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Supplementary Material

Theoretical Investigation of Main-Group Element Hydride Insertion into Phosphorus-Heterocyclic Carbenes (PHCs)

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Cartesian coordinates (Å) and electronic energies for M06-2X/def2-TZVP optimised geometries

All energies given in hartree.

Reactants

PHC^{H}
Ee(M06-2X)= -854.646226520
Ee(RI-SCS-MP2) = -853.34987544

C	1.52948400	0.95948700	-0.00485900
C	-0.99689300	-0.29970000	-0.00672700
P	-0.11141500	1.29434700	0.09551200
H	-0.67360900	2.37691900	-0.59175800
P	1.44643700	-0.74679700	-0.13092900
H	2.16760400	-1.40141300	0.87594400
N	-0.17621400	-1.27666800	0.09144200
C	-2.48414900	-0.45572800	-0.03144800
H	-2.95792800	0.22566900	0.67598000
H	-2.86822700	-0.22063200	-1.02597400
H	-2.75031700	-1.48147200	0.21516800

PHC^{Me}
Ee(M06-2X) = -933.286140574
Ee(RI-SCS-MP2) = -931.81067815

C	-0.48170000	-1.52327700	-0.05201700
C	0.61137400	1.06532000	-0.01256000
P	-1.48348900	-0.19730700	-0.48823800
P	0.93151200	-0.69993700	0.25991500
N	-0.63972500	1.27660900	-0.19928700
C	-3.00718000	-0.06649200	0.49973600
H	-3.57743400	0.79390100	0.15480200
H	-3.58599200	-0.97473300	0.34461000
H	-2.77419100	0.04383700	1.55691500
C	2.60329200	-1.32791200	-0.06777700
H	3.33164500	-0.73411700	0.48272500
H	2.64644100	-2.35925200	0.27714700
H	2.82915200	-1.29220300	-1.13193900
C	1.63819200	2.14931700	0.09571100
H	2.31860500	2.11450800	-0.75820900
H	1.14811700	3.12064300	0.11573400
H	2.23750700	2.02806900	0.99951000

PHC^{Ph}
Ee(M06-2X) = -1316.74334111
Ee(RI-SCS-MP2) = -1314.4087411

C	-0.06918600	-0.93238600	0.88361100
C	0.60309500	1.64832000	0.01691700
P	-1.15399000	-0.00212500	0.08902400
P	1.20334500	0.24990100	1.06275100
N	-0.64060200	1.55165100	-0.32655600
C	1.40884500	2.87416500	-0.26782100
H	2.33287300	2.60076500	-0.78283900
H	0.83679200	3.56577600	-0.88273500
H	1.68908000	3.36849800	0.66380000
C	-2.91349800	-0.19322400	-0.04006900
C	-3.69201200	0.80684100	-0.62129100
C	-3.49876800	-1.37515400	0.41522900
C	-5.06048100	0.61854000	-0.74162200
H	-3.22388400	1.71938000	-0.96601300
C	-4.86606700	-1.55031100	0.28733800
H	-2.87862900	-2.13825400	0.86883700
C	-5.64708300	-0.55586400	-0.29010800
H	-5.66999100	1.39311000	-1.18805400
H	-5.32499700	-2.46365800	0.64206500
H	-6.71582100	-0.69670900	-0.38548600
C	2.76310700	-0.30492400	0.31603700
C	2.83648900	-1.49688100	-0.40192600
C	3.91138000	0.46858700	0.48416800
C	4.04425500	-1.89979600	-0.95345600
H	1.94573100	-2.10062400	-0.51867300
C	5.11168700	0.07051700	-0.08537200
H	3.86902900	1.37925100	1.07085600
C	5.18015800	-1.11590700	-0.80342700
H	4.09601400	-2.82799500	-1.50793100
H	5.99708100	0.67924400	0.04504100
H	6.11908700	-1.43213400	-1.23884700

NHC^{Me}
Ee(M06-2X) = -360.134511368
Ee(RI-SCS-MP2) = -359.38455427

C	0.61265600	-1.20497900	0.00013100
C	-0.61878000	0.68252300	0.00010100
N	0.61061900	1.09039200	-0.00008200
N	1.32913100	-0.07384900	-0.00006600
N	-0.65588100	-0.68828500	-0.00000300
C	-1.82013400	1.55457800	0.00015200
H	-2.43587900	1.37050700	-0.88176300
H	-2.43591800	1.37034900	0.88200600
H	-1.50560400	2.59466900	0.00024800
C	-1.86202500	-1.48689800	-0.00008900
H	-2.46145100	-1.28307200	0.88778100
H	-2.46151000	-1.28282800	-0.88786300
H	-1.56108800	-2.53001500	-0.00024000
C	2.77068800	0.01546300	-0.00009500
H	3.10969700	0.54842200	-0.88731900
H	3.10979900	0.54777400	0.88748300
H	3.16044000	-0.99773400	-0.00047100

SiH_4
Ee(M06-2X) = -291.853373354
Ee(RI-SCS-MP2) = -291.40184095

Si	2.57357300	0.00853700	0.31387900
H	1.63211300	0.07240300	-0.88882600
H	1.75568300	0.03004200	1.54850200
H	3.33498700	-1.25565300	0.21783600
H	3.46349700	1.18989400	0.26144900

SiH_2Ph_2
Ee(M06-2X) = -753.950317492
Ee(RI-SCS-MP2) = -752.453536

Si	0.00000600	1.57398100	0.00001800
H	-0.10112400	2.44282700	1.19540500
C	-1.53267400	0.50356000	-0.05670700
C	-1.56285600	-0.66197200	-0.82765900
C	-2.68266500	0.85314100	0.65386000
C	-2.70475200	-1.44703800	-0.89294900
H	-0.67893100	-0.96555000	-1.37867800
C	-3.82882300	0.07144600	0.59199000

H	-2.68410600	1.74628300	1.26889400
C	-3.84053900	-1.07932800	-0.18308400
H	-2.70942300	-2.34661400	-1.49517600
H	-4.71039200	0.35806600	1.15109900
H	-4.73183700	-1.69186000	-0.23115000
C	1.53268300	0.50357000	0.05664800
C	2.68268200	0.85311800	-0.65391700
C	1.56284800	-0.66193200	0.82765300
C	3.82882800	0.07140400	-0.59200800
H	2.68413500	1.74622700	-1.26899500
C	2.70473200	-1.44700600	0.89299100
H	0.67889500	-0.96548400	1.37864700
C	3.84053300	-1.07932500	0.18311800
H	4.71039800	0.35798400	-1.15113800
H	2.70938900	-2.34655700	1.49525400
H	4.73182200	-1.69186600	0.23122300
H	0.10109500	2.44298200	-1.19526500

BH_3
Ee(M06-2X) = -26.58593247
Ee(RI-SCS-MP2) = -26.5176983

B	0.00000000	0.00000000	0.00000000
H	0.00000000	1.18732400	0.00000000
H	1.02825300	-0.59366200	0.00000000
H	-1.02825300	-0.59366200	0.00000000

BH_2NMe_3
Ee(M06-2X) = -160.569620809
Ee(RI-SCS-MP2) = -160.2630698

B	-2.85847034	1.69056150	-0.02197238
H	-1.67847034	1.69056150	-0.02197238
H	-3.44847034	0.66865153	-0.02197238
N	-3.64847034	3.05888164	-0.02197238
C	-3.29332525	3.82972752	-1.22220927
H	-3.48763969	3.24126085	-2.09447579
H	-3.87914171	4.72440852	-1.25777576
H	-2.25468745	4.08460484	-1.18801771
C	-3.29336516	3.82970447	1.17829112
H	-3.84680499	4.74537250	1.19079759
H	-3.52920913	3.25844579	2.05175614
H	-2.24560350	4.04637001	1.16598044

SiH_4 + PHC^H

SiH_4-PHC^H **T1**
Ee(M06-2X) = -1146.48217077
Ee(RI-SCS-MP2) = -1144.726794

C	0.651927	0.810421	1.112151
C	-1.475417	-0.327982	-0.299198
P	-0.377468	-0.662986	1.200078
H	-1.232531	-0.277534	2.252052
P	-0.154318	1.770383	-0.095506
H	0.780731	2.188409	-1.057375
N	-1.208313	0.714736	-0.972784
Si	2.506505	-0.765714	-0.506108
H	2.005230	0.225657	0.570958
H	1.412886	-1.041440	-1.457374
H	3.634824	-0.111200	-1.199093
H	2.932086	-1.997424	0.183855
C	-2.498432	-1.332694	-0.728227
H	-2.021620	-2.300055	-0.898622
H	-3.239753	-1.476098	0.061070
H	-2.996391	-1.002887	-1.637391

SiH_4-PHC^H **B**
Ee(M06-2X) = -1146.62568626
Ee(RI-SCS-MP2) = -1144.876234

C	-1.01173800	-0.05102000	-0.69089600
C	1.51991900	-0.00993000	0.23552200
P	0.45752300	-1.17645100	-0.79225400
H	0.99031800	-0.71509800	-2.02533500
P	-0.32188400	1.65389600	-0.37274400
H	-1.05544900	1.99379700	0.79106400
N	1.11108000	1.16666900	0.44617100
Si	-2.16162700	-0.62546700	0.67770700
H	-1.52694900	-0.06800700	-1.65255500
H	-1.37832200	-0.68096700	1.93126100
H	-3.26632000	0.34476500	0.83317600
H	-2.71947100	-1.96329900	0.38537000
C	2.82085200	-0.52167300	0.77235800
H	2.64227300	-1.37516000	1.42932200
H	3.45116200	-0.87671600	-0.04670300
H	3.33919000	0.26459300	1.31636800

SiH_4-PHC^H **T2**
Ee(M06-2X) = -1146.51573500
Ee(RI-SCS-MP2) = -1144.771151

C	-1.470749	0.512084	-0.647342
C	1.541570	-0.101124	0.188056
P	0.532482	-1.370668	-0.496590
H	1.560121	-1.933814	-1.307161
P	-0.233023	1.627540	-0.278300
H	-0.687114	2.815725	0.299383
N	1.059997	1.086472	0.520256
Si	-2.275449	-0.708940	0.494838
H	-2.089344	0.859189	-1.474446
H	-1.461924	-0.876525	1.713604
H	-3.572759	-0.093628	0.874079
H	-2.542459	-2.014083	-0.137636
C	3.021739	-0.297011	0.405314
H	3.579925	0.365996	-0.259237
H	3.265379	-0.015916	1.430824
H	3.337223	-1.323870	0.238235

SiH_4-PHC^H **C**
Ee(M06-2X) = -1146.55308923
Ee(RI-SCS-MP2) = -1144.804632

C	1.93750200	0.73053100	-0.10401400
C	-1.63430100	0.01403500	0.07659400
P	-1.14217500	-1.38495200	-0.75324200
P	0.52423900	1.52651900	-0.27466700
N	-0.97714700	1.21612800	-0.07712900
Si	2.29817400	-1.00908200	0.43919200
H	-2.16652800	-2.22439300	-0.25857900
H	0.66375900	2.86532500	-0.62257000
H	3.72210500	-1.01856600	0.83916100
H	2.09248100	-1.97601500	-0.65581800
H	1.47724100	-1.39308700	1.60197600
H	2.77472600	1.39733600	-0.28867600
C	-2.83995300	0.13423200	0.96434900
H	-3.39223300	-0.79817600	1.03537900
H	-2.52514000	0.44624000	1.96281000
H	-3.49125300	0.91929300	0.57458800

SiH_4-PHC^H **T3**

Ee(M06-2X) = -1146.49017677

Ee(RI-SCS-MP2) = -1144.733147

C	-1.91502300	0.50407000	-0.08009100
C	1.40225900	0.19336600	-0.00826100
P	0.68757400	-1.22081200	0.84593300
P	-0.73839000	1.65107400	0.12492700
N	0.84685400	1.37644400	-0.04326100
Si	-1.43787200	-1.25592700	-0.47099900
H	1.50234900	-2.18672200	0.20964700
H	-0.94088800	2.76159100	0.93837700
H	-2.61658100	-2.07608900	-0.88458200
H	-1.97475400	-1.09716500	1.00170200
H	-0.61692300	-1.37112200	-1.71927700
H	-2.95417600	0.80791200	-0.04544100
C	2.74240400	0.06507900	-0.67476900
H	2.58419500	-0.36789800	-1.66751300
H	3.19626900	1.04713200	-0.79474800
H	3.40713600	-0.59878700	-0.12551700

SiH_4-PHC^H **D**

Ee(M06-2X) = -1146.63800624

Ee(RI-SCS-MP2) = -1144.885092

C	1.83513300	-0.36132600	0.58546900
C	-1.33595700	-0.33809000	0.08772200
P	-0.74722900	1.20397000	-0.76241300
P	0.91722700	-1.56323700	-0.49681600
N	-0.67002200	-1.41628800	0.14199100
Si	1.23149500	1.39614700	0.32263600
H	-1.48736200	2.13037400	0.00136800
H	1.25741700	-2.73618300	0.20826300
H	1.70323700	-0.63909000	1.63179300
H	2.89655300	-0.42396600	0.33963100
H	1.07816200	2.10535400	1.61028700
H	2.15684700	2.15988400	-0.53937400
C	-2.73994400	-0.29950800	0.63060900
H	-2.78727200	0.36365900	1.49685100
H	-3.43088400	0.09294600	-0.11818200
H	-3.04281900	-1.30247200	0.92416000

SiH_4 + PHC^{Me}

PHC^{Me} **T1**

Ee(M06-2X) = -1225.11939168

Ee(RI-SCS-MP2) = -1223.183247

C	0.45112800	0.23712800	-1.23407000
C	-1.26261600	-0.44848200	0.84041400
P	0.46415000	-1.40648400	-0.67887700
P	-0.92800900	0.96684100	-0.35587400
N	-0.48514900	-1.45212200	0.77368000
C	2.14431300	-1.88816000	-0.17471500
H	2.15140900	-2.91595700	0.18208600
H	2.79391700	-1.80192900	-1.04436100
H	2.50229100	-1.22830200	0.61878500
C	-2.32816000	0.84399900	-1.55143900
H	-3.24431800	1.15650500	-1.05094800
H	-2.12969900	1.52706600	-2.37503700
H	-2.44269300	-0.16668900	-1.93838100
C	-2.31931900	-0.31339500	1.89262300
H	-3.29905700	-0.18268500	1.42589300
H	-2.33917600	-1.19462000	2.53037000
H	-2.13275500	0.57660500	2.49705900
H	1.67462700	0.91239500	-0.68191000
Si	2.13541300	1.69265700	0.60094100
H	3.60806400	1.60317000	0.70892800
H	1.69576500	3.08108300	0.38128800
H	1.50770700	1.10911600	1.80169200

SiH_4-PHC^{Me} **B**

Ee(M06-2X) = -1225.26027846

Ee(RI-SCS-MP2) = -1223.329634

C	-1.76864100	-0.14514900	0.09441600
P	-0.57806200	1.19436000	0.67094800
P	0.39666600	-1.28175000	-0.66997500
N	-1.30718200	-1.20455300	-0.42052200
C	0.87581400	0.06419600	0.53497900
C	0.78382500	-2.77002200	0.32998300
H	0.42016000	-3.65616400	-0.18841700
H	1.86746400	-2.84904600	0.42858200
H	0.32760700	-2.71495500	1.31894400
C	-0.51420100	2.11091100	-0.93870300
H	-0.28258200	1.46466100	-1.78625200
H	-1.48400900	2.58240600	-1.10129700
H	0.23145000	2.90398500	-0.87748300
C	-3.23931400	0.09484300	0.25609600
H	-3.52956300	1.01580200	-0.25609500
H	-3.80717800	-0.73913400	-0.15022700
H	-3.47970200	0.23143100	1.31229000
Si	2.49746200	0.88901900	0.08258500
H	3.58405900	-0.11253100	0.15390200
H	2.43368600	1.42513900	-1.29185900
H	2.80491100	1.99236700	1.01895000
H	0.99553400	-0.37617400	1.53120800

SiH_4-PHC^{Me} **T2**

Ee(M06-2X) = -1225.15117874

Ee(RI-SCS-MP2) = -1223.226879

C	1.30812300	0.75160200	-0.74135400
C	-1.17783500	-0.85308200	0.41534000
P	1.18748700	-0.93569400	-0.49146200
P	-1.32409800	0.84412400	-0.01198600
N	0.00012500	-1.45857500	0.46941400
C	2.74044200	-1.79895300	-0.12485600
H	2.53391700	-2.86565100	-0.06868400
H	3.44099200	-1.60322800	-0.93529100
H	3.16992400	-1.44898200	0.81227600
C	-2.99234600	0.86340600	-0.82002200
H	-3.76387100	0.75717300	-0.05330800
H	-3.13206800	1.83252700	-1.29684900
H	-3.12278400	0.07485300	-1.55991600
C	-2.38555100	-1.71981300	0.67405400
H	-3.19737900	-1.18460100	1.16466600
H	-2.76785200	-2.11704400	-0.27113600
H	-2.08234700	-2.56340400	1.29226400
H	1.83599000	0.97336600	-1.66877100
Si	1.40728800	2.07093200	0.55001800
H	2.84575000	2.43637000	0.65527600
H	0.65197300	3.29448100	0.21518700
H	0.97702200	1.54571100	1.86089500

SiH_4-PHC^{Me} **C**

Ee(M06-2X) = -1225.18928864

Ee(RI-SCS-MP2) = -1223.260252

C	-1.83570600	1.10116500	-0.07420900
C	0.96358800	-0.94087800	0.28988400
P	1.67912000	-0.15929700	-1.02959000
P	-1.60005200	-0.51611100	-0.09342400

N	-0.35254700	-1.38118700	0.19615000
Si	-0.58914600	2.39272900	0.36845900
H	-1.34297200	3.56615200	0.86565700
H	0.23411000	2.81482000	-0.78417800
H	0.30551300	1.92090500	1.44665900
C	3.39207700	0.22274400	-0.42650400
H	3.96560300	-0.68203900	-0.22424900
H	3.90216600	0.77300100	-1.21657600
H	3.37944200	0.84664700	0.46740700
C	-3.02253500	-1.55455000	-0.43065500
H	-3.92039000	-0.94501400	-0.49120900
H	-2.86036000	-2.08291800	-1.36867700
H	-3.11323400	-2.28609000	0.37022900
C	1.60424300	-1.29977400	1.59778800
H	2.67236800	-1.10432400	1.61901900
H	1.12527100	-0.72993100	2.39962300
H	1.42383000	-2.35655700	1.80381400
H	-2.85149600	1.39432400	-0.31160900

SiH_4-PHC^{Me} **T3**

Ee(M06-2X) = -1225.14749014

Ee(RI-SCS-MP2) = -1223.209578

C	1.37282700	1.41012300	0.25619300
C	-0.62103000	-1.19438100	-0.00251400
P	1.77058300	-0.21003900	0.36995900
P	-1.45158900	0.21934800	0.70989200
N	0.67844700	-1.33568000	-0.07345200
C	3.38401600	-0.77530200	-0.21489600
H	3.37413100	-0.84935300	-1.30143700
H	4.14217400	-0.06157200	0.10139900
H	3.59488300	-1.75264100	0.21423700
C	-3.15472300	0.07600700	0.00820100
H	-3.65445400	-0.82826300	0.35309800
H	-3.72884300	0.93103700	0.36442700
H	-3.15299600	0.09214100	-1.08233600
C	-1.43177100	-2.34890700	-0.53118300
H	-1.96003100	-2.04681400	-1.43922300
H	-0.76932500	-3.17923600	-0.76511900
H	-2.18562000	-2.66998900	0.18842800
H	2.11084600	2.16385300	0.49576500
Si	-0.27265600	1.94181300	-0.49755400
H	-0.80865700	3.16295000	0.13024500
H	1.00466200	2.45660000	-1.30720500
H	-0.97954700	1.60079300	-1.76493500

SiH_4-PHC^{Me} **D**

Ee(M06-2X) = -1225.27000455

Ee(RI-SCS-MP2) = -1223.335661

C	-0.52408100	1.21949100	0.03904400
C	1.35339100	-1.34649500	0.51498000
H	1.54311500	-1.05594900	1.55139200
H	-1.08874900	-2.06881400	1.63715900
N	0.74521700	1.28702300	0.05077100
P	1.77797600	0.07896300	-0.59796900
P	-1.46651700	-0.15660200	-0.76223200
C	3.33580100	0.62863500	0.19404300
H	3.20000600	0.77814900	1.26555100
H	4.11087100	-0.11877500	0.01990600
H	3.65026600	1.56718700	-0.26141800
C	-3.10578000	-0.10823500	0.10328200
H	-3.67742100	-0.98008000	-0.21548300
H	-3.02268500	-0.12373600	1.18899700
H	-3.65767200	0.77897400	-0.20498600
Si	-0.44176400	-1.85160000	0.32145200
H	2.00639400	-2.18435300	0.26512800
H	-0.58093800	-3.08561400	-0.48062100
C	-1.32579900	2.37255800	0.58516000
H	-2.02378700	2.74664500	-0.16726900
H	-1.91719900	2.05933600	1.44792200
H	-0.64708700	3.16912600	0.88196300

SiH_4 + PHC^{Ph}

SiH_4-PHC^{Ph} **T1**

Ee(M06-2X) = -1608.5782271

Ee(RI-SCS-MP2) = -1605.782851

C	0.01535100	-0.89493600	0.51678900
C	0.71878900	1.59433900	-0.52358500
P	-0.75174400	-0.36148600	-0.94425800
P	1.22158200	0.37628700	0.82240300
N	-0.32315100	1.30132800	-1.18870700
C	1.44946400	2.88996100	-0.67580300
H	2.48851300	2.69337800	-0.95270200
H	0.98049500	3.50524900	-1.44061800
H	1.46424700	3.42652400	0.27488900
C	-2.54231600	-0.38744900	-0.74073900
C	-3.33971100	0.65001400	-1.22522400
C	-3.13401800	-1.46972000	-0.08782600
C	-4.71322300	0.60635400	-1.04086600
H	-2.87732300	1.49126900	-1.72446700
C	-4.50984600	-1.50739300	0.08612400
H	-2.51357200	-2.27543200	0.28744000
C	-5.30070900	-0.46964900	-0.38714000
H	-5.32763600	1.41903400	-1.40632500
H	-4.96283400	-2.34724800	0.59679500
H	-6.37337300	-0.49836400	-0.24683900
C	2.84543500	-0.25003700	0.28183600
C	2.99584100	-1.45576900	-0.40159600
C	3.97262900	0.52198200	0.56352500
C	4.25662600	-1.87448800	-0.80111900
H	2.12461400	-2.06282300	-0.61174800
C	5.22893000	0.10868800	0.14454200
H	3.86749800	1.44594700	1.12091500
C	5.37281000	-1.09227700	-0.53623000
H	4.36574500	-2.81362400	-1.32815400
H	6.09641900	0.71780600	0.36340600
H	6.35359200	-1.42085100	-0.85457900
H	-0.98159500	-0.78856000	1.64883200
Si	-1.69572400	0.31716000	2.50625700
H	-1.77565500	1.55668800	1.71115800
H	-3.04356700	-0.13971700	2.90155400
H	-0.82726000	0.50147800	3.68548900

SiH_4-PHC^{Ph} **B**

Ee(M06-2X) = -1608.71676352

Ee(RI-SCS-MP2) = -1605.927943

C	-0.01490300	0.90544700	0.52543800
C	0.50116100	-1.69949600	0.03046400
P	-1.07399700	-0.29084300	1.51211800
P	0.83365900	-0.06019600	-0.80402800
N	-0.35743700	-1.76111400	0.95851300
C	1.20355500	-2.91516200	-0.49451400
H	2.28353100	-2.80099300	-0.37611200
H	0.86689300	-3.80270600	0.03610700
H	1.00879300	-3.02328400	-1.56380600
C	-2.61326600	-0.29359600	0.51151600
C	-2.76814800	-0.98632400	-0.68777600

C	-3.65653100	0.51129900	0.96654600
C	-3.93471100	-0.85675200	-1.42631200
H	-1.97713300	-1.63277300	-1.04664800
C	-4.82003300	0.65094900	0.22180600
H	-3.55385500	1.03533100	1.91036500
C	-4.95900500	-0.03234800	-0.97723000
H	-4.04493300	-1.39862300	-2.35689500
H	-5.61919800	1.28535300	0.58276500
H	-5.86685400	0.06906600	-1.55775300
C	2.60550900	0.14362800	-0.36900200
C	3.10367700	-0.15107400	0.90176100
C	3.48335300	0.59894900	-1.34875900
C	4.45018100	0.00912400	1.18433800
H	2.43243400	-0.51411500	1.67378900
C	4.83403400	0.76571500	-1.06510800
H	3.10518000	0.82532700	-2.33846800
C	5.31761600	0.47033400	0.19964200
H	4.82624500	-0.22647600	2.17160900
H	5.50572600	1.12526200	-1.83382000
H	6.36937400	0.59660200	0.42160300
H	0.74096900	1.27125900	1.22599600
Si	-0.92257800	2.40235900	-0.16336300
H	-1.81638600	2.00106300	-1.26670800
H	-1.70938600	3.05614200	0.90591700
H	0.07687300	3.36975100	-0.66866300

SiH_4-PHC^{Ph} **T2**

Ee(M06-2X) = -1608.62691123

Ee(RI-SCS-MP2) = -1605.843788

C	-0.93240700	1.74127800	0.64662900
C	0.64283700	-0.17702000	-1.34873200
P	-1.62365500	0.74135400	-0.52074300
P	1.55515000	0.88415200	-0.29589700
N	-0.68214200	-0.11022200	-1.49659600
C	1.28805300	-1.22982700	-2.22372700
H	0.91258100	-2.22130100	-1.96307000
H	0.99148900	-1.03191000	-3.25478000
H	2.37220400	-1.23062400	-2.15795100
C	-2.99508700	-0.28710300	-0.01205900
C	-3.11852700	-1.60588700	-0.44932900
C	-3.96546900	0.26359600	0.82462700
C	-4.20251700	-2.36536400	-0.03866200
H	-2.36289500	-2.01992700	-1.10297600
C	-5.03538200	-0.50939700	1.24704900
H	-3.88589400	1.29831800	1.13703600
C	-5.15673000	-1.82274800	0.81291600
H	-4.29857700	-3.38867300	-0.37742400
H	-5.78195200	-0.08212500	1.90342300
H	-5.99800800	-2.42254300	1.13485000
C	2.97285000	-0.15953900	0.18220200
C	2.86042000	-1.51046900	0.52524500
C	4.22174600	0.45505400	0.30245900
C	3.96810100	-2.23077300	0.94140000
H	1.89265400	-1.99456500	0.46823600
C	5.33276700	-0.26472400	0.71882000
H	4.32094100	1.50679900	0.05940600
C	5.20840100	-1.60988200	1.03587300
H	3.86519300	-3.27683000	1.20065700
H	6.29495100	0.22503500	0.79646100
H	6.07278700	-2.17267600	1.36393200
Si	-0.24389100	3.41142400	0.19215300
H	-1.42927900	1.69124200	1.61801000
H	0.92569800	3.76003600	1.01964600
H	0.09515000	3.44655000	-1.24258900
H	-1.30432800	4.41906000	0.44450800

SiH_4-PHC^{Ph} **C**

Ee(M06-2X) = -1608.64795617

Ee(RI-SCS-MP2) = -1605.857756

C	-1.41286600	2.00871000	-0.34198100
C	0.65745800	-0.62524500	0.63447400
P	-1.68412500	0.45514200	0.08523800
P	1.44755000	-0.50840800	-0.86553100
N	-0.72875900	-0.61772100	0.65941800
C	1.26210400	-0.84303600	1.99063000
H	1.15640800	0.06833800	2.58715200
H	0.69613000	-1.62554500	2.49862200
H	2.31252900	-1.11485400	1.94505300
C	-3.34814700	-0.17406300	-0.00938800
C	-3.55336800	-1.54727800	0.11229700
C	-4.42868800	0.68384400	-0.20639200
C	-4.83938100	-2.05714700	0.02879100
H	-2.70257400	-2.19543500	0.27483500
C	-5.71045000	0.16556100	-0.29002500
H	-4.27286800	1.75191100	-0.27982100
C	-5.91530600	-1.20345900	-0.17417400
H	-5.00124700	-3.12279200	0.12148900
H	-6.55038500	0.83039000	-0.44090400
H	-6.91825400	-1.60504200	-0.23898500
C	3.22295500	-0.49620000	-0.42450700
C	3.77777700	0.45582900	0.43444000
C	4.07945000	-1.40149400	-1.05273900
C	5.14211900	0.48057100	0.68167800
H	3.13033500	1.18280200	0.91152000
C	5.44544500	-1.37908000	-0.80661500
H	3.66949300	-2.13491400	-1.73764300
C	5.97967800	-0.43946100	0.06354900
H	5.55429400	1.22336100	1.35297500
H	6.09289900	-2.09562400	-1.29589500
H	7.04484700	-0.41856600	0.25447600
Si	0.19187100	2.89864200	-0.12757700
H	-2.26271700	2.52712700	-0.76690100
H	0.87986600	2.43018900	1.09542800
H	1.10487900	2.73607100	-1.27839800
H	-0.12256100	4.33630900	0.03130400

SiH_4-PHC^{Ph} **T3**

Ee(M06-2X) = -1608.58306451

Ee(RI-SCS-MP2) = -1605.786411

C	1.10853800	1.96537200	-0.46067000
C	-0.49116100	-0.99055500	-0.45321700
P	1.70343100	0.42857400	-0.61243000
P	-1.27233600	0.09573300	0.76921800
N	0.76439700	-0.88381000	-0.78356100
C	-1.22187800	-2.17037900	-1.03440600
H	-1.62009600	-1.89942900	-2.01533000
H	-0.51273400	-2.98459600	-1.17803200
H	-2.05419500	-2.49120000	-0.41214400
C	3.33744700	-0.04321400	-0.08794100
C	3.71626100	-1.38486500	-0.10648100
C	4.24904300	0.93692700	0.30502800
C	5.00349000	-1.73756400	0.26968200
H	3.00117100	-2.13709900	-0.41064000
C	5.53070500	0.57290200	0.68060200
H	3.95247000	1.97776500	0.33038200
C	5.91077400	-0.76360500	0.66228900
H	5.29624400	-2.77918000	0.25830100
H	6.23388200	1.33371800	0.99258900

H	6.91317200	-1.04444600	0.95746800
C	-3.06092400	-0.14450600	0.45670100
C	-3.64167700	-0.07813700	-0.81287500
C	-3.89383900	-0.34254800	1.55933700
C	-5.01147800	-0.22325500	-0.97312200
H	-3.01768300	0.09530400	-1.68025900
C	-5.26588900	-0.48157400	1.40071500
H	-3.45826400	-0.39272300	2.55035000
C	-5.82693700	-0.42542500	0.13316200
H	-5.44488600	-0.17243200	-1.96388800
H	-5.89518400	-0.63805600	2.26744200
H	-6.89605500	-0.53689700	0.00630000
Si	-0.73035800	2.22720200	-0.31781800
H	1.78168100	2.81266200	-0.50284600
H	-1.44838800	1.76892800	-1.55696100
H	0.05907900	2.42645800	1.05483900
H	-1.13725100	3.66501700	-0.34783600

SiH_4-PHC^{Ph} **D**

Ee(M06-2X) = -1608.72573366

Ee(RI-SCS-MP2) = -1605.931984

C	1.15654400	-1.44956000	0.76998300
C	-0.48056700	0.89556000	-0.68764000
P	1.70450100	-0.59909500	-0.79076900
P	-1.56028100	-0.59291200	-0.92166400
N	0.78862400	0.83724200	-0.68258200
C	-1.15672500	2.24175700	-0.66373500
H	-1.63260500	2.41548900	0.30273000
H	-0.41204100	3.01432000	-0.84333800
H	-1.94377500	2.29556200	-1.41822700
C	3.33150200	0.01857800	-0.22972800
C	3.54139900	1.30242100	0.26559100
C	4.40828000	-0.86364500	-0.30838300
C	4.80694800	1.68970700	0.68584800
H	2.71019200	1.99384200	0.30884200
C	5.66956000	-0.47996600	0.12221700
H	4.25969500	-1.85770200	-0.71787200
C	5.87093500	0.80064300	0.62006300
H	4.96265500	2.69133200	1.06650200
H	6.49683600	-1.17518700	0.05876500
H	6.85597000	1.10660500	0.94817400
C	-3.16661600	-0.09553800	-0.18772700
C	-3.31044500	0.37645100	1.11904600
C	-4.30246100	-0.19474900	-0.99005700
C	-4.55345600	0.74871400	1.60426600
H	-2.44111300	0.45473300	1.76156700
C	-5.55129200	0.17053000	-0.50268200
H	-4.20539100	-0.55915600	-2.00561600
C	-5.67789600	0.64462800	0.79351600
H	-4.64757900	1.11609700	2.61810000
H	-6.42281700	0.08615600	-1.13880500
H	-6.64919100	0.93191200	1.17480000
Si	-0.64882600	-1.93683600	0.65766300
H	1.31848900	-0.77082100	1.61045800
H	-0.80458600	-3.33225000	0.19856900
H	1.77987300	-2.33367800	0.91319400
H	-1.33898000	-1.77532600	1.95597800

SiH_4 + NHC^{Me}

SiH_4-NHC^{Me} **T1**

Ee(M06-2X) = -651.954749029

Ee(RI-SCS-MP2) = -650.7467983

C	-1.60811300	0.26688000	-0.01328000
N	-0.65053100	-0.70216700	-0.22592700
C	0.56842200	-0.07938000	-0.19246200
N	0.25843200	1.23121600	-0.21275100
H	1.18542600	-0.48941800	1.47284000
N	-1.08057000	1.44426000	0.00259000
Si	2.25800700	-0.86152300	0.05167600
H	2.82536500	-0.99113300	-1.34941700
H	3.25138900	0.03516300	0.68305000
H	2.18674700	-2.27969500	0.46995100
C	-3.05700700	-0.02035800	0.12430400
H	-3.58852700	0.92089300	0.23335500
H	-3.43525900	-0.54276900	-0.75575600
H	-3.25080600	-0.64107000	1.00000500
C	-0.80423000	-2.11870900	0.00009000
H	-0.45707200	-2.35658900	1.01161200
H	-1.84948000	-2.39434500	-0.11271600
H	-0.20685200	-2.67543400	-0.71952000
C	1.19414100	2.28773700	0.07408800
H	1.49280200	2.23498700	1.12635500
H	2.07429600	2.17302900	-0.55601400
H	0.70927300	3.23751200	-0.13103900

SiH_4-NHC^{Me} **B**

Ee(M06-2X) = -652.008996243

Ee(RI-SCS-MP2) = -650.807143

C	0.63924200	-0.12140800	0.34892600
C	-1.50467200	0.27482100	-0.19786300
N	-0.95877600	1.42384800	-0.26438900
N	0.43887100	1.21367000	-0.22288200
N	-0.59208700	-0.78165300	-0.08718700
C	-2.96645400	0.03760200	-0.32075600
H	-3.17120500	-0.63790200	-1.15378800
H	-3.37034800	-0.41540300	0.58614600
H	-3.46430700	0.98686500	-0.49711700
C	-0.96686100	-1.97963700	0.63097100
H	-1.07561900	-1.79549800	1.70956500
H	-1.90567400	-2.36718600	0.23989300
H	-0.20411300	-2.74483500	0.48900000
C	1.11195300	2.27641800	0.49176900
H	0.85270900	3.22549700	0.02872000
H	0.81985300	2.30253900	1.55149700
H	2.18994700	2.13052100	0.42357900
Si	2.19826400	-0.93526300	-0.35440600
H	0.64781100	-0.06801900	1.46575600
H	2.04878500	-1.07170200	-1.81359800
H	3.37363800	-0.10072300	-0.02725600
H	2.38752700	-2.26830400	0.26220600

SiH_4-NHC^{Me} **T2**

Ee(M06-2X) = -651.956972613

Ee(RI-SCS-MP2) = -650.7561962

C	0.81049600	-0.71424700	-0.36541000
N	0.82865500	0.30900400	0.48073900
C	-1.21119300	0.53214900	0.40797300
N	-1.37772700	-0.68201700	-0.09565800
H	-1.74447700	0.70509800	1.34398100
N	-0.32064700	-1.18880100	-0.86049400
Si	-0.54481200	2.00501800	-0.53471200
H	0.19815800	1.63935100	-1.74942900
H	-1.72149400	2.80567600	-0.98747600
H	0.18299700	2.87354200	0.41093000
C	2.06933000	-1.37897200	-0.83231000
H	1.82703000	-2.11721100	-1.59149100

H	2.76577200	-0.64334100	-1.23782600
H	2.56084900	-1.87540600	0.00640400
C	1.95590900	0.55065900	1.35171000
H	2.10455600	-0.24527300	2.08881300
H	2.88288300	0.66374100	0.77975000
H	1.78841400	1.48422200	1.88937200
C	-2.04287900	-1.72982500	0.66154000
H	-2.32362100	-2.51847800	-0.03227800
H	-1.36244600	-2.14240000	1.41289800
H	-2.93319700	-1.32566400	1.13919600

SiH_4-NHC^{Me} **C**

Ee(M06-2X) = -651.985054082

Ee(RI-SCS-MP2) = -650.780468

C	-0.52866900	-1.04732400	0.06104100
N	-1.11931600	0.09218500	-0.19755800
C	1.30422900	1.07171800	-0.12913300
N	1.60035700	-0.18514600	-0.03690500
H	2.17049700	1.69439900	-0.33504600
N	0.78801900	-1.24154100	0.18862000
Si	-0.36446300	1.93601900	0.20794300
H	-1.14978100	1.84407500	1.47106100
H	0.37957700	3.21869900	0.56664100
H	-1.09689900	2.44174500	-0.97907400
C	-1.30864300	-2.32549700	0.22266400
H	-1.74013500	-2.62940900	-0.73243500
H	-0.64342900	-3.10906800	0.57140100
H	-2.12827200	-2.19255600	0.92913200
C	-2.56177600	0.10926300	-0.36155300
H	-2.92591400	-0.72687800	-0.95807800
H	-3.07256500	0.09594000	0.60668800
H	-2.83803400	1.03556800	-0.86535800
C	2.98582800	-0.65629900	-0.17122500
H	3.64654500	0.19027700	-0.32577000
H	3.24392100	-1.19024300	0.73971800
H	3.02774000	-1.34646700	-1.00994800

SiH_4-NHC^{Me} **T3**

Ee(M06-2X) = -651.968046812

Ee(RI-SCS-MP2) = -650.7575047

C	0.57004500	-0.97915100	-0.03102300
N	1.18046100	0.22630100	-0.23280700
C	-1.33706500	1.04806900	-0.37588800
N	-1.63307400	-0.22416200	-0.16068600
H	-2.14632000	1.68014900	-0.72135400
N	-0.70282200	-1.22552000	0.04440500
Si	0.27811400	1.72344800	0.20698100
H	-1.19413900	2.06018800	0.98687000
H	0.61831900	2.86422700	-0.66750700
H	0.97058400	1.93676400	1.51245400
C	1.43220900	-2.20032800	0.14066300
H	0.79126300	-3.05543000	0.32857700
H	2.02063100	-2.38593800	-0.75923900
H	2.12828500	-2.07759900	0.97146200
C	2.63631100	0.29637100	-0.16484400
H	3.02931100	0.07055000	0.83007100
H	3.09868600	-0.37812100	-0.88508800
H	2.94301100	1.31154700	-0.41894500
C	-2.98576600	-0.69223300	0.08510200
H	-3.68886100	0.03389400	-0.31624700
H	-3.11902300	-1.65706100	-0.39807100
H	-3.15170600	-0.80414400	1.15883200

SiH_4-NHC^{Me} **D**

Ee(M06-2X) = -652.048406152

Ee(RI-SCS-MP2) = -650.8421442

C	-0.59294100	0.97843300	0.04386500
N	-1.17132900	-0.27477000	-0.12804800
C	1.41256100	-0.98654200	0.55194200
N	1.54527800	0.18781600	-0.31650600
H	2.23870900	-1.66688700	0.34281800
N	0.66025600	1.22960800	-0.00341700
Si	-0.22004500	-1.71814200	0.04014300
H	-0.12571800	-2.47265500	-1.22738200
H	-0.85802000	-2.60436800	1.04463100
C	-1.50509400	2.14158100	0.30664400
H	-2.07755400	1.99430100	1.22435300
H	-0.89786800	3.03610900	0.40316900
H	-2.21732700	2.27866600	-0.50899800
H	1.46110300	-0.71062700	1.61670500
C	2.89533800	0.72629700	-0.29697300
H	2.93631400	1.59699000	-0.94720600
H	3.19643200	1.02577300	0.71597600
H	3.58433800	-0.03194300	-0.66818800
C	-2.61145100	-0.37885300	-0.32125200
H	-3.17312500	0.04762700	0.51221000
H	-2.93161500	0.10914300	-1.24413100
H	-2.88494900	-1.43222300	-0.39552000

SiH_2Ph_2 + PHC^H

SiH_2Ph_2-PHC^H **T1**

Ee(M06-2X) = -1608.582626

Ee(RI-SCS-MP2) =-1605.782283

C	-2.12201600	0.28715000	1.51973700
C	-3.88521100	0.22171900	-0.58274800
P	-2.79020600	-0.91693200	0.42174400
H	-3.71132300	-1.57681500	1.25690400
P	-2.45533200	1.86106500	0.74187300
H	-3.29992700	2.35631300	1.75584800
N	-3.68546500	1.46231100	-0.41787300
Si	0.46854600	0.07114100	-0.11846900
H	-0.38640400	0.18130800	1.13499600
H	-0.43128500	0.32950200	-1.26873700
C	1.81652200	1.35618400	-0.10832700
C	3.08320300	1.07530300	0.41097000
C	1.56581200	2.64326800	-0.59343400
C	4.06980400	2.05026600	0.44498900
H	3.30235500	0.08168200	0.78650600
C	2.54937100	3.62120900	-0.55735600
H	0.59132600	2.88337200	-1.00445800
C	3.80234100	3.32430500	-0.03812400
H	5.04743200	1.81708400	0.84703300
H	2.34037200	4.61320500	-0.93672700
H	4.57182200	4.08537100	-0.01250300
C	1.14747800	-1.66553900	-0.10405400
C	0.76512400	-2.56679400	0.89154300
C	2.05424800	-2.09427100	-1.07758100
C	1.26939200	-3.86067800	0.91255500
H	0.06637500	-2.25295100	1.65984100
C	2.56003900	-3.38562400	-1.05983400
H	2.37575500	-1.41041200	-1.85620800
C	2.16591000	-4.27040500	-0.06390900
H	0.96403900	-4.54761500	1.69140100
H	3.26213100	-3.70269300	-1.82031200
H	2.56062900	-5.27833500	-0.04864100

C	-4.85260200	-0.32729700	-1.58534500
H	-4.31137300	-0.84211200	-2.38164500
H	-5.51043200	-1.06126700	-1.11515700
H	-5.44631400	0.47744600	-2.01321400

SiH_2Ph_2-PHC^H **B**

Ee(M06-2X) = -1608.72401553

Ee(RI-SCS-MP2) = -1605.930939

C	1.25530200	-0.01750200	0.25469000
C	3.94617100	0.14705900	0.14436100
P	2.49502200	1.22741200	-0.33961600
H	2.55826400	2.07262400	0.79251600
P	2.14523500	-1.65219700	-0.03662600
H	1.89246200	-2.24663200	1.21861000
N	3.74402000	-1.09284200	0.28829500
Si	-0.37184600	0.02264100	-0.68282100
H	1.08753900	0.10398300	1.32635100
H	-0.05535500	-0.05972000	-2.12721200
C	-1.40768200	-1.46609700	-0.21558400
C	-2.35345100	-1.39617300	0.81067400
C	-1.21648600	-2.69522600	-0.85440400
C	-3.07961600	-2.51625500	1.19198900
H	-2.53290300	-0.45101000	1.31220200
C	-1.93977200	-3.81792800	-0.47621900
H	-0.49363000	-2.77725400	-1.65902500
C	-2.87176600	-3.72884200	0.54902000
H	-3.80985700	-2.44262500	1.98780500
H	-1.77960100	-4.76071800	-0.98347000
H	-3.43863700	-4.60288400	0.84345900
C	-1.32749900	1.58396600	-0.29467900
C	-0.85780300	2.55605200	0.58903700
C	-2.57312900	1.79156200	-0.89665200
C	-1.59973900	3.69921700	0.86161600
H	0.10031500	2.42564900	1.08023300
C	-3.31769600	2.93027200	-0.63116800
H	-2.97021400	1.04866700	-1.58093300
C	-2.82968200	3.88763200	0.25002100
H	-1.21685600	4.44118500	1.55061300
H	-4.27831300	3.07300800	-1.10935300
H	-3.40944100	4.77744600	0.45954300
C	5.30742200	0.76280600	0.25668800
H	5.59492200	1.20628000	-0.69908500
H	5.30076500	1.56602500	0.99635600
H	6.03695200	0.00741800	0.54013200

SiH_2Ph_2-PHC^H **T2**

Ee(M06-2X) = -1608.63147979

Ee(RI-SCS-MP2) = -1605.843365

C	0.87971500	-0.65592300	1.04544800
C	3.77333200	-0.47262900	-0.29947200
P	2.73755100	0.93472500	-0.37531200
H	3.79433300	1.87009800	-0.22035300
P	1.98105500	-1.91818300	0.85892700
H	2.31249200	-2.59339700	2.03669800
N	3.38935600	-1.67429600	0.12390800
Si	-0.26987600	-0.11971400	-0.32799700
H	0.40074300	-0.65683200	2.02877600
H	0.35934200	-0.41333200	-1.63187700
C	-1.81087300	-1.18767700	-0.21167600
C	-2.95550600	-0.76831300	0.46972800
C	-1.81495900	-2.46317900	-0.78287300
C	-4.06614300	-1.59536100	0.57914200
H	-2.98497200	0.22098300	0.91349600
C	-2.92171300	-3.29293700	-0.67884700
H	-0.93964000	-2.81394700	-1.32062300
C	-4.05013000	-2.85852000	0.00487800
H	-4.94537300	-1.25231700	1.10964000
H	-2.90709600	-4.27591200	-1.13229200
H	-4.91624600	-3.50284800	0.08642700
C	-0.78064700	1.66591800	-0.12631700
C	-0.25112700	2.50169000	0.85763100
C	-1.77093800	2.18199900	-0.96737800
C	-0.69281100	3.81111300	0.99707300
H	0.52323600	2.12871400	1.51810800
C	-2.20920100	3.49182600	-0.83882500
H	-2.21215100	1.55060900	-1.73199200
C	-1.66977100	4.30840900	0.14663300
H	-0.27148500	4.44405300	1.76768200
H	-2.97209500	3.87518400	-1.50428300
H	-2.01173300	5.33020700	0.25125500
C	5.22354200	-0.41594900	-0.72424400
H	5.58036500	0.60493600	-0.83369500
H	5.84058900	-0.95285700	-0.00391900
H	5.32675000	-0.91820400	-1.68807900

SiH_2Ph_2-PHC^H **C**

Ee(M06-2X) = -1608.65323946

Ee(RI-SCS-MP2) = -1605.862713

C	0.06512400	-0.94330600	2.24854600
C	-0.40176800	-2.45677600	-1.08616700
P	0.94189200	-1.56742300	-1.60821700
P	-0.15225200	-2.41611600	1.57503100
N	-0.44681200	-3.00679100	0.18218000
Si	0.10942400	0.79207100	1.59008700
H	0.44999300	-1.32219400	-2.91278700
H	-0.16497400	-3.45048600	2.50431500
H	0.19804200	1.65274800	2.79307000
H	0.12681300	-1.06186800	3.32761700
C	-1.44620900	1.25288200	0.65974300
C	-2.30472200	0.30211500	0.10718000
C	-1.75307500	2.60375500	0.47068400
C	-3.42603400	0.68314100	-0.61785900
H	-2.10498500	-0.75421000	0.24817500
C	-2.87138500	2.99179200	-0.25334400
H	-1.10930300	3.36720500	0.89621000
C	-3.70917100	2.02915800	-0.80094300
H	-4.08077500	-0.07040700	-1.03740500
H	-3.09199400	4.04311200	-0.38732700
H	-4.58360600	2.32826400	-1.36462900
C	1.61136600	1.08842600	0.51385300
C	2.85223800	0.57601600	0.89746800
C	1.52690800	1.78197500	-0.69405200
C	3.97194100	0.73802000	0.09598600
H	2.94204100	0.02061700	1.82524500
C	2.64555600	1.94966100	-1.49955400
H	0.57153500	2.17198300	-1.02677300
C	3.86797800	1.42280900	-1.10795900
H	4.92369300	0.32420000	0.40394000
H	2.56001500	2.48082200	-2.43908700
H	4.73861400	1.54343400	-1.73995400
C	-1.60657600	-2.81896000	-1.90762900
H	-1.70327700	-3.90639000	-1.93952200
H	-2.50961200	-2.43257100	-1.42692200
H	-1.54410200	-2.42688200	-2.91857700

SiH_2Ph_2-PHC^H **T3**

Ee(M06-2X) = -1608.61430755

Ee(RI-SCS-MP2) = -1605.817582

C	-0.04256500	-1.90754100	1.44857100
C	-2.01085600	-1.26353000	-1.09974400
P	-0.28634700	-1.24874500	-1.55707900
P	-1.54016700	-2.54716300	1.09055100
N	-2.49281800	-1.85180800	-0.02703800
Si	0.44727400	-0.28361000	0.62948700
H	-0.40229700	-0.25231500	-2.55033100
H	-2.36103700	-2.95956500	2.14078600
H	0.42515800	-0.18513600	2.21605000
H	0.58478300	-2.35042500	2.20960700
C	-0.71996900	1.17929100	0.45300600
C	-1.82430700	1.28167600	1.29795900
C	-0.56909300	2.13490500	-0.55638800
C	-2.76762200	2.28918500	1.12704600
H	-1.94974000	0.56631000	2.10475500
C	-1.48919700	3.16034100	-0.71127400
H	0.27691500	2.07175400	-1.23355200
C	-2.59890100	3.23243200	0.12504600
H	-3.62792800	2.34116300	1.78219100
H	-1.34873800	3.90017800	-1.48930300
H	-3.32553500	4.02419500	-0.00474400
C	2.24952200	-0.00193500	0.24074400
C	3.03469800	-0.96635100	-0.39247400
C	2.84371400	1.20695100	0.60932500
C	4.37947300	-0.73325100	-0.64371500
H	2.58833600	-1.90678800	-0.69682200
C	4.18486800	1.44875700	0.34553500
H	2.25170100	1.96735400	1.10763100
C	4.95478600	0.47655700	-0.27826900
H	4.97741700	-1.49284000	-1.13096100
H	4.63018600	2.39318300	0.63128300
H	6.00201600	0.66176600	-0.48053600
C	-3.01704700	-0.52721500	-1.93872500
H	-2.79351100	-0.60420100	-3.00151000
H	-4.01994100	-0.89580100	-1.73075400
H	-2.96720600	0.53135900	-1.65928500

SiH_2Ph_2-PHC^H **D**

Ee(M06-2X) = -1608.73968993

Ee(RI-SCS-MP2) = -1605.944408

C	0.55956500	-0.92826800	1.71506700
C	2.64485400	-1.44139200	-0.67037900
P	1.01854400	-1.18581700	-1.52289800
P	1.42476900	-2.53761600	1.38903800
N	2.76690500	-2.00838000	0.45828800
Si	-0.08239000	-0.11212600	0.14763400
H	1.37892300	-0.07132100	-2.31022400
H	2.11664100	-2.62531500	2.61476400
H	-0.27842700	-1.11626500	2.39091000
H	1.24740800	-0.23789700	2.20618600
C	-1.90876000	-0.44180600	-0.07843700
C	-2.48291400	-1.60302900	0.44626000
C	-2.71797000	0.41034200	-0.83471500
C	-3.82175500	-1.89893700	0.23213200
H	-1.87654700	-2.29545300	1.02103000
C	-4.05787800	0.11954500	-1.04978600
H	-2.29817500	1.31587700	-1.25948300
C	-4.61161300	-1.03528000	-0.51418200
H	-4.24833800	-2.80348000	0.64626200
H	-4.66998500	0.79322900	-1.63574800
H	-5.65670400	-1.26314500	-0.68042100
C	0.25345900	1.73188100	0.17776300
C	-0.67964200	2.60662000	0.74303300
C	1.46315600	2.26427500	-0.27305400
C	-0.41517800	3.96533000	0.84719400
H	-1.62775300	2.22376900	1.10477100
C	1.73384400	3.62139200	-0.16880900
H	2.20799200	1.60964500	-0.71236700
C	0.79235700	4.47462000	0.38990200
H	-1.15171700	4.62660900	1.28549700
H	2.67784200	4.01356600	-0.52501300
H	0.99937100	5.53415800	0.46894700
C	3.87753300	-1.06564900	-1.45092900
H	3.93716800	0.01846200	-1.56976600
H	4.76186700	-1.42135100	-0.92618100
H	3.84149300	-1.49904200	-2.45251700

SiH_2Ph_2 + PHC^{Me}

SiH_2Ph_2-PHC^{Me} **T1**

Ee(M06-2X) = -1687.22093556

Ee(RI-SCS-MP2) = -1684.23694023

C	1.68405600	-0.62501800	1.11599100
C	3.52108400	-0.33889300	-0.88945300
P	2.36774100	0.65724300	0.17118700
P	2.07538400	-2.13215900	0.21340700
N	3.32126700	-1.59086400	-0.88231100
Si	-0.90424700	-0.11427900	-0.35657600
H	0.01904300	-0.55164300	0.78409300
H	-0.16081400	-0.33783000	-1.61697500
C	-2.46460700	-1.13563800	-0.26748200
C	-3.73914300	-0.57120000	-0.34908300
C	-2.35972900	-2.52306000	-0.12278900
C	-4.87538900	-1.36782800	-0.29065100
H	-3.84763600	0.50182600	-0.46079500
C	-3.49223400	-3.32100700	-0.06470600
H	-1.37972500	-2.98482200	-0.05550900
C	-4.75246900	-2.74252400	-0.14829100
H	-5.85651500	-0.91503600	-0.35657200
H	-3.39367500	-4.39317700	0.04709200
H	-5.63778300	-3.36385600	-0.10198700
C	-1.22774400	1.70490400	-0.12022000
C	-1.96962300	2.15129700	0.97866300
C	-0.71029600	2.65902600	-0.99956700
C	-2.19262700	3.50375500	1.18823500
H	-2.37948100	1.43185400	1.68006400
C	-0.93196700	4.01478300	-0.79433100
H	-0.12724400	2.33784400	-1.85483600
C	-1.67334000	4.43725700	0.29956400
H	-2.76935200	3.83155300	2.04362400
H	-0.52649200	4.74043600	-1.48779800
H	-1.84768600	5.49347000	0.46097400
C	4.54063300	0.32754000	-1.76384900
H	4.05033200	0.99134400	-2.47871800
H	5.21396000	0.94059000	-1.16044900
H	5.11739300	-0.42215600	-2.30118300
C	3.20167100	-2.87404100	1.46885600
H	2.60521900	-3.25827300	2.29369400
H	3.73829600	-3.69216300	0.98948700
H	3.91613800	-2.13948100	1.84023200
C	3.34951800	1.79268900	1.22911500
H	3.79267300	2.56853300	0.60604400
H	2.66258400	2.26198500	1.93111400
H	4.12772800	1.26643600	1.77772100

SiH_2Ph_2-PHC^{Me} **B**

Ee(M06-2X) = -1687.36246943

Ee(RI-SCS-MP2) = -1684.38865402

C	0.91135000	-0.52259200	0.27869200
C	3.59083600	-0.75343400	0.22666300
P	1.51732600	-2.28876500	0.19610900
P	2.33478600	0.54796900	-0.21229600
N	3.21901700	-1.96044800	0.31740200
C	1.45385300	-2.62142500	-1.61350300
H	2.03147700	-3.52507800	-1.80707000
H	0.42026500	-2.80421900	-1.91216800
H	1.86396400	-1.79959900	-2.20240600
C	2.46660300	1.69335100	1.22628600
H	3.37989400	2.28248900	1.14015500
H	1.61775700	2.37875300	1.18850200
H	2.46176000	1.16191200	2.17850100
C	5.03157400	-0.35145900	0.34389000
H	5.33827700	0.21356400	-0.53880200
H	5.16698400	0.30243600	1.20889100
H	5.65933200	-1.23235800	0.45778400
H	0.68721400	-0.33803500	1.33649700
Si	-0.61640600	-0.03522500	-0.69707700
H	-0.34866300	-0.20300700	-2.14398600
C	-2.11728700	-1.02503300	-0.18088300
C	-2.06782500	-2.02666600	0.79013600
C	-3.35251600	-0.74479200	-0.77597300
C	-3.21114200	-2.73035200	1.15139200
H	-1.12813000	-2.27163500	1.27288800
C	-4.49521700	-1.44382000	-0.42002600
H	-3.42360000	0.03611400	-1.52644000
C	-4.42433700	-2.44042600	0.54620900
H	-3.15141100	-3.50505000	1.90507800
H	-5.44113600	-1.21312000	-0.89321900
H	-5.31529800	-2.98793300	0.82618800
C	-0.92910900	1.78467900	-0.37525100
C	-1.67552700	2.19562200	0.73211100
C	-0.33302700	2.76734100	-1.17067800
C	-1.81492600	3.54191800	1.04217400
H	-2.16034200	1.45340800	1.35819900
C	-0.47012100	4.11504000	-0.86580700
H	0.25184600	2.47587800	-2.03637700
C	-1.20945200	4.50312400	0.24375000
H	-2.39743800	3.84158400	1.90410300
H	-0.00255500	4.86230800	-1.49430100
H	-1.31771200	5.55337200	0.48296200

SiH_2Ph_2-PHC^{Me} **T2**

Ee(M06-2X) = -1687.27192138

Ee(RI-SCS-MP2) = -1684.30325822

C	-0.48495900	0.48128500	-1.34413100
C	-3.26927400	1.14090800	-0.03877400
P	-1.93641200	-0.27921700	-1.72975300
P	-1.88581200	2.13311200	0.38101800
N	-3.28272400	0.20961000	-0.98945400
C	-1.95655900	-2.08593800	-1.69322000
H	-1.87813200	-2.44824000	-0.66821500
H	-2.89921600	-2.41601200	-2.12698500
H	-1.12653800	-2.47010900	-2.28456800
C	-2.29678900	2.55516600	2.14181800
H	-2.54658600	1.68584300	2.74965300
H	-1.42731700	3.04847000	2.57536700
H	-3.13064900	3.25984800	2.18081000
C	-4.56820000	1.25330000	0.73064300
H	-5.36100700	0.78257900	0.15337900
H	-4.48112400	0.72671600	1.68435200
H	-4.83900400	2.28545200	0.94930900
H	-0.45141900	1.52722600	-1.61610100
Si	1.13073500	-0.41156300	-1.10234600
H	1.63529400	-1.05582600	-2.34198800
C	0.84420000	-1.80281000	0.11962300
C	1.34975200	-3.08284100	-0.11117900
C	0.09097100	-1.58807100	1.27780100
C	1.11194600	-4.11994300	0.78282400
H	1.93008100	-3.27817200	-1.00680700
C	-0.15009000	-2.61944500	2.17343900
H	-0.32543000	-0.60343000	1.46954900
C	0.35979700	-3.88857000	1.92526300
H	1.50916900	-5.10754700	0.58554200
H	-0.73762300	-2.43709400	3.06437400
H	0.16883600	-4.69524700	2.62150000
C	2.42148100	0.80309800	-0.50806300
C	3.76608700	0.42058700	-0.51896400
C	2.10010400	2.07365400	-0.02896600
C	4.75812700	1.27684200	-0.06590800
H	4.04495000	-0.56123500	-0.88821900
C	3.09083400	2.93614800	0.42341900
H	1.06483700	2.39637500	-0.00403600
C	4.41973600	2.53877300	0.40590300
H	5.79412700	0.96331100	-0.08260900
H	2.82380100	3.91962600	0.78885100
H	5.19209700	3.21081700	0.75772100

SiH_2Ph_2-PHC^{Me} **C**

Ee(M06-2X) = -1687.2943014

Ee(RI-SCS-MP2) = -1684.32106358

C	-0.38174400	-1.74290200	-1.62060800
C	-1.63262200	-0.59239200	1.54512800
P	-1.53880400	-2.21525500	-0.56252300
P	-0.11343200	-0.77828600	2.26501600
N	-2.11985900	-1.60028400	0.72372500
C	-2.40148500	-3.73989500	-0.95481400
H	-2.20890600	-4.46693300	-0.16772400
H	-3.46982900	-3.53250500	-0.98085800
H	-2.06733600	-4.12303700	-1.91533600
C	0.06428300	0.75033200	3.30208300
H	-0.63869000	0.75424800	4.13565200
H	1.07400600	0.75239000	3.71242700
H	-0.07074400	1.66133400	2.71887800
C	-2.61029100	0.52609200	1.73595900
H	-2.27504000	1.26765700	2.45516800
H	-2.77955200	1.01808400	0.77391200
H	-3.56607600	0.10976800	2.06218900
H	-0.24105100	-2.46197800	-2.42062800
Si	0.53134000	-0.14064700	-1.71487000
H	0.78277400	0.08336200	-3.16019400
C	2.18731800	-0.15533500	-0.84425700
C	3.04448600	0.94012900	-0.98623500
C	2.61550700	-1.23078400	-0.06669400
C	4.28501900	0.96518300	-0.36564700
H	2.73883500	1.78963500	-1.58954000
C	3.85712000	-1.21309000	0.55544600
H	1.96321100	-2.08657100	0.06391700
C	4.69204000	-0.11469000	0.40773000
H	4.93474600	1.82270900	-0.48631700
H	4.17030900	-2.05501800	1.15965400
H	5.65964500	-0.09910600	0.89326600
C	-0.51316700	1.30398500	-1.12274200
C	-1.71125700	1.60204100	-1.77778600

C	-0.10745900	2.14304400	-0.08397700
C	-2.47440000	2.70453800	-1.41610600
H	-2.05111300	0.96713500	-2.59007200
C	-0.86641600	3.24650900	0.28428200
H	0.81534800	1.92950800	0.44459400
C	-2.04960600	3.53113300	-0.38435900
H	-3.39760000	2.91988300	-1.93906300
H	-0.53277300	3.88725300	1.09140900
H	-2.64033300	4.39293700	-0.10101700

SiH_2Ph_2-PHC^{Me} **T3**
Ee(M06-2X) = -1687.25178464
Ee(RI-SCS-MP2) = -1684.27453739

C	0.39162200	2.01050500	-1.07860000
C	1.95687700	0.52609500	1.40925500
P	1.95159600	2.26579100	-0.52935400
P	0.21688200	0.73078700	1.72425500
N	2.62429700	1.19856100	0.49677700
C	3.23133700	2.78595900	-1.69230400
H	4.05953400	3.22385700	-1.13905300
H	3.58707800	1.92189200	-2.25267000
H	2.80985400	3.52178300	-2.37428900
C	-0.18454100	-0.70178700	2.81636100
H	0.17075300	-0.53198000	3.83295400
H	-1.27209800	-0.78286600	2.85067000
H	0.22354200	-1.64107900	2.44299200
C	2.75669100	-0.48634000	2.17987100
H	2.50775700	-0.48736800	3.24074300
H	2.52410500	-1.48194500	1.78507000
H	3.81909900	-0.29658000	2.04208600
H	-0.07146200	2.70502400	-1.76562100
Si	-0.46280900	0.40601100	-0.61739100
H	-0.30039500	0.62269600	-2.19598200
C	-2.31832600	0.39763400	-0.40020400
C	-3.08485800	-0.53921300	-1.09746400
C	-2.97379600	1.30331100	0.43551000
C	-4.46532700	-0.57628000	-0.95741400
H	-2.59559800	-1.24765400	-1.75767600
C	-4.35558000	1.27822300	0.56721200
H	-2.39600100	2.03435000	0.99083800
C	-5.10245000	0.33521500	-0.12612700
H	-5.04422700	-1.31250900	-1.50048500
H	-4.84949800	1.99140100	1.21494100
H	-6.17944400	0.31070600	-0.01883500
C	0.35369000	-1.28451200	-0.72407300
C	1.57207300	-1.42784700	-1.39236700
C	-0.17950600	-2.40693300	-0.08386800
C	2.25124800	-2.63899600	-1.39626100
H	1.99256700	-0.58109500	-1.92620400
C	0.48431700	-3.62634900	-0.10388800
H	-1.12902800	-2.32792900	0.43642500
C	1.70775200	-3.74218500	-0.75202100
H	3.20010300	-2.72523100	-1.91072600
H	0.04798400	-4.48702000	0.38770300
H	2.23010200	-4.69019200	-0.76209400

SiH_2Ph_2-PHC^{Me} **D**
Ee(M06-2X) = -1687.367725
Ee(RI-SCS-MP2) = -1684.39172721

C	-0.90173700	-0.14719000	-1.61394700
C	-2.64711600	-0.90779400	1.00354900
P	-2.58998900	0.51988400	-1.27828100
P	-1.02637800	-0.29197200	1.76635500
N	-3.17070800	-0.57211000	-0.09677600
C	-3.49391900	-0.16870500	-2.71520200
H	-4.55898000	0.02287700	-2.58963600
H	-3.15318900	0.33234600	-3.62223500
H	-3.32968100	-1.24283200	-2.80576200
C	-1.52192000	1.48897500	1.98884400
H	-2.25288900	1.53788800	2.79564200
H	-0.63766400	2.05225900	2.28631700
H	-1.94460600	1.94400500	1.09340300
C	-3.38362200	-1.86512100	1.90435400
H	-3.56576400	-1.39861000	2.87597300
H	-4.32725200	-2.16196100	1.45105800
H	-2.76506500	-2.74555100	2.09396800
H	-0.45217800	0.42876600	-2.42795200
Si	0.22439600	-0.07627800	-0.11182700
H	-0.98819700	-1.18843300	-1.93930300
C	1.48628700	-1.45912200	-0.17876300
C	1.35595800	-2.62543100	0.57691300
C	2.57518300	-1.35681600	-1.05064200
C	2.27638200	-3.65955600	0.46223000
H	0.53263200	-2.72627400	1.27610000
C	3.49880400	-2.38517100	-1.16707600
H	2.70880400	-0.45610900	-1.64136200
C	3.34826800	-3.54025400	-0.41029400
H	2.15939100	-4.55561700	1.05830500
H	4.33669400	-2.28630600	-1.84541000
H	4.06857400	-4.34361700	-0.49802200
C	1.09970900	1.57421000	-0.02636800
C	2.30148700	1.70598900	0.67569900
C	0.53651100	2.72174700	-0.59285500
C	2.92173600	2.94080900	0.80597900
H	2.76201000	0.83011800	1.12055800
C	1.15372100	3.95863600	-0.46447000
H	-0.40092400	2.65343700	-1.13551300
C	2.34751700	4.06908100	0.23550300
H	3.85371100	3.02309400	1.35061000
H	0.70331000	4.83610900	-0.91068200
H	2.83071200	5.03266600	0.33511400

SiH_2Ph_2 + NHC^{Me}

SiH_2Ph_2-NHC^{Me} **T1**
Ee(M06-2X) = -1114.06103392
Ee(RI-SCS-MP2) = -1111.81014992

C	2.34304000	-2.68459100	0.18891200
N	2.10765100	-1.40035100	-0.25799700
C	0.74186300	-1.27644600	-0.42497000
N	0.31113600	-2.56544100	-0.37780800
H	0.23808200	-0.48267900	0.97040200
N	1.27646200	-3.40287300	0.13502100
Si	-0.28059000	0.27448000	-0.65875900
H	-0.44701700	0.47832600	-2.14494600
C	3.67686700	-3.17690900	0.61375400
H	3.58814000	-4.22561900	0.88354800
H	4.40338200	-3.07860200	-0.19465900
H	4.04689400	-2.61734500	1.47379100
C	3.00282700	-0.28426200	-0.07386700
H	2.76475900	0.23545900	0.85985100
H	4.02634400	-0.64978900	-0.04475400
H	2.89851100	0.42042800	-0.89599800
C	-1.06348300	-2.98441300	-0.28643500
H	-1.48453800	-2.70345100	0.68420300
H	-1.64626700	-2.50895300	-1.07259500
H	-1.08894200	-4.06410400	-0.40414300

C	0.61332200	1.86674200	-0.19929200
C	1.07125700	2.69902800	-1.22304600
C	0.79576800	2.29034000	1.11934600
C	1.71676500	3.89756100	-0.94382100
H	0.92096600	2.40364600	-2.25576300
C	1.42632500	3.49253100	1.40590400
H	0.44598300	1.66113600	1.92981000
C	1.89563400	4.29529200	0.37314800
H	2.07467600	4.52180900	-1.75292300
H	1.55201600	3.80603000	2.43470600
H	2.39257800	5.23117100	0.59565600
C	-2.08156000	0.09887500	-0.13742900
C	-2.49879800	-0.01451000	1.19099900
C	-3.06444400	0.13824400	-1.12955400
C	-3.84529600	-0.09867700	1.51561800
H	-1.75452600	-0.04972100	1.97785100
C	-4.41393200	0.04543000	-0.81278300
H	-2.76824600	0.23997300	-2.16778200
C	-4.80611000	-0.07424700	0.51259700
H	-4.14703900	-0.18362600	2.55207500
H	-5.15771700	0.06824800	-1.59931400
H	-5.85679300	-0.14432800	0.76461300

SiH_2Ph_2-NHC^{Me} **B**

Ee(M06-2X) = -1114.1090272

Ee(RI-SCS-MP2) = -1111.86357670

C	3.02404500	-1.81975200	0.03002900
N	2.30615700	-0.61450600	0.11409000
C	0.90953900	-1.05853500	0.19905300
N	0.99623400	-2.37066200	-0.45591300
H	0.63749000	-1.18429100	1.27607500
N	2.31452900	-2.83239900	-0.27086400
Si	-0.30533400	0.05877200	-0.75294500
H	-0.09687900	-0.17869800	-2.19535100
C	4.50013400	-1.86032700	0.20084100
H	4.85385900	-2.86282400	-0.02296500
H	4.97841100	-1.14783700	-0.47427700
H	4.78737000	-1.59986800	1.22084500
C	2.72534100	0.33742100	1.12728000
H	2.61063300	-0.07618000	2.13982100
H	3.76792500	0.60776000	0.96881200
H	2.12860500	1.24392700	1.05334000
C	0.01768100	-3.33622400	-0.00554200
H	0.04916700	-3.46909000	1.08639000
H	-0.98036000	-3.00266900	-0.29014500
H	0.22679600	-4.28926900	-0.48573700
C	0.03361200	1.86338500	-0.38942000
C	1.04138200	2.52804500	-1.09569500
C	-0.64573400	2.56524300	0.60826500
C	1.36921800	3.84450800	-0.80527600
H	1.58270700	2.00571200	-1.87727600
C	-0.32019600	3.88283200	0.90394000
H	-1.44709800	2.08213300	1.15671300
C	0.69019400	4.52233100	0.19950400
H	2.15131500	4.34377000	-1.36305800
H	-0.85817900	4.41190200	1.68026200
H	0.94356900	5.54988900	0.42722200
C	-2.05157900	-0.40186600	-0.26713400
C	-2.39851300	-0.60554400	1.07272200
C	-3.04892300	-0.55540000	-1.23290100
C	-3.69430000	-0.94464700	1.43554300
H	-1.64634500	-0.50583600	1.84884500
C	-4.34701600	-0.89562100	-0.87620600
H	-2.80802800	-0.41306200	-2.28042000
C	-4.67091400	-1.09012600	0.45906900
H	-3.94193000	-1.09965200	2.47791600
H	-5.10493500	-1.01198900	-1.64032800
H	-5.68168800	-1.35801600	0.73893000

SiH_2Ph_2-NHC^{Me} **T2**

Ee(M06-2X) = -1114.05755867

Ee(RI-SCS-MP2) = -1111.81230889

C	0.20953500	-1.93842100	-0.81011400
C	1.90380400	-1.04090000	0.78267100
N	2.42113100	-1.53571000	-0.34434900
N	1.44230600	-2.37641200	-0.90396800
N	0.62660000	-1.14923200	1.08479300
C	2.86410700	-0.28014800	1.64432100
H	2.53028500	0.75811400	1.72743300
H	2.90036700	-0.70432100	2.64880300
H	3.85405100	-0.31040500	1.19807000
C	0.14768700	-0.80956200	2.40464900
H	0.42055700	0.21878100	2.67115500
H	-0.94005800	-0.86819200	2.42334600
H	0.53438000	-1.47674300	3.18365000
C	1.76206000	-3.78526700	-0.74702900
H	1.03530100	-4.39055000	-1.28585700
H	2.75683700	-3.95164700	-1.15285000
H	1.76061200	-4.04508000	0.31595400
Si	-0.36924300	-0.18466000	-1.20655300
H	-0.55177800	-2.71955900	-0.84018900
H	-0.46319700	-0.13970000	-2.69119700
C	-2.10234700	-0.05145200	-0.51423800
C	-2.88926800	1.04306300	-0.88667600
C	-2.66307100	-0.99578900	0.34718900
C	-4.18529500	1.19166600	-0.41544100
H	-2.48137000	1.79558300	-1.55418300
C	-3.96193200	-0.85541700	0.82006900
H	-2.07699300	-1.84998600	0.66643400
C	-4.72431400	0.23937600	0.43983300
H	-4.77569200	2.04784700	-0.71579000
H	-4.37737200	-1.59995300	1.48735900
H	-5.73588800	0.35141000	0.80864000
C	0.67177500	1.27173300	-0.67077400
C	1.88679400	1.56366900	-1.29416900
C	0.25399200	2.08956400	0.38185000
C	2.66810500	2.62936800	-0.86863400
H	2.24027600	0.93791400	-2.10527900
C	1.02780000	3.16278300	0.80465100
H	-0.68659200	1.88363500	0.88146000
C	2.23878400	3.43115600	0.18081200
H	3.61274200	2.83384300	-1.35610800
H	0.68701200	3.78679700	1.62122500
H	2.84634900	4.26441700	0.51051000

SiH_2Ph_2-NHC^{Me} **C**

Ee(M06-2X) = -1114.08651741

Ee(RI-SCS-MP2) = -1111.83950561

C	-0.52613900	-2.16315200	-1.00175400
N	-0.13229900	-0.91702600	-0.87674700
C	0.01856200	-1.54529200	1.68512600
N	-0.31389200	-2.70778900	1.22605700
H	0.25486800	-1.56630300	2.74519400
N	-0.65373200	-3.06920200	-0.03095700
Si	0.08624600	0.15231200	0.81175400
H	0.19227000	0.83571900	2.17638700
C	-0.89475800	-2.72827500	-2.34805100
H	-1.14893900	-3.77735900	-2.23880800

H	-1.74814500	-2.19029900	-2.76465400
H	-0.06848300	-2.62293600	-3.05153100
C	-0.02638000	-0.12025200	-2.09673100
H	0.76552200	-0.49432800	-2.74958500
H	-0.96581100	-0.09926800	-2.65244400
H	0.22137500	0.90413500	-1.82825600
C	-0.36955800	-3.88790200	2.10060000
H	-1.37928400	-4.28771900	2.05501500
H	0.32300300	-4.62859600	1.70927900
H	-0.10826900	-3.60359100	3.11430300
C	-1.47603200	1.14972900	0.34956400
C	-1.56361800	2.46943300	0.80261000
C	-2.57208900	0.64563200	-0.35500100
C	-2.66757600	3.26466100	0.52956100
H	-0.75344300	2.87866500	1.39616500
C	-3.69877600	1.42016800	-0.60264500
H	-2.55911200	-0.37863400	-0.71127400
C	-3.74354800	2.73827100	-0.17239600
H	-2.69618300	4.28975900	0.87744300
H	-4.54111200	0.99475500	-1.13418600
H	-4.61477800	3.34859200	-0.37406000
C	1.82202600	0.70347100	0.26498200
C	2.69298100	-0.10312400	-0.47091000
C	2.29245300	1.95605700	0.66734600
C	3.97422600	0.32160300	-0.79869700
H	2.36685400	-1.08651400	-0.79179000
C	3.55946500	2.40328400	0.31916400
H	1.65728600	2.58997800	1.27608400
C	4.40661900	1.58278600	-0.41337500
H	4.63481300	-0.33046900	-1.35676100
H	3.89144100	3.38611300	0.62971900
H	5.40098500	1.92146200	-0.67562100

SiH_2Ph_2-NHC^{Me} **T3**

Ee(M06-2X) = -1114.07037045

Ee(RI-SCS-MP2) = -1111.81780779

C	-1.98268200	1.41040100	1.01073800
N	-0.76027700	0.82435000	1.12745500
C	-0.46297900	1.76955900	-1.31160000
N	-1.69780400	2.20843500	-1.15811300
H	0.08721100	2.17391900	-2.15418100
N	-2.47920000	2.00566800	-0.03414300
Si	0.07989800	0.25980100	-0.38068700
H	-0.21854900	0.19093700	-2.03693200
C	-2.91123400	1.38846600	2.19450300
H	-3.85339700	1.84552000	1.91018900
H	-3.08915900	0.36893600	2.54015100
H	-2.47998900	1.94555800	3.02783700
C	-0.37105900	0.24180600	2.40602800
H	0.64822200	-0.13293500	2.31640000
H	-0.37925500	0.99292900	3.19679500
H	-1.00536100	-0.59560500	2.70959700
C	-2.45596900	2.84825900	-2.22061500
H	-1.76771000	3.18466000	-2.99205200
H	-3.16319400	2.13508000	-2.64777900
H	-3.00617100	3.68926500	-1.80550800
C	-0.47837700	-1.56250100	-0.33226100
C	0.20052200	-2.50713100	-1.11190100
C	-1.59857200	-2.00530900	0.37153600
C	-0.19260900	-3.83506600	-1.15374900
H	1.04824000	-2.18987000	-1.71144100
C	-2.01764100	-3.33067300	0.31738900
H	-2.17829000	-1.30311900	0.96025500
C	-1.30768900	-4.25205100	-0.43537400
H	0.35944400	-4.54448700	-1.75755600
H	-2.89900800	-3.64115700	0.86470900
H	-1.62522900	-5.28626300	-0.47378800
C	1.92964100	0.37986900	-0.11700700
C	2.56630900	1.62119700	-0.21771900
C	2.71072300	-0.72341900	0.23978200
C	3.92995900	1.75335900	0.00447600
H	1.98548900	2.50307300	-0.46128500
C	4.07416900	-0.59649600	0.47001100
H	2.24826300	-1.69738300	0.34820200
C	4.68777000	0.64195800	0.34625700
H	4.40042100	2.72459800	-0.08268000
H	4.65750400	-1.46562000	0.74657600
H	5.75121100	0.74220500	0.52273600

SiH_2Ph_2-NHC^{Me} **D**

Ee(M06-2X) = -1114.15372915

Ee(RI-SCS-MP2) = -1111.90453022

C	1.46609600	-2.20368700	0.80071100
N	0.61418100	-1.13739700	1.06750200
C	0.83342500	-0.95344100	-1.67781900
N	2.17495400	-1.27984900	-1.18475900
H	0.93119800	-0.24864200	-2.50531200
N	2.18796300	-2.32493200	-0.24848800
Si	0.01230300	-0.12994600	-0.21973300
C	1.55721700	-3.30471500	1.81715100
H	0.58459700	-3.77386900	1.97700700
H	2.25974000	-4.04835600	1.45404500
H	1.90282700	-2.92688000	2.78101800
H	0.31640600	-1.84896800	-2.05764700
C	3.07884900	-1.63385900	-2.26582900
H	4.05218400	-1.87809000	-1.84643000
H	2.71063600	-2.49899700	-2.83410600
H	3.18037700	-0.77994400	-2.93502900
C	0.05221900	-0.98916500	2.40467100
H	-0.57546700	-1.83658100	2.68936600
H	0.83413000	-0.86313100	3.15623700
H	-0.57252600	-0.09527100	2.43002300
C	0.57742900	1.63359100	0.00960800
C	1.63880300	1.93061700	0.86673600
C	0.00049700	2.68174500	-0.71417300
C	2.10310900	3.23190000	1.00628600
H	2.11227900	1.12876100	1.42218500
C	0.46431700	3.98284100	-0.58373500
H	-0.82520600	2.48120300	-1.38974800
C	1.51551600	4.25886400	0.28125400
H	2.92650500	3.44400000	1.67636600
H	0.00710600	4.78136900	-1.15407000
H	1.87719900	5.27376500	0.38730100
C	-1.86073800	-0.19692900	-0.24599300
C	-2.66243000	0.82919400	0.26085700
C	-2.49709600	-1.34576400	-0.72914500
C	-4.04688500	0.71737200	0.27894800
H	-2.20039600	1.72993800	0.64963200
C	-3.87925600	-1.46257000	-0.71657300
H	-1.90419000	-2.16638300	-1.11887600
C	-4.65666100	-0.42757200	-0.21306000
H	-4.64924500	1.52415500	0.67685400
H	-4.35090600	-2.35884800	-1.09888200
H	-5.73564100	-0.51527100	-0.20281900

BH_3 + PHC^{Me}

BH_3-PHC^{Me} **T1**

Ee(M06-2X) = -959.8848574
Ee(RI-SCS-MP2) = -958.33001382

C	0.56025000	-0.56920700	-0.86930300
P	0.77990100	1.08233300	-0.14783400
P	-1.50495600	0.01463100	0.36221700
N	-0.65545000	-0.97005200	-0.75533300
C	-0.62776100	1.43774300	0.69131700
C	-3.18066300	0.22485400	-0.30824000
H	-3.15006900	0.72871300	-1.27213800
H	-3.64227100	-0.75456600	-0.41776600
H	-3.75128900	0.82200200	0.40004600
C	2.43995100	1.47630100	0.47931900
H	2.69064600	0.84374400	1.32928300
H	3.17207300	1.33554600	-0.31473400
H	2.44426400	2.51971900	0.78867600
C	1.61360500	-1.31627400	-1.62752100
H	1.17291400	-2.18077200	-2.12015200
H	2.08302800	-0.67477600	-2.37505500
H	2.40049900	-1.65594500	-0.94903100
B	0.90032100	-2.27225700	2.10208900
H	-0.09555500	-2.76526700	1.68874900
H	1.12767800	-1.12571600	1.88065800
H	1.67816500	-2.91597900	2.72918000

BH_3-PHC^{Me} **B**

Ee(M06-2X) = -960.008264826
Ee(RI-SCS-MP2) = -958.44955076

C	0.98966900	-0.96628300	0.02271600
P	0.84193600	0.79376200	0.61678100
P	-1.43781300	-0.56553900	-0.76282200
N	-0.02477500	-1.51907000	-0.49312600
C	-0.65950600	1.14125500	-0.39169300
C	-2.29383900	-0.95358200	0.82371500
H	-3.22688500	-0.39177100	0.88971200
H	-2.53433700	-2.01665100	0.80895400
H	-1.67594800	-0.73578900	1.69508700
C	2.16840100	1.57640400	-0.40380700
H	2.09714700	2.65908000	-0.30499400
H	3.14150600	1.27129300	-0.01802600
H	2.09431000	1.30528100	-1.45738200
C	2.26804200	-1.71205800	0.26615600
H	2.14275200	-2.76501300	0.02462700
H	3.06458800	-1.29420500	-0.35427500
H	2.57763400	-1.60121900	1.30724300
B	-1.73571200	2.01776800	0.28653600
H	-1.90560100	1.94793000	1.46306300
H	-2.43706500	2.73400800	-0.35752800
H	-0.38455300	1.49394600	-1.38919400

BH_3-PHC^{Me} **T2**

Ee(M06-2X) = -959.927011866
Ee(RI-SCS-MP2) = -958.37495131

C	-1.32672300	1.27581900	-0.45643800
C	1.00379800	-0.80880100	-0.20082800
P	-1.54434100	-0.41603800	-0.46215000
P	1.40121300	0.88865000	-0.39895400
N	-0.21561200	-1.32142800	-0.32431000
C	2.06340300	-1.81346200	0.20138300
H	1.69784600	-2.81387800	-0.01958600
H	3.01270300	-1.65213800	-0.30775200
H	2.24990800	-1.74803400	1.27614100
B	-2.07240700	2.18126700	0.50817700
H	-0.81576200	1.66195700	-1.32460500
H	-2.88433200	1.73420000	1.25911000
H	-1.81701500	3.34253700	0.55528700
C	2.91554700	1.00099200	0.66139800
H	2.78629900	0.56738400	1.65213900
H	3.75236300	0.50130700	0.16686900
H	3.17353700	2.05418100	0.76389500
C	-2.70999100	-1.09738000	0.74378200
H	-2.76045700	-2.17064700	0.56898500
H	-2.36205600	-0.91393700	1.75929200
H	-3.69100300	-0.65145400	0.60028100

BH_3-PHC^{Me} **C**

Ee(M06-2X) = -959.968697365
Ee(RI-SCS-MP2) = -958.40866184

C	0.64356500	1.00768300	-0.03132600
P	1.38202800	-0.52761400	-0.57165400
P	-1.67750600	-0.06598700	-0.01217500
N	-0.65558000	1.20115300	0.01785100
C	-1.21853800	-1.59813600	0.26302300
C	-3.36999500	0.51720700	-0.08817700
H	-4.03831800	-0.33817800	-0.01820300
H	-3.54844200	1.20693200	0.73518100
H	-3.53178600	1.03931400	-1.02984000
C	3.06263600	-0.47354800	0.18034400
H	3.55248800	-1.41381300	-0.07248200
H	3.66465000	0.33880600	-0.22426000
H	3.01559300	-0.39687900	1.26689600
C	1.49998800	2.19995500	0.27473200
H	0.88731900	3.09502400	0.35664400
H	2.02334400	2.03125900	1.21976500
H	2.26263800	2.33548500	-0.49306200
B	0.35153000	-1.98003100	0.34096800
H	0.57720100	-2.95833500	-0.32569200
H	0.69470500	-2.13089200	1.49201100
H	-2.00176100	-2.33160400	0.42911900

BH_3-PHC^{Me} **T3**

Ee(M06-2X) = -959.955383238
Ee(RI-SCS-MP2) = -958.39221520

C	0.77941100	1.06555600	-0.17016100
C	-1.10933400	-1.47984600	-0.47580100
H	-0.06742900	-1.28153600	-2.10842700
N	-0.46095700	1.18856700	0.11425700
P	-1.50459300	-0.08825200	0.40029300
P	1.74502300	-0.54304100	-0.34486300
C	-3.16113500	0.57920600	0.08283900
H	-3.19970200	1.03783300	-0.90337600
H	-3.88176600	-0.23435200	0.14912200
H	-3.39317600	1.32586400	0.83923000
C	1.76460300	-0.94452100	1.47264200
H	2.41727700	-0.25072500	2.00249700
H	0.77781900	-0.93141100	1.93848200
H	2.18035800	-1.94715000	1.57719800
C	1.56763600	2.31924600	-0.40209100
H	2.43421900	2.32517100	0.26474400
H	1.96651000	2.31048000	-1.41861500
H	0.95942600	3.20723400	-0.24099100
B	0.32229500	-1.71765100	-0.99891400
H	0.67482500	-2.85399500	-1.15562400
H	-1.90666600	-2.20757000	-0.62548600

BH_3-PHC^{Me} **D**

Ee(M06-2X) = -960.019851856

Ee(RI-SCS-MP2) = -958.45886378

C	0.63365300	1.01940700	-0.13779100
C	-1.21971200	-1.46121700	-0.56576600
H	-1.27275400	-1.00392900	-1.55756400
N	-0.57241100	1.13396700	0.22126500
P	-1.65381500	-0.11100700	0.65523400
P	1.52859000	-0.57939300	-0.53114400
C	-3.16917600	0.54433700	-0.14251600
H	-2.99485800	0.77527100	-1.19344500
H	-3.95875800	-0.20257400	-0.05722100
H	-3.48253700	1.44631700	0.38126700
C	2.84190200	-0.64343000	0.76875200
H	3.67645700	-0.00027000	0.49542200
H	2.47009500	-0.35979700	1.75169100
H	3.20606100	-1.66980500	0.81266300
C	1.48943200	2.24842200	-0.29711200
H	2.35780200	2.19203600	0.36407700
H	1.86694700	2.31201200	-1.31957000
H	0.91077100	3.13715900	-0.05515100
B	0.22256800	-1.86087900	-0.13788300
H	0.49790300	-2.89254700	0.38663600
H	-1.96131200	-2.25636400	-0.48297700

BH_3 + PHC^{Ph}

BH_3-PHC^{Ph} **T1**

Ee(M06-2X) = -1343.05605681

Ee(RI-SCS-MP2) = -1340.98336880

C	-0.08487700	-0.92379400	0.26447500
C	0.46574100	1.72347500	-0.07073500
P	-1.12849600	-0.06175400	-0.86651400
P	1.07398900	0.25359300	0.89902200
N	-0.64641500	1.59279500	-0.68583700
C	1.18925800	3.03201100	0.03242500
H	2.19953100	2.93241400	-0.38213200
H	0.64603900	3.80304500	-0.51744100
H	1.29161400	3.33093800	1.08143300
C	-2.87019400	-0.13382300	-0.34714200
C	-3.64289100	1.03349600	-0.35324600
C	-3.44666500	-1.36179700	-0.00535500
C	-4.98878800	0.96696400	0.00022200
H	-3.19037800	1.98390900	-0.61920600
C	-4.79278400	-1.41263800	0.34875300
H	-2.84846400	-2.26798400	-0.00022500
C	-5.56560300	-0.25235800	0.35122100
H	-5.58581800	1.87424400	0.00418500
H	-5.23606800	-2.36505500	0.62420100
H	-6.61519200	-0.29811400	0.62658300
C	2.75546500	-0.16878700	0.32824700
C	2.98170700	-1.10343000	-0.68895400
C	3.83886900	0.47619800	0.93520600
C	4.28399100	-1.37864100	-1.09681100
H	2.14451600	-1.62196700	-1.14784800
C	5.13868500	0.20847200	0.51033300
H	3.66888200	1.18090300	1.74610000
C	5.36161000	-0.72021700	-0.50435200
H	4.45560900	-2.10996900	-1.88096000
H	5.97521400	0.71407500	0.98342200
H	6.37523800	-0.93764600	-0.82807000
B	-0.16497400	-2.41611100	0.71499800
H	-0.93902400	-2.08862900	1.65057400
H	0.85258100	-2.84394800	1.20872200
H	-0.76803400	-3.14359500	-0.03680700

BH_3-PHC^{Ph} **B**

Ee(M06-2X) = -1343.17310232

Ee(RI-SCS-MP2) = -1341.04725759

C	-0.17628500	-0.82949200	0.78315600
C	0.33043200	1.60394200	-0.35364800
P	-0.98974800	-0.55956700	-0.89715700
P	0.96359200	0.62548400	1.12534900
N	-0.53905200	1.10758400	-1.13550200
C	0.88903700	2.98685200	-0.54622300
H	1.97858300	2.93938300	-0.66323800
H	0.44863000	3.44702100	-1.43292000
H	0.68363900	3.60519900	0.33464400
C	-2.73895700	-0.32966400	-0.36741300
C	-3.16383400	0.77492100	0.38029100
C	-3.66428700	-1.32361000	-0.69706800
C	-4.48825800	0.87820700	0.79565000
H	-2.45695300	1.56415700	0.62793200
C	-4.99041200	-1.22664600	-0.27349500
H	-3.34801800	-2.17614100	-1.29431700
C	-5.40310300	-0.12547900	0.47240800
H	-4.80873000	1.74232100	1.37096700
H	-5.70022100	-2.00674300	-0.53384900
H	-6.43638700	-0.04433700	0.79764700
C	2.57788700	0.06115700	0.40027800
C	2.77233300	-0.19376600	-0.96515400
C	3.65195500	-0.11468800	1.28034700
C	4.01213300	-0.61796400	-1.43397400
H	1.95135500	-0.06642200	-1.66854900
C	4.89265300	-0.54833200	0.81215800
H	3.51411800	0.08896100	2.33994000
C	5.07350800	-0.79853600	-0.54556200
H	4.14953300	-0.81280300	-2.49367900
H	5.71479500	-0.68527000	1.50855200
H	6.03893800	-1.13316400	-0.91395500
B	0.74059500	-2.09188100	0.91345600
H	-0.92179400	-0.78167100	1.58668800
H	1.05991000	-2.48501400	1.99614800
H	1.14652500	-2.65933400	-0.05416400

BH_3-PHC^{Ph} **T2**

Ee(M06-2X) = -1343.07991211

Ee(RI-SCS-MP2) = -1340.96622482

C	-0.72435400	-1.77809700	0.36223800
C	0.69563500	1.03809900	0.78037300
P	-1.36202700	-0.21877700	-0.04507100
P	1.55845300	-0.50066200	1.05423900
N	-0.61572600	1.08366400	0.58773400
C	1.39529400	2.38244500	0.81391200
H	1.33182400	2.87578400	-0.16273900
H	0.87165800	3.01685500	1.53665600
H	2.44482600	2.30785800	1.10399600
C	-3.13979000	0.01387800	-0.10329100
C	-3.65604900	1.30532500	-0.28429200
C	-4.00445100	-1.08629700	-0.05619300
C	-5.02939800	1.48810200	-0.39681600
H	-2.97829000	2.15341400	-0.32325900
C	-5.37717300	-0.89329300	-0.19341100
H	-3.60448800	-2.08314700	0.10387300
C	-5.89216300	0.39064500	-0.35945400
H	-5.42927400	2.49006500	-0.52198400

H	-6.04477700	-1.74893600	-0.15569700
H	-6.96371300	0.53879200	-0.45598500
C	3.14395000	-0.17133400	0.20521500
C	3.23698300	0.52590700	-1.01059400
C	4.30914300	-0.73453800	0.74872400
C	4.46433200	0.68328800	-1.64569800
H	2.33783600	0.93844400	-1.46277700
C	5.54048200	-0.57049300	0.11798200
H	4.24839300	-1.29881400	1.67695200
C	5.61893600	0.13993100	-1.07872500
H	4.52248300	1.22390600	-2.58608200
H	6.43650300	-1.00006900	0.55656400
H	6.57737200	0.26348800	-1.57477700
B	-0.76483600	-2.86140100	-0.70427400
H	-0.46983400	-1.99057900	1.39327000
H	-1.18252000	-2.60338000	-1.79770900
H	-0.39837400	-3.97215100	-0.46041100

BH_3-PHC^{Ph} **C**

Ee(M06-2X) = -1343.13025784

Ee(RI-SCS-MP2) = -1341.00710822

C	-0.59517600	-0.90851200	-0.17223400
P	-1.46227600	0.54621600	-0.83817100
P	1.59473500	0.44183200	-0.07857900
N	0.70480000	-0.94805600	-0.01561300
C	0.92207600	1.90517100	0.23227900
C	-1.33580900	-2.18231000	0.12335100
H	-0.63068100	-3.00566700	0.25552600
H	-1.92509700	-2.05339400	1.03913900
H	-2.04677400	-2.41201000	-0.67644900
B	-0.68335500	2.07931000	0.20402100
H	-0.98833400	3.05478500	-0.44181000
H	-1.07683700	2.17003200	1.35013200
H	1.58264200	2.73855700	0.47118100
C	3.33605600	0.05790500	0.01164300
C	3.74582100	-1.26053600	0.23902500
C	4.28001800	1.07710200	-0.16356600
C	5.10665100	-1.54916300	0.30689700
H	3.00035500	-2.03950500	0.36292500
C	5.63553200	0.77764400	-0.08477700
H	3.95785400	2.09503600	-0.36796300
C	6.04917800	-0.53452300	0.14933800
H	5.42971900	-2.57029300	0.48533800
H	6.36999400	1.56596100	-0.21729200
H	7.10889600	-0.76561500	0.20314600
C	-3.18357000	0.23089100	-0.26209000
C	-3.58086900	0.45024000	1.06288300
C	-4.13053000	-0.24166500	-1.17851700
C	-4.88913800	0.18646300	1.46390700
H	-2.86103800	0.83531700	1.78018800
C	-5.44005600	-0.50835900	-0.77918900
H	-3.83672600	-0.40040200	-2.21386400
C	-5.82057200	-0.29641900	0.54430400
H	-5.18262600	0.36090600	2.49557100
H	-6.16204400	-0.87743900	-1.50234600
H	-6.84067500	-0.50074800	0.85750000

BH_3-PHC^{Ph} **T3**

Ee(M06-2X) = -1343.12743315

Ee(RI-SCS-MP2) = -1340.99734337

C	0.93871100	-1.78280000	0.23186200
C	-0.57956300	0.88575300	-0.44961600
P	1.63330300	-0.48400500	-0.63448600
P	-1.51185200	-0.65347900	-0.87357600
N	0.71101000	0.92007200	-0.43065400
C	-1.31077900	2.16736600	-0.16025500
H	-1.89170100	2.06409700	0.76309400
H	-0.59969700	2.99039100	-0.06213100
H	-2.02741500	2.38304000	-0.96023400
C	3.31675700	-0.05182300	-0.12747000
C	3.62374700	1.21964900	0.36514400
C	4.32221800	-1.01409000	-0.27024500
C	4.93546800	1.51328900	0.73301800
H	2.83638700	1.96062800	0.45950500
C	5.62680600	-0.71656200	0.11322400
H	4.08974500	-1.99226800	-0.68673700
C	5.93481300	0.54861500	0.61267600
H	5.17545700	2.49998600	1.11841300
H	6.40422700	-1.46717000	0.00705400
H	6.95515000	0.78435700	0.90045700
C	-3.17571400	-0.28425300	-0.17469600
C	-3.51858900	-0.53166400	1.16051100
C	-4.14955600	0.24886300	-1.02890000
C	-4.79694000	-0.23556000	1.63111800
H	-2.78170800	-0.95856000	1.83574000
C	-5.42516600	0.55534200	-0.55834200
H	-3.90424000	0.42191500	-2.07479100
C	-5.75116000	0.31358900	0.77513800
H	-5.04779400	-0.43523500	2.66938200
H	-6.16550200	0.97277700	-1.23508000
H	-6.74644600	0.54449900	1.14439100
H	-0.52131000	-1.38658300	1.55078500
H	1.61273400	-2.53451400	0.65000600
B	-0.60406200	-1.85847500	0.39613500
H	-1.11275400	-2.94751200	0.45598500

BH_3-PHC^{Ph} **D**

Ee(M06-2X) = -1343.18922879

Ee(RI-SCS-MP2) = -1341.05943668

C	-1.00101200	-1.45524600	-0.87336400
C	0.52083100	0.59811700	0.92478500
P	-1.67800500	-0.86372300	0.76422900
P	1.53006000	-0.93103400	0.56935500
N	-0.75147500	0.57808900	0.98314100
C	1.27384600	1.87486700	1.19798300
H	1.81812800	2.20541700	0.30660400
H	0.56384200	2.64624800	1.50394500
H	2.01784100	1.72281500	1.98825200
C	-3.26053400	-0.11782300	0.19858800
C	-3.39974500	1.23367600	-0.13154800
C	-4.36774900	-0.96547900	0.08094000
C	-4.62461400	1.72277900	-0.58406300
H	-2.54677400	1.89712600	-0.01920800
C	-5.58842100	-0.47902800	-0.38356100
H	-4.27866300	-2.01400800	0.36174700
C	-5.71862400	0.86846500	-0.71639700
H	-4.72473000	2.77552300	-0.83451400
H	-6.43925400	-1.14867000	-0.47303300
H	-6.67094000	1.25264200	-1.07073000
C	3.15597900	-0.31945600	-0.01622200
C	3.34750800	0.22127300	-1.29574000
C	4.24902800	-0.38810900	0.85588400
C	4.60028700	0.68452400	-1.68946400
H	2.51049100	0.28556000	-1.98694900
C	5.50272700	0.08115800	0.46525100
H	4.11656700	-0.81478200	1.84730100
C	5.67958700	0.61759000	-0.80821300

H	4.73356900	1.10121200	-2.68373000
H	6.34026000	0.02267500	1.15438800
H	6.65579200	0.98097600	-1.11590200
H	-1.28672100	-0.75155000	-1.67404400
H	-1.47730100	-2.40918300	-1.13488500
B	0.55962400	-1.57292900	-0.91457300
H	1.13470800	-2.07646400	-1.83127400

BH_2NMe_2 + PHC^{Me}

BH_2NMe_2-PHC^{Me} **T1**

Ee(M06-2X) = -1093.93231292

Ee(RI-SCS-MP2) = -1092.08485313

C	-2.24336200	-0.69279600	0.03053800
P	-0.46321700	-0.98906300	0.39138600
P	-1.20582000	1.52854900	-0.66020900
N	-2.53978600	0.51192200	-0.24120800
C	0.17553900	0.46611800	-0.26878800
C	-1.18390500	2.77593200	0.68408600
H	-0.24535700	3.32214400	0.59819100
H	-2.01603800	3.46239000	0.54137400
H	-1.25192500	2.30373100	1.66236900
C	0.26532000	-2.48967100	-0.34174500
H	1.34219600	-2.36278800	-0.21826000
H	-0.08055900	-3.37613300	0.18554500
H	0.02112800	-2.55224600	-1.40073700
C	-3.26441800	-1.76487600	0.24740400
H	-4.26512700	-1.34878400	0.15515000
H	-3.13484900	-2.55949400	-0.49116200
H	-3.14079600	-2.21409900	1.23479300
B	1.66498200	0.74367000	-0.61755300
H	1.36833600	0.39372200	-1.79160200
H	1.95731800	1.92864100	-0.70180600
N	2.66703800	-0.19277400	0.01562500
C	2.91856700	0.13382600	1.40718900
H	3.57106700	-0.61459600	1.86769100
H	3.40307500	1.11798700	1.52707800
H	1.98249500	0.15407000	1.97048700
C	3.92048700	-0.24634400	-0.71083400
H	4.44625500	0.72360500	-0.71460800
H	4.59327500	-0.98513800	-0.26411300
H	3.74001100	-0.53082600	-1.74830600

BH_2NMe_2-PHC^{Me} **B**

Ee(M06-2X) = -1094.02976107

Ee(RI-SCS-MP2) = -1092.18659310

C	-2.22870500	0.19456400	0.24622800
P	-0.87036300	-1.07483400	0.36393500
P	-0.36750400	1.58917400	-0.86831900
N	-1.96391600	1.33826800	-0.22865200
C	0.17020200	-0.21445200	-0.88632700
C	0.41454000	2.20975500	0.68168500
H	1.49436200	2.27248700	0.53844900
H	0.03265500	3.21253700	0.87262500
H	0.19349200	1.57801000	1.54278500
C	-1.62544700	-2.43441200	-0.63191800
H	-0.86595500	-3.19105200	-0.82697600
H	-2.42321400	-2.90334300	-0.05538400
H	-2.02573600	-2.07458300	-1.58064900
C	-3.57945800	-0.13763200	0.80997400
H	-4.21122800	0.74776400	0.81690300
H	-4.05550000	-0.91302900	0.20479800
H	-3.48019100	-0.53381700	1.82263500
B	1.74778500	-0.32691300	-0.97020900
H	2.22147600	-0.29841200	-2.06812800
H	-0.19908800	-0.53432200	-1.86739400
N	2.66995100	-0.39747200	0.07352100
C	2.38480200	-0.41629300	1.49620000
H	2.84864000	-1.29120200	1.96150800
H	2.79566500	0.47602700	1.97932600
H	1.31717000	-0.45812700	1.68216700
C	4.10041700	-0.43712700	-0.18154400
H	4.59690100	0.41718700	0.28889800
H	4.53909500	-1.34821800	0.23616700
H	4.29019400	-0.41044500	-1.25079200

BH_2NMe_2-PHC^{Me} **T2**

Ee(M06-2X) = -1093.94565638

Ee(RI-SCS-MP2) = -1092.10517582

C	2.17568600	-0.42434200	0.04795000
P	1.77020400	1.12561400	-0.66680600
P	-0.09175200	-1.47395200	-0.58512800
N	1.41833500	-1.51837200	-0.01664000
C	-0.69175600	-0.02582800	-1.20266600
C	-1.12056100	-2.33325900	0.63116400
H	-0.82563700	-3.38091400	0.65335000
H	-0.98421100	-1.90557200	1.62315900
H	-2.16326600	-2.25603800	0.32542700
C	2.79468000	2.25780700	0.39279800
H	2.53979100	3.28232300	0.12372100
H	2.62596700	2.12427900	1.46123000
H	3.85822500	2.11656300	0.18764600
C	3.44438900	-0.60337200	0.85464500
H	4.31193900	-0.15403800	0.37208100
H	3.33432700	-0.13056400	1.83361700
H	3.62111200	-1.66622300	1.00460100
B	-2.18490200	0.42903000	-1.09903300
H	-2.84751600	0.55958200	-2.08350500
H	-0.15325400	0.28855200	-2.08732700
N	-2.79815900	0.70656300	0.12283900
C	-2.13021700	0.72773700	1.41032100
H	-2.30188500	1.68976700	1.90160100
H	-2.52338800	-0.05500900	2.06753800
H	-1.05795500	0.59317400	1.28387300
C	-4.19612800	1.08534600	0.21874300
H	-4.73570900	0.39689300	0.87622900
H	-4.29471400	2.09158500	0.63643600
H	-4.65387400	1.06367300	-0.76662900

BH_2NMe_2-PHC^{Me} **C**

Ee(M06-2X) = -1093.96737435

Ee(RI-SCS-MP2) = -1092.12310689

C	0.30912000	1.52505600	0.25020200
P	1.22022300	0.99995900	-1.08082200
P	-1.94922300	0.11317100	-0.12918800
N	-1.04827000	1.28792000	0.32744500
C	-1.67717000	-1.45484400	-0.51273400
C	-3.66056100	0.65577600	-0.17295700
H	-4.31617600	-0.19434600	-0.34321200
H	-3.89501400	1.13132500	0.77761500
H	-3.78235200	1.39049600	-0.96714500
C	2.93050100	1.62889400	-0.71609100
H	3.57565300	1.30331400	-1.53190400
H	2.97000100	2.71742300	-0.67211100
H	3.33110000	1.22042600	0.21251300
C	0.79962600	2.33894700	1.41452800

H	0.20049200	3.24897000	1.48832400
H	0.63798400	1.77801700	2.33930600
H	1.84976200	2.60605800	1.34217200
B	-0.31437300	-2.18694200	-0.66004100
H	-0.12634400	-2.84322900	-1.64078200
H	-2.58362100	-1.94662800	-0.85206200
N	0.70460200	-2.16069900	0.29117400
C	0.64297800	-1.50852000	1.58224200
H	1.32551000	-0.65291100	1.61562300
H	-0.36557300	-1.15899500	1.78863700
H	0.93643900	-2.21026200	2.36883300
C	2.00650100	-2.74555400	0.03524100
H	2.77621600	-1.96631800	0.01853300
H	2.26929300	-3.46226600	0.81924800
H	2.00320000	-3.25239000	-0.92615900

BH_2NMe_2-PHC^{Me} **T3**

Ee(M06-2X) = -1093.71595624

Ee(RI-SCS-MP2) = -1092.08524181

C	-1.28918100	1.39944100	0.07315600
C	-0.16688600	-1.63728500	-0.08158200
H	0.87896300	-1.13713200	-1.58749800
N	-2.14696400	0.43641300	0.22579900
P	-1.75145000	-1.17055600	0.25457700
P	0.32485500	1.28703000	-0.78115100
C	-3.14492700	-2.11315200	-0.43634500
H	-3.29643800	-1.84782700	-1.48539600
H	-2.92859200	-3.18049500	-0.35319300
H	-4.04714400	-1.87818800	0.13126600
C	1.36016800	2.35842600	0.34223100
H	1.37688300	1.99149700	1.37174700
H	2.38710000	2.35329500	-0.03210100
H	1.00384800	3.39188300	0.31913500
C	-1.73071800	2.76533300	0.54117200
H	-1.43345000	3.55129100	-0.15889900
H	-2.81483500	2.77168600	0.67454500
H	-1.26123400	2.98339300	1.50874800
B	0.96445600	-0.61797700	-0.43508400
H	0.07034000	-2.69346800	0.05612300
N	2.29741900	-0.69161100	0.20465500
C	2.60104100	-1.81332800	1.06314200
H	2.76171200	-2.75680500	0.50482400
H	3.51664300	-1.61426700	1.63526200
H	1.78409300	-1.97526000	1.77420100
C	3.42551800	-0.32236400	-0.62465300
H	3.16357800	0.52708700	-1.26484700
H	4.28640100	-0.03474900	-0.00566100
H	3.74551600	-1.14521700	-1.29012300

BH_2NMe_2-PHC^{Me} **D**

Ee(M06-2X) = -1094.03537698

Ee(RI-SCS-MP2) = -1092.18967147

C	1.55407800	-1.15856100	-0.20281100
C	0.00886300	1.47834500	-0.64750600
H	0.50608600	1.33757400	-1.61473200
N	2.10416900	-0.09540900	0.20660000
P	1.32517500	1.35889500	0.64811800
P	-0.27244500	-1.48321400	-0.50655100
C	2.56587500	2.52494900	-0.03339600
H	2.77498800	2.31018500	-1.08200700
H	2.18811400	3.54348500	0.06332300
H	3.48667800	2.43871900	0.54214900
C	-0.62042700	-2.15645600	1.19848400
H	-0.03457600	-3.06345800	1.34511800
H	-0.37115200	-1.44265000	1.98297300
H	-1.67217400	-2.42507100	1.28220500
C	2.41130700	-2.37025200	-0.46924100
H	2.01899200	-3.24485300	0.05538300
H	2.38797300	-2.60757100	-1.53496400
H	3.43532300	-2.18147000	-0.15383100
B	-1.01646600	0.30776900	-0.40380600
H	-0.41310900	2.48381100	-0.62913700
N	-2.38124300	0.48201700	-0.15499500
C	-3.03142700	1.76697100	0.03741700
H	-3.76309700	1.95172300	-0.75464600
H	-3.56233100	1.77750400	0.99359600
H	-2.30870900	2.57559800	0.04254600
C	-3.33248800	-0.61065400	-0.04104000
H	-2.91265700	-1.53312200	-0.43642900
H	-3.63298200	-0.76974100	0.99926600

BH_2NMe_2 + PHC^{Ph}

BH_2NMe_2-PHC^{Ph} **T1**

Ee(M06-2X) = -1114.15372915

Ee(RI-SCS-MP2) = -1474.64203580

C	-0.35735300	0.77682100	-0.03148700
C	-0.66021300	-1.93341500	0.51887800
P	-1.50546600	0.37978100	1.33828400
P	-0.04646300	-0.80677500	-0.86572200
N	-1.37982800	-1.39794300	1.42115000
C	-0.49192900	-3.42383000	0.40493400
H	0.55623900	-3.69848300	0.24197900
H	-0.86916400	-3.91578500	1.30427500
H	-1.05727400	-3.78224200	-0.46373100
C	-3.06800500	0.48220000	0.35732200
C	-4.01749100	-0.54531800	0.40609200
C	-3.35316700	1.64029500	-0.37762100
C	-5.22751400	-0.41764300	-0.27504500
H	-3.80568400	-1.44614900	0.97471900
C	-4.56237900	1.76166100	-1.05812600
H	-2.61607000	2.43703100	-0.43032800
C	-5.50392400	0.73393400	-1.00894800
H	-5.95562900	-1.22309200	-0.22968400
H	-4.76824600	2.66102400	-1.63218100
H	-6.44735400	0.83126100	-1.53871900
C	1.78213500	-0.97108700	-0.77893800
C	2.43669700	-1.47312100	0.35572600
C	2.55339000	-0.49143700	-1.84374500
C	3.82891500	-1.48558600	0.42558300
H	1.85608900	-1.83624700	1.20158400
C	3.94550600	-0.48338700	-1.76505400
H	2.05854500	-0.11133900	-2.73487800
C	4.58637500	-0.98111400	-0.63115000
H	4.31992500	-1.88199300	1.31013200
H	4.53026300	-0.09843100	-2.59644700
H	5.67138500	-0.98604100	-0.57552500
B	1.80121500	1.24572300	1.32774100
H	0.73240300	1.01359700	0.65485800
H	1.89507600	0.74497200	2.39777800
N	2.65363200	2.10685300	0.69296800
C	2.39787800	2.71879200	-0.60780900
H	1.42533800	2.39321200	-0.98236600
H	2.40177700	3.81030200	-0.50529300
H	3.18335600	2.42834100	-1.31438900
C	3.94595800	2.46199300	1.26876200
H	4.74957000	2.11210200	0.61010500

H	4.02529300	3.54973400	1.37831500
H	4.06112500	1.99359900	2.24758800

BH_2NMe_2-PHC^{Ph} **B**

Ee(M06-2X) = -1477.151946

Ee(RI-SCS-MP2) = -1474.79003843

C	-0.24152100	0.55045300	-0.27718400
C	-0.01640100	-2.11053600	-0.81585200
P	-1.08941800	-0.57787600	0.96674100
P	0.87794100	-0.52783500	-1.31143000
N	-0.90542200	-2.07764500	0.09350700
C	0.35904400	-3.38199300	-1.52365700
H	1.42229100	-3.59865200	-1.36055200
H	-0.24118800	-4.21391800	-1.14927900
H	0.21522100	-3.27354600	-2.60432700
C	-2.85449800	-0.21334200	0.59543000
C	-3.48648900	-0.63897500	-0.57892500
C	-3.57964800	0.54222300	1.52153800
C	-4.81729000	-0.30984500	-0.82200000
H	-2.93677800	-1.24399800	-1.29656200
C	-4.90957600	0.88357800	1.27367700
H	-3.10288900	0.85873800	2.44710500
C	-5.52994900	0.45570100	0.10238600
H	-5.30171900	-0.65300200	-1.73214700
H	-5.46193300	1.47259900	2.00041500
H	-6.56862500	0.71030700	-0.08875700
C	2.37088900	-0.67514800	-0.22217000
C	2.43585900	-1.47567200	0.92523900
C	3.48362500	0.10470800	-0.56293400
C	3.58386700	-1.48786700	1.71521700
H	1.58563000	-2.08864700	1.21579400
C	4.62771800	0.10321000	0.23378800
H	3.45126600	0.72078800	-1.45972900
C	4.67926300	-0.69499100	1.37482300
H	3.61782400	-2.11250300	2.60326900
H	5.48004700	0.71791900	-0.04177900
H	5.57110000	-0.70283200	1.99481300
B	0.62171900	1.71319400	0.38212900
H	-1.00005400	0.93452700	-0.97211300
H	0.97260300	1.62489300	1.52326300
N	1.05066300	2.83935700	-0.32774700
C	0.77695400	3.11059100	-1.72869600
H	0.11518600	2.35395900	-2.15136100
H	0.30466200	4.09482700	-1.84335200
H	1.71021700	3.11349900	-2.30834200
C	1.91533100	3.84536700	0.26701400
H	2.87898900	3.88284000	-0.25938700
H	1.45452200	4.83967000	0.20103200
H	2.09742500	3.60545500	1.31519200

BH_2NMe_2-PHC^{Ph} **T2**

Ee(M06-2X) = -1477.1068029

Ee(RI-SCS-MP2) = -1474.74624204

C	-0.14421000	-0.12143300	-1.74398100
C	0.47884000	-2.43542600	-0.27897000
P	-1.56626600	-1.39780100	-1.51319400
P	1.10362500	-0.81011200	-0.62516300
N	-0.70627100	-2.68405900	-0.71968000
C	1.26468800	-3.46178400	0.48956200
H	2.16051800	-3.76050400	-0.06494500
H	1.58200200	-3.05713300	1.45695800
H	0.63451200	-4.33840900	0.65297000
B	-0.69032500	1.37297000	-1.70643900
H	0.18758100	-0.29884600	-2.77413600
H	-1.08973200	1.79393000	-2.75605900
N	-0.79457900	2.24016700	-0.61894400
C	-1.41471900	3.54951900	-0.75834300
H	-2.35145000	3.58482700	-0.18452100
H	-0.75009500	4.33192500	-0.37014000
H	-1.63148000	3.75479100	-1.80724300
C	-0.49665100	1.94225600	0.77401100
H	-1.42752700	1.91780100	1.35700600
H	-0.00786300	0.97295000	0.87385300
H	0.15790600	2.71740900	1.19374900
C	-2.43001900	-0.68095400	-0.03991700
C	-2.21670900	-1.10389900	1.27496000
C	-3.37656600	0.32339200	-0.28244700
C	-2.92163000	-0.52044200	2.32833700
H	-1.50402900	-1.89941600	1.47293700
C	-4.07076300	0.91754600	0.76874000
H	-3.57308100	0.64458300	-1.30516400
C	-3.84382700	0.49423300	2.07939500
H	-2.74848000	-0.86016100	3.34583500
H	-4.80032600	1.69696200	0.56556400
H	-4.39168500	0.94776100	2.90070000
C	2.58691900	-0.01246100	-0.04179700
C	2.74621100	1.36817700	-0.25072500
C	3.60026600	-0.72367900	0.62340100
C	3.89330700	2.01488000	0.19966700
H	1.97108000	1.93399100	-0.76277700
C	4.73388400	-0.06048200	1.08022000
H	3.50898800	-1.79478000	0.77750700
C	4.89079200	1.30985200	0.87134900
H	4.00309200	3.08173800	0.02575300
H	5.50664200	-0.62413800	1.59540400
H	5.78173200	1.82003100	1.22390900

BH_2NMe_2-PHC^{Ph} **C**

Ee(M06-2X) = -1477.07580405

Ee(RI-SCS-MP2) = -1474.72254617

C	-0.50304300	-0.81750100	0.48846900
P	-1.40511400	-0.31910900	-0.88540500
P	1.85015600	0.36956500	-0.13283300
N	0.85889100	-0.63238300	0.55543400
C	1.68051700	1.88356200	-0.76511300
C	-1.01052100	-1.57974700	1.68882300
H	-0.29701400	-2.37891600	1.91474500
H	-1.04119100	-0.92131600	2.56694100
H	-2.00244600	-2.00510300	1.53455700
B	0.33611700	2.66107000	-0.90370400
H	0.06807900	3.16167600	-1.95831900
H	2.56793300	2.24578800	-1.28124200
C	3.50528400	-0.32440900	-0.08853700
C	3.65708200	-1.69269200	0.15978300
C	4.62997600	0.48133500	-0.29769300
C	4.93223000	-2.25075900	0.18894100
H	2.77397500	-2.29899400	0.33721300
C	5.90068500	-0.08485300	-0.27106700
H	4.51846400	1.54857800	-0.46615300
C	6.05226800	-1.45025700	-0.02924200
H	5.05052900	-3.31279000	0.38152200
H	6.77291800	0.54163400	-0.43177600
H	7.04581700	-1.88856200	-0.00594700
C	-3.14102900	-0.74586000	-0.44705000
C	-3.77270100	-0.25776900	0.70699400
C	-3.91150600	-1.47712300	-1.36145000
C	-5.11807400	-0.51893100	0.95524700

H	-3.20147300	0.33349900	1.42035200
C	-5.25926700	-1.73912800	-1.11797800
H	-3.44822800	-1.85055900	-2.27220000
C	-5.86609300	-1.26312000	0.04281600
H	-5.58442300	-0.13553100	1.85886900
H	-5.83535700	-2.31594300	-1.83640400
H	-6.91633900	-1.46474500	0.23328200
N	-0.57725800	2.83320000	0.14222800
C	-0.38635300	2.39960500	1.51299200
H	0.66086400	2.15241700	1.69470200
H	-0.67861800	3.20301600	2.20113600
H	-1.00117800	1.51549100	1.73569500
C	-1.89753800	3.39968400	-0.08234300
H	-2.67363100	2.64171900	0.09328100
H	-2.07705300	4.24120600	0.59948900
H	-1.98077800	3.74729800	-1.11283900

BH_2NMe_2-PHC^{Ph} **T3**

Ee(M06-2X) = -1477.05390042

Ee(RI-SCS-MP2) = -1474.68860243

C	-1.02620400	1.36291000	-0.09059900
C	0.31340500	-1.47542900	-0.35234900
P	-1.81681700	-0.01196100	-0.67976700
P	1.35418500	-0.08193100	-0.98272600
N	-0.97893200	-1.42975700	-0.32210800
C	0.96087800	-2.75952100	0.08523900
H	1.58361700	-2.57952700	0.96875600
H	0.19513800	-3.50453400	0.31162300
H	1.62838400	-3.13457900	-0.69836400
C	-3.52354700	-0.27570700	-0.14827700
C	-3.90067700	-1.45408100	0.50261300
C	-4.47257600	0.71489600	-0.42246800
C	-5.22625200	-1.62292000	0.89781800
H	-3.15637900	-2.22005700	0.69472700
C	-5.79151300	0.54183100	-0.01390800
H	-4.18438900	1.61598400	-0.95991300
C	-6.16915600	-0.62780500	0.64604400
H	-5.52109800	-2.53509800	1.40819400
H	-6.52649300	1.31402800	-0.22045400
H	-7.20053500	-0.76567800	0.95704500
C	2.98590400	-0.47392400	-0.22591800
C	3.36124600	-0.02045100	1.04519300
C	3.89366000	-1.24653700	-0.96119100
C	4.60544900	-0.35855500	1.57523800
H	2.68160000	0.60974900	1.61204600
C	5.13416400	-1.59284400	-0.42847700
H	3.62306100	-1.57911800	-1.96150800
C	5.49080100	-1.15039700	0.84427600
H	4.88553100	-0.00052100	2.56221400
H	5.82292200	-2.19977800	-1.00961200
H	6.45893300	-1.41320900	1.26169500
H	0.32776400	0.87797700	1.31315200
H	-1.63857800	2.23878700	0.14432600
B	0.54720100	1.33704300	0.15961500
N	1.34217900	2.59721300	0.22865400
C	1.71587500	3.19650900	-1.03648800
H	0.84573800	3.61043100	-1.58579400
H	2.42665200	4.01655700	-0.87264400
H	2.19725000	2.45878900	-1.68668200
C	0.83382100	3.59617200	1.14384900
H	1.58416400	4.38043800	1.30895200
H	-0.08346000	4.09861500	0.77230200
H	0.59925500	3.13684100	2.10984000

BH_2NMe_2-PHC^{Ph} **D**

Ee(M06-2X) = -1477.16060418

Ee(RI-SCS-MP2) = -1474.79481965

C	-1.06171800	1.23766600	-0.00915100
C	0.21845400	-1.51456000	-0.65451600
P	-1.88032900	0.00654800	-1.15273000
P	1.35219400	-0.13744800	-1.19567000
N	-1.05521400	-1.43282200	-0.67507000
C	0.86607700	-2.82829800	-0.28991000
H	1.41004700	-2.74402400	0.65717200
H	0.09219100	-3.59371900	-0.20032200
H	1.59520500	-3.12650600	-1.05221900
C	-3.45998700	-0.23834400	-0.24308300
C	-3.66230600	-1.26339800	0.68603600
C	-4.49894700	0.66422500	-0.49768000
C	-4.87994000	-1.37183700	1.35715600
H	-2.86437500	-1.97826400	0.86590000
C	-5.71111500	0.56341000	0.18202400
H	-4.36246300	1.44884500	-1.24065100
C	-5.90380400	-0.45766800	1.11187400
H	-5.02964100	-2.17378600	2.07512600
H	-6.50793300	1.27328600	-0.02215700
H	-6.85125100	-0.54542000	1.63623100
C	2.86067600	-0.47681200	-0.18719600
C	2.90247100	-0.29423700	1.20238300
C	4.01325600	-0.93339600	-0.83573500
C	4.06358800	-0.56470900	1.92196000
H	2.01663000	0.06021700	1.72656200
C	5.17810400	-1.20752000	-0.11762500
H	3.99762800	-1.07445200	-1.91416800
C	5.20530900	-1.02286100	1.26238000
H	4.07781200	-0.42038400	2.99879400
H	6.06290100	-1.56285500	-0.63839400
H	6.11081900	-1.23482700	1.82357200
H	-1.22939900	0.89662100	1.02427000
H	-1.58724400	2.19271700	-0.12883100
B	0.49164200	1.36786800	-0.30011900
N	1.23069700	2.51328800	0.01892100
C	0.68852200	3.62744700	0.78503300
H	1.32514400	3.82570300	1.65680500
H	0.65661800	4.53891200	0.17420900
H	-0.31685000	3.40271600	1.14018800
C	2.62548300	2.73948400	-0.33536600
H	2.74030400	3.75737400	-0.72714600
H	3.28100000	2.62721300	0.53849400
H	2.95355700	2.03996700	-1.10532500

Cartesian coordinates (Å) and electronic energies for M06-2X/6-31+G(d) optimised geometries.

SiH_2Ph_2 + PHC^{Ph}

PHC^{Ph}
Ee(M06-2X) = -1316.4527662
Ee(RI-SCS-MP2) =-1314.4093540

C	-0.06918600	-0.93238600	0.88361100
C	0.60309500	1.64832000	0.01691700
P	-1.15399000	-0.00212500	0.08902400
P	1.20334500	0.24990100	1.06275100
N	-0.64060200	1.55165100	-0.32655600
C	1.40884500	2.87416500	-0.26782100
H	2.33287300	2.60076500	-0.78283900
H	0.83679200	3.56577600	-0.88273500
H	1.68908000	3.36849800	0.66380000
C	-2.91349800	-0.19322400	-0.04006900
C	-3.69201200	0.80684100	-0.62129100
C	-3.49876800	-1.37515400	0.41522900
C	-5.06048100	0.61854000	-0.74162200
H	-3.22388400	1.71938000	-0.96601300
C	-4.86606700	-1.55031100	0.28733800
H	-2.87862900	-2.13825400	0.86883700
C	-5.64708300	-0.55586400	-0.29010800
H	-5.66999100	1.39311000	-1.18805400
H	-5.32499700	-2.46365800	0.64206500
H	-6.71582100	-0.69670900	-0.38548600
C	2.76310700	-0.30492400	0.31603700
C	2.83648900	-1.49688100	-0.40192600
C	3.91138000	0.46858700	0.48416800
C	4.04425500	-1.89979600	-0.95345600
H	1.94573100	-2.10062400	-0.51867300
C	5.11168700	0.07051700	-0.08537200
H	3.86902900	1.37925100	1.07085600
C	5.18015800	-1.11590700	-0.80342700
H	4.09601400	-2.82799500	-1.50793100
H	5.99708100	0.67924400	0.04504100
H	6.11908700	-1.43213400	-1.23884700

SiH_2Ph_2
Ee(M06-2X) = -753.763852911 (s)
Ee(RI-SCS-MP2) = -752.4535360

Si	-0.00001000	1.58332600	0.00003400
H	0.10338200	2.45567700	-1.19752000
H	-0.10360600	2.45553500	1.19768800
C	1.53757500	0.50723100	0.05825200
C	1.57110100	-0.65565400	0.84346600
C	2.68832200	0.84847400	-0.66610100
C	2.71702500	-1.44549900	0.90969700
H	0.68783100	-0.95341400	1.40622100
C	3.83832200	0.06173300	-0.60474600
H	2.68866600	1.73852800	-1.29226100
C	3.85359000	-1.08633700	0.18501500
H	2.72311900	-2.34204600	1.52326400
H	4.71914300	0.34229900	-1.17548500
H	4.74716400	-1.70246100	0.23232100
C	-1.53749600	0.50706900	-0.05828300
C	-2.68834600	0.84856800	0.66582400
C	-1.57100600	-0.65596800	-0.84322400
C	-3.83839700	0.06192400	0.60447000
H	-2.68869500	1.73877000	1.29177400
C	-2.71699000	-1.44575500	-0.90943000
H	-0.68772000	-0.95397400	-1.40582600
C	-3.85363100	-1.08633700	-0.18502500
H	-4.71929500	0.34272100	1.17497700
H	-2.72302900	-2.34245900	-1.52277000
H	-4.74722900	-1.70242400	-0.23234500

SiH_2Ph_2-PHC^{Ph} **T1**
Ee(M06-2X) = -2070.21292172
Ee(RI-SCS-MP2) = -2066.8505034

C	-0.20044300	-0.88878000	-0.36889600
C	-1.25887600	-2.98328500	1.07246200
P	0.33510900	-2.49802700	-0.80538300
P	-1.37882700	-1.12105000	0.93818600
N	-0.31942600	-3.55410800	0.41996000
C	-2.13564900	-3.71738300	2.04252700
H	-2.02740000	-3.29611600	3.04773300
H	-3.18706000	-3.60340200	1.75291800
H	-1.87564800	-4.77769200	2.05704800
C	2.14264700	-2.59379500	-0.66623400
C	2.74635500	-3.23289300	0.42164800
C	2.92853600	-1.96235700	-1.63561400
C	4.13487800	-3.22320300	0.54056200
H	2.13276900	-3.73148000	1.16616900
C	4.31437500	-1.94327100	-1.49928600
H	2.46085900	-1.47854000	-2.48912000
C	4.91834600	-2.57405100	-0.41236500
H	4.60427200	-3.71912800	1.38522500
H	4.92058400	-1.43816500	-2.24526400
H	5.99949600	-2.56197500	-0.31012200
C	-3.04238000	-0.68197000	0.32291400
C	-3.55345400	-1.20798600	-0.87099800
C	-3.80035700	0.23104600	1.05966700
C	-4.81307000	-0.82123600	-1.31755400
H	-2.95889000	-1.90803900	-1.45433100
C	-5.06238500	0.61657100	0.60853800
H	-3.39312000	0.65911500	1.97198000
C	-5.56794900	0.09173500	-0.57741500
H	-5.20532500	-1.22712500	-2.24558000
H	-5.64143800	1.33666600	1.17945700
H	-6.54883000	0.39624200	-0.93131700
H	1.30372900	-0.08680900	0.62485400
Si	0.95623700	0.95277400	-0.46297100
H	1.35336600	0.65035100	-1.86179100
C	-0.63687200	1.96919700	-0.35928000
C	-0.88190900	2.86658800	0.68795000
C	-1.62534900	1.82304700	-1.34525400
C	-2.07917500	3.58406600	0.75693900
H	-0.12563100	3.01716900	1.45647400
C	-2.80969500	2.55263400	-1.29849100
H	-1.46882800	1.10972100	-2.15372300
C	-3.04050900	3.43289500	-0.24012800
H	-2.25364500	4.26915200	1.58263000

H	-3.55966600	2.42474200	-2.07491700
H	-3.96888800	3.99649700	-0.19311800
C	2.31711900	2.19231000	0.10197900
C	3.38602900	1.76331100	0.89913800
C	2.32091100	3.53060700	-0.32321500
C	4.42158400	2.62733000	1.25997800
H	3.41189700	0.73037000	1.24724400
C	3.34947100	4.40257900	0.03100500
H	1.50213800	3.90267000	-0.93864000
C	4.40394700	3.95102700	0.82568500
H	5.23897400	2.26934000	1.88101400
H	3.32826300	5.43508800	-0.30873800
H	5.20568800	4.62901900	1.10615700

SiH_2Ph_2-PHC^{Ph} **B**

Ee(M06-2X) = -2070.35498565

Ee(RI-SCS-MP2) = -2066.9529337

C	0.33095700	-0.43680200	0.37652500
C	1.14835500	-2.76530700	-0.34040200
P	-0.82890400	-1.74192900	1.04477900
P	1.62789800	-1.01170900	-0.76954300
N	0.13296800	-3.03014400	0.37813200
C	2.01010100	-3.85579100	-0.90828000
H	3.04177600	-3.74127700	-0.55510100
H	1.62212500	-4.82933700	-0.60063400
H	2.03274700	-3.79325100	-2.00245200
C	-2.33453300	-1.94885800	-0.04901000
C	-2.33533800	-2.56273200	-1.30920200
C	-3.54347300	-1.44159800	0.44216400
C	-3.50130800	-2.63312900	-2.06704000
H	-1.42375700	-2.99847500	-1.70444700
C	-4.71356000	-1.51025300	-0.31590500
H	-3.57557100	-0.99177400	1.43418400
C	-4.69399300	-2.10130300	-1.57518000
H	-3.48038400	-3.11022800	-3.04323600
H	-5.63889000	-1.10550600	0.08441300
H	-5.60337200	-2.15966200	-2.16700700
C	3.19841500	-0.93360600	0.20025000
C	3.31455800	-1.48109200	1.48350700
C	4.30222700	-0.30016800	-0.37400400
C	4.51523200	-1.39314000	2.18020400
H	2.45798700	-1.97769300	1.93606300
C	5.50655400	-0.20456200	0.32607600
H	4.21960400	0.12456400	-1.37201600
C	5.61359300	-0.75109400	1.60198200
H	4.59698300	-1.82324000	3.17462400
H	6.35725600	0.29688100	-0.12691600
H	6.55004100	-0.67924400	2.14793300
H	0.43146000	0.49753300	0.89305400
Si	-0.66599800	0.91064300	-0.70535700
H	-1.22429200	0.44676000	-1.99560300
C	0.52227500	2.33916600	-0.97957400
C	1.44969800	2.37240100	-2.03948000
C	0.50944900	3.42164900	-0.08280100
C	2.32145800	3.44853900	-2.19574700
H	1.48681600	1.56181500	-2.75099400
C	1.38354100	4.49698000	-0.23774000
H	-0.19097800	3.42633300	0.74246800
C	2.28991400	4.51052000	-1.29382900
H	3.02334100	3.45977500	-3.01723200
H	1.35714600	5.31973500	0.46142400
H	2.96605500	5.34378800	-1.41489500
C	-1.98084100	1.53388700	0.46474400
C	-3.18624500	2.03083100	-0.05160000
C	-1.86375000	1.38380500	1.85859700
C	-4.21738000	2.42689300	0.79702500
H	-3.32192200	2.11564900	-1.12212100
C	-2.89458600	1.77501700	2.71080800
H	-0.96605200	0.95983300	2.29304900
C	-4.07106400	2.30271600	2.17908300
H	-5.13442000	2.81995700	0.38250000
H	-2.78419800	1.66138400	3.77907900
H	-4.87274700	2.60443200	2.83638800

SiH_2Ph_2-PHC^{Ph} **T2**

Ee(M06-2X) = -2070.24136315

Ee(RI-SCS-MP2) = -2066.8932984

C	-0.71669600	-0.25876700	-1.31348200
C	-0.04987300	-1.97408700	1.35029900
P	1.04962100	-0.77999000	0.63958900
P	-1.71313900	-1.39522200	-0.48538300
N	-1.33183300	-1.93872900	1.00282200
C	-3.48639100	-1.31577800	-0.73613600
C	-4.30861500	-2.30382200	-0.17515300
C	-4.04390700	-0.31653400	-1.54308900
C	-5.67786400	-2.27745500	-0.41179400
H	-3.86865800	-3.07646700	0.44929000
C	-5.41466900	-0.31470400	-1.79491800
H	-3.41049700	0.46580100	-1.95262500
C	-6.23262200	-1.28929800	-1.22855800
H	-6.31519600	-3.03564600	0.03386400
H	-5.84384400	0.46241700	-2.42053200
H	-7.30194300	-1.27873200	-1.41800500
C	2.66043500	-1.62659500	0.52980400
C	3.80118600	-0.80878300	0.55954100
C	2.82088500	-3.00494400	0.31614600
C	5.07263400	-1.35874800	0.41509300
H	3.68506900	0.26668600	0.68738900
C	4.09128000	-3.55480200	0.17713800
H	1.94436700	-3.64495900	0.25130100
C	5.21909300	-2.73256600	0.22928300
H	5.94645300	-0.71369600	0.44105300
H	4.20479600	-4.62344600	0.01743500
H	6.20957100	-3.16400500	0.11481000
Si	-0.23994200	1.52170800	-1.04011600
H	-0.81214800	-0.46428200	-2.38839500
H	-0.86127400	2.24109900	-2.19329900
C	1.62065000	1.80671400	-1.18383400
C	2.36207700	1.07702600	-2.12550100
C	2.29999400	2.74548300	-0.39542000
C	3.73261900	1.27732800	-2.27916800
H	1.86794600	0.32167700	-2.73539900
C	3.67193200	2.95333500	-0.54611900
H	1.75685800	3.31282500	0.35848900
C	4.39051400	2.21975900	-1.48962100
H	4.28856700	0.69188800	-3.00651500
H	4.18020300	3.68454200	0.07699200
H	5.45933400	2.37843400	-1.60599800
C	-0.95452300	2.32849800	0.49897400
C	-1.34575000	1.64110400	1.65670500
C	-1.13047000	3.72206200	0.47322900
C	-1.88539800	2.32015700	2.74881600
H	-1.23539200	0.56137900	1.72338500
C	-1.65871600	4.40778200	1.56525200
H	-0.85382500	4.28451600	-0.41789100
C	-2.03855300	3.70442700	2.70754600
H	-2.18568600	1.76397000	3.63244400
H	-1.78041900	5.48668500	1.52192600

H	-2.45762300	4.23263300	3.55963700
C	0.33289200	-2.98627200	2.40590100
H	0.24033100	-4.00684900	2.01532600
H	1.35062400	-2.84167100	2.77449300
H	-0.36570300	-2.89256000	3.24399100

SiH_2Ph_2-PHC^{Ph} **C**

Ee(M06-2X) = -2070.27283203

Ee(RI-SCS-MP2) = -2066.9197841

C	-1.83417400	1.24212600	0.68395100
C	-0.30365900	-1.89475400	-0.44444300
N	-1.62544200	-1.58000700	-0.19098100
H	-0.54312600	2.85286900	2.35526000
H	-2.66354400	1.94382900	0.76528800
P	0.64288900	-0.87130200	-1.43673000
P	-2.33062600	-0.21969800	0.10860800
C	0.07369200	-3.22661900	0.14866100
H	0.22963500	-3.11615800	1.23027600
H	-0.76383700	-3.91764500	0.00749200
H	0.97916000	-3.64466700	-0.29214300
Si	-0.19966700	1.91539500	1.25115900
C	2.30440400	-1.64774100	-1.39250600
C	3.00732700	-1.84791400	-2.58820800
C	2.94686400	-1.94461100	-0.18217400
C	4.30411100	-2.35968900	-2.57677300
C	4.24240600	-2.45370300	-0.16793200
C	4.92463700	-2.66599500	-1.36645100
H	4.83015000	-2.51805000	-3.51427400
H	4.72114100	-2.67715500	0.78241900
C	-4.09965100	-0.42363800	-0.13208900
C	-5.02081700	0.46157500	0.43869000
C	-4.54605000	-1.49660000	-0.91151800
C	-6.38276300	0.27783400	0.22038100
C	-5.91023600	-1.67190400	-1.12686700
C	-6.82775900	-0.78561000	-0.56434400
H	-7.09655400	0.96287500	0.66752100
H	-6.25529100	-2.50332200	-1.73394600
H	2.42451000	-1.77092000	0.75515500
H	5.93699600	-3.06015300	-1.35669700
H	2.53224600	-1.60750400	-3.53705900
H	-4.68536100	1.28187100	1.06596700
H	-7.89147900	-0.92626100	-0.73273700
H	-3.81919400	-2.18546500	-1.33079900
C	0.65171400	2.95962800	-0.05844600
C	0.37252500	2.83354900	-1.42531700
C	1.58320600	3.93100200	0.33952900
C	1.01612900	3.63639900	-2.36582300
H	-0.35509300	2.09817500	-1.76000600
C	2.23329700	4.73418000	-0.59601400
H	1.79930800	4.07369200	1.39806700
C	1.95124700	4.58417800	-1.95310400
H	0.78847300	3.52047900	-3.42194300
H	2.95178700	5.47958900	-0.26605600
H	2.45346200	5.20941700	-2.68627700
C	0.94876200	0.61887300	1.99201900
C	2.33654000	0.82273700	2.00172200
C	0.44206600	-0.49308200	2.68119900
C	3.18711000	-0.03430500	2.69988300
H	2.76541200	1.65756200	1.45085000
C	1.28897300	-1.36145400	3.36947500
H	-0.63042100	-0.68539400	2.68840100
C	2.66410500	-1.12604400	3.39034600
H	4.25893000	0.14450300	2.69239200
H	0.87471700	-2.21761700	3.89598300
H	3.32344200	-1.79554800	3.93625300

SiH_2Ph_2-PHC^{Ph} **T3**

Ee(M06-2X) = -2070.21695937

Ee(RI-SCS-MP2) = -2066.8573642

C	-1.44930700	1.10488100	-0.06996300
C	-0.69540200	-2.18059200	-0.24812500
P	-2.41465800	-0.21655100	-0.14816600
P	0.37175900	-1.33641300	-1.42528700
N	-1.90459100	-1.74887600	0.05623200
C	-0.33936200	-3.51003900	0.36519500
H	0.07215300	-3.33361300	1.36751000
H	-1.25014400	-4.10450000	0.47606700
H	0.40652300	-4.05466200	-0.21621600
C	-4.19965300	-0.15440200	-0.09997800
C	-4.93142600	-1.30451900	0.21700300
C	-4.85482000	1.04861300	-0.38752300
C	-6.32182400	-1.23863900	0.25682800
H	-4.40778800	-2.23147600	0.42866100
C	-6.24367000	1.10240500	-0.34265500
H	-4.28457300	1.93410900	-0.65529100
C	-6.97723800	-0.03969900	-0.01930400
H	-6.89351600	-2.12757800	0.50516800
H	-6.75370200	2.03422400	-0.56650600
H	-8.06180900	0.00505300	0.01221400
C	2.02093400	-2.10988100	-1.17941100
C	2.60729300	-2.35086400	0.07252000
C	2.75914000	-2.41323800	-2.33266500
C	3.88630500	-2.89432900	0.16350800
H	2.06946500	-2.10140100	0.98367700
C	4.04387200	-2.94645900	-2.24184900
H	2.31832500	-2.23505300	-3.31100700
C	4.60910000	-3.19127900	-0.99189000
H	4.32278500	-3.07115700	1.14292500
H	4.59898900	-3.17560700	-3.14709000
H	5.60919400	-3.60887100	-0.91669700
Si	0.43396400	1.01862800	-0.51463900
H	-1.91059900	2.08623300	0.03457500
H	-0.17284600	1.45095300	-1.85870600
C	1.26360000	2.77928400	-0.49400700
C	1.51288500	3.42139700	-1.71611300
C	1.53544600	3.50845900	0.67699300
C	2.03083700	4.71560400	-1.77911200
H	1.29031900	2.89677500	-2.64457800
C	2.01877600	4.81524600	0.62791700
H	1.36147600	3.05202700	1.64900700
C	2.27908400	5.41916500	-0.60253900
H	2.23072500	5.17645000	-2.74319200
H	2.19947100	5.36111900	1.55059300
H	2.67035900	6.43236200	-0.64281200
C	1.19869400	0.47377000	1.17925200
C	2.57764500	0.61178600	1.40581500
C	0.44514200	-0.14984100	2.18399700
C	3.17884700	0.15674000	2.57839700
H	3.20035800	1.08710800	0.64913100
C	1.03405600	-0.60212300	3.36686800
H	-0.62705800	-0.28274500	2.05705400
C	2.40673600	-0.45634400	3.56474800
H	4.25020200	0.27552600	2.71949600
H	0.41963100	-1.06790400	4.13360000
H	2.86805700	-0.81218800	4.48208300

SiH_2Ph_2-PHC^{Ph} **D**
Ee(M06-2X) = -2070.3639612
Ee(RI-SCS-MP2) = -2066.9985042

C	-1.49769200	0.41292300	0.68994600
C	-0.68664600	-1.75987500	-1.54536600
P	-2.50372700	0.06437700	-0.84846400
P	0.64724800	-0.46913000	-1.68641800
N	-1.90347200	-1.49994900	-1.25607300
C	-0.33486700	-3.16283700	-1.98843000
H	0.19935700	-3.70350400	-1.20130400
H	-1.25867100	-3.69658500	-2.22244800
H	0.31859900	-3.14556900	-2.86722900
C	-4.08780100	-0.42607300	-0.05236200
C	-4.43995800	-1.75407300	0.20426700
C	-4.97107700	0.59709700	0.31065300
C	-5.65216500	-2.04951100	0.82719600
H	-3.76385000	-2.54822100	-0.09868800
C	-6.17728500	0.30176000	0.94187300
H	-4.71820800	1.63372300	0.09148400
C	-6.52028100	-1.02487800	1.20122000
H	-5.91938900	-3.08504500	1.02040100
H	-6.85311500	1.10537000	1.22084700
H	-7.46412200	-1.25837200	1.68578900
C	2.20538200	-1.36364300	-1.28585500
C	2.33322200	-2.28318300	-0.23431500
C	3.34380000	-1.03870200	-2.03231100
C	3.56160800	-2.86712900	0.05512700
H	1.47044100	-2.52607800	0.38189800
C	4.58146500	-1.61073600	-1.73344300
H	3.26069300	-0.32804600	-2.85136800
C	4.69158500	-2.52757500	-0.69192600
H	3.64181200	-3.57181100	0.87818400
H	5.45535200	-1.34217400	-2.32020500
H	5.65324800	-2.97623800	-0.45926800
Si	0.29446700	0.74901000	0.22182400
H	-1.59920200	-0.44184700	1.37047300
H	-1.91716400	1.29933400	1.18097600
C	0.54534000	2.55759200	-0.22632900
C	0.16891700	3.05539100	-1.48316000
C	1.05844600	3.46132000	0.71754200
C	0.29729100	4.40965200	-1.78672700
H	-0.22833100	2.37807500	-2.23628700
C	1.19237700	4.81598600	0.41644600
H	1.36511600	3.10441400	1.69917300
C	0.81166200	5.29162800	-0.83727500
H	-0.00186900	4.77515300	-2.76506700
H	1.59587900	5.49899200	1.15885300
H	0.91682600	6.34685900	-1.07404100
C	1.52123900	0.24798400	1.54853300
C	2.87323000	0.59639800	1.39304000
C	1.17026900	-0.56607600	2.63362200
C	3.84150300	0.13844600	2.28168900
H	3.17772500	1.22056400	0.55369100
C	2.13594700	-1.02585600	3.53008000
H	0.13227800	-0.85437700	2.78551800
C	3.47323700	-0.67841000	3.35159900
H	4.88320400	0.40979000	2.13489400
H	1.84302800	-1.65430700	4.36666100
H	4.22682800	-1.04100300	4.04527300

SiH_4 + PHC^{Ar}

PHC^{Ar}
Ee(M06-2X) = -2259.48697878
Ee(RI-SCS-MP2) = -2255.61545

C	-0.08643900	-0.05828100	-1.01973000
C	0.58238800	-0.13142500	1.69793900
P	-1.25393000	0.32003200	0.12722500
P	1.19625600	-0.44677300	0.03750700
N	-0.69924100	0.11372700	1.72010100
C	1.39849800	-0.29230400	2.94692700
H	2.46344300	-0.13414700	2.74686600
H	1.05950500	0.42169800	3.70233200
H	1.27496300	-1.30284200	3.35438200
C	-3.05116500	0.12324300	-0.02562700
C	-3.84768800	1.30191600	-0.02438000
C	-3.64855500	-1.17178500	-0.09153500
C	-5.23986500	1.14486300	-0.03155700
C	-5.04248900	-1.22696200	-0.09492100
C	-5.85826500	-0.09778100	-0.05084200
H	-5.86453300	2.02370000	-0.01912400
H	-5.53031400	-2.19076900	-0.12981400
C	2.97469000	-0.13432700	-0.20896400
C	3.84117600	-1.26904400	-0.19369100
C	3.50358400	1.18729600	-0.24947700
C	5.21438500	-1.03197800	-0.11198200
C	4.89550200	1.32609900	-0.16229800
C	5.76494200	0.24636100	-0.06671900
H	5.89447100	-1.87165500	-0.07794400
H	5.32007900	2.31716500	-0.16319500
C	2.67312200	2.48205900	-0.46266400
C	2.02108400	2.43919900	-1.85897100
C	1.60368500	2.71698400	0.62714000
C	3.56271700	3.74124000	-0.44535800
H	2.79452800	2.39400100	-2.63476000
H	1.35176800	1.58658900	-1.98864400
H	1.43549600	3.35418300	-2.01446600
H	1.99573100	2.49660500	1.62719500
H	1.30630800	3.77207800	0.61188800
H	0.69244100	2.14043800	0.46830700
H	2.92785100	4.61083000	-0.64047900
H	4.04702900	3.89651400	0.52596200
H	4.33000200	3.72250800	-1.22603400
C	7.28207600	0.41285700	0.05339600
C	7.76406500	-0.26034600	1.35034000
C	7.96369000	-0.25626300	-1.15348800
C	7.70750600	1.88487100	0.09027300
H	7.28780500	0.19582600	2.22518500
H	7.53451800	-1.33065600	1.36057100
H	8.84996300	-0.14825800	1.45186600
H	7.62511200	0.19731300	-2.09141100
H	9.05133600	-0.13668900	-1.08534700
H	7.74618400	-1.32835300	-1.19939900
H	8.79650200	1.94634400	0.19099400
H	7.42937500	2.41269300	-0.82893200
H	7.26448000	2.41448300	0.94135500
C	3.37409900	-2.74939700	-0.28702000
C	2.66656700	-3.21093300	1.00464800
C	2.48375700	-2.97569300	-1.52663400
C	4.56831100	-3.70871500	-0.46581900
H	3.28987800	-2.99058500	1.87947700
H	1.68973000	-2.74682400	1.15104800

H	2.51027500	-4.29558800	0.96423500
H	3.02898400	-2.70117600	-2.43669300
H	2.22422300	-4.03889600	-1.59375800
H	1.54889300	-2.41331300	-1.51283400
H	4.17862500	-4.72102300	-0.61109500
H	5.17162300	-3.45724800	-1.34487300
H	5.21955100	-3.73677200	0.41463100
C	-2.88395200	-2.51539900	-0.23080900
C	-2.28296700	-2.60848200	-1.64758200
C	-1.78213900	-2.70994900	0.83525000
C	-3.82798800	-3.72461800	-0.07722400
H	-3.08086000	-2.58487400	-2.39905700
H	-1.58450900	-1.79632100	-1.86078500
H	-1.74320200	-3.55834300	-1.75184000
H	-2.10051400	-2.35071300	1.81926200
H	-1.55498000	-3.77876600	0.91932500
H	-0.84361100	-2.21941700	0.57361600
H	-3.23327100	-4.63892100	-0.16451400
H	-4.32329500	-3.73996200	0.90100500
H	-4.59011600	-3.76758700	-0.86157900
C	-3.29511300	2.75514200	-0.02855400
C	-2.54419800	3.07857800	1.27970100
C	-2.41327300	3.01370300	-1.26929800
C	-4.42663800	3.79855400	-0.11599400
H	-3.19979600	2.91208400	2.14200200
H	-1.64124800	2.48729200	1.43263700
H	-2.24942200	4.13495900	1.27358400
H	-2.98788700	2.82924900	-2.18416100
H	-2.09712500	4.06386500	-1.27262900
H	-1.51230500	2.40039600	-1.31130000
H	-3.97289200	4.79412200	-0.15006500
H	-5.02960400	3.68220200	-1.02314500
H	-5.08906600	3.77349100	0.75611200
C	-7.37948900	-0.26835100	-0.04122800
C	-8.11624700	1.07347100	0.03244700
C	-7.81726200	-0.98941100	-1.32814100
C	-7.78758700	-1.11026700	1.18086000
H	-7.85955000	1.62829800	0.94200800
H	-7.89443900	1.70654100	-0.83411700
H	-9.19699100	0.89560800	0.04483100
H	-7.35796800	-1.97950500	-1.41454000
H	-8.90557900	-1.12180600	-1.33410700
H	-7.53604800	-0.40864800	-2.21339800
H	-8.87649200	-1.23473500	1.20466100
H	-7.33654100	-2.10750300	1.15555200
H	-7.47585200	-0.62250800	2.11096100

SiH_4-PHC^{Ar} **T1**

Ee(M06-2X) = -2551.28209255

Ee(RI-SCS-MP2) = -2546.950592

C	0.28525000	0.15805500	0.22663400
C	-0.71572500	-0.14502000	-2.32148300
N	0.49915800	0.20704700	-2.54418400
H	1.53669700	-1.42301300	2.96787600
H	1.07493200	-1.29414700	0.78477200
P	-1.14181900	-0.44508700	-0.57329000
P	1.24939900	0.83325800	-1.10639700
C	-1.67745100	-0.50690000	-3.41626100
H	-2.71082400	-0.29409100	-3.12265900
H	-1.42818200	0.04873200	-4.32302300
H	-1.60559500	-1.57962000	-3.63314000
Si	0.94946200	-0.34534400	2.06801700
C	-2.84516200	-0.12002000	0.00229600
C	-3.60418300	-1.28905900	0.32850700
C	-3.44559400	1.17202200	0.04495800
C	-4.96384100	-1.12325400	0.59554400
C	-4.81800200	1.23515400	0.32191300
C	-5.59862900	0.11549600	0.57886000
H	-5.56586500	-1.98891500	0.83150800
H	-5.30128800	2.19846700	0.33975500
C	2.98876900	0.36356700	-0.76788800
C	3.70918200	1.39743500	-0.11037000
C	3.50217100	-0.97311200	-0.77323700
C	4.76319200	1.02246200	0.73864100
C	4.54954200	-1.25595900	0.09794000
C	5.14864000	-0.29612600	0.91909600
H	5.28283100	1.79142800	1.29007800
H	4.92600700	-2.26930700	0.14881900
C	-3.03631500	-2.73752700	0.43261500
C	-2.70881400	-3.31717800	-0.95810400
C	-1.80438500	-2.81160700	1.36264600
C	-4.06984900	-3.70154100	1.05258200
H	-3.58421900	-3.25585900	-1.61536800
H	-1.87420500	-2.80559700	-1.44175300
H	-2.43228200	-4.37363800	-0.85707800
H	-1.98386300	-2.26394700	2.29462200
H	-1.60488400	-3.85835900	1.61834100
H	-0.88899400	-2.42595600	0.90644900
H	-3.60235900	-4.68435300	1.16353800
H	-4.39469100	-3.37385600	2.04641700
H	-4.95203300	-3.83805800	0.41843500
C	-7.10006000	0.19786000	0.86447700
C	-7.86036600	-0.62182700	-0.19286500
C	-7.38510400	-0.38091000	2.26187100
C	-7.62527500	1.63710800	0.82576500
H	-7.67829100	-0.22422200	-1.19737200
H	-7.55660500	-1.67353800	-0.18542000
H	-8.93814800	-0.58115900	0.00331600
H	-6.84287500	0.17749000	3.03266300
H	-8.45720000	-0.31960300	2.48237900
H	-7.08848100	-1.43221000	2.33543300
H	-8.70123000	1.63641700	1.03046600
H	-7.14427400	2.26630900	1.58330200
H	-7.47441900	2.09935300	-0.15631000
C	-2.70497500	2.52630400	-0.12194500
C	-1.70871900	2.71282900	1.03876400
C	-1.99094300	2.66121700	-1.48317500
C	-3.67156200	3.72588700	-0.04497300
H	-2.24108100	2.72108000	1.99686900
H	-0.95168300	1.92765000	1.07863400
H	-1.19264700	3.67437700	0.92616100
H	-2.61670900	2.28197900	-2.30017400
H	-1.78981800	3.71988200	-1.68173200
H	-1.02749700	2.15649600	-1.51199700
H	-3.08355200	4.64365800	-0.14169400
H	-4.40823000	3.71934600	-0.85682100
H	-4.19871900	3.78206100	0.91293300
C	3.07611800	-2.07501800	-1.77491100
C	1.69314000	-2.68094600	-1.48278800
C	3.13292000	-1.48865200	-3.19978400
C	4.06100900	-3.25999000	-1.76648900
H	1.67165600	-3.13028400	-0.48314400
H	0.88460500	-1.95714000	-1.54534100
H	1.48563200	-3.46829300	-2.21834500
H	4.14607000	-1.12969700	-3.41651900
H	2.88608200	-2.27090700	-3.92812800
H	2.43343900	-0.66584400	-3.34656300
H	3.77990800	-3.94685600	-2.57165300

H	5.09269100	-2.93894900	-1.94773700
H	4.02713600	-3.82810800	-0.83052400
C	3.45180000	2.92398300	-0.28411200
C	3.23386500	3.28342800	-1.76829400
C	2.28979200	3.43611500	0.59108200
C	4.69255000	3.73742300	0.14525500
H	4.09110500	2.95551200	-2.36724300
H	2.33139600	2.84685200	-2.19833100
H	3.14524800	4.37164500	-1.86691000
H	2.44742700	3.15266000	1.63794600
H	2.25163500	4.53142800	0.53591500
H	1.31816500	3.05027000	0.27701100
H	4.53884600	4.78210700	-0.14357700
H	4.84836200	3.72778200	1.22862700
H	5.60565600	3.38271000	-0.34540500
C	6.22071500	-0.72246200	1.92268400
C	5.60970400	-1.75300800	2.88873800
C	7.40640700	-1.35777800	1.17525600
C	6.74547000	0.45790300	2.74667400
H	4.75491700	-1.32477700	3.42342100
H	5.25921300	-2.64461700	2.35892400
H	6.35833500	-2.06975900	3.62457400
H	7.85125700	-0.64327100	0.47376500
H	8.17901300	-1.66707500	1.88913400
H	7.10149600	-2.24291600	0.60750200
H	7.48323000	0.09736300	3.47168400
H	7.23883700	1.20739100	2.11716500
H	5.93969900	0.94884000	3.30396900
H	-0.34184300	-0.08044500	2.76457400
H	1.93907400	0.75389200	2.20261800

SiH_4-PHC^{Ar} **B**

Ee(M06-2X) = -2551.39004679

Ee(RI-SCS-MP2) = -2547.070464

C	-0.43384300	0.21703200	-0.47791500
C	0.93551000	0.19717700	1.81627500
N	-0.28439600	0.19664300	2.21406200
H	-2.46332300	0.61721100	-2.31806400
H	-0.53703600	-0.87617000	-0.51350900
P	1.22513000	0.85930600	0.09869500
P	-1.33876900	0.93609000	1.02646700
C	2.08088600	-0.13309400	2.72739200
H	2.74387800	-0.87658800	2.27066300
H	2.68327800	0.76766300	2.90181300
H	1.70094900	-0.50164100	3.68307000
Si	-1.05205800	1.00627800	-2.07912400
C	2.89101400	0.20060800	-0.44500400
C	3.33082400	-1.15199400	-0.59855200
C	3.87712100	1.23468200	-0.39581500
C	4.68427300	-1.43668800	-0.43848100
C	5.21851500	0.85871200	-0.20687800
C	5.64262400	-0.45969000	-0.16726400
H	5.01571200	-2.46455300	-0.51691000
H	5.96016300	1.63414000	-0.09269900
C	-3.04246500	0.20991400	0.88200100
C	-3.95121200	1.19793000	0.40253400
C	-3.44955800	-1.16015500	0.84092200
C	-5.00169900	0.77712200	-0.43246600
C	-4.51040200	-1.50053400	0.00780400
C	-5.24324400	-0.55667600	-0.72072900
H	-5.64487000	1.52650900	-0.87134200
H	-4.79347400	-2.54286300	-0.07766200
C	2.40815400	-2.32812100	-0.97183000
C	1.57606000	-2.74631500	0.24405100
C	1.53068200	-1.93122200	-2.17070200
C	3.18170400	-3.58069400	-1.42236300
H	2.23246900	-3.10223500	1.04735100
H	0.98816700	-1.92179300	0.63845800
H	0.88969900	-3.55918100	-0.02117100
H	2.14614200	-1.85354900	-3.07456700
H	0.75896300	-2.69073600	-2.34725500
H	1.04105600	-0.97087900	-2.03472600
H	2.45887200	-4.31463900	-1.79551500
H	3.88331800	-3.36056000	-2.23447800
H	3.72922500	-4.05844300	-0.60302600
C	7.09477700	-0.86493100	0.08795800
C	7.14586200	-1.80004300	1.30898100
C	7.64623800	-1.60372500	-1.14410100
C	7.99548100	0.34299200	0.36706800
H	6.75551300	-1.29660400	2.20049100
H	6.55424500	-2.70698700	1.14693900
H	8.18020500	-2.10302400	1.50965300
H	7.60397600	-0.96323100	-2.03189000
H	8.69109900	-1.88973100	-0.97481600
H	7.08027000	-2.51611400	-1.35898400
H	9.01561200	-0.00143900	0.56886700
H	8.03952000	1.02401400	-0.49048300
H	7.65512000	0.90898000	1.24163800
C	3.62667100	2.76344600	-0.60392800
C	2.67378300	3.01418800	-1.79098700
C	3.13518400	3.47779100	0.67196300
C	4.93704600	3.48294000	-1.00082200
H	3.05963300	2.53238900	-2.69699100
H	1.65924500	2.65832400	-1.61424500
H	2.60869900	4.09187500	-1.98061200
H	3.79935200	3.24674600	1.51375900
H	3.16245100	4.56295600	0.51326000
H	2.11646000	3.20145000	0.94437200
H	4.68903900	4.50376200	-1.30762700
H	5.64387500	3.56765400	-0.16904900
H	5.43918300	2.99124200	-1.84116500
C	-2.88260200	-2.24352800	1.78229100
C	-1.49269600	-2.71181600	1.35173900
C	-2.82619400	-1.67212500	3.21178500
C	-3.78771500	-3.48640600	1.83283600
H	-1.49078300	-3.01610100	0.29751100
H	-0.76039400	-1.92352100	1.50030400
H	-1.17656600	-3.57188000	1.95586800
H	-3.82482500	-1.35688900	3.53639000
H	-2.46844800	-2.44415900	3.90398200
H	-2.14794700	-0.81978400	3.28389500
H	-3.41044700	-4.15874300	2.61072000
H	-4.82356000	-3.23170800	2.08314000
H	-3.78242700	-4.04785800	0.89170100
C	-3.95253500	2.70100200	0.82423500
C	-3.58149500	2.85039000	2.31397200
C	-3.05990300	3.59981300	-0.05191900
C	-5.38337300	3.27539200	0.70830600
H	-4.24119200	2.23394600	2.93539900
H	-2.54874600	2.57519500	2.53175200
H	-3.71010700	3.89699700	2.61389700
H	-3.27687500	3.43714000	-1.11464800
H	-3.26966400	4.65243600	0.17608800
H	-1.99714300	3.42076800	0.11787500
H	-5.40456400	4.25353500	1.19962900
H	-5.69313900	3.43642400	-0.32931300
H	-6.12292500	2.63340600	1.19927100
C	-6.30942000	-1.02155900	-1.71281100

C	-5.63578600	-1.89937300	-2.78241300
C	-7.38275400	-1.84443100	-0.97935900
C	-6.99802000	0.15242500	-2.41662500
H	-4.86722400	-1.33348000	-3.32068600
H	-5.15661400	-2.77774900	-2.33778600
H	-6.37869200	-2.25072300	-3.50824000
H	-7.87150600	-1.24298400	-0.20492800
H	-8.14814700	-2.18253600	-1.68795300
H	-6.95713700	-2.73158500	-0.49912700
H	-7.72092400	-0.23049000	-3.14524900
H	-7.54551900	0.78641000	-1.70983500
H	-6.27717300	0.77739000	-2.95612200
H	-0.23226600	0.55545200	-3.23143500
H	-0.94253300	2.47917000	-1.98066700

SiH_4-PHC^{Ar} **T2**

Ee(M06-2X) = -2551.32502808

Ee(RI-SCS-MP2) = -2547.024762

C	0.98624000	0.71792300	1.51807600
C	-0.84199600	0.49320200	-0.96097600
N	0.44027300	0.64571000	-1.25894100
H	0.23338000	3.39182200	1.73386800
H	1.57467900	-0.02682500	2.07617900
P	-1.46957400	0.96463600	0.62478100
P	1.57448100	0.93611100	-0.11220000
C	-1.71017500	-0.07920500	-2.06032200
H	-2.16616500	-1.01710400	-1.71994700
H	-2.53075900	0.59013300	-2.33361200
H	-1.09250900	-0.27528800	-2.93979600
Si	0.57457700	2.21561400	2.56559200
C	-3.22371000	0.31620800	0.52897000
C	-3.63878900	-0.96915300	0.97269400
C	-4.15741000	1.14774900	-0.15567100
C	-4.82658400	-1.49344800	0.46261700
C	-5.32243700	0.54249600	-0.65376200
C	-5.64696400	-0.78825100	-0.41869000
H	-5.13155400	-2.49005600	0.75822200
H	-6.00679300	1.13883700	-1.23908100
C	3.19867300	0.16145100	-0.46975400
C	4.30253300	1.05723400	-0.35455400
C	3.43689700	-1.24406700	-0.58544600
C	5.57376500	0.51029200	-0.12877400
C	4.73401400	-1.70098400	-0.35379500
C	5.80644900	-0.85650000	-0.06709000
H	6.41104500	1.17711900	0.00657000
H	4.92905700	-2.76399400	-0.39452600
C	-2.88776400	-1.77607800	2.05653100
C	-1.61514400	-2.42068800	1.49744200
C	-2.53352600	-0.85554400	3.23902500
C	-3.75802100	-2.90693800	2.63228000
H	-1.84144500	-3.02755300	0.61259500
H	-0.88260600	-1.66483000	1.22168800
H	-1.15697300	-3.07218500	2.25273100
H	-3.43684700	-0.39632700	3.65609700
H	-2.04550400	-1.43778200	4.02961600
H	-1.84662300	-0.05284400	2.95889200
H	-3.22969800	-3.35985200	3.47785300
H	-4.72287600	-2.53733400	2.99702800
H	-3.94102100	-3.70403300	1.90375700
C	-6.88633000	-1.46292300	-1.01137800
C	-6.44947600	-2.70953500	-1.80087400
C	-7.83772800	-1.88507000	0.12220700
C	-7.65382900	-0.53783100	-1.96250200
H	-5.77167600	-2.43385600	-2.61635600
H	-5.93072800	-3.43072000	-1.16117700
H	-7.32392800	-3.21002500	-2.23329800
H	-8.15362700	-1.01439400	0.70723400
H	-8.73204500	-2.36418800	-0.29364200
H	-7.36336900	-2.59659900	0.80584600
H	-8.50651100	-1.07795100	-2.38811200
H	-8.04640800	0.34413000	-1.44394800
H	-7.02356700	-0.19927500	-2.79256600
C	-4.04017800	2.69585800	-0.30161600
C	-3.71200600	3.32170700	1.07052300
C	-3.02513700	3.16604000	-1.36183100
C	-5.38977700	3.31606400	-0.71923500
H	-4.46514500	3.02811900	1.81047400
H	-2.72965100	3.03221500	1.44788200
H	-3.72462700	4.41463800	0.98523700
H	-3.26387600	2.74089800	-2.34335700
H	-3.08271500	4.25754200	-1.45168800
H	-1.99341700	2.91113500	-1.11395300
H	-5.29960400	4.40608600	-0.67310700
H	-5.66996300	3.06122600	-1.74694100
H	-6.20340200	3.01872800	-0.04900900
C	2.38927400	-2.27876300	-1.05317100
C	1.17870200	-2.35494900	-0.11715000
C	1.94629000	-1.91023100	-2.48331900
C	2.96390900	-3.70485200	-1.12622300
H	1.48955600	-2.53869400	0.91866400
H	0.57321900	-1.45313300	-0.14212600
H	0.52907600	-3.18280000	-0.42498300
H	2.80460900	-1.94377500	-3.16450400
H	1.20250900	-2.63611200	-2.83539600
H	1.50367200	-0.91414000	-2.52943700
H	2.17912300	-4.37187800	-1.49695400
H	3.80843600	-3.78010300	-1.81930000
H	3.27658300	-4.07913900	-0.14451600
C	4.22620500	2.60059400	-0.55828700
C	3.47196300	2.92541500	-1.86416900
C	3.60456500	3.35676900	0.63706500
C	5.63431400	3.20545600	-0.74195400
H	3.97883500	2.46472500	-2.71966000
H	2.43496300	2.58376600	-1.86682000
H	3.46066600	4.01092900	-2.01685600
H	3.98325700	2.96661800	1.58856900
H	3.87649100	4.41699800	0.57334100
H	2.51557400	3.30555000	0.65284900
H	5.52214400	4.25606500	-1.02716200
H	6.22323800	3.18476800	0.18139000
H	6.19995600	2.70382500	-1.53415400
C	7.18124600	-1.45432900	0.23961900
C	7.06701200	-2.37165800	1.47010600
C	7.66325100	-2.27733000	-0.96840200
C	8.23103600	-0.37825200	0.53836600
H	6.72477400	-1.80788700	2.34474600
H	6.36198100	-3.19157100	1.30008700
H	8.04382100	-2.81074000	1.70390600
H	7.73896400	-1.64803500	-1.86185600
H	8.65200800	-2.70355900	-0.76236900
H	6.98254400	-3.10434100	-1.19443900
H	9.18632800	-0.85783100	0.77697300
H	8.39701500	0.27922900	-0.32248200
H	7.94418500	0.23969700	1.39660500
H	1.77322300	2.56725100	3.37788500
H	-0.53502300	1.92766900	3.50648200

SiH_4-PHC^{Ar} **C**

Ee(M06-2X) =-2551.35916465

Ee(RI-SCS-MP2) = -2547.049742

C	1.77462000	1.63320700	1.72460100
C	-0.84451700	0.36775600	-0.53878600
N	0.52225800	0.45304300	-0.67633100
H	1.32136000	3.75444300	3.28391400
H	2.78566900	1.62281400	2.13198800
P	-1.59477300	0.37841400	0.99962500
P	1.68802600	0.77956700	0.31688200
C	-1.51718800	0.17976800	-1.87423700
H	-1.23436500	1.00843100	-2.53485900
H	-1.14097900	-0.74398900	-2.33336900
H	-2.60439600	0.12754700	-1.80329400
Si	0.52641900	2.73032000	2.55667300
C	-3.37211300	0.04092600	0.55170100
C	-3.82807600	-1.30408800	0.41600600
C	-4.24837000	1.11323700	0.23012400
C	-5.05693900	-1.52034600	-0.21184600
C	-5.46981500	0.81162200	-0.39093100
C	-5.87605600	-0.48779600	-0.66491000
H	-5.40142800	-2.53480900	-0.36423800
H	-6.12371900	1.62115500	-0.67889300
C	3.29237100	0.13520000	-0.20547500
C	4.27649000	1.04715100	-0.65509200
C	3.61319700	-1.23097700	0.06468200
C	5.60825400	0.60364500	-0.66344200
C	4.95708000	-1.58918900	-0.00141400
C	5.97709200	-0.68632800	-0.31507800
H	6.38159000	1.30191100	-0.95028100
H	5.24069400	-2.61022000	0.21453700
C	-3.06695200	-2.55796000	0.93127300
C	-1.87459200	-2.92430900	0.02585300
C	-2.60508300	-2.37055000	2.38995300
C	-3.97898700	-3.80227800	0.95281900
H	-2.20477400	-3.04395400	-1.01326600
H	-1.08334000	-2.17423200	0.04901700
H	-1.44485100	-3.87897900	0.35705500
H	-3.45957500	-2.12259800	3.03014300
H	-2.16651000	-3.30695300	2.75555900
H	-1.85205800	-1.59021200	2.51118900
H	-3.43917400	-4.62232000	1.43726200
H	-4.89983300	-3.62581300	1.51998800
H	-4.24568000	-4.14570300	-0.05227400
C	-7.18189000	-0.81960400	-1.39193100
C	-6.86273800	-1.64924200	-2.64806200
C	-8.09661000	-1.63468600	-0.46106200
C	-7.94157600	0.43764800	-1.82909600
H	-6.21463300	-1.08597900	-3.32872700
H	-6.35323700	-2.58475100	-2.39544200
H	-7.78691800	-1.90203700	-3.18130400
H	-8.33953100	-1.06262000	0.44119900
H	-9.03323700	-1.88387700	-0.97422700
H	-7.62490200	-2.57215800	-0.14861100
H	-8.85392800	0.14675300	-2.36137000
H	-8.23915900	1.05114800	-0.97114400
H	-7.34256900	1.05725800	-2.50608600
C	-3.95683200	2.61089300	0.52447400
C	-3.52275800	2.80799700	1.98942100
C	-2.91016100	3.19714000	-0.44416700
C	-5.21848600	3.48124500	0.35649900
H	-4.31002400	2.45888400	2.66768400
H	-2.60170100	2.28062100	2.24229300
H	-3.35337400	3.87445700	2.18110900
H	-3.21577500	3.02253200	-1.48299300
H	-2.83599600	4.28084600	-0.28981500
H	-1.91703200	2.76962900	-0.30279900
H	-4.98687700	4.49737200	0.69253600
H	-5.54335200	3.55491500	-0.68695900
H	-6.05556600	3.11289200	0.96002100
C	2.56664800	-2.34521600	0.32670500
C	1.60182600	-2.04052300	1.49261000
C	1.77085600	-2.58103800	-0.97350400
C	3.24119800	-3.68247500	0.68305800
H	2.13856500	-1.67931800	2.37693600
H	0.81545700	-1.32100900	1.24956700
H	1.07633400	-2.96259800	1.76742600
H	2.44679000	-2.88783300	-1.78013500
H	1.03831200	-3.38234300	-0.81624200
H	1.23601100	-1.68285000	-1.29280500
H	2.46081600	-4.43057400	0.85204100
H	3.87523600	-4.05877400	-0.12608900
H	3.83971100	-3.61191200	1.59897800
C	4.04274800	2.49645000	-1.16580100
C	2.62309700	2.77705200	-1.69708600
C	4.37365500	3.50557900	-0.05207700
C	4.98490000	2.77199500	-2.36191500
H	2.25486400	1.96941900	-2.33811400
H	1.89056700	2.95696400	-0.90680400
H	2.64944200	3.69534600	-2.29309500
H	5.39083300	3.35532700	0.32680400
H	4.30270700	4.52710000	-0.44464900
H	3.67489100	3.41463900	0.78530100
H	4.73738100	3.74759800	-2.79171200
H	6.04007200	2.81322700	-2.08139200
H	4.86432600	2.01335000	-3.14303900
C	7.43235500	-1.15983100	-0.30046800
C	7.77824600	-1.69308800	1.10082700
C	7.60999500	-2.28622200	-1.33417600
C	8.41396100	-0.03379300	-0.64205000
H	7.65181900	-0.91103400	1.85736100
H	7.14462100	-2.54048600	1.38181400
H	8.82056800	-2.03142100	1.12654500
H	7.35345000	-1.93552900	-2.33980800
H	8.65197300	-2.62664700	-1.34307100
H	6.97727500	-3.14979600	-1.10543000
H	9.43846000	-0.41868300	-0.60055500
H	8.24895300	0.35877400	-1.65188100
H	8.34144500	0.79630800	0.06980500
H	-0.32493100	2.02061200	3.53805200
H	-0.33434500	3.43040200	1.57395000

SiH_4-PHC^{Ar} **T3**

Ee(M06-2X) =-2551.28417174

Ee(RI-SCS-MP2) = -2546.967348

C	1.19240000	-0.39202800	1.97702900
C	-0.78317800	-0.21258600	-0.66134800
N	0.45909700	-0.52473400	-0.81166800
H	-1.21565100	1.47383100	3.41494800
H	1.95105100	-0.62986700	2.72546300
P	-1.53253000	0.66597700	0.75874700
P	1.63442800	-0.67729300	0.36976600
C	-1.66076200	-0.35822600	-1.88513400
H	-1.03536900	-0.63338200	-2.73689800
H	-2.42206600	-1.12991900	-1.72213000
H	-2.19891900	0.57219500	-2.09770600
Si	-0.44865900	0.34627000	2.74246100
C	-3.33898600	0.30964600	0.55180200

C	-3.87789700	-1.01361400	0.60962900
C	-4.12361400	1.36394500	0.01319700
C	-5.05772700	-1.26611500	-0.08794200
C	-5.31660100	1.02878900	-0.64906000
C	-5.76891300	-0.27660600	-0.77067800
H	-5.45228000	-2.27346200	-0.11293400
H	-5.89997500	1.81583000	-1.10305900
C	3.30979500	-0.23320500	-0.21809300
C	3.80395000	1.09557100	-0.18871000
C	4.20626900	-1.33081200	-0.44867000
C	5.19699400	1.27557900	-0.23559200
C	5.56761000	-1.04971600	-0.52624300
C	6.09628300	0.23455400	-0.38028400
H	5.58203000	2.28229400	-0.14614100
H	6.26525200	-1.85924900	-0.68989700
C	-3.30704900	-2.15312900	1.49224400
C	-1.89470500	-2.64113700	1.09869300
C	-3.35823200	-1.66427300	2.95387600
C	-4.19099900	-3.41562700	1.44416100
H	-1.82077900	-2.79345800	0.01508400
H	-1.08844100	-1.97566700	1.40269000
H	-1.70701800	-3.60729600	1.58151800
H	-4.40152300	-1.59729300	3.28349500
H	-2.83005000	-2.36414300	3.61225600
H	-2.91789700	-0.67399600	3.08470400
H	-3.79918100	-4.13831200	2.16726500
H	-5.22990500	-3.20872000	1.72018600
H	-4.17479200	-3.89495200	0.45809100
C	-7.02067900	-0.65593700	-1.56425000
C	-6.63415300	-1.67225700	-2.65319700
C	-8.05811400	-1.28870000	-0.62017600
C	-7.66766600	0.55478700	-2.24594600
H	-5.89433200	-1.24387300	-3.33866200
H	-6.20694800	-2.58378200	-2.22288500
H	-7.51838200	-1.95728200	-3.23548900
H	-8.33785600	-0.58861600	0.17479000
H	-8.96273600	-1.55562800	-1.17914600
H	-7.67498300	-2.19943500	-0.14849700
H	-8.54080300	0.22650800	-2.82032300
H	-8.01106000	1.29695700	-1.51640400
H	-6.97667200	1.04520700	-2.94094200
C	-3.77717000	2.87762900	0.10562700
C	-3.28592100	3.25751500	1.51668100
C	-2.74999500	3.29975900	-0.96345600
C	-5.02948200	3.74747100	-0.13447000
H	-4.00982700	2.93681000	2.27484000
H	-2.31636200	2.82756200	1.76793700
H	-3.18392400	4.34704000	1.58341200
H	-3.11470100	3.04183500	-1.96541500
H	-2.61249900	4.38781100	-0.92694400
H	-1.77590500	2.83003500	-0.81206000
H	-4.77846500	4.78860400	0.09193400
H	-5.37058000	3.72371800	-1.17463200
H	-5.86201500	3.45353500	0.51452900
C	3.78205800	-2.81638800	-0.62876600
C	3.43067800	-3.47260700	0.72296900
C	2.62209200	-2.96207100	-1.63274600
C	4.93208100	-3.66080600	-1.21601800
H	4.25934800	-3.35173400	1.43033400
H	2.52789300	-3.05788300	1.17417500
H	3.26719900	-4.54671100	0.57270400
H	2.88445100	-2.49509600	-2.58901200
H	2.43643900	-4.02723800	-1.81285400
H	1.67896200	-2.52641300	-1.30257900
H	4.54817000	-4.66201900	-1.43511600
H	5.31772500	-3.23849900	-2.15058600
H	5.76329400	-3.78602900	-0.51442900
C	3.01282800	2.42767200	-0.10775000
C	1.50226700	2.33584900	-0.34130600
C	3.24852700	3.06127000	1.27544700
C	3.53419600	3.38393800	-1.20619200
H	1.25737400	1.79327500	-1.25958400
H	0.97495500	1.88502800	0.49954600
H	1.10310100	3.35206500	-0.43526400
H	4.31074900	3.25701300	1.45625600
H	2.70913800	4.01314300	1.34660100
H	2.88116600	2.40278900	2.07004400
H	2.94802600	4.30880300	-1.18245200
H	4.58261700	3.66473300	-1.08282000
H	3.41693600	2.93232100	-2.19758600
C	7.61229700	0.43879300	-0.41338900
C	8.25637400	-0.36436400	0.73019700
C	8.16383200	-0.05887200	-1.76124800
C	8.00374000	1.91093300	-0.24740200
H	7.87871300	-0.02781800	1.70192000
H	8.04923500	-1.43555500	0.63969100
H	9.34434200	-0.22967700	0.71787300
H	7.71100400	0.49106400	-2.59356400
H	9.24940200	0.08851700	-1.80075700
H	7.96485800	-1.12474700	-1.91328600
H	9.09507100	2.00253400	-0.26715700
H	7.60395400	2.53104800	-1.05791200
H	7.65307400	2.31884800	0.70738700
H	-0.69467100	-0.75112600	3.72091500
H	0.92554800	1.20527800	2.71312700

SiH_4-PHC^{Ar} **D**

Ee(M06-2X) = -2551.416501

Ee(RI-SCS-MP2) = -2547.096025

C	1.58384000	-0.13508600	1.69288000
C	-0.82602200	-0.13443700	-0.70658300
N	0.43166400	-0.07336400	-0.96325800
H	-0.37056200	0.29063100	3.67213600
H	2.13625400	-1.07762100	1.66766000
P	-1.51369000	0.46634700	0.88982700
P	1.57842700	0.71634800	0.02542000
C	-1.77374600	-0.53833800	-1.81078700
H	-2.29273700	-1.47051300	-1.57408600
H	-2.54754900	0.22563500	-1.95127700
H	-1.20520400	-0.66015100	-2.73534200
Si	-0.12698100	-0.46031800	2.41674900
C	-3.34373100	0.15375800	0.75563700
C	-3.98500900	-1.12473700	0.67308800
C	-4.07928400	1.31568200	0.37746200
C	-5.16599500	-1.21419100	-0.05859600
C	-5.26042200	1.13118900	-0.36111900
C	-5.78415700	-0.11664900	-0.66203600
H	-5.63160600	-2.18068800	-0.17595600
H	-5.78138500	2.00208400	-0.71980100
C	3.29632800	0.23133200	-0.51750600
C	4.21622600	1.31130600	-0.39194500
C	3.81550300	-1.10107800	-0.66472300
C	5.55853900	1.01139300	-0.09323800
C	5.16046000	-1.30448200	-0.36711700
C	6.03970400	-0.28251100	0.00294000
H	6.24251700	1.82482300	0.07830800
H	5.55832800	-2.30549900	-0.42339700
C	-3.50796500	-2.40995100	1.43668900

C	-2.25224800	-3.04363300	0.79902900
C	-3.30756900	-2.03565700	2.92508200
C	-4.58679000	-3.52253200	1.43843300
H	-2.49870500	-3.42602000	-0.18484900
H	-1.44439400	-2.34483800	0.69301500
H	-1.90901800	-3.87279300	1.40826100
H	-4.26266700	-1.76015800	3.35722500
H	-2.91006100	-2.88279900	3.47311000
H	-2.64259000	-1.20004400	3.05730200
H	-4.23510700	-4.32942800	2.07213100
H	-5.52794700	-3.16520400	1.83783100
H	-4.75132600	-3.93352700	0.44992600
C	-7.03798000	-0.32482500	-1.54826100
C	-6.67564100	-1.27380300	-2.71281800
C	-8.16968600	-0.94417300	-0.69746800
C	-7.55134200	0.99879900	-2.14823600
H	-5.88101300	-0.84708500	-3.31404500
H	-6.34720600	-2.23921300	-2.34903300
H	-7.54311300	-1.42831800	-3.34627900
H	-8.42459300	-0.28733700	0.12623600
H	-9.05394000	-1.09014800	-1.30952200
H	-7.87881500	-1.90462100	-0.29085900
H	-8.40434900	0.79189900	-2.78498200
H	-7.87259600	1.68683100	-1.37474700
H	-6.78899800	1.47849600	-2.75141000
C	-3.71861900	2.80833400	0.76179500
C	-3.24383800	2.89259800	2.23301700
C	-2.68083300	3.42871800	-0.20215700
C	-4.98221700	3.70881200	0.69087500
H	-4.00055500	2.48004100	2.89119700
H	-2.31574400	2.37282900	2.39606500
H	-3.09224600	3.93393900	2.49691400
H	-3.03782400	3.36178400	-1.22463500
H	-2.54692600	4.47846000	0.04108900
H	-1.72525900	2.93673700	-0.13079100
H	-4.72963800	4.67414000	1.11399800
H	-5.31017700	3.88247500	-0.32607700
H	-5.80126900	3.28960400	1.26289600
C	3.02640100	-2.31673200	-1.28494600
C	1.91868700	-2.87010400	-0.36341600
C	2.43834500	-1.86126700	-2.64170300
C	3.96202400	-3.51219200	-1.59323400
H	2.33958100	-3.19415700	0.58278100
H	1.14660600	-2.14507600	-0.18672000
H	1.45892400	-3.73078100	-0.83902000
H	3.23727000	-1.52206300	-3.29205300
H	1.94109000	-2.70104600	-3.11940700
H	1.72350500	-1.06852300	-2.50136400
H	3.37690500	-4.26928700	-2.10308000
H	4.77700600	-3.22398600	-2.24578300
H	4.36559100	-3.96194500	-0.69307200
C	3.88299600	2.84205100	-0.63084900
C	2.93210300	3.01637900	-1.84072000
C	3.31936500	3.53002800	0.63463200
C	5.17059800	3.62141200	-1.01752400
H	3.36950300	2.56031800	-2.72155900
H	1.96102300	2.58368400	-1.67414800
H	2.79615000	4.07549100	-2.03433800
H	4.00192400	3.39120300	1.46672600
H	3.21954300	4.59606900	0.45279000
H	2.35138700	3.13961000	0.90383900
H	4.87879900	4.61510000	-1.33776100
H	5.84927000	3.74142500	-0.18277400
H	5.69348400	3.13885600	-1.83427800
C	7.49476800	-0.62543200	0.41086900
C	7.46428700	-1.58785000	1.61940000
C	8.21651700	-1.29860000	-0.77831200
C	8.29517000	0.62815300	0.81542900
H	6.96139700	-1.12198400	2.45915700
H	6.94568500	-2.50734200	1.37906200
H	8.47715900	-1.83839200	1.91856400
H	8.23609500	-0.63168200	-1.63255500
H	9.23872700	-1.53893800	-0.50322700
H	7.72177900	-2.21544700	-1.07312600
H	9.29106100	0.32954400	1.12416500
H	8.39638800	1.31824300	-0.01427600
H	7.82450300	1.14307400	1.64521200
H	-0.25174200	-1.90377900	2.70835000
H	2.13183600	0.54486100	2.35551000

Conformational Studies

Table 1: *Relative electronic and free energies of PHC(Me) model.*

PHC-Me				
Conformers	**Ee(M06-2X)**	**Ee+TCG**	**ΔEe (kJ mol^{-1})**	**ΔG (kJ mol^{-1})**
(R)(R)	-933.2861406640	-933.192350	0.0	0.0
(S)(S)	-933.2861406560	-933.192347	2.10E-05	7.88E-03
(R)(S)	-933.2861405700	-933.192343	2.26E-04	1.05E-02
(S)(R)	-933.2861405750	-933.192334	-1.31E-05	2.36E-02

Molecular Orbital Energies

Table 2: *Molecular orbital energies computed at the BP86/def2-TZVP level of theory.*

	LUMO (a.u.)	HOMO (a.u.)	HOMO-1 (a.u.)	HOMO-LUMO (eV)	HOMO – HOMO-1 (eV)	S-T Gap (eV)
NHC(Me)	-0.01461	-0.18375	-0.22784	4.60	1.20	4.41
PHC(H)	-0.11231	-0.21540	-0.23455	2.81	0.52	2.41
PHC(Me)	-0.09091	-0.19753	-0.20773	2.90	0.28	2.76
PHC(Ph)	-0.09943	-0.19521	-0.20346	2.61	0.22	2.56
PHC(Ar)[a]	-0.06551	-0.18479	-0.18978	3.25	0.14	3.06

[a] PHC^{Ar} calculated using BP86/6-31+G(d)).