270 -0.006603
  6 -1.957793 -0.131217 0.002802

6 -1.400226 1.163335 0.005055
6 -0.044593 1.376218 -0.002266
6 0.846748 0.286777 -0.012323
6 0.318527 -1.013715 -0.013291
5 -3.462209 -0.359993 0.010769
7 2.189973 0.512422 -0.027257
6 3.184431 -0.526769 0.023946
1 -2.066432 2.017780 0.012805
1 0.352811 2.384479 -0.001787
1 0.979100 -1.869040 -0.019273
1 -1.435412 -2.212278 -0.007741
1 -4.217573 0.569350 0.018846
1 -3.905756 -1.472373 0.009047
1 2.497958 1.463531 0.036075
1 4.170948 -0.069864 0.017264
1 3.095900 -1.134344 0.929403
1 3.115257 -1.190382 -0.841602

- $Me_2NC_6H_4BH_2$

  E_{tot} = -391.6479876 au

  6 0.000000 0.000000 -2.292369
  6 0.000000 1.191752 -1.547519
  6 0.000000 1.207514 -0.171643
  6 0.000000 0.000000 0.557918
  6 0.000000 -1.207514 -0.171643
  6 0.000000 -1.191752 -1.547519
  1 0.000000 2.137012 -2.077504
  1 0.000000 2.156266 0.343008
  7 0.000000 0.000000 1.923466
  1 0.000000 -2.156266 0.343008
  1 0.000000 -2.137012 -2.077504
  5 0.000000 0.000000 -3.814095
  1 0.000000 1.032578 -4.420884
  1 0.000000 -1.032578 -4.420884
  6 0.000000 -1.248591 2.651374
  6 0.000000 1.248591 2.651374
  1 0.000000 -1.041774 3.717627
  1 -0.885571 -1.849218 2.425472
  1 0.885571 -1.849218 2.425472
  1 0.000000 1.041774 3.717627
  1 0.885571 1.849218 2.425472
  1 -0.885571 1.849218 2.425472

*** Geometries of $XC_6H_4BH_2\cdots SiH_4$ ***

- $NCC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -641.7970898 au

  6 0.024255 -0.189663 0.054721
  6 -0.041844 -0.084039 1.449716
  6 1.163048 -0.025840 2.161553
  6 2.384422 -0.076116 1.517592
  6 2.418045 -0.187409 0.128179
  6 1.236012 -0.242483 -0.608233
  5 -1.404798 -0.069617 2.185358
  6 3.680554 -0.245953 -0.549346
  7 4.691564 -0.293197 -1.091698
  1 1.134984 0.053747 3.240729
  1 3.310071 -0.033584 2.074183
  1 1.278751 -0.327859 -1.684943
  1 -0.894800 -0.237626 -0.515185
  1 -1.440996 0.023504 3.374623
  1 -2.420452 -0.124576 1.560871
  1 -1.519700 -2.541302 2.552900
  14 -0.839718 -3.487149 1.630687
  1 -1.281634 -3.207714 0.247716
  1 0.622564 -3.299860 1.740228
  1 -1.207086 -4.870145 2.006514

- $O_2NC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -754.0707291 au

  6 -0.423438 1.378957 0.898551
  6 -1.158234 1.243831 -0.285976
  6 -0.570568 0.549691 -1.350759
  6 0.695809 0.002224 -1.245420
  6 1.376888 0.159931 -0.052282
  6 0.844582 0.841945 1.027179
  5 -2.595979 1.814089 -0.402522
  7 2.727668 -0.424055 0.075480
  8 3.172578 -1.021909 -0.880712
  8 3.307282 -0.269584 1.128979
  1 -1.122025 0.432845 -2.274641
  1 1.155301 -0.538034 -2.058796
  1 1.418230 0.937401 1.936314
  1 -0.860558 1.909785 1.734275
  1 -3.205682 1.689797 -1.420691
  1 -3.080691 2.403805 0.514509
  1 -3.744098 -0.178077 0.499364
  14 -3.156973 -1.539544 0.395649
  1 -2.848579 -1.819467 -1.022856
  1 -1.918539 -1.590804 1.201163
  1 -4.138621 -2.523222 0.902624

- $H_2BC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -574.99653 au

  6 -0.422078 1.189605 1.050511
  6 0.294538 1.351006 -0.143420
  6 -0.134536 0.638272 -1.271579
  6 -1.226886 -0.207770 -1.205946
  6 -1.938350 -0.375910 -0.009979
  6 -1.514131 0.344277 1.116040
  5 1.551561 2.249708 -0.201303
  5 -3.151153 -1.329825 0.066291
  1 0.408564 0.749126 -2.202069

1 -1.539931 -0.755595 -2.086245
1 -2.052550 0.227717 2.048546
1 -0.103463 1.731424 1.932519
1 2.170142 2.349312 -1.218241
1 1.909069 2.844170 0.770879
1 -3.496582 -1.939572 -0.901046
1 -3.746803 -1.462165 1.093205
1 2.989667 -0.133930 0.657292
14 2.448436 -1.444088 0.223495
1 1.097508 -1.635113 0.793342
1 2.382385 -1.475995 -1.253813
1 3.350521 -2.518432 0.697990

- $HCOC_6H_4BH_2\cdots SiH_4$

  E_{tot} =HF=-662.8869833 au

  6 0.003543 1.140043 -1.083619
  6 0.820473 1.291698 0.048187
  6 0.356774 0.786586 1.268522
  6 -0.868794 0.148270 1.355526
  6 -1.655922 0.005088 0.218828
  6 -1.219769 0.505656 -1.005960
  5 2.214700 1.954784 -0.057995
  6 -2.964086 -0.687278 0.325988
  8 -3.717822 -0.864401 -0.593046
  1 0.973337 0.891648 2.152259
  1 -1.218703 -0.244329 2.303126
  1 -1.851125 0.382347 -1.875689
  1 0.349724 1.523582 -2.035165
  1 2.903097 2.056917 0.912393
  1 2.599718 2.377271 -1.106095
  1 -3.216670 -1.046774 1.343075
  1 3.395376 -0.265362 -0.684732
  14 2.848472 -1.553926 -0.190023
  1 2.745950 -1.497392 1.284246
  1 1.511218 -1.774707 -0.780122
  1 3.765245 -2.647314 -0.583451

- $HOOCC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -738.1496463 au

  6 -0.751297 0.718283 -1.314517
  6 -1.354182 1.350442 -0.219474
  6 -0.620762 1.440434 0.971774
  6 0.653635 0.916252 1.070432
  6 1.225669 0.286287 -0.030645
  6 0.524008 0.188651 -1.228059
  5 -2.799043 1.889475 -0.308815
  6 2.598451 -0.272045 0.123058
  8 3.248502 -0.214172 1.131807
  8 3.055919 -0.861006 -0.993890
  1 -1.068508 1.923102 1.831199
  1 1.220189 0.979453 1.988982
  1 0.975727 -0.301911 -2.077798
  1 -1.300849 0.635648 -2.243675
  1 -3.302685 2.414986 0.637829
  1 -3.417431 1.778061 -1.324567
  1 3.940353 -1.187388 -0.796233
  1 -3.511437 -0.826654 0.749780
  14 -2.617504 -1.936780 0.343970
  1 -1.257741 -1.697040 0.873286
  1 -3.149561 -3.208670 0.883977
  1 -2.576285 -2.010442 -1.133030

- $F_3CC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -886.6389567 au

  6 0.203906 -0.353484 1.249947
  6 -1.079107 -0.875936 1.263909
  6 -1.667727 -1.396934 0.106589
  6 -0.912656 -1.383234 -1.074738
  6 0.367264 -0.865673 -1.102762
  6 0.919672 -0.349278 0.063684
  5 -3.117641 -1.927968 0.119887
  6 2.304068 0.242130 0.000547
  9 3.168427 -0.591573 -0.593162
  9 2.312847 1.379769 -0.710012
  9 2.794936 0.528482 1.209146
  14 -2.828787 1.967610 -0.187878
  1 -1.347254 -1.779958 -1.983337
  1 0.938408 -0.857611 -2.021125
  1 0.643611 0.049447 2.150650
  1 -1.643018 -0.873893 2.187990
  1 -3.605833 -2.360735 -0.880137
  1 -3.754752 -1.902331 1.129502
  1 -3.737178 0.928004 -0.726654
  1 -1.456875 1.732468 -0.687308
  1 -3.302032 3.300170 -0.625706
  1 -2.842254 1.902090 1.290174

- $HCCC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -625.7018994 au

  6 0.194565 1.303641 1.084575
  6 0.935994 1.367225 -0.103859
  6 0.364502 0.809225 -1.256154
  6 -0.879715 0.209867 -1.228326
  6 -1.596563 0.152175 -0.031010
  6 -1.050164 0.707808 1.128843
  5 2.344132 1.989571 -0.132372
  6 -2.881018 -0.473533 0.007852
  1 0.917154 0.842865 -2.186742
  1 -1.307127 -0.221572 -2.122811
  1 -1.609878 0.660664 2.052672
  1 0.614150 1.725397 1.989345
  1 2.972344 2.006875 -1.148664

1 2.815861 2.453020 0.862704
6 -3.956981 -0.999419 0.040237
1 -4.911901 -1.465432 0.068893
1 3.187041 -0.833040 0.731255
14 2.332126 -1.911690 0.183017
1 0.953087 -1.763670 0.695230
1 2.332709 -1.828849 -1.294114
1 2.882416 -3.222394 0.598913

- $FCCC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -724.9232651 au

  6 -0.971834 -0.829987 1.252937
  6 -1.612910 -1.290333 0.094081
  6 -0.863227 -1.325245 -1.090385
  6 0.455086 -0.916325 -1.124133
  6 1.071062 -0.454968 0.041994
  6 0.346248 -0.417225 1.235165
  5 -3.095698 -1.702704 0.112242
  6 2.434590 -0.022557 0.013368
  1 -1.334343 -1.674473 -2.000715
  1 1.019805 -0.944471 -2.045752
  1 0.825983 -0.059478 2.135682
  1 -1.528089 -0.789905 2.181150
  1 -3.625241 -2.084406 -0.888518
  1 -3.724271 -1.638413 1.126528
  6 3.570368 0.338611 -0.011181
  9 4.782132 0.723667 -0.037162
  1 -3.522489 1.201769 -0.755677
  14 -2.541465 2.149641 -0.178124
  1 -1.188778 1.840955 -0.689396
  1 -2.917594 3.529341 -0.563872
  1 -2.561473 2.032799 1.296473

- $ClC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -1009.1764021 au

  6 -0.408757 0.844456 -1.254400
  6 -0.974442 1.397856 -0.097422
  6 -0.247890 1.284219 1.096087
  6 0.977417 0.646102 1.144007
  6 1.495076 0.107679 -0.024917
  6 0.815636 0.201932 -1.229959
  5 -2.357919 2.069967 -0.127534
  17 3.027174 -0.706412 0.022991
  1 -0.660982 1.700571 2.006288
  1 1.528537 0.558675 2.069280
  1 1.241820 -0.226645 -2.125614
  1 -0.948242 0.914419 -2.190612
  1 -2.823144 2.530645 0.871745
  1 -2.974220 2.129009 -1.149434
  1 -3.264592 -0.742445 0.824134
  14 -2.497569 -1.824505 0.164722
  1 -1.090329 -1.784803 0.617533
  1 -3.099116 -3.130505 0.519000
  1 -2.558366 -1.640148 -1.301980

- $HSC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -947.7682681 au

  6 0.445178 0.862224 1.252144
  6 1.025544 1.401466 0.095005
  6 0.295951 1.286122 -1.097796
  6 -0.935305 0.664707 -1.141023
  6 -1.483879 0.132004 0.025900
  6 -0.786341 0.237701 1.227725
  5 2.410358 2.060898 0.126138
  16 -3.053754 -0.656673 -0.098733
  1 0.714881 1.690159 -2.011138
  1 -1.473949 0.585176 -2.076404
  1 -1.204108 -0.171702 2.138044
  1 0.981667 0.931400 2.190482
  1 2.885517 2.509996 -0.874494
  1 3.023172 2.124476 1.150678
  1 -3.165335 -1.006098 1.188074
  1 3.241616 -0.875822 -0.872926
  14 2.425271 -1.886465 -0.162791
  1 1.011017 -1.772274 -0.578682
  1 2.933290 -3.238181 -0.493723
  1 2.539812 -1.669695 1.296465

- $FC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -648.8124006 au

  6 -0.374994 1.146967 1.086561
  6 0.313238 1.386531 -0.112673
  6 -0.122549 0.704666 -1.258894
  6 -1.185762 -0.178296 -1.220848
  6 -1.822004 -0.378315 -0.009650
  6 -1.440620 0.269470 1.151505
  5 1.522866 2.331326 -0.160022
  9 -2.846418 -1.233003 0.041721
  1 0.393311 0.869572 -2.196427
  1 -1.523803 -0.710904 -2.098263
  1 -1.972519 0.075958 2.072090
  1 -0.056818 1.658818 1.986029
  1 2.112469 2.501472 -1.185614
  1 1.882464 2.897544 0.828968
  1 3.050180 -0.176848 0.762700
  14 2.496866 -1.420023 0.177969
  1 1.124958 -1.641686 0.683740
  1 2.474201 -1.297317 -1.296227
  1 3.358994 -2.562031 0.560054

- $C_6H_5BH_2\cdots SiH_4$

  E_{tot} = -549.5637124 au

6 -0.017799 0.210693 0.128995
6 -0.083086 0.042214 1.519665
6 1.118333 0.095512 2.241208
6 2.328788 0.313311 1.606814
6 2.361497 0.482198 0.228603
6 1.189159 0.429271 -0.513119
5 -1.431824 -0.153344 2.234481
1 1.090243 -0.029605 3.316719
1 3.245953 0.355474 2.179067
1 3.306382 0.656450 -0.269913
1 1.220815 0.561935 -1.586347
1 -0.934199 0.176251 -0.447379
1 -1.470277 -0.287853 3.421474
1 -2.448657 -0.167489 1.606144
1 -1.348447 2.843913 2.582034
14 -0.682042 3.553562 1.465355
1 -1.352309 3.201351 0.194544
1 -0.796261 5.014024 1.687200
1 0.744374 3.169014 1.407949

- $MeC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -588.883232 au

  6 1.373282 0.374312 -1.134583
  6 0.262578 1.195281 -1.087460
  6 -0.442980 1.404929 0.106293
  6 0.029689 0.750188 1.252767
  6 1.140318 -0.071934 1.208386
  6 1.828490 -0.271826 0.013496
  5 -1.701027 2.283875 0.148097
  6 3.049138 -1.145830 -0.031224
  1 -0.496527 0.886281 2.189806
  1 1.478783 -0.573268 2.107055
  1 1.895193 0.222840 -2.071692
  1 -0.080399 1.682171 -1.992327
  1 -2.300900 2.428509 1.172414
  1 -2.091184 2.825833 -0.843669
  1 3.176568 -1.600686 -1.012714
  1 3.945476 -0.558007 0.177979
  1 2.996565 -1.939784 0.712696
  1 -3.068886 -0.382761 -0.775690
  14 -2.412846 -1.566356 -0.174769
  1 -1.022865 -1.675145 -0.666540
  1 -2.419281 -1.435505 1.298769
  1 -3.170661 -2.781591 -0.555850

- $HOC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -624.7972614 au

  6 -0.320305 1.111729 1.114009
  6 0.357636 1.401092 -0.079942
  6 -0.112766 0.775940 -1.247900
  6 -1.186213 -0.088399 -1.234581
  6 -1.829600 -0.354279 -0.028817
  6 -1.397387 0.249727 1.150004
  5 1.570037 2.333615 -0.101417
  8 -2.872282 -1.211188 -0.059131
  1 0.390226 0.976013 -2.185986
  1 -1.540797 -0.570375 -2.134930
  1 -1.903904 0.036685 2.084381
  1 0.016305 1.573948 2.033817
  1 2.146836 2.550050 -1.126537
  1 1.952057 2.848593 0.908205
  1 -3.232703 -1.326245 0.821179
  1 3.035134 -0.346751 0.898018
  14 2.455854 -1.479529 0.141142
  1 1.050103 -1.689929 0.548662
  1 2.523257 -1.189187 -1.307691
  1 3.241418 -2.702823 0.428389

- $MeOC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -664.0957802 au

  6 -0.182473 1.119689 -1.142718
  6 -1.028979 1.392181 -0.061137
  6 -0.573185 1.008426 1.214653
  6 0.640766 0.389958 1.397201
  6 1.457466 0.128285 0.293599
  6 1.043769 0.498292 -0.985618
  5 -2.392981 2.052854 -0.264620
  8 2.623532 -0.485391 0.562491
  6 3.495012 -0.790032 -0.504529
  1 -1.202383 1.201041 2.074965
  1 0.986450 0.091780 2.377287
  1 1.661592 0.303667 -1.849349
  1 -0.501442 1.399502 -2.139431
  1 -3.111225 2.257379 0.669863
  1 -2.753038 2.365926 -1.361532
  1 4.356722 -1.278007 -0.058808
  1 3.024624 -1.469388 -1.219281
  1 3.820525 0.115262 -1.022363
  1 -3.165624 -0.998290 -1.068529
  14 -2.466403 -1.879349 -0.106264
  1 -1.009345 -1.841538 -0.355170
  1 -2.755974 -1.431739 1.273344
  1 -2.958852 -3.266649 -0.278830

- $H_2NC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -604.9324796 au

  6 -0.019388 -0.003731 0.025298
  6 0.003536 -0.012817 1.426385
  6 1.205592 -0.010372 2.096251
  6 2.439556 0.002624 1.422053
  6 2.386759 0.007474 0.017035
  6 1.195418 0.005202 -0.672442

5 3.764478 0.032452 2.175641
7 -1.212794 0.039231 -0.651999
14 2.428481 3.550782 1.046067
1 3.316084 0.019492 -0.539629
1 1.187429 0.017151 -1.755574
1 -0.930983 -0.015068 1.974178
1 1.203660 -0.013175 3.179627
1 4.800303 0.062195 1.576487
1 3.779964 0.030970 3.372386
1 -1.211587 -0.200205 -1.626528
1 -2.047271 -0.213087 -0.154989
1 2.968752 3.195823 2.377440
1 1.119718 2.895627 0.838435
1 2.258870 5.021977 0.973526
1 3.381123 3.125599 -0.002828

- $HMeNC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -644.2379807 au

  6 0.892549 0.221675 -1.045733
  6 -0.362800 0.748009 -1.266136
  6 -1.119620 1.350876 -0.249034
  6 -0.523399 1.401340 1.027336
  6 0.724054 0.886217 1.272502
  6 1.460024 0.280220 0.236598
  5 -2.515559 1.901069 -0.507399
  7 2.698123 -0.225566 0.493919
  6 3.489370 -0.946885 -0.468608
  1 -1.073563 1.857500 1.841659
  1 1.153828 0.938026 2.265968
  1 1.433753 -0.238947 -1.859794
  1 -0.786032 0.686642 -2.261721
  1 -3.140570 2.409235 0.378358
  1 -3.003039 1.825594 -1.598388
  1 3.001554 -0.230441 1.448785
  1 4.415160 -1.264283 0.004816
  1 2.972726 -1.836409 -0.841451
  1 3.748301 -0.317586 -1.323319
  1 -3.312838 -1.002774 0.807377
  14 -2.353802 -1.964916 0.221129
  1 -0.995138 -1.714594 0.747599
  1 -2.771908 -3.340616 0.584815
  1 -2.359131 -1.837615 -1.252504

- $Me_2NC_6H_4BH_2\cdots SiH_4$

  E_{tot} = -683.5414743 au

  6 -1.166409 -0.311459 0.047256
  6 -0.535873 -0.815831 -1.109865
  6 0.742727 -1.318216 -1.045004
  6 1.481957 -1.358156 0.149845
  6 0.833769 -0.858515 1.292485
  6 -0.443917 -0.350007 1.258311
  5 2.906160 -1.893826 0.198874
  7 -2.431242 0.198519 -0.004355
  6 -3.049642 0.733432 1.187629
  6 -3.143458 0.252162 -1.261062
  14 2.570935 2.016865 -0.257441
  1 1.364305 -0.867063 2.237319
  1 -0.884794 0.024535 2.169449
  1 -1.050010 -0.807062 -2.058807
  1 1.200754 -1.692113 -1.953133
  1 3.516848 -1.898229 1.228865
  1 3.430795 -2.310846 -0.793301
  1 -4.124195 0.689601 -1.098607
  1 -2.618746 0.865557 -1.999193
  1 -3.287364 -0.744680 -1.686390
  1 -4.046448 1.089868 0.944848
  1 -3.146182 -0.026246 1.967923
  1 -2.481691 1.573504 1.597699
  1 3.420940 1.143738 -1.096484
  1 1.143324 1.784585 -0.563444
  1 2.835859 1.745281 1.172165
  1 2.906497 3.432502 -0.546199

*** Geometries of $XC_6H_4BH_2\cdots SiMeH_3$ ***

- $NCC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -681.1279825 au

  6 -0.017298 0.077898 -0.024514
  6 0.005873 -0.019818 1.354311
  6 1.211418 -0.093349 2.062076
  6 2.404315 -0.059556 1.329861
  6 2.403117 0.038706 -0.048433
  6 1.186528 0.105388 -0.726085
  5 1.225397 -0.227482 3.609448
  6 1.173854 0.202508 -2.156634
  7 1.163790 0.279520 -3.302386
  14 0.767084 -3.428774 2.784425
  1 3.348325 -0.116789 1.856556
  1 3.328854 0.062157 -0.606116
  1 -0.952926 0.131397 -0.563277
  1 -0.928721 -0.045618 1.899849
  1 2.264308 -0.248186 4.196713
  1 0.198773 -0.218728 4.217967
  1 1.276461 -2.448870 3.789724
  1 -0.614512 -3.026691 2.433071
  1 1.623068 -3.315071 1.581245
  6 0.812338 -5.153567 3.501539
  1 0.441510 -5.880022 2.777734
  1 1.829661 -5.436029 3.772712
  1 0.191828 -5.219865 4.395314

- $O_2NC_6H_4BH_2\cdots SiMeH_3$

E_{tot} = -793.4017694 au

6 -1.365200 0.585501 -1.162326
6 -0.183357 1.300774 -1.093166
6 0.489331 1.488663 0.119847
6 -0.071866 0.932810 1.275143
6 -1.252635 0.212418 1.231884
6 -1.875534 0.052246 0.007717
5 1.827625 2.283820 0.179984
7 -3.133151 -0.717803 -0.052858
8 -3.663393 -0.842803 -1.136308
8 -3.559418 -1.179434 0.984378
14 3.076166 -0.718435 0.010067
1 0.431337 1.065607 2.224099
1 -1.690401 -0.221549 2.117707
1 -1.888646 0.434696 -2.093932
1 0.233096 1.721550 -1.999239
1 2.354772 2.481139 1.232187
1 2.254093 2.804666 -0.805518
1 3.217883 0.754157 -0.213667
1 2.602683 -0.908744 1.399813
1 2.040004 -1.204740 -0.928786
6 4.721197 -1.554768 -0.276254
1 4.636255 -2.630338 -0.117466
1 5.069799 -1.390190 -1.295829
1 5.477605 -1.170607 0.408141

- $H_2BC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -614.3270501 au

  6 2.081744 0.040243 -1.183849
  6 1.090893 1.002388 -1.120381
  6 0.468158 1.318256 0.094305
  6 0.882841 0.633683 1.244061
  6 1.872453 -0.330854 1.180982
  6 2.493110 -0.650637 -0.034667
  5 -0.666651 2.375184 0.158864
  5 3.592944 -1.730552 -0.106272
  14 -2.488486 -0.465761 0.050761
  1 0.411516 0.863498 2.191785
  1 2.176267 -0.852786 2.080173
  1 2.550261 -0.191566 -2.132567
  1 0.781764 1.520259 -2.020085
  1 -1.171213 2.648849 1.205989
  1 -0.990882 2.966752 -0.826655
  1 3.926493 -2.314971 0.881162
  1 4.115561 -1.988085 -1.149496
  1 -2.437837 0.983382 -0.300441
  1 -1.468286 -1.163289 -0.765062
  1 -2.132684 -0.593316 1.482973
  6 -4.202613 -1.137458 -0.277924
  1 -4.256549 -2.196183 -0.022108
  1 -4.948523 -0.608281 0.315403
  1 -4.468066 -1.030492 -1.329848

- $HCOC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -702.217661 au

  6 -1.738256 0.244188 -1.066093
  6 -0.635540 1.065539 -1.187066
  6 0.082162 1.495952 -0.060306
  6 -0.354405 1.071954 1.199511
  6 -1.458957 0.247205 1.330719
  6 -2.150537 -0.168696 0.199017
  5 1.338781 2.394300 -0.207388
  6 -3.328313 -1.055933 0.355460
  8 -3.993444 -1.474408 -0.554233
  14 2.798833 -0.631916 0.075025
  1 0.187055 1.391003 2.081079
  1 -1.788267 -0.079319 2.310330
  1 -2.292778 -0.091806 -1.932078
  1 -0.308973 1.383526 -2.169288
  1 1.921546 2.769724 0.764696
  1 1.683094 2.770367 -1.286911
  1 -3.570929 -1.323333 1.403113
  1 2.906607 0.750721 -0.475452
  1 2.475084 -0.514890 1.516088
  1 1.675974 -1.304964 -0.617337
  6 4.409382 -1.545450 -0.182529
  1 4.345341 -2.558246 0.216628
  1 4.651891 -1.615414 -1.243041
  1 5.231130 -1.035329 0.320349

- $HOOCC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -777.4801869 au

  6 -1.191097 0.250469 1.205874
  6 -0.027531 0.996310 1.275077
  6 0.522884 1.596493 0.136495
  6 -0.145933 1.424703 -1.082449
  6 -1.309141 0.683727 -1.165127
  6 -1.832129 0.092836 -0.018867
  5 1.846117 2.401029 0.217006
  6 -3.083607 -0.702011 -0.153869
  8 -3.503410 -1.227953 1.009302
  8 -3.677272 -0.871960 -1.184977
  14 3.053823 -0.754329 0.025968
  1 0.263212 1.878116 -1.976475
  1 -1.825347 0.547855 -2.105277
  1 -1.603358 -0.210418 2.091633
  1 0.473591 1.114376 2.227541
  1 2.289205 2.924459 -0.760498
  1 2.389201 2.555549 1.269181
  1 -4.310392 -1.717786 0.818264
  1 3.312519 0.687804 -0.254628
  1 1.922119 -1.183631 -0.827241

6 4.593150 -1.755588 -0.326457
1 2.656099 -0.869195 1.448442
1 4.419194 -2.813005 -0.124459
1 4.891395 -1.656144 -1.370303
1 5.424331 -1.424857 0.296571

- $F_3CC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -925.9695534 au

  6 -1.506363 0.210716 0.034607
  6 -0.852099 0.443656 1.233109
  6 0.328197 1.170049 1.230219
  6 0.874431 1.670972 0.045085
  6 0.184248 1.421705 -1.148858
  6 -0.993356 0.700670 -1.161084
  5 2.215463 2.448325 0.048121
  6 -2.785353 -0.582964 -0.009396
  9 -3.191284 -0.972369 1.202139
  9 -3.784545 0.126907 -0.553313
  9 -2.648593 -1.689214 -0.755699
  14 3.336166 -0.751594 0.065798
  1 0.588308 1.797753 -2.080152
  1 -1.514663 0.513019 -2.090120
  1 -1.259045 0.059831 2.157244
  1 0.843570 1.347832 2.165509
  1 2.655537 2.886597 -0.971590
  1 2.777047 2.666755 1.078753
  1 3.639278 0.661009 -0.306539
  1 2.184950 -1.195335 -0.753531
  6 4.838677 -1.824375 -0.228208
  1 2.942621 -0.762139 1.494113
  1 4.629901 -2.860415 0.040490
  1 5.134541 -1.800878 -1.277177
  1 5.683823 -1.483832 0.370239

- $HCCC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -665.0321517 au

  6 1.716259 0.408633 -1.182344
  6 0.628251 1.258410 -1.147249
  6 -0.028082 1.561274 0.053295
  6 0.462218 0.972958 1.226638
  6 1.548797 0.119753 1.208657
  6 2.184475 -0.170848 -0.000412
  5 -1.268658 2.480291 0.076621
  6 3.306584 -1.056148 -0.028522
  14 -2.705423 -0.670371 0.058004
  1 -0.028582 1.187772 2.167673
  1 1.914700 -0.330605 2.121009
  1 2.212024 0.181054 -2.115913
  1 0.267395 1.697315 -2.069112
  1 -1.811399 2.729706 1.111245
  1 -1.666411 2.977893 -0.934077
  1 -2.931925 0.749896 -0.330148
  1 -1.575695 -1.189630 -0.747097
  1 -2.324472 -0.692513 1.489902
  6 -4.260448 -1.668909 -0.233932
  6 4.246910 -1.798353 -0.051747
  1 5.081360 -2.456350 -0.072211
  1 -5.090667 -1.277894 0.354635
  1 -4.548637 -1.642162 -1.285053
  1 -4.108268 -2.711360 0.047688

- $FCCC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -764.2534773 au

  6 1.695150 -0.342220 0.012194
  6 1.012586 -0.532079 1.215498
  6 -0.197794 -1.198279 1.223054
  6 -0.770059 -1.694496 0.044252
  6 -0.065005 -1.496233 -1.150527
  6 1.146217 -0.833382 -1.174829
  5 -2.143206 -2.398182 0.055475
  6 2.947043 0.351081 -0.005276
  6 3.989783 0.928637 -0.020424
  9 5.102638 1.545314 -0.036368
  14 -3.019823 0.971427 0.057002
  6 -4.361638 2.243351 -0.230632
  1 -0.485695 -1.866825 -2.077039
  1 1.677267 -0.685356 -2.105049
  1 1.439644 -0.151100 2.132933
  1 -0.722577 -1.334447 2.160427
  1 -2.610566 -2.819425 -0.960223
  1 -2.728140 -2.556475 1.085164
  1 -3.492797 -0.374827 -0.369423
  1 -1.800063 1.295206 -0.718908
  1 -2.666777 0.893672 1.494198
  1 -4.027930 3.233807 0.080507
  1 -4.630211 2.294098 -1.286063
  1 -5.260032 1.996506 0.335531

- $ClC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -1048.5066753 au

  6 -1.408318 0.118089 1.211611
  6 -0.359102 1.019475 1.225590
  6 0.100085 1.634802 0.053806
  6 -0.549035 1.309495 -1.144497
  6 -1.600278 0.412231 -1.182641
  6 -2.016843 -0.177409 0.001573
  5 1.304186 2.596775 0.074368
  17 -3.329925 -1.313891 -0.032853
  14 2.778133 -0.616011 0.062265
  1 -0.213535 1.766965 -2.066839
  1 -2.092764 0.164342 -2.111957
  1 -1.752643 -0.355420 2.119803

1 0.125719 1.248453 2.166301
1 1.680464 3.109293 -0.937050
1 1.850961 2.851793 1.105494
1 3.035427 0.779403 -0.387894
1 1.601826 -1.128172 -0.679118
6 4.285929 -1.680290 -0.244741
1 2.448805 -0.572569 1.506884
1 4.109063 -2.704997 0.083566
1 4.535487 -1.704509 -1.305776
1 5.150499 -1.296518 0.297336

- $HSC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -987.0982942 au

  6 -1.296453 0.176713 1.209655
  6 -0.325645 1.159228 1.215258
  6 0.084041 1.802228 0.038921
  6 -0.542296 1.411201 -1.153492
  6 -1.513617 0.431312 -1.178264
  6 -1.894628 -0.196325 0.007840
  5 1.206014 2.849438 0.047927
  16 -3.132754 -1.445896 -0.093684
  14 2.647162 -0.637145 0.069017
  1 -0.248225 1.885654 -2.081596
  1 -1.976767 0.145298 -2.113779
  1 -1.585717 -0.304301 2.134770
  1 0.140245 1.433337 2.153765
  1 1.543895 3.378470 -0.969389
  1 1.748201 3.140946 1.072830
  1 -3.170622 -1.747581 1.209365
  1 3.014101 0.658733 -0.558114
  1 1.349200 -1.081149 -0.492048
  6 3.982042 -1.911397 -0.247781
  1 2.482184 -0.410654 1.525429
  1 4.937952 -1.584682 0.162441
  1 3.725146 -2.865420 0.213672
  1 4.113461 -2.079233 -1.317098

- $FC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -688.142586 au

  6 2.201279 -0.748450 -0.009400
  6 1.927527 -0.092588 -1.195932
  6 1.096204 1.010702 -1.152226
  6 0.536546 1.467196 0.050283
  6 0.855221 0.765862 1.222219
  6 1.683837 -0.341050 1.206093
  5 -0.432985 2.659710 0.074439
  9 2.998436 -1.820170 -0.039537
  14 -2.475880 -0.348982 0.070640
  6 -4.093042 -1.234476 -0.250863
  1 0.432865 1.095271 2.163115
  1 1.929479 -0.889670 2.104160
  1 2.358345 -0.453218 -2.119101
  1 0.862705 1.532642 -2.071678
  1 -0.918380 3.018756 1.105865
  1 -0.698613 3.239574 -0.936206
  1 -2.542042 1.045393 -0.441911
  1 -1.349989 -1.038750 -0.602713
  1 -2.193144 -0.287440 1.524814
  1 -4.920950 -0.725306 0.243092
  1 -4.309388 -1.273573 -1.318777
  1 -4.055010 -2.258134 0.122976

- $C_6H_5BH_2\cdots SiMeH_3$

  E_{tot} = -588.8938116 au

  6 -0.050902 -0.270397 -0.016036
  6 0.011122 -0.019170 1.344367
  6 1.239653 0.129132 2.002369
  6 2.408073 0.009584 1.237331
  6 2.355221 -0.242598 -0.122569
  6 1.123177 -0.380488 -0.748487
  5 1.303811 0.449562 3.509699
  14 0.728278 3.584818 2.097944
  1 3.368402 0.124290 1.725122
  1 3.267366 -0.329413 -0.697980
  1 1.078207 -0.574544 -1.812488
  1 -1.008364 -0.378507 -0.508175
  1 -0.904583 0.072969 1.915513
  1 2.360536 0.568199 4.055395
  1 0.297739 0.547721 4.147405
  1 1.355510 2.915418 3.270506
  1 -0.667739 3.099626 1.989680
  6 0.769088 5.442292 2.324968
  1 1.473224 3.179704 0.883336
  1 0.309653 5.946036 1.473859
  1 0.227292 5.736815 3.224057
  1 1.794694 5.800977 2.415559

- $MeC_6H_4BH_2\cdots SiMeH_3$

  E_{tot} = -628.2131496 au

  6 2.118712 -0.746831 0.001288
  6 1.839452 -0.059135 -1.178981
  6 1.057649 1.079774 -1.162276
  6 0.518632 1.580627 0.031655
  6 0.812397 0.880712 1.209733
  6 1.594408 -0.259996 1.196097
  5 -0.400240 2.811136 0.040165
  6 2.986667 -1.972706 -0.015902
  14 -2.440115 -0.366395 0.084658
  1 0.405024 1.237196 2.147991
  1 1.797681 -0.787626 2.120096
  1 2.236078 -0.430218 -2.116395
  1 0.843336 1.594232 -2.091216

1 -0.872417 3.203412 1.066444
1 -0.648642 3.385534 -0.978782
1 2.838458 -2.550098 -0.927934
1 4.041528 -1.693182 0.026852
1 2.781807 -2.617821 0.837334
1 -2.580775 0.990292 -0.504098
1 -1.244060 -1.014679 -0.502911
1 -2.232341 -0.215149 1.545027
6 -3.979151 -1.378916 -0.254100
1 -4.861198 -0.903777 0.176095
1 -4.144365 -1.488690 -1.326306
1 -3.889889 -2.376746 0.176690

- $HOC_6H_4BH_2 \cdots SiMeH_3$

  E_{tot} = -664.1271704 au

  6 1.837725 -0.174700 -1.175826
  6 1.122098 1.005285 -1.163075
  6 0.615285 1.551482 0.025458
  6 0.874064 0.845606 1.212774
  6 1.586044 -0.334688 1.222921
  6 2.066995 -0.848267 0.021909
  5 -0.219332 2.833760 0.019887
  8 2.753342 -2.010403 0.075110
  14 -2.429573 -0.279790 0.057664
  1 0.492893 1.238268 2.147344
  1 1.777005 -0.876803 2.138532
  1 2.215855 -0.581884 -2.106597
  1 0.938870 1.521123 -2.097608
  1 -0.666490 3.267422 1.040935
  1 -0.431587 3.410286 -1.006437
  1 3.029591 -2.271775 -0.804279
  1 -2.538759 1.034448 -0.624778
  1 -1.248778 -0.995744 -0.481161
  1 -2.217795 -0.033703 1.504325
  6 -3.989829 -1.280444 -0.212724
  1 -4.861479 -0.757264 0.181461
  1 -4.157165 -1.461191 -1.274961
  1 -3.922509 -2.247341 0.286982

- $MeOC_6H_4BH_2 \cdots SiMeH_3$

  E_{tot} = -703.4256099 au

  6 1.562372 0.288529 -1.003345
  6 0.600984 1.268902 -1.174535
  6 -0.101829 1.825185 -0.099299
  6 0.218095 1.345941 1.184913
  6 1.168914 0.372580 1.381647
  6 1.845849 -0.165453 0.284112
  5 -1.195713 2.871345 -0.319376
  8 2.753306 -1.118152 0.566716
  6 3.467245 -1.713637 -0.494067
  14 -2.643466 -0.651418 0.041632
  1 -0.308332 1.750427 2.040659
  1 1.408453 0.001685 2.368594
  1 2.075709 -0.115940 -1.862760
  1 0.378581 1.611748 -2.177770
  1 -1.805280 3.313682 0.610069
  1 -1.451019 3.253122 -1.424004
  1 4.128005 -2.445458 -0.038725
  1 2.794393 -2.218751 -1.191180
  1 4.064418 -0.975678 -1.035041
  1 -3.004536 0.514131 -0.804225
  1 -1.297277 -1.126948 -0.356815
  1 -2.591845 -0.201275 1.453259
  6 -3.912279 -2.014914 -0.161360
  1 -4.904731 -1.670407 0.130614
  1 -3.962975 -2.348467 -1.198293
  1 -3.659030 -2.876328 0.457527

- $H_2NC_6H_4BH_2 \cdots SiMeH_3$

  E_{tot} = -644.262168 au

  6 -0.017944 -0.012560 0.035530
  6 -0.002937 -0.042198 1.435547
  6 1.230175 -0.043496 2.100537
  6 2.402227 -0.012524 1.379888
  6 2.416934 0.022469 -0.025391
  6 1.166042 0.018124 -0.666363
  7 -1.178738 -0.025977 2.146779
  5 3.721360 0.099122 -0.811286
  14 2.081516 3.558826 -0.284552
  1 1.134685 0.048324 -1.748795
  1 -0.966765 -0.005768 -0.487122
  1 1.251023 -0.061398 3.183479
  1 3.346278 -0.007960 1.911372
  1 3.705026 0.152981 -2.007010
  1 4.772650 0.108468 -0.239120
  1 -2.021837 -0.279767 1.664994
  1 -1.147033 -0.300861 3.111544
  1 3.503023 3.137440 -0.218918
  1 1.337109 2.904322 0.816763
  6 1.955047 5.423896 -0.147671
  1 1.520816 3.102028 -1.579223
  1 2.500486 5.912422 -0.955644
  1 0.915002 5.747808 -0.199138
  1 2.369774 5.773604 0.798291

- $HMeNC_6H_4BH_2 \cdots SiMeH_3$

  E_{tot} = -683.5675761 au

  6 1.848811 -0.082276 0.261885
  6 1.347223 0.152714 -1.027124
  6 0.381113 1.117346 -1.223058
  6 -0.138404 1.891095 -0.173917
  6 0.387611 1.638870 1.108960

6 1.349593 0.686225 1.330149
5 -1.235008 2.921978 -0.405246
7 2.806643 -1.023452 0.496747
6 3.295634 -1.937621 -0.502232
14 -2.580093 -0.709420 -0.049317
1 0.012634 2.212812 1.947925
1 1.731911 0.513688 2.329409
1 1.710163 -0.423625 -1.866101
1 -0.000149 1.277045 -2.224599
1 -1.665064 3.565513 0.508303
1 -1.679875 3.095962 -1.503223
1 3.034751 -1.212156 1.454033
1 4.021102 -2.604743 -0.043138
1 2.494082 -2.545898 -0.932657
1 3.796621 -1.406992 -1.315100
1 -3.110957 0.562995 0.498255
1 -1.275239 -1.000660 0.590102
6 -3.791379 -2.103809 0.272777
1 -2.372507 -0.541982 -1.507866
1 -4.754959 -1.899250 -0.194870
1 -3.416096 -3.046067 -0.128076
1 -3.957796 -2.235756 1.342404

- $Me_2NC_6H_4BH_2 \cdots SiMeH_3$

  E_{tot} = -722.8710449 au

  6 0.928358 0.512813 1.227974
  6 1.570445 0.171916 0.019505
  6 1.086198 0.756989 -1.169307
  6 0.017536 1.622196 -1.135865
  6 -0.641110 1.967589 0.056406
  6 -0.138527 1.381452 1.230309
  7 2.623705 -0.696901 0.000497
  6 3.248455 -1.055666 -1.252309
  5 -1.847774 2.896016 0.070305
  6 3.086493 -1.305333 1.226894
  14 -2.777574 -0.889647 0.012052
  1 -0.616058 1.615135 2.174500
  1 1.263876 0.089634 2.162469
  1 1.546260 0.526124 -2.117992
  1 -0.335525 2.048085 -2.067666
  1 -2.402399 3.153596 1.099896
  1 -2.256313 3.374011 -0.948703
  1 4.056536 -1.756074 -1.062109
  1 2.541527 -1.534071 -1.936423
  1 3.672957 -0.183238 -1.756425
  1 3.924204 -1.961039 1.007748
  1 3.427220 -0.555545 1.946004
  1 2.304974 -1.904229 1.703620
  1 -3.352656 0.221893 -0.784156
  1 -1.378776 -1.118457 -0.420465
  1 -2.779858 -0.494034 1.440997
  6 -3.796589 -2.445555 -0.226400
  1 -4.828574 -2.288140 0.088666
  1 -3.807147 -2.747205 -1.274329
  1 -3.388835 -3.271569 0.357395