SUPPORTING INFORMATION

Highly Variable Zr–CH_2–Ph Bond Angles in Tetrabenzylzirconium: Analysis of Benzyl Ligand Coordination Modes

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Table 1. Cartesian coordinates for geometry optimized structures of $Zr(CH_2Ph)_4$.

$Zr(CH_2Ph)_4$

-1130.45218388542 Hartrees

atom	x	y	z
Zr	8.239323671	-0.001254698	2.409602562
C	8.408181668	1.779462771	0.961024838
C	9.793685028	1.711548268	0.424362307
C	10.11996669	0.892273825	-0.678722049
C	11.43119607	0.76519128	-1.136445741
C	12.47090716	1.454263199	-0.508661548
C	12.17113022	2.285016414	0.575437801
C	10.86039267	2.410924793	1.031283312
H	7.650418188	1.640357353	0.181928176
H	8.196583218	2.716196455	1.487962588
H	9.325742696	0.357735524	-1.193682187
H	11.6392377	0.128222596	-1.992931495
H	12.96485749	2.842847656	1.066251952
H	10.64601442	3.07001395	1.869884263
C	8.026067124	-1.798951135	0.985384539
C	6.649932662	-1.719203573	0.42541138
C	6.361478019	-0.949435018	-0.722942095
C	5.061660477	-0.813634813	-1.208340697
C	3.994787328	-1.443954882	-0.564270942
C	4.25594105	-2.225106319	0.565232999
C	5.556471752	-2.359914588	1.049037421
H	8.797285067	-1.711278854	0.212474909
H	8.205485624	-2.722848923	1.546876067

H	7.176965569	-0.46109036	-1.250585424
H	4.882996654	-0.215734418	-2.098811792
H	3.440792935	-2.73732238	1.070712828
H	5.74065847	-2.982144752	1.922386957
C	9.973434724	0.280391229	3.873892737
C	10.40455202	-1.088075177	3.543857508
C	9.895421584	-2.210253458	4.24639133
C	10.17705415	-3.509869375	3.837270671
C	10.96244126	-3.741324375	2.703320547
C	11.46562759	-2.654806143	1.987907182
C	11.18736892	-1.348289456	2.391009006
H	9.647427593	0.418432737	4.907514297
H	10.6645853	1.064413099	3.560428747
H	9.291856773	-2.043405763	5.135598132
H	9.783891164	-4.348476102	4.406187553
H	12.07933418	-2.821277227	1.106532096
H	11.60004026	-0.51274943	1.830499745
C	6.543166054	-0.283721741	3.918810219
C	6.109994752	1.086464214	3.599554483
C	6.642429382	2.20635256	4.288690634
C	6.3561766	3.507326445	3.886732768
C	5.542951376	3.742412986	2.773359671
C	5.017734567	2.658377695	2.070439204
C	5.300947505	1.350657558	2.465798585
H	6.892432162	-0.424808582	4.944271799
H	5.84179065	-1.06465741	3.620237691
H	7.267278662	2.036721499	5.162588659
H	6.767115833	4.344064665	4.445792351

H	4.382543976	2.827837882	1.205140585
H	4.870679903	0.516712525	1.916062678
H	2.981518298	-1.338320265	-0.941115837
H	5.321275229	4.759030158	2.461861866
H	13.49262465	1.356349948	-0.864233324
H	11.17979063	-4.756933924	2.385383395

$Zr(CH_2Ph)_4$ S_4 symmetry constraint

-1130.45107676578 Hartrees

atom	x	y	z
Zr	0	0	0
C	0.024388962	1.766166116	-1.441227395
C	1.488920578	1.991580032	-1.554773266
C	2.283239191	1.210177905	-2.422851049
C	3.670977098	1.341525614	-2.454196056
C	4.311909422	2.259462814	-1.620402009
C	3.543975047	3.052836497	-0.763254858
C	2.157680853	2.921649677	-0.729520324
H	-0.431169736	1.454122799	-2.388251164
H	-0.519170443	2.627825262	-1.043412213
H	1.798001452	0.50368469	-3.092833095
H	4.252322898	0.728639395	-3.138555422
H	4.029987367	3.780655869	-0.118428779
H	1.571948909	3.546160905	-0.058497355
C	-0.024388962	-1.766166116	-1.441227395
C	-1.488920578	-1.991580032	-1.554773266
C	-2.283239191	-1.210177905	-2.422851049
C	-3.670977098	-1.341525614	-2.454196056

C	-4.311909422	-2.259462814	-1.620402009
C	-3.543975047	-3.052836497	-0.763254858
C	-2.157680853	-2.921649677	-0.729520324
H	0.431169736	-1.454122799	-2.388251164
H	0.519170443	-2.627825262	-1.043412213
H	-1.798001452	-0.50368469	-3.092833095
H	-4.252322898	-0.728639395	-3.138555422
H	-4.029987367	-3.780655869	-0.118428779
H	-1.571948909	-3.546160905	-0.058497355
C	1.766166116	-0.024388962	1.441227395
C	1.991580032	-1.488920578	1.554773266
C	1.210177905	-2.283239191	2.422851049
C	1.341525614	-3.670977098	2.454196056
C	2.259462814	-4.311909422	1.620402009
C	3.052836497	-3.543975047	0.763254858
C	2.921649677	-2.157680853	0.729520324
H	1.454122799	0.431169736	2.388251164
H	2.627825262	0.519170443	1.043412213
H	0.50368469	-1.798001452	3.092833095
H	0.728639395	-4.252322898	3.138555422
H	3.780655869	-4.029987367	0.118428779
H	3.546160905	-1.571948909	0.058497355
C	-1.766166116	0.024388962	1.441227395
C	-1.991580032	1.488920578	1.554773266
C	-1.210177905	2.283239191	2.422851049
C	-1.341525614	3.670977098	2.454196056
C	-2.259462814	4.311909422	1.620402009
C	-3.052836497	3.543975047	0.763254858

C	-2.921649677	2.157680853	0.729520324
H	-1.454122799	-0.431169736	2.388251164
H	-2.627825262	-0.519170443	1.043412213
H	-0.50368469	1.798001452	3.092833095
H	-0.728639395	4.252322898	3.138555422
H	-3.780655869	4.029987367	0.118428779
H	-3.546160905	1.571948909	0.058497355
H	-5.393133968	-2.361472658	-1.643710932
H	-2.361472658	5.393133968	1.643710932
H	5.393133968	2.361472658	-1.643710932
H	2.361472658	-5.393133968	1.643710932

$Zr(CH_2Ph)_4$ Monoclinic Zr–CH_2–Ph angle constraints

-1130.45052426791 Hartrees

atom	x	y	z
Zr	0.12881304	0.045019238	-0.371135449
C	-0.074928406	0.242016527	1.925901307
C	1.385375669	0.330237541	1.852148639
C	-0.244929732	-2.25623909	-0.35744257
C	-1.587428264	-1.825296213	-0.747437242
C	-1.315551441	1.694787989	-1.102992374
C	-0.811869851	2.979917232	-0.551537439
C	2.043175968	0.411763005	-1.621901312
C	1.629522031	-0.274462248	-2.868424769
H	-0.582623785	1.162685791	2.21278003
H	-0.468529218	-0.635351274	2.438338472
C	2.025983581	1.544438601	1.488810865
H	1.438873944	2.457646547	1.428491806

C	3.408815179	1.599478227	1.292734096
H	3.872408411	2.550351453	1.044352942
C	4.190025911	0.452182965	1.409579451
H	5.264130396	0.499106344	1.255816396
C	3.574760714	-0.766134858	1.725003177
H	4.173691861	-1.66873391	1.816661043
C	2.201661721	-0.832265685	1.929016756
H	1.739138936	-1.779638789	2.192701661
H	0.323415165	-2.774734284	-1.128200114
H	-0.168488157	-2.730133846	0.620886161
C	-1.866418931	-1.429682891	-2.082344501
H	-1.124789859	-1.609325497	-2.856493077
C	-3.115764903	-0.907128865	-2.434323097
H	-3.307169286	-0.642023298	-3.470662699
C	-4.106632155	-0.72650318	-1.474275056
H	-5.075784323	-0.322242265	-1.751539829
C	-3.841525355	-1.075367985	-0.142344287
H	-4.608604734	-0.940851544	0.616146983
C	-2.607693756	-1.598809941	0.218739126
H	-2.421698143	-1.883260905	1.25083286
H	-1.31680196	1.686227918	-2.19814239
H	-2.326066705	1.450949128	-0.758086827
C	0.18449722	3.730042247	-1.214639808
H	0.534540636	3.397315763	-2.189200901
C	0.721715838	4.889916401	-0.658315653
H	1.48606253	5.43993946	-1.202190185
C	0.281302186	5.349415709	0.585002261
H	0.701136138	6.251523925	1.020728775

C	-0.719744098	4.636779979	1.251602015
H	-1.08825118	4.989377114	2.211864714
C	-1.255670973	3.477322805	0.693807761
H	-2.041236084	2.941782425	1.222369799
H	2.190338938	1.487929084	-1.749341638
H	2.92119326	-0.029260475	-1.142854595
C	0.862613598	0.383967463	-3.857633695
H	0.638123897	1.440404635	-3.733936263
C	0.407738958	-0.280836861	-4.995566221
H	-0.174720996	0.26174987	-5.736195397
C	0.701019853	-1.631872041	-5.19043742
H	0.344139037	-2.15182571	-6.074924549
C	1.472178775	-2.302653113	-4.235795084
H	1.723632488	-3.350361768	-4.381310292
C	1.928526645	-1.637381876	-3.100861359
H	2.537797096	-2.170795545	-2.37458598

$Zr(CH_2Ph)_4$ Orthorhombic Zr–CH_2–Ph angle constraints

-1130.44909871992 Hartrees

atom	x	y	z
Zr	0.013625841	-0.073732513	-0.116797268
C	-0.046798658	0.04592766	2.173687535
C	1.424648697	0.101357619	2.134185943
C	1.974531075	-0.435547444	-1.307325335
C	1.446031281	0.157910549	-2.556628475
C	-0.574049737	2.132002168	-0.360749492
C	-1.985708593	1.741151186	-0.542523595
C	-1.438667745	-1.822726596	-0.585385927

C	-0.661101185	-2.939074655	0.015252873
C	2.110128935	1.340660568	2.038885838
C	3.487039632	1.392977543	1.852909063
C	4.232949252	0.214031621	1.737334159
C	3.580907731	-1.016059594	1.81199071
C	2.198137221	-1.078444092	1.995277366
C	1.744430251	1.490528372	-2.931816295
C	1.194086846	2.069921044	-4.069709308
C	0.321220996	1.342842173	-4.888145919
C	0.019898232	0.024090064	-4.550796592
C	0.570183673	-0.557431805	-3.406787003
C	-2.464877013	1.303153677	-1.800611972
C	-3.760861354	0.803870227	-1.947121235
C	-4.615157382	0.715705903	-0.849300226
C	-4.163282707	1.142173404	0.404838254
C	-2.874475713	1.640545124	0.557166249
C	-0.845985655	-3.339745952	1.35826712
C	-0.069207731	-4.341922728	1.938932995
C	0.925148451	-4.989314824	1.200415836
C	1.111443103	-4.63035147	-0.136840912
C	0.331917937	-3.631130346	-0.716329315
H	-0.525629315	0.94108479	2.572296302
H	-0.451953739	-0.860880309	2.625096176
H	1.709269293	-2.046511263	2.071115971
H	4.149743538	-1.938140601	1.726102448
H	5.308872595	0.258873613	1.594372405
H	3.985554608	2.357815854	1.802549465
H	1.544277958	2.262847809	2.141677023

H	2.8396859	0.08591257	-0.892447833
H	2.163036981	-1.509752284	-1.371916285
H	2.427957149	2.06610326	-2.311692648
H	1.450494786	3.094441555	-4.327886734
H	-0.106876062	1.796507423	-5.777422596
H	-0.641036031	-0.563295909	-5.183429499
H	0.348107361	-1.597452648	-3.184313937
H	-0.386885405	2.730077625	0.533618706
H	-0.120672214	2.587495228	-1.242707626
H	-1.818439109	1.384538749	-2.671383623
H	-4.103064918	0.484779072	-2.928224305
H	-5.622354079	0.32556122	-0.965040986
H	-4.823389555	1.089173734	1.267083535
H	-2.540259671	1.977953431	1.534849955
H	-2.39889148	-1.643421737	-0.091802161
H	-1.595955631	-1.934180171	-1.661475637
H	-1.62717483	-2.862297593	1.945214021
H	-0.245781798	-4.623355565	2.97421811
H	1.531988765	-5.768303169	1.652952102
H	1.863548958	-5.136902383	-0.736822342
H	0.4804947	-3.38857946	-1.765682018

Table 2. Cartesian coordinates for geometry optimized structures of $Zr(CH_2Ph)_4$ in which one of the benzyl Zr–C–C angles is constrained.

Zr–CH_2–Ph angle fixed at 70˚

-1130.44071569975 Hartrees

atom	x	y	z
Zr	0.047195395	0.002602372	-0.003736116
C	-0.021975409	-0.061637785	2.47559592
C	1.346317784	-0.04787493	2.020563106
C	-1.166306385	1.86261403	-0.61002917
C	-0.56699064	3.016628782	0.105738653
C	0.508310203	3.749377238	-0.443395804
C	1.128943375	4.776274052	0.2666766
C	0.697685405	5.113274196	1.55242138
C	-0.379054318	4.415492561	2.107685474
C	-0.999955026	3.388708121	1.397935272
H	-1.103479546	1.966158895	-1.699647988
H	-2.211356927	1.688841074	-0.329620208
H	0.846064577	3.508452658	-1.447933705
H	1.950929223	5.322609615	-0.190332816
H	-0.740734112	4.676606364	3.099386165
H	-1.843610546	2.863700995	1.840763265
C	1.808228674	-0.321141652	-1.453094082
C	1.311580786	0.191249323	-2.752890742
C	1.672560123	1.472312726	-3.227006987
C	1.136589943	1.99132774	-4.401254708
C	0.217138655	1.250024781	-5.151099649
C	-0.13778268	-0.026536302	-4.716769123

C	0.403376166	-0.549148348	-3.540572215
H	2.750554245	0.129305344	-1.13719387
H	1.920203044	-1.412825759	-1.45634935
H	2.394209186	2.055868604	-2.659753465
H	1.440201609	2.97908601	-4.739549788
H	-0.831732874	-0.626049536	-5.301026901
H	0.142847426	-1.560898618	-3.236906575
C	2.072431828	-1.255285378	1.76342119
C	3.402571656	-1.235192078	1.36296024
C	4.069696353	-0.02382659	1.137184384
C	3.362783812	1.16644126	1.286442657
C	2.02201816	1.165954421	1.685810503
H	-0.410055175	-0.989392466	2.884606788
H	-0.430725466	0.856159882	2.886300767
H	1.590966714	-2.206279886	1.975702201
H	3.929111604	-2.176729223	1.228816092
H	3.851146167	2.11907949	1.098745033
H	1.521862784	2.11337355	1.862864273
C	-0.918300933	-2.057416324	-0.180352542
C	-2.287449028	-1.502403626	-0.294650642
C	-3.06384757	-1.222441789	0.854963086
C	-4.294988371	-0.580995565	0.759073335
C	-4.794643858	-0.189147482	-0.486489712
C	-4.051159992	-0.460353452	-1.63558885
C	-2.817689784	-1.104000684	-1.543285456
H	-0.761440185	-2.681754619	0.702781417
H	-0.583367348	-2.585141245	-1.07849004
H	-2.688863894	-1.524520355	1.828864707

H	-4.870279948	-0.386806859	1.660705664
H	-4.431813816	-0.168443962	-2.610773242
H	-2.2533	-1.30960119	-2.449115222
H	-0.203178293	1.658219467	-6.065747653
H	-5.754339362	0.314484881	-0.558712224
H	1.181526134	5.913207209	2.105626043
H	5.113482962	-0.01621763	0.839056253

Zr–CH_2–Ph angle fixed at 75˚

-1130.44613926602 Hartrees

atom	x	y	z
Zr	0.048867803	0.023738073	0.023213987
C	-0.00409472	0.010185991	2.415136385
C	1.409088103	-0.002533269	2.069716212
C	-1.11898328	1.899390394	-0.613493588
C	-0.503218798	3.030318839	0.125934512
C	0.609141138	3.731436452	-0.389813159
C	1.242355619	4.734759141	0.343189864
C	0.788123379	5.077673736	1.619174574
C	-0.324060007	4.410391533	2.14191168
C	-0.957715377	3.408157736	1.409247407
H	-1.029301839	2.008057111	-1.700491448
H	-2.173297655	1.74880795	-0.355521916
H	0.96581513	3.485407908	-1.386463447
H	2.092882547	5.257372353	-0.088476396
H	-0.702954506	4.676282466	3.125861709
H	-1.827895711	2.906369868	1.826946777
C	1.855715978	-0.290177091	-1.372546212

C	1.431229489	0.236214749	-2.692596263
C	1.856673279	1.501805916	-3.153421916
C	1.388483292	2.035972729	-4.350105071
C	0.47616454	1.325246495	-5.136816284
C	0.059274505	0.062971314	-4.715512067
C	0.53210047	-0.474482485	-3.516988453
H	2.796241006	0.134625422	-1.017135081
H	1.944943147	-1.384644052	-1.378442154
H	2.574744977	2.061221807	-2.557912563
H	1.740754672	3.011482239	-4.67669475
H	-0.629974541	-0.513944525	-5.327466832
H	0.223158574	-1.475423921	-3.223101061
C	2.111780865	-1.224611872	1.849401189
C	3.454511673	-1.235966883	1.489367453
C	4.149767973	-0.038370795	1.284725223
C	3.470675543	1.170803497	1.425561827
C	2.121040214	1.197874197	1.785570334
H	-0.406964	-0.900991848	2.851510686
H	-0.398373227	0.931989891	2.834776074
H	1.597794651	-2.163566716	2.040720247
H	3.965819434	-2.187490605	1.368463097
H	3.990227805	2.1108313	1.25977055
H	1.628810537	2.153347782	1.940835575
C	-0.910748788	-2.03165529	-0.227613707
C	-2.278490169	-1.47351532	-0.338361742
C	-3.060494968	-1.214454616	0.812232955
C	-4.291482659	-0.571299512	0.721896102
C	-4.784314797	-0.156613273	-0.518781581

C	-4.033332351	-0.404500553	-1.66872059
C	-2.800437213	-1.049248757	-1.582055935
H	-0.760366689	-2.669665033	0.647712734
H	-0.570279922	-2.545836913	-1.130771813
H	-2.692029416	-1.537340836	1.782293894
H	-4.871946231	-0.394980508	1.623925444
H	-4.408364881	-0.093334921	-2.640129078
H	-2.229026614	-1.235376525	-2.487929713
H	0.108980332	1.744969173	-6.068957102
H	-5.744271807	0.347095732	-0.587038006
H	1.281697709	5.858920491	2.190191377
H	5.200947041	-0.053211138	1.013015505

Zr–CH_2–Ph angle fixed at 80˚

-1130.44933814005 Hartrees

atom	x	y	z
Zr	0.063714149	0.011641506	0.026066796
C	-0.023935525	0.01257061	2.361370211
C	1.425428056	-0.001599451	2.161522386
C	-1.065577973	1.881751218	-0.675180226
C	-0.442930594	3.012226782	0.059160744
C	0.696792983	3.67763821	-0.443395452
C	1.32950593	4.685665344	0.28290718
C	0.847040622	5.066975373	1.53684046
C	-0.288685784	4.431976855	2.048081357
C	-0.921921289	3.424753446	1.322551552
H	-0.949323995	1.970031011	-1.761498824
H	-2.127669372	1.75547648	-0.437490332

H	1.074789205	3.401214305	-1.423842675
H	2.201536921	5.181804656	-0.13679037
H	-0.685548159	4.727405249	3.016377454
H	-1.811274748	2.948047059	1.729242228
C	1.945152097	-0.305971078	-1.260322252
C	1.643602449	0.273582257	-2.592683827
C	2.204762112	1.501536411	-3.006149308
C	1.852649537	2.092439421	-4.216530043
C	0.923843008	1.479312083	-5.062927921
C	0.372088498	0.254498721	-4.687249837
C	0.730118368	-0.341185447	-3.476799972
H	2.877330791	0.064883948	-0.828262158
H	1.987745264	-1.403817247	-1.293206703
H	2.935057574	1.986239916	-2.362025667
H	2.309005148	3.036183107	-4.505679192
H	-0.33416434	-0.247392655	-5.344260019
H	0.314324242	-1.312924014	-3.217929188
C	2.136146232	-1.224467646	2.005272691
C	3.498887384	-1.240722728	1.728597261
C	4.204177189	-0.044345232	1.558633243
C	3.522536493	1.168472715	1.659339837
C	2.154448036	1.197495746	1.935926884
H	-0.447114683	-0.892075088	2.796775055
H	-0.439045884	0.929783367	2.775452058
H	1.606674186	-2.16162193	2.161116881
H	4.016636667	-2.192570693	1.643284243
H	4.055301727	2.105805729	1.523204492
H	1.650030641	2.153177602	2.045498493

C	-0.897141406	-2.032254287	-0.30484378
C	-2.267421449	-1.473789499	-0.381861859
C	-3.028943981	-1.239117238	0.787165801
C	-4.258520569	-0.588384014	0.733410351
C	-4.770952415	-0.143892119	-0.488372407
C	-4.041909629	-0.371156653	-1.657083523
C	-2.810690073	-1.022518299	-1.606622414
H	-0.736007479	-2.698526695	0.547882529
H	-0.566084638	-2.516883052	-1.227459851
H	-2.646423685	-1.586482882	1.743263595
H	-4.821327331	-0.429525254	1.649758428
H	-4.433136117	-0.037414611	-2.614505378
H	-2.255706329	-1.191455651	-2.526402417
H	0.646504635	1.943891389	-6.004798126
H	-5.728679104	0.366981986	-0.528222354
H	1.340561925	5.852421242	2.102498229
H	5.269589042	-0.061686477	1.348508977

Zr–CH_2–Ph angle fixed at 85˚

-1130.45091947076 Hartrees

atom	x	y	z
Zr	0.013858277	0.003087549	-0.033703918
C	-0.056250275	-0.006457284	2.266277252
C	1.41079053	-0.004730469	2.182874871
C	-1.088577837	1.86814393	-0.771903751
C	-0.461696783	2.996952193	-0.036297392
C	0.700458036	3.635116373	-0.521757595
C	1.331945763	4.644188507	0.204346243

C	0.826155445	5.052342354	1.440373952
C	-0.329794873	4.441449191	1.935602586
C	-0.961715872	3.432909303	1.210695123
H	-0.953825741	1.945587297	-1.856982773
H	-2.155856051	1.75793862	-0.549932531
H	1.097964068	3.33842922	-1.488470254
H	2.221217083	5.120300025	-0.202240263
H	-0.743378312	4.756940724	2.890465935
H	-1.866805686	2.975418482	1.604614953
C	1.947220409	-0.296469731	-1.23634854
C	1.784666086	0.323938468	-2.576627418
C	2.45126888	1.519585218	-2.918735098
C	2.242480886	2.144351672	-4.146215946
C	1.357588422	1.59754967	-5.079542187
C	0.700846217	0.405639184	-4.771101292
C	0.914753584	-0.222788474	-3.543987441
H	2.854818191	0.031365022	-0.722843616
H	1.966814118	-1.394676682	-1.299208805
H	3.149573596	1.95242861	-2.205807116
H	2.777572967	3.062026295	-4.379156904
H	0.023707873	-0.043795307	-5.493468089
H	0.41514847	-1.166954382	-3.334933313
C	2.138472517	-1.218663913	2.067719386
C	3.513991948	-1.220542978	1.859603482
C	4.212714721	-0.015605618	1.73186816
C	3.516333397	1.191274511	1.81455678
C	2.136932937	1.203474511	2.021944328
H	-0.487560804	-0.914529497	2.691487508

H	-0.500030428	0.896372791	2.686906327
H	1.609400056	-2.161988885	2.184525645
H	4.04618849	-2.165981797	1.794415975
H	4.047958997	2.134048328	1.716327609
H	1.614179847	2.152331102	2.103762045
C	-0.93628532	-2.025640231	-0.463266458
C	-2.3197256	-1.492976198	-0.470822152
C	-3.042361281	-1.316809705	0.732475664
C	-4.284923902	-0.688118738	0.747421292
C	-4.849352128	-0.209978234	-0.437650546
C	-4.159686778	-0.381739158	-1.639781934
C	-2.916194711	-1.010256657	-1.657733147
H	-0.737614532	-2.733201952	0.348197761
H	-0.624569132	-2.456177527	-1.418865457
H	-2.619942939	-1.69236788	1.660845557
H	-4.816111495	-0.573184142	1.688880009
H	-4.592323819	-0.022133539	-2.56964319
H	-2.391883366	-1.13671028	-2.602354556
H	1.192139092	2.087550765	-6.034821685
H	-5.816370535	0.284485365	-0.424160918
H	1.318042881	5.839652009	2.005027269
H	5.286937142	-0.020390244	1.570701755

Zr–CH_2–Ph angle fixed at 90˚

-1130.45155743985 Hartrees

atom	x	y	z
Zr	0.019570618	0.017308068	-0.035783396
C	-0.038383889	-0.002367809	2.243555561

C	1.436640789	0.003315411	2.281108616
C	-1.079184132	1.875795782	-0.787227896
C	-0.48247602	3.000396191	-0.020209099
C	0.69133428	3.648725244	-0.461494095
C	1.292603976	4.654811082	0.293987898
C	0.743521923	5.049094508	1.515673137
C	-0.424544986	4.427451155	1.96711774
C	-1.026101398	3.422177452	1.213162938
H	-0.90410216	1.962442625	-1.866117607
H	-2.153504598	1.760518002	-0.606749445
H	1.121045441	3.363788373	-1.417975544
H	2.192087308	5.139161512	-0.078821886
H	-0.871220391	4.731910216	2.910507949
H	-1.940690088	2.955389337	1.572930235
C	1.998189403	-0.23881822	-1.163975693
C	1.874200146	0.365221647	-2.516640281
C	2.522586181	1.574251643	-2.845679181
C	2.341891046	2.183505251	-4.085594183
C	1.505657962	1.606628642	-5.04497369
C	0.869449782	0.400344827	-4.749804408
C	1.054488398	-0.212059285	-3.509963903
H	2.874013832	0.117302517	-0.613915131
H	2.04911641	-1.337203908	-1.213831997
H	3.184124884	2.030611394	-2.112751468
H	2.860948472	3.112999362	-4.30732701
H	0.230556167	-0.072319904	-5.491985634
H	0.570752601	-1.166325245	-3.310048993
C	2.173368417	-1.206031168	2.22970799

C	3.559980826	-1.205846536	2.112481833
C	4.261527624	0.000577621	2.029586535
C	3.557931065	1.2058127	2.074709169
C	2.168344598	1.212783986	2.190554752
H	-0.489920066	-0.912061976	2.648754628
H	-0.507464821	0.891054412	2.660484476
H	1.639291541	-2.151205395	2.304392593
H	4.097346805	-2.150232557	2.083168302
H	4.093488189	2.149779928	2.017526223
H	1.63649592	2.160094892	2.232904089
C	-0.919487946	-2.004894925	-0.515721177
C	-2.295576845	-1.458673145	-0.594918519
C	-3.06421172	-1.247107175	0.57367089
C	-4.299720917	-0.605548801	0.523210474
C	-4.810003607	-0.149828314	-0.694489188
C	-4.073305955	-0.355697872	-1.863186125
C	-2.836873902	-0.995925987	-1.8158724
H	-0.770331739	-2.710035225	0.308443244
H	-0.563976887	-2.443356086	-1.452052669
H	-2.68517871	-1.607340109	1.526886043
H	-4.868151427	-0.464035521	1.438903902
H	-4.463895009	-0.01310168	-2.817794406
H	-2.27484017	-1.147153249	-2.734702598
H	1.361607432	2.08474276	-6.009698868
H	-5.771781502	0.353484105	-0.732336837
H	1.211827987	5.833950123	2.103161255
H	5.343737946	-0.000888508	1.934936103

Zr–CH_2–Ph angle fixed at 95˚

-1130.45122471032 Hartrees

atom	x	y	z
Zr	-0.013323261	0.020058983	-0.030591062
C	-0.01870516	0.006901129	2.237298414
C	1.455719094	0.006359565	2.369819303
C	-1.110653928	1.876837059	-0.784801025
C	-0.509362892	3.001974435	-0.020063272
C	0.667920983	3.643499129	-0.461749989
C	1.271735064	4.65035778	0.29091211
C	0.721298045	5.052528582	1.50912846
C	-0.450178414	4.437514132	1.960764164
C	-1.053804457	3.431016989	1.210232737
H	-0.93340301	1.960744237	-1.863849683
H	-2.186127523	1.768349509	-0.607153243
H	1.098292939	3.354077192	-1.416632863
H	2.174063556	5.129298629	-0.081918251
H	-0.898199136	4.748570536	2.901376217
H	-1.971139411	2.969576777	1.5702024
C	1.989855608	-0.215465451	-1.108489557
C	1.915295106	0.377318387	-2.470801171
C	2.579553071	1.580362327	-2.788004503
C	2.449036933	2.175281475	-4.041503391
C	1.649153808	1.588919695	-5.025544329
C	0.996728057	0.388684668	-4.740271773
C	1.130870425	-0.208599588	-3.486742841
H	2.837754242	0.157683097	-0.525713232
H	2.060695111	-1.313539152	-1.146803693

H	3.214340445	2.043085962	-2.035704091
H	2.979414021	3.100509757	-4.254033768
H	0.384723769	-0.090623342	-5.500583027
H	0.634508738	-1.157704146	-3.292972408
C	2.187023324	-1.204289206	2.353877322
C	3.578911223	-1.209412755	2.32749305
C	4.288314285	-0.005715624	2.310035412
C	3.58721677	1.202318028	2.331918984
C	2.193692958	1.212991124	2.356978631
H	-0.489346386	-0.900623017	2.629988731
H	-0.502345913	0.895030487	2.652277934
H	1.645671773	-2.148135084	2.37609097
H	4.113330434	-2.155883545	2.318988075
H	4.129261567	2.144416295	2.327814542
H	1.662158233	2.161567691	2.374408447
C	-0.952090439	-1.996986979	-0.527539475
C	-2.332246319	-1.456534718	-0.579101362
C	-3.079646979	-1.253055156	0.604556439
C	-4.31931059	-0.617253772	0.579959218
C	-4.854766227	-0.159856334	-0.626084605
C	-4.138797379	-0.357799955	-1.809254226
C	-2.898612744	-0.991867715	-1.787662635
H	-0.787610966	-2.711031819	0.286216415
H	-0.609455566	-2.423591725	-1.474111535
H	-2.682285459	-1.616650477	1.549205476
H	-4.870967571	-0.48228765	1.506833814
H	-4.549126992	-0.014105136	-2.755175306
H	-2.353527174	-1.138073668	-2.717497475

H	1.544367272	2.05541984	-6.000995361
H	-5.819818628	0.338318401	-0.644228105
H	1.191172295	5.838490727	2.093881306
H	5.37434935	-0.01022142	2.284775251

Zr–CH_2–Ph angle fixed at 100˚

-1130.45057973266 Hartrees

atom	x	y	z
Zr	0.004008791	0.005517905	0.008894382
C	0.010237296	0.018310809	2.271005417
C	1.473146842	0.003009305	2.524912181
C	-1.105885385	1.841110417	-0.772933754
C	-0.543561524	2.969943716	0.016266538
C	0.648870053	3.616509576	-0.374872766
C	1.217094751	4.624402153	0.404122252
C	0.614101996	5.022855684	1.598240471
C	-0.572938812	4.402797865	1.99939331
C	-1.140654042	3.395084839	1.22318317
H	-0.886606098	1.929261336	-1.844107374
H	-2.186171897	1.721767315	-0.638181085
H	1.120893577	3.33007063	-1.310971742
H	2.132896396	5.106630146	0.070560174
H	-1.061091965	4.710718641	2.920840409
H	-2.069793296	2.928688437	1.54446395
C	2.037372911	-0.173627203	-1.01073633
C	2.011757182	0.406128806	-2.381984863
C	2.676167934	1.612076282	-2.685631931
C	2.593899331	2.189894386	-3.951652943

C	1.844267768	1.582845604	-4.962509473
C	1.192766092	0.378771298	-4.688907783
C	1.278035687	-0.200731669	-3.422726322
H	2.846604789	0.229510066	-0.392972912
H	2.145784672	-1.269586922	-1.035699891
H	3.273966929	2.091094707	-1.913393878
H	3.124014669	3.117933006	-4.152021433
H	0.619577805	-0.117714751	-5.468184279
H	0.782261149	-1.152202071	-3.237761592
C	2.188099013	-1.213253189	2.591452758
C	3.575837965	-1.231796914	2.709985135
C	4.295017093	-0.035577609	2.762189129
C	3.606730823	1.178743574	2.703350372
C	2.218451309	1.201514085	2.58346198
H	-0.494147454	-0.879277791	2.648304345
H	-0.489791498	0.91060909	2.659577116
H	1.638542719	-2.152305436	2.563089775
H	4.098178484	-2.183566725	2.764323368
H	4.155229168	2.115955608	2.752706439
H	1.696481288	2.154731709	2.540975234
C	-0.891631026	-2.034943411	-0.472960047
C	-2.269753687	-1.500548883	-0.584477836
C	-3.049911648	-1.25660003	0.570341769
C	-4.285176047	-0.616531978	0.489725543
C	-4.783277961	-0.195923974	-0.745209828
C	-4.035233673	-0.435563021	-1.900604062
C	-2.79938002	-1.073392317	-1.823303012
H	-0.751942684	-2.725978632	0.365187913

H	-0.512934944	-2.482354409	-1.395952234
H	-2.682211643	-1.591802162	1.53746137
H	-4.862440504	-0.449031836	1.395412348
H	-4.416665914	-0.120704577	-2.868335303
H	-2.228207789	-1.25139128	-2.731684842
H	1.778472766	2.034840366	-5.947926621
H	-5.744370233	0.306250149	-0.807046391
H	1.055867266	5.80977864	2.203253563
H	5.377451278	-0.050007617	2.85315047

Zr–CH_2–Ph angle fixed at 105˚

-1130.45301579180 Hartrees

atom	x	y	z
Zr	0.005548798	0.446246884	-0.333320427
C	0.139217395	0.465098395	1.964025966
C	1.505729994	-0.030198419	2.273893025
C	-1.66591179	1.480439302	-1.502107474
C	-2.056427317	2.131753888	-0.24036149
C	-1.473058279	3.359164685	0.166848905
C	-1.718166452	3.896273819	1.426974994
C	-2.539577265	3.223224043	2.338232099
C	-3.11690998	2.008956418	1.965582521
C	-2.875016799	1.4630094	0.704085787
H	-1.302362917	2.162224431	-2.274527398
H	-2.399173094	0.775395628	-1.897258028
H	-0.839666734	3.897448509	-0.534616361
H	-1.266521862	4.846240553	1.70105694
H	-3.759409615	1.476485084	2.661698495

H	-3.34447907	0.522051502	0.426104182
C	1.786991259	1.691187653	-1.044094118
C	2.194132167	0.543396572	-1.871525635
C	1.707930597	0.379048104	-3.193485257
C	1.96965877	-0.775946579	-3.923354645
C	2.710971516	-1.818856384	-3.357750393
C	3.189881466	-1.687172836	-2.05433895
C	2.930777323	-0.531868098	-1.315411827
H	1.500500804	2.580645125	-1.610232187
H	2.475803174	1.934407025	-0.233148909
H	1.139946455	1.187205769	-3.64856361
H	1.596213336	-0.864564871	-4.940369672
H	3.769957322	-2.488840385	-1.604703323
H	3.326754187	-0.438956815	-0.306700925
C	1.78821234	-1.410975485	2.358794611
C	3.081247964	-1.881977215	2.582068055
C	4.143779455	-0.988263309	2.730326186
C	3.887761517	0.384449382	2.664028271
C	2.594813158	0.853086864	2.441337046
H	-0.643918822	-0.196710579	2.348970985
H	-0.04639799	1.478069654	2.337064595
H	0.973760724	-2.12470314	2.262894362
H	3.257777918	-2.953120773	2.646734923
H	4.701483462	1.094223871	2.791571966
H	2.412234893	1.924889244	2.403129464
C	-0.261693777	-1.790672514	-0.804285192
C	-1.667042109	-2.114194184	-0.441969395
C	-2.031620965	-2.442277058	0.88205463

C	-3.358718627	-2.672577263	1.241940855
C	-4.376652613	-2.584794061	0.290065616
C	-4.039266547	-2.278291794	-1.031797866
C	-2.711998511	-2.048817497	-1.38988372
H	0.464305743	-2.342951043	-0.197325949
H	-0.03793104	-1.974987	-1.860914764
H	-1.254956579	-2.531752119	1.637488856
H	-3.596807844	-2.928079137	2.271705385
H	-4.815984867	-2.222735114	-1.79068771
H	-2.467821817	-1.82146014	-2.425540914
H	2.913602153	-2.719962513	-3.929579004
H	-5.411079205	-2.763755594	0.569061014
H	-2.727731373	3.643848962	3.321598643
H	5.152074451	-1.35391462	2.903747988

Zr–CH_2–Ph angle fixed at 110˚

-1130.45264466609 Hartrees

atom	x	y	z
Zr	0.013507868	0.054110989	0.003934337
C	0.014171337	0.105227399	2.300392211
C	1.408671622	0.009818924	2.811227394
C	-1.859899292	0.417261307	-1.253792111
C	-2.547102839	0.841941433	-0.022214198
C	-2.492468587	2.187690889	0.422162836
C	-3.007603549	2.564190109	1.658737721
C	-3.581363892	1.61115554	2.506175057
C	-3.637937138	0.278854922	2.09686528
C	-3.123258768	-0.106728629	0.858871412

H	-1.733190386	1.207915988	-1.997699746
H	-2.250696905	-0.498001506	-1.701631741
H	-2.057731035	2.939833025	-0.232403467
H	-2.962161921	3.606323961	1.964445747
H	-4.083779259	-0.470208067	2.745825432
H	-3.187974864	-1.147355125	0.549370434
C	1.290054243	1.858868726	-0.582398717
C	2.079242132	0.941942696	-1.420891137
C	1.694543234	0.650080422	-2.754753358
C	2.342047889	-0.332518153	-3.497841232
C	3.38517179	-1.074326535	-2.934583751
C	3.772275858	-0.817780003	-1.618985775
C	3.126521394	0.163975465	-0.867176987
H	0.738703188	2.623861525	-1.13422645
H	1.831875116	2.283192456	0.264843319
H	0.892126673	1.227513027	-3.208355273
H	2.032345705	-0.52094116	-4.522580201
H	4.580945224	-1.388100088	-1.169967356
H	3.448142795	0.36027362	0.153325152
C	2.010498065	-1.236716634	3.086605242
C	3.335437152	-1.334282814	3.506530128
C	4.112042191	-0.185447193	3.670013182
C	3.535726486	1.061818204	3.417580625
C	2.20986257	1.156897271	2.996937721
H	-0.607059099	-0.730345617	2.642380648
H	-0.482286702	1.034934442	2.605138004
H	1.420510095	-2.143565968	2.980568074
H	3.761694001	-2.313337941	3.71224606

H	4.121767855	1.967504717	3.554155985
H	1.77413644	2.137785708	2.818430846
C	0.627257992	-2.122999825	-0.399059794
C	-0.593409757	-2.936400259	-0.155656903
C	-0.933785749	-3.388814522	1.137684588
C	-2.112806288	-4.09124966	1.381877075
C	-2.998882816	-4.36947852	0.339765795
C	-2.678554865	-3.944174521	-0.952594045
C	-1.499043159	-3.243113463	-1.194933914
H	1.436130862	-2.364706367	0.299945748
H	1.010111287	-2.220141996	-1.421054432
H	-0.250705894	-3.197420453	1.960818797
H	-2.336423206	-4.428097218	2.391365472
H	-3.351051481	-4.164837969	-1.777969088
H	-1.261336764	-2.927984288	-2.208849802
H	3.887807694	-1.841892385	-3.51586556
H	-3.918518636	-4.916124714	0.528842002
H	-3.980002705	1.906768535	3.472347169
H	5.145684791	-0.260418365	3.995965461

Zr–CH_2–Ph angle fixed at 115˚

-1130.45197546406 Hartrees

atom	x	y	z
Zr	-0.013497162	0.005303075	-0.008924114
C	0.020498606	0.037176772	2.281373285
C	1.378246136	0.022435905	2.890493182
C	-1.940079729	0.236012912	-1.215373885
C	-2.644011028	0.581679135	0.0321197

C	-2.691325835	1.918571673	0.502102579
C	-3.220039186	2.229437708	1.751243684
C	-3.70680614	1.218017154	2.584955152
C	-3.665374768	-0.106468452	2.148329298
C	-3.137444263	-0.42590978	0.897373721
H	-1.887296289	1.049874261	-1.94375933
H	-2.265917139	-0.696508511	-1.679712657
H	-2.323972753	2.715019614	-0.141218659
H	-3.253076777	3.265711686	2.077595503
H	-4.044797283	-0.900492133	2.786059889
H	-3.123631493	-1.462038834	0.56713207
C	1.108055299	1.925529191	-0.546297176
C	1.973859028	1.072437907	-1.373589832
C	1.6225257	0.747260875	-2.710206701
C	2.350173111	-0.186877329	-3.443035052
C	3.439689419	-0.848502544	-2.866954999
C	3.791839772	-0.56141065	-1.547042889
C	3.066341021	0.369944409	-0.803146408
H	0.506195449	2.649000344	-1.100819343
H	1.599745792	2.380338534	0.315573775
H	0.786684242	1.265342968	-3.17478623
H	2.066777607	-0.399757446	-4.470524584
H	4.635139622	-1.070014838	-1.08778918
H	3.359693043	0.590770823	0.220778846
C	2.023401271	-1.186717924	3.223747203
C	3.318619131	-1.207349083	3.737063219
C	4.019360608	-0.016264646	3.937228293
C	3.397824955	1.194844244	3.625221986

C	2.101565324	1.213259599	3.111518814
H	-0.572244132	-0.828678016	2.602556792
H	-0.546279838	0.933116088	2.56946349
H	1.491735203	-2.125315623	3.086449268
H	3.781530094	-2.15926256	3.986296811
H	3.924540405	2.132332314	3.786680133
H	1.629052155	2.166900378	2.885138573
C	0.803874158	-2.101791842	-0.408723417
C	-0.356419086	-3.012441046	-0.229717626
C	-0.718626959	-3.505255019	1.042478151
C	-1.846112975	-4.305446953	1.223383472
C	-2.656354104	-4.641465776	0.137272185
C	-2.31283892	-4.173589703	-1.134460764
C	-1.184844035	-3.376430085	-1.313803789
H	1.590925749	-2.27720669	0.33398092
H	1.246823645	-2.161945048	-1.408474865
H	-0.091668053	-3.268810973	1.898350035
H	-2.088342711	-4.672911744	2.217819756
H	-2.92610384	-4.436759118	-1.992794266
H	-0.92696712	-3.028416273	-2.311919093
H	4.00559022	-1.575740008	-3.441445048
H	-3.535395064	-5.264353957	0.27700909
H	-4.115296642	1.462307266	3.561301275
H	5.029908787	-0.031396957	4.335815277

Zr–CH_2–Ph angle fixed at 120˚

-1130.45088939287 Hartrees

atom	x	y	z
Zr	-0.013294868	-0.005670968	-0.01424887
C	0.004990463	0.003611492	2.26955337
C	1.299556236	-0.000854923	3.003251569
C	-1.952988199	0.201731904	-1.204074333
C	-2.670108099	0.530468018	0.041272427
C	-2.729113792	1.862191035	0.523522461
C	-3.272065868	2.158122926	1.770499345
C	-3.763380804	1.136235152	2.588305957
C	-3.714183542	-0.183546888	2.137154005
C	-3.172210042	-0.487458885	0.888857963
H	-1.908945006	1.022239655	-1.926225662
H	-2.266950517	-0.73011467	-1.678112033
H	-2.3580608	2.666939631	-0.107357527
H	-3.312028994	3.190819913	2.107405856
H	-4.098596217	-0.985290362	2.762112224
H	-3.149462502	-1.519977036	0.548017264
C	1.072890138	1.948977738	-0.496449944
C	1.987774351	1.125447144	-1.299377243
C	1.689770148	0.798797261	-2.648390439
C	2.46614214	-0.111807425	-3.361246186
C	3.552485668	-0.748605524	-2.752457588
C	3.85193321	-0.460716703	-1.41928439
C	3.077857123	0.446891143	-0.696131022
H	0.472106315	2.662438849	-1.064919759

H	1.521820875	2.407056473	0.386918179
H	0.857841142	1.298963651	-3.139332661
H	2.22287105	-0.325424926	-4.398879748
H	4.691829452	-0.950498643	-0.933925972
H	3.329697826	0.667611098	0.338888611
C	1.915663122	-1.203812536	3.403572909
C	3.157410002	-1.213680066	4.035916518
C	3.830955176	-0.017577642	4.291175579
C	3.236410911	1.187685782	3.911647247
C	1.994058623	1.195162943	3.278538292
H	-0.605597693	-0.86664836	2.546556074
H	-0.594382951	0.889601406	2.525387845
H	1.403463961	-2.146060085	3.222867545
H	3.599825244	-2.161336808	4.334057804
H	3.742328235	2.129086749	4.112423267
H	1.541436059	2.144335148	2.998624535
C	0.866509646	-2.085619356	-0.417455878
C	-0.277971785	-3.022540379	-0.276179001
C	-0.658565023	-3.53716309	0.98205322
C	-1.774476432	-4.360052109	1.128742864
C	-2.553570016	-4.698882729	0.021213084
C	-2.190663778	-4.210749038	-1.237470875
C	-1.074619202	-3.390104793	-1.382903256
H	1.635069828	-2.24834118	0.347503224
H	1.339616616	-2.128113948	-1.404142185
H	-0.054461133	-3.298579658	1.853629161
H	-2.031867571	-4.743160978	2.113320255
H	-2.779361062	-4.476111009	-2.112201953

H	-0.801536461	-3.025871402	-2.371258947
H	4.156058439	-1.457675912	-3.311105741
H	-3.423495967	-5.339667669	0.134286251
H	-4.182319315	1.368454478	3.563176145
H	4.799930201	-0.024544276	4.782579908

Zr–CH_2–Ph angle fixed at 125˚

-1130.44955329804 Hartrees

atom	x	y	z
Zr	0.076420293	0.239031916	-0.012299226
C	0.067766781	0.584176521	2.238163344
C	1.036444548	-0.012781664	3.196828345
C	-1.864953839	0.20221003	-1.206546842
C	-2.657662318	0.399806342	0.021774489
C	-2.903192528	1.699171288	0.530639878
C	-3.509849555	1.889071532	1.769336102
C	-3.885337258	0.790383455	2.5471011
C	-3.659366185	-0.500586821	2.063425974
C	-3.050194341	-0.697662096	0.825968354
H	-1.925688225	1.032934064	-1.916073197
H	-2.029335451	-0.755940955	-1.704718641
H	-2.625785848	2.562326547	-0.071252588
H	-3.689000113	2.898015096	2.13154429
H	-3.955067794	-1.362231212	2.656147489
H	-2.880661274	-1.708255083	0.464156478
C	1.078207736	2.170155456	-0.722875523
C	1.911438227	1.375333673	-1.646625567
C	1.418330581	0.976898056	-2.914701247

C	2.130732721	0.09458278	-3.724373437
C	3.353222682	-0.431224862	-3.296450892
C	3.858227463	-0.054666256	-2.049420992
C	3.148830348	0.824858745	-1.233458953
H	0.375136822	2.846692632	-1.216828188
H	1.640715349	2.694483279	0.053404518
H	0.475119025	1.388472786	-3.266244416
H	1.730015599	-0.182762102	-4.695953418
H	4.809230614	-0.453916573	-1.70711913
H	3.559134351	1.111872069	-0.267748978
C	0.637115894	-0.992407222	4.126665434
C	1.554505949	-1.592983155	4.988274957
C	2.903443697	-1.235013702	4.949375197
C	3.318642874	-0.257673545	4.042936257
C	2.400107268	0.343529059	3.184092039
H	-0.960194056	0.481450715	2.605995017
H	0.252468776	1.672039441	2.147635331
H	-0.411407088	-1.278194056	4.171399893
H	1.212698028	-2.344027845	5.696596316
H	4.363817995	0.040483247	4.006542525
H	2.740188422	1.115040389	2.494760053
C	1.149120947	-1.751340678	-0.312464311
C	0.135525959	-2.801103461	-0.028519847
C	-0.123963362	-3.231877272	1.290197758
C	-1.113587941	-4.175993664	1.562269581
C	-1.877811332	-4.721399831	0.529036045
C	-1.633315917	-4.312519643	-0.78522947
C	-0.644941954	-3.369376696	-1.058502871

H	1.971760185	-1.761748517	0.414227363
H	1.568865135	-1.822208862	-1.321475286
H	0.469500887	-2.827198271	2.105863325
H	-1.282144018	-4.493116796	2.588705393
H	-2.212820468	-4.735943831	-1.602032891
H	-0.458973697	-3.069508463	-2.087926492
H	3.905447579	-1.120547422	-3.928134363
H	-2.64627731	-5.459512766	0.741811707
H	-4.354571945	0.939615948	3.515364463
H	3.618477727	-1.705925874	5.618161268

Zr–CH_2–Ph angle fixed at 130˚

-1130.44774207696 Hartrees

atom	x	y	z
Zr	0.049594726	0.080294513	0.021126878
C	-0.000924395	0.086043138	2.289231692
C	1.104781416	-0.084319821	3.271500227
C	-1.585037772	-1.019837111	-1.117622701
C	-2.255833169	-1.525189734	0.100391297
C	-3.236745754	-0.751485172	0.764898906
C	-3.763115417	-1.148187619	1.991225108
C	-3.325802781	-2.32907134	2.597777747
C	-2.368294273	-3.11590988	1.952842276
C	-1.836392164	-2.722413862	0.726142949
H	-2.203810794	-0.334583434	-1.706282203
H	-1.166068241	-1.803168792	-1.755409914
H	-3.591972754	0.165095439	0.297793971
H	-4.516882798	-0.534356459	2.477438602

H	-2.029962676	-4.042432231	2.409398774
H	-1.090891156	-3.345413997	0.237929384
C	-0.305519173	2.290343529	-0.439021257
C	0.634297552	2.250626431	-1.582782001
C	0.236153675	1.713962267	-2.830648905
C	1.151084277	1.52498676	-3.864962549
C	2.494846783	1.861254981	-3.689304789
C	2.909959697	2.401511075	-2.469232485
C	1.999034741	2.589493733	-1.432815869
H	-1.347203236	2.467851244	-0.725862803
H	-0.008699705	2.978516506	0.357061672
H	-0.809982687	1.46130928	-2.987338479
H	0.811365902	1.115359892	-4.81271066
H	3.951891783	2.674138064	-2.323671634
H	2.337461064	3.011900729	-0.489062912
C	1.199184284	-1.241687248	4.067512922
C	2.255327618	-1.42426008	4.959932294
C	3.253375253	-0.4562836	5.084578131
C	3.174817196	0.701553151	4.30812785
C	2.117812936	0.883576424	3.418111984
H	-0.854960337	-0.54491782	2.568127616
H	-0.374079584	1.129697306	2.329869157
H	0.426897239	-2.002725918	3.982338257
H	2.296820139	-2.32761265	5.564009738
H	3.940571792	1.468447077	4.397270401
H	2.068177352	1.797492443	2.828100694
C	2.077106983	-0.775674095	-0.558130512
C	1.948422051	-2.248749264	-0.387916452

C	2.122875649	-2.859513141	0.872187149
C	1.94391792	-4.231992303	1.042391999
C	1.584907452	-5.040505102	-0.037625912
C	1.412194123	-4.456216455	-1.295735944
C	1.590305989	-3.084832388	-1.467343059
H	2.80453199	-0.339208958	0.139303346
H	2.347780471	-0.483686951	-1.5785447
H	2.408845614	-2.248981524	1.724345609
H	2.092673806	-4.671421705	2.025780022
H	1.142630764	-5.074333466	-2.148691493
H	1.463546633	-2.646873307	-2.455409545
H	3.208138649	1.709232006	-4.494084334
H	1.448540105	-6.110259874	0.095746908
H	-3.733006798	-2.63562093	3.557090415
H	4.077148145	-0.599883851	5.778288507

Zr–CH_2–Ph angle fixed at 135˚

-1130.44617833927 Hartrees

atom	x	y	z
Zr	0.069822612	0.009407574	-0.097401159
C	0.362737852	0.639730843	2.059671891
C	1.101529586	0.085673274	3.227061672
C	-1.171091075	-1.790978559	-0.710777655
C	-1.807957347	-2.085835009	0.597696934
C	-2.960750541	-1.386314744	1.023091185
C	-3.53073591	-1.619407057	2.272975593
C	-2.966735834	-2.556268314	3.142282308
C	-1.820129903	-3.249099629	2.747137474

C	-1.242915615	-3.013439788	1.500537489
H	-1.89705544	-1.472923875	-1.469628236
H	-0.566693751	-2.614876167	-1.098372997
H	-3.426803712	-0.673221494	0.345958503
H	-4.424409192	-1.074096058	2.565917021
H	-1.370276169	-3.979221294	3.414913433
H	-0.353039337	-3.563419044	1.204228773
C	-1.200528675	1.780132802	-0.803264257
C	-0.188432683	2.051150422	-1.840605212
C	-0.188187758	1.329033399	-3.060569445
C	0.855962021	1.447884406	-3.975921489
C	1.945636122	2.279664723	-3.703932408
C	1.968048926	3.003218595	-2.508428672
C	0.926536223	2.888019569	-1.590175013
H	-2.175114372	1.472845136	-1.19129129
H	-1.307431751	2.569223235	-0.054876822
H	-1.036638538	0.68865634	-3.293222203
H	0.817961345	0.887660551	-4.906523322
H	2.805656726	3.659675044	-2.287999695
H	0.955857741	3.464886898	-0.668088109
C	0.460628808	-0.710211086	4.194295303
C	1.166810398	-1.247174074	5.269601753
C	2.534435167	-1.006507736	5.413638082
C	3.186111833	-0.213412053	4.467764646
C	2.479599027	0.324835752	3.392953442
H	-0.69423225	0.813273651	2.324911971
H	0.777657535	1.633259876	1.801093789
H	-0.603025138	-0.908555991	4.095968927

H	0.643248974	-1.855562524	6.003283898
H	4.249521071	-0.009471563	4.567594216
H	3.000804234	0.948833814	2.66929001
C	2.244629006	-0.218450639	-0.744760734
C	2.434109394	-1.689462646	-0.648456242
C	2.617545974	-2.322929115	0.60045629
C	2.703953451	-3.713046611	0.700682474
C	2.607816707	-4.51320028	-0.438158625
C	2.434054178	-3.904160917	-1.685143584
C	2.349224105	-2.518676645	-1.788482459
H	2.833227715	0.326635661	0.004450116
H	2.462185886	0.186216638	-1.73727104
H	2.711369679	-1.716246569	1.498107415
H	2.85438842	-4.169016544	1.676118458
H	2.368700386	-4.515177874	-2.582137591
H	2.219210788	-2.058220898	-2.765674114
H	2.760714286	2.368142237	-4.415899767
H	2.674262786	-5.594718135	-0.358972619
H	-3.415335479	-2.74356587	4.113902286
H	3.08295831	-1.42572192	6.25266142

Zr–CH_2–Ph angle fixed at 140˚

-1130.44459250456 Hartrees

atom	x	y	z
Zr	-0.024167821	-0.023038138	-0.022410595
C	0.013544119	0.062407891	2.236131738
C	0.982988291	0.005738306	3.362063604
C	0.625707093	-1.780260486	-1.306270589

C	0.712854006	-2.757062287	-0.194476415
C	-0.433141917	-3.451573328	0.261143981
C	-0.367483827	-4.328395745	1.341950233
C	0.841267116	-4.534802524	2.011036314
C	1.979889969	-3.842790158	1.592848778
C	1.918689033	-2.961668811	0.51471777
H	-0.159860428	-2.025882137	-2.030415773
H	1.574857393	-1.610593834	-1.819755412
H	-1.374848954	-3.321640214	-0.268286368
H	-1.261597563	-4.86035388	1.657163329
H	2.924475424	-3.989800842	2.109730971
H	2.815597426	-2.437325072	0.194303916
C	-2.294011592	0.042313644	-0.337714519
C	-2.098875562	1.286627454	-1.101776653
C	-1.730339874	1.250140271	-2.470588907
C	-1.376921649	2.408459837	-3.159451196
C	-1.36070438	3.6445172	-2.50724519
C	-1.716357669	3.706879405	-1.157576886
C	-2.070891863	2.551505887	-0.463716509
H	-2.66454914	-0.798917778	-0.928938256
H	-2.867335282	0.158641899	0.584930301
H	-1.751038461	0.297237415	-2.995433228
H	-1.111651857	2.345182364	-4.211486712
H	-1.713877807	4.662327966	-0.639729423
H	-2.355678941	2.619001845	0.584297828
C	1.253808394	-1.19410492	4.045141392
C	2.183022129	-1.239233663	5.083304889
C	2.870832871	-0.088288155	5.472729831

C	2.610222467	1.112991272	4.811533691
C	1.679742859	1.1584677	3.774226815
H	-0.782127285	-0.690576103	2.38664062
H	-0.500907948	1.044353557	2.251357507
H	0.728825004	-2.099347042	3.752831043
H	2.368581513	-2.180662251	5.595123309
H	3.131086657	2.020913825	5.106145852
H	1.481293424	2.105135564	3.275234965
C	1.308864798	1.778106742	-0.463283854
C	2.638950897	1.152520594	-0.688516958
C	3.42313222	0.691471464	0.391222859
C	4.634952037	0.031371631	0.176550741
C	5.100579779	-0.191981418	-1.119396557
C	4.341419327	0.263246385	-2.202518476
C	3.134305314	0.923150718	-1.990777488
H	1.287111323	2.386532546	0.449900479
H	0.96740375	2.387989996	-1.304633312
H	3.085817336	0.865827513	1.410085598
H	5.218379501	-0.303522535	1.030743421
H	4.697063693	0.105422367	-3.217870112
H	2.557686039	1.276469017	-2.843150714
H	-1.080734107	4.545620858	-3.044420517
H	6.043045097	-0.706418018	-1.285701253
H	0.893975523	-5.224224611	2.849040218
H	3.594383396	-0.125579244	6.282565082

Table 3. Cartesian coordinates for geometry optimized structures of $Me_3Zr(CH_2Ph)$ with constraints on the Zr-CH_2-Ph angle.

$Me_3Zr(CH_2Ph)$

-437.283341934335 Hartrees

atom	x	y	z
Zr	0.113483541	0.104001631	0.066811591
C	-0.115254907	0.324843588	2.330333834
C	1.319481817	0.066236403	2.574140802
C	2.275059752	1.104650201	2.476745482
C	3.641622639	0.839012105	2.532041863
C	4.102237398	-0.471207855	2.679652977
C	3.176817748	-1.512358295	2.789085906
C	1.810073889	-1.250692049	2.734004362
H	-0.443014008	1.331613285	2.608798044
H	-0.785946804	-0.425964982	2.759785334
H	1.93022831	2.13168521	2.372930803
H	4.351028342	1.658997467	2.458828057
H	3.522642025	-2.53473286	2.917161269
H	1.100511167	-2.070464015	2.828296195
H	5.167712163	-0.677630556	2.718392333
C	-0.496426227	2.03618294	-0.884661982
H	-1.310416685	1.871099605	-1.605606813
H	-0.86537819	2.745052876	-0.128844966
H	0.33187208	2.518268637	-1.421279726
C	2.091500616	-0.453779789	-0.839221145
H	2.366772351	0.323794784	-1.568987626
H	2.935517195	-0.590141792	-0.154266363

H	1.957160471	-1.388258954	-1.406569199
C	-1.323296854	-1.470977598	-0.618695053
H	-1.818207209	-1.16811757	-1.55271115
H	-0.827005392	-2.433625427	-0.802925958
H	-2.109135435	-1.63605269	0.132916321

Zr–CH_2–Ph angle fixed at 70˚

-437.271306173114 Hartrees

atom	x	y	z
Zr	0.043435159	-0.029761754	-0.003305304
C	-0.029361222	-0.081793088	2.493372767
C	1.33814498	-0.012330245	2.041181953
C	1.987729438	1.231702894	1.76259118
C	3.312605277	1.284879331	1.33623915
C	4.049582301	0.11514128	1.120748654
C	3.415465933	-1.114756474	1.296202412
C	2.083080546	-1.184645412	1.70573177
H	-0.476760645	0.813865527	2.915414272
H	-0.391286731	-1.028362596	2.88478307
H	1.457836215	2.157067717	1.978318969
H	3.777912101	2.254768883	1.180408542
H	3.958538392	-2.037433287	1.109621338
H	1.628959005	-2.157835276	1.881668199
H	5.086093611	0.164656417	0.803335835
C	-0.894527849	1.907300948	-0.614684557
H	-1.746532168	1.717106455	-1.285082021
H	-1.277619814	2.461577523	0.254335945
H	-0.188984782	2.559186052	-1.146762779

C	1.722482805	-0.29429182	-1.477637612
H	1.430081515	0.301017892	-2.358743487
H	2.733656257	-0.000969599	-1.182049742
H	1.753209359	-1.346987093	-1.796550875
C	-1.310046188	-1.725396484	-0.571213448
H	-1.418615735	-1.770103376	-1.665476091
H	-0.948212761	-2.707854392	-0.238038019
H	-2.311592136	-1.576083968	-0.141971402

Zr–CH_2–Ph angle fixed at 75˚

-437.276960772433 Hartrees

atom	x	y	z
Zr	0.00808651	0.00521133	-0.066373457
C	0.020370868	-0.036233525	2.347354406
C	1.422636083	-0.018594559	1.964194316
C	2.10895253	1.199377517	1.686691879
C	3.440441105	1.20933498	1.274030179
C	4.137308537	0.014433807	1.077319212
C	3.470272621	-1.196518068	1.27756351
C	2.138077952	-1.218662484	1.685524313
H	-0.38097987	0.871056024	2.794836145
H	-0.362865294	-0.961007925	2.773765306
H	1.600785497	2.142441267	1.878502083
H	3.938373811	2.161294596	1.109808786
H	3.991674161	-2.136082562	1.115280157
H	1.651271114	-2.173184724	1.874120612
H	5.176126904	0.027002111	0.762696193
C	-1.061354537	1.871880898	-0.687589692

H	-1.807112763	1.631474442	-1.46062976
H	-1.598060082	2.329242359	0.15604472
H	-0.38217741	2.626572875	-1.106121621
C	1.71414201	-0.128174827	-1.523032967
H	1.527712117	0.650803752	-2.280373903
H	2.747121627	-0.033949727	-1.178041631
H	1.610480069	-1.098340206	-2.035106031
C	-1.234030289	-1.762916552	-0.661692092
H	-1.524297927	-1.682491379	-1.719674007
H	-0.702272211	-2.716635148	-0.539421779
H	-2.155815269	-1.813243007	-0.064562214

Zr–CH_2–Ph angle fixed at 80˚

-437.280722429046 Hartrees

atom	x	y	z
Zr	0.011145839	0.00545859	-0.033429256
C	0.006968297	-0.00570493	2.322289639
C	1.447425791	-0.005980531	2.07092661
C	2.158863422	1.202250075	1.836461266
C	3.508313181	1.196493617	1.488268995
C	4.196795784	-0.008427495	1.327303841
C	3.51202723	-1.212235746	1.512114266
C	2.162477127	-1.215741626	1.858177181
H	-0.401791946	0.904441159	2.762051625
H	-0.401774085	-0.916075927	2.761274537
H	1.64799726	2.150935903	1.988349149
H	4.026105641	2.140822596	1.342972868
H	4.032999675	-2.157436101	1.385184921

H	1.653077801	-2.16264598	2.02445712
H	5.248873597	-0.009364169	1.059208642
C	-1.058411229	1.859701363	-0.689960861
H	-1.799413865	1.619661938	-1.466848266
H	-1.597810973	2.323926709	0.148382307
H	-0.371633162	2.609020229	-1.106227105
C	1.791841961	-0.104514649	-1.40304974
H	1.677142864	0.710452601	-2.136049681
H	2.803154675	-0.053259611	-0.989380686
H	1.699608672	-1.048202544	-1.964781968
C	-1.192031523	-1.775780176	-0.666319482
H	-1.595848555	-1.629929851	-1.678760247
H	-0.593805599	-2.69732042	-0.680642147
H	-2.041920428	-1.936083959	0.012603391

Zr–CH_2–Ph angle fixed at 85˚

-437.282785010368 Hartrees

atom	x	y	z
Zr	0.011197847	0.000892112	-0.012939065
C	-0.002492517	-0.002214998	2.305265965
C	1.460943104	-0.001756022	2.185936464
C	2.181460691	1.205688048	1.995011067
C	3.548957846	1.200864976	1.726279856
C	4.245451392	-0.005007546	1.612802093
C	3.555869729	-1.209292139	1.778201978
C	2.188828863	-1.211339739	2.045963345
H	-0.435107464	0.90570586	2.731329268
H	-0.434029228	-0.905516583	2.741428351

H	1.65855581	2.153715505	2.104310783
H	4.073507568	2.144608319	1.603435066
H	4.086495054	-2.154013938	1.695626643
H	1.670445585	-2.156716177	2.191741653
H	5.310368423	-0.006411067	1.401015176
C	-1.04047262	1.856384882	-0.692949075
H	-1.833185319	1.611514384	-1.414801467
H	-1.514106595	2.373459364	0.154291883
H	-0.354421919	2.563457685	-1.178432025
C	1.859624705	-0.102866462	-1.289127613
H	1.81417144	0.741006021	-1.996185984
H	2.842134639	-0.090696049	-0.807069944
H	1.785478889	-1.022717683	-1.891417591
C	-1.187451169	-1.771499934	-0.676824477
H	-1.728395999	-1.546139178	-1.60745324
H	-0.556438813	-2.650564201	-0.866231773
H	-1.933461279	-2.048510629	0.081957623

Zr–CH_2–Ph angle fixed at 90˚

-437.283115301503 Hartrees

atom	x	y	z
Zr	0.011563792	0.004814089	-0.004378827
C	-0.005170252	0.010507691	2.290461262
C	1.469618486	0.001803564	2.301237057
C	2.209516351	1.204398342	2.197824548
C	3.592446155	1.192535567	2.030641368
C	4.285691892	-0.017500097	1.94970731
C	3.578559342	-1.217952534	2.054347879

C	2.19588935	-1.210913638	2.221839477
H	-0.457952737	0.915632217	2.705288497
H	-0.468409135	-0.886021811	2.712174298
H	1.684157616	2.154760931	2.270234974
H	4.1321927	2.133147537	1.960110982
H	4.107663826	-2.165825433	2.002527082
H	1.659604377	-2.153555348	2.312089799
H	5.363082405	-0.025024103	1.813801942
C	-1.102677769	1.81413037	-0.709800948
H	-1.920852099	1.519841092	-1.383152688
H	-1.551066852	2.355019371	0.136305657
H	-0.458546776	2.516842388	-1.255344159
C	1.923067165	-0.025360539	-1.186459965
H	1.924383583	0.854959597	-1.848513445
H	2.867872479	-0.035740645	-0.632919799
H	1.899716784	-0.912098562	-1.839527131
C	-1.122283484	-1.799182047	-0.690965645
H	-1.843864263	-1.526459442	-1.474492272
H	-0.45766843	-2.569952218	-1.104006471
H	-1.688049616	-2.249701995	0.137384368

Zr–CH_2–Ph angle fixed at 95˚

-437.283289471904 Hartrees

atom	x	y	z
Zr	0.07399033	0.109936661	-0.009603444
C	-0.016892708	0.344016065	2.256988086
C	1.421401229	0.069084232	2.472845899

C	2.38468033	1.098243966	2.368005886
C	3.749086121	0.818603985	2.400323743
C	4.198349084	-0.497245461	2.534108749
C	3.264213176	-1.529122206	2.653464692
C	1.899503159	-1.252659486	2.621498383
H	-0.323699855	1.354981254	2.546148155
H	-0.68352424	-0.394037182	2.715779262
H	2.048675355	2.129026678	2.272317102
H	4.465734203	1.631735072	2.320157257
H	3.601346964	-2.555494778	2.771924077
H	1.183102088	-2.065555341	2.723132075
H	5.262180564	-0.714661367	2.554840353
C	-0.604154885	2.027848262	-0.943284236
H	-1.446674829	1.850475024	-1.627320717
H	-0.946172631	2.738390519	-0.176639471
H	0.195417286	2.514104814	-1.518600094
C	2.021350124	-0.422084683	-0.994011857
H	2.266116128	0.359450108	-1.73007574
H	2.884886335	-0.546321716	-0.331492527
H	1.885283841	-1.358662751	-1.556785217
C	-1.376026283	-1.487904628	-0.606284411
H	-2.003110294	-1.153231891	-1.445166604
H	-0.866927759	-2.409926205	-0.918823831
H	-2.047267456	-1.74065659	0.227427386

Zr–CH_2–Ph angle fixed at 100˚

-437.283034611721 Hartrees

atom	x	y	z
Zr	-0.014745254	-0.001283793	-0.001882439
C	0.01125399	-0.003822684	2.270554666
C	1.476764015	-0.000746836	2.511714301
C	2.207240817	1.206397875	2.550688673
C	3.597845399	1.208138942	2.638936494
C	4.304394698	0.004353861	2.689705386
C	3.600200551	-1.201905163	2.665236934
C	2.209776847	-1.205155478	2.576967529
H	-0.492593502	0.889076695	2.659674311
H	-0.489094312	-0.897700911	2.66152732
H	1.66927376	2.152048118	2.521573665
H	4.132815785	2.153717234	2.670189296
H	4.137262088	-2.14541773	2.717194066
H	1.673846551	-2.152294216	2.567450753
H	5.38852065	0.006186708	2.755793744
C	-1.099199598	1.825115362	-0.703896215
H	-1.933765979	1.550895281	-1.365062693
H	-1.519304808	2.386894842	0.143057774
H	-0.440479438	2.504064048	-1.262791864
C	1.962220867	-0.045727612	-1.062671004
H	2.038882469	0.835329169	-1.71831227
H	2.84521623	-0.062542519	-0.413990484
H	2.000784643	-0.933288768	-1.712960619
C	-1.159049462	-1.791640433	-0.699927585

H	-1.904314126	-1.509264728	-1.45715242
H	-0.496480523	-2.544427951	-1.148923766
H	-1.696312505	-2.270010268	0.131752494

Zr–CH_2–Ph angle fixed at 105˚

-437.282949961212 Hartrees

atom	x	y	z
Zr	0.05747326	0.126426602	-0.013116674
C	-0.001479567	0.282563362	2.246097436
C	1.395459341	0.017644964	2.687209944
C	2.348361764	1.05487947	2.755969735
C	3.683270556	0.791902541	3.059171067
C	4.108593663	-0.515530421	3.302483731
C	3.178219123	-1.55614982	3.248037778
C	1.843658645	-1.294437841	2.944731333
H	-0.348240573	1.287729663	2.520732812
H	-0.71671543	-0.450620747	2.64146311
H	2.029996932	2.080482075	2.578863886
H	4.39419226	1.612625223	3.108347201
H	3.493619544	-2.577444043	3.445478782
H	1.128994748	-2.114654043	2.913616191
H	5.149008215	-0.720335088	3.53756729
C	-0.523740939	2.101957192	-0.887444804
H	-1.425848942	2.007286748	-1.508702694
H	-0.73809784	2.841754642	-0.102692666
H	0.27594006	2.509902703	-1.52139374
C	2.035482714	-0.446992155	-0.896984807
H	1.913644759	-1.313815305	-1.563637252

H	2.423614349	0.381116195	-1.508937014
H	2.798016189	-0.698122314	-0.149866545
C	-1.436859886	-1.402869973	-0.670497124
H	-2.136134115	-0.984775874	-1.408556612
H	-0.942726427	-2.268672385	-1.133393739
H	-2.031530552	-1.771666511	0.17781192

Zr–CH_2–Ph angle fixed at 110˚

-437.282375541434 Hartrees

atom	x	y	z
Zr	-0.005420505	-0.003305744	-0.004429833
C	0.008157245	-0.021928121	2.257173892
C	1.411499572	-0.008128063	2.758600944
C	2.109499651	1.202979394	2.936129805
C	3.449811996	1.215526636	3.318840279
C	4.134218863	0.018087832	3.535546926
C	3.457390568	-1.192429665	3.371536923
C	2.117475108	-1.205629151	2.988737877
H	-0.557717182	0.861676495	2.585821001
H	-0.542607347	-0.91444385	2.586093778
H	1.586397383	2.144926683	2.781950793
H	3.96090382	2.165512249	3.452324636
H	3.97486352	-2.132213665	3.546434832
H	1.601178492	-2.156722989	2.873289849
H	5.178697461	0.027927255	3.833297569
C	-0.99618822	1.876635715	-0.702178229
H	-1.887054332	1.647984788	-1.304360767
H	-1.317789969	2.505510959	0.140355703

H	-0.317624659	2.475822352	-1.325599182
C	2.020821605	-0.118826951	-0.947511419
H	2.068968073	-0.954917978	-1.660695659
H	2.234361106	0.802944698	-1.508768067
H	2.822284109	-0.256083203	-0.210573098
C	-1.204241145	-1.746516908	-0.729199815
H	-2.006208749	-1.417259116	-1.405157503
H	-0.575517777	-2.459506276	-1.281078171
H	-1.673900448	-2.290430667	0.102936434

Zr–CH_2–Ph angle fixed at 115˚

-437.281991883099 Hartrees

atom	x	y	z
Zr	-0.006037356	0.002093943	-0.000450648
C	0.006284616	0.013676149	2.25686883
C	1.360907996	0.004511749	2.879642239
C	2.055849154	1.20356286	3.129992508
C	3.352093784	1.194496762	3.642419346
C	3.994140998	-0.013734727	3.91986675
C	3.31908408	-1.212797797	3.683020968
C	2.022966268	-1.203981966	3.17059007
H	-0.567522986	0.909316388	2.541124399
H	-0.588475086	-0.862203953	2.55818692
H	1.565212944	2.153946726	2.928429555
H	3.86150144	2.136310211	3.829799852
H	3.802957658	-2.16121943	3.902139975
H	1.507077764	-2.146891765	2.999507059
H	5.004192597	-0.020832054	4.319218709

C	-0.972233564	1.885259654	-0.724982965
H	-1.880400206	1.659813024	-1.302123746
H	-1.260294043	2.549601107	0.101942529
H	-0.292563971	2.446864542	-1.381766414
C	2.035064627	-0.145862349	-0.899796503
H	2.121011121	-1.021325437	-1.559485039
H	2.270777925	0.745059797	-1.499688377
H	2.801690436	-0.236209956	-0.118223611
C	-1.219103354	-1.741277216	-0.703395942
H	-2.051496292	-1.410006048	-1.340475901
H	-0.600289353	-2.429695335	-1.296604161
H	-1.646997569	-2.313733789	0.131752169

Zr–CH_2–Ph angle fixed at 120˚

-437.281369743157 Hartrees

atom	x	y	z
Zr	-0.001520631	-0.001459188	-0.000856717
C	0.004748148	-0.008860633	2.251136865
C	1.297806438	-0.002852565	2.992932564
C	1.945885387	1.204201052	3.316688499
C	3.185451678	1.210670811	3.954128502
C	3.815602821	0.010200212	4.286729237
C	3.185899121	-1.196781225	3.97704175
C	1.946377271	-1.203223561	3.339677404
H	-0.60763011	0.872501742	2.503307001
H	-0.600273359	-0.895204727	2.502917398
H	1.463366207	2.148595075	3.072176625
H	3.659469107	2.158656283	4.195620817

H	3.660604352	-2.139689971	4.236460824
H	1.464854324	-2.152435488	3.112550334
H	4.781362502	0.015151551	4.783829076
C	-0.974880986	1.885558991	-0.707920614
H	-1.894758656	1.664201019	-1.267951147
H	-1.243604465	2.555079718	0.12115712
H	-0.303588186	2.440487763	-1.379017344
C	2.04910099	-0.136609535	-0.875194606
H	2.160357389	-1.015484364	-1.526121939
H	2.295819807	0.753159952	-1.471858539
H	2.794540305	-0.217834353	-0.071214893
C	-1.206147547	-1.747001924	-0.713738527
H	-2.059806206	-1.412242848	-1.320107496
H	-0.590897516	-2.40630678	-1.342812806
H	-1.602663689	-2.352101141	0.113536671

Zr–CH_2–Ph angle fixed at 125˚

-437.280389927622 Hartrees

atom	x	y	z
Zr	0.008457768	0.00306103	-0.004051767
C	0.003197006	0.026384401	2.241749586
C	1.221742481	0.009362815	3.099661173
C	1.858893682	1.2037145	3.483923213
C	3.027400167	1.186945451	4.243712113
C	3.594647883	-0.025092315	4.641439376
C	2.97437741	-1.219886562	4.271512363
C	1.805957477	-1.202671885	3.511653587
H	-0.607506565	0.924448567	2.439862629

H	-0.646899887	-0.83865026	2.460196794
H	1.423971599	2.156852859	3.189446597
H	3.494740889	2.125817293	4.529743011
H	3.400018298	-2.171595973	4.579409905
H	1.329519617	-2.142285867	3.238680546
H	4.504535151	-0.038277379	5.234636576
C	-0.984745151	1.876875775	-0.721624662
H	-1.929563556	1.644285747	-1.233454003
H	-1.212534677	2.575727977	0.095103804
H	-0.340389242	2.404305727	-1.439755303
C	2.05616146	-0.122225382	-0.88361321
H	2.184087399	-1.01689004	-1.509358621
H	2.284817632	0.755132226	-1.505229458
H	2.805234268	-0.166037494	-0.079272674
C	-1.19889837	-1.754541285	-0.686769425
H	-2.076661604	-1.421239381	-1.25894972
H	-0.601625123	-2.402172487	-1.344773089
H	-1.560997469	-2.372112513	0.146808952

Zr–CH_2–Ph angle fixed at 130˚

-437.279210029928 Hartrees

atom	x	y	z
Zr	0.01610755	0.010582654	-0.00704215
C	0.006587175	0.055698159	2.233007942
C	1.142633194	0.017402564	3.196714276
C	1.772123724	1.1991714	3.628677073
C	2.860943106	1.161518778	4.498147161
C	3.354134421	-0.059564889	4.961018019

C	2.740705484	-1.242110569	4.54415013
C	1.651980864	-1.204031086	3.674544165
H	-0.597607079	0.970167784	2.379355423
H	-0.685502596	-0.78771565	2.413277469
H	1.394377527	2.159638336	3.283531741
H	3.323754266	2.091463858	4.818590973
H	3.108854773	-2.200793209	4.900575669
H	1.179512201	-2.134403417	3.365498095
H	4.20162925	-0.089026061	5.639805748
C	-1.017357727	1.861337649	-0.729892504
H	-2.009908269	1.617404357	-1.135191458
H	-1.157058081	2.609981705	0.062060962
H	-0.438568701	2.335506335	-1.535634379
C	2.062208403	-0.088772532	-0.89019493
H	2.215081999	-0.996292087	-1.490990805
H	2.278183326	0.777987313	-1.530583227
H	2.805199708	-0.096985981	-0.078214732
C	-1.166811263	-1.775359836	-0.660622456
H	-2.125001441	-1.466400685	-1.102463455
H	-0.615867154	-2.339592825	-1.426958014
H	-1.388905738	-2.466690889	0.163928412

Zr–CH_2–Ph angle fixed at 135˚

-437.277792768735 Hartrees

atom	x	y	z
Zr	0.0015372	0.00104772	0.00523887
C	0.00177762	0.00036353	2.237064241
C	1.054429816	-0.000459938	3.289489578

C	1.584514951	1.202646763	3.789860199
C	2.59705321	1.201980976	4.747641653
C	3.110753827	-0.002123639	5.23219152
C	2.595581439	-1.205362749	4.747119645
C	1.582998831	-1.204423217	3.789354819
H	-0.661920157	0.879259188	2.357532931
H	-0.661908948	-0.878687941	2.356255833
H	1.189676308	2.149410496	3.426830442
H	2.984200134	2.147264159	5.119416546
H	2.981568979	-2.151262568	5.11851204
H	1.186840223	-2.150535652	3.426085442
H	3.898779741	-0.002756593	5.979819843
C	-1.12950962	1.810797029	-0.67708386
H	-2.113473155	1.52452999	-1.075646696
H	-1.295628256	2.546836127	0.121189795
H	-0.581058601	2.316685311	-1.484981065
C	2.03760178	0.022583332	-0.904794123
H	2.22671438	-0.864778304	-1.524899625
H	2.204509772	0.911076936	-1.529708652
H	2.789894043	0.034047791	-0.101215152
C	-1.090018749	-1.831812903	-0.678485109
H	-2.070473157	-1.565363796	-1.098722844
H	-0.518171098	-2.337065215	-1.470456091
H	-1.259572267	-2.562153223	0.124241292

Zr–CH_2–Ph angle fixed at 140˚

-437.276235185670 Hartrees

atom	x	y	z
Zr	0.012801808	0.000118432	0.005138619
C	0.004957528	-0.002688323	2.229709136
C	0.95763678	-0.001207136	3.373240996
C	1.434448203	1.202814948	3.921789631
C	2.348789595	1.204433196	4.973696722
C	2.814960778	0.001473604	5.506750013
C	2.352264866	-1.202844804	4.973727927
C	1.437863438	-1.203877361	3.921876131
H	-0.67339608	0.872761869	2.302237869
H	-0.667872569	-0.882517818	2.300192707
H	1.075734389	2.148830717	3.521298025
H	2.695837425	2.150672421	5.380951424
H	2.702073931	-2.148057288	5.381001764
H	1.081779332	-2.150920378	3.52148538
H	3.525886362	0.002529116	6.328097981
C	-1.127483141	1.810143626	-0.663286202
H	-2.134894056	1.526865337	-1.001019898
H	-1.241013813	2.576939172	0.114474586
H	-0.613434932	2.277065989	-1.516247234
C	2.033969169	0.020477331	-0.938192922
H	2.211179276	-0.865729305	-1.563445605
H	2.193694686	0.910380408	-1.56289426
H	2.799793731	0.027706531	-0.147210458
C	-1.094231307	-1.828050254	-0.669087219

H	-2.101024763	-1.559841055	-1.020649847
H	-0.563148613	-2.291353286	-1.513548607
H	-1.207120184	-2.593150471	0.110406657

Zr–CH_2–Ph angle fixed at 145˚

-437.274482014419 Hartrees

atom	x	y	z
Zr	0.004845506	1.85854E-05	0.001936022
C	0.000365823	0.000600254	2.218449545
C	0.850985098	0.000385121	3.438500748
C	1.279148121	1.203660551	4.027210556
C	2.09660327	1.20348175	5.156098145
C	2.511609347	-0.000369413	5.728021732
C	2.096299586	-1.20382732	5.155576309
C	1.278901465	-1.203252243	4.026688873
H	-0.683314597	0.877529397	2.24279009
H	-0.683484287	-0.87621637	2.242805562
H	0.959816012	2.150203812	3.596065092
H	2.40834116	2.148948702	5.592616917
H	2.40777071	-2.149565933	5.591683142
H	0.959344745	-2.149514096	3.59509726
H	3.146879469	-0.000641524	6.609213332
C	-1.128966061	1.816508004	-0.663961879
H	-2.16875573	1.562650988	-0.915742697
H	-1.154872576	2.621814522	0.082175939
H	-0.660240332	2.222987633	-1.572374374
C	2.018602193	0.01074862	-0.958020084
H	2.188149453	-0.87604955	-1.584562479

H	2.179282838	0.900268074	-1.58303036
H	2.789251715	0.013880668	-0.171675498
C	-1.109127743	-1.828859152	-0.663313525
H	-2.150400469	-1.586009227	-0.919729434
H	-0.632965184	-2.233425758	-1.568718839
H	-1.129814305	-2.632119085	0.085209618

Zr–CH_2–Ph angle fixed at 150˚

-437.272492615933 Hartrees

atom	x	y	z
Zr	0.002132319	-0.000196116	0.004910061
C	0.001216729	-0.001012345	2.2126168
C	0.74386091	-0.000484476	3.500148566
C	1.117563258	1.203604604	4.123027938
C	1.833264457	1.20419208	5.319031068
C	2.198046924	0.000673552	5.924826381
C	1.836352534	-1.203450721	5.318400445
C	1.12072832	-1.203989392	4.122372508
H	-0.689505274	0.873807585	2.191384938
H	-0.687064154	-0.877733335	2.190693005
H	0.836734094	2.14961706	3.664872842
H	2.104986306	2.149977397	5.780805347
H	2.110450492	-2.148792011	5.779677343
H	0.842350845	-2.150413015	3.663620779
H	2.75387709	0.001127257	6.858154129
C	-1.134365154	1.816598597	-0.658630851
H	-2.178509633	1.563661208	-0.892824892
H	-1.146785845	2.630527872	0.078239007

H	-0.677412482	2.211102055	-1.578307356
C	2.009387859	0.011649057	-0.970855975
H	2.174058237	-0.8748031	-1.599262952
H	2.164678465	0.901444012	-1.596910638
H	2.786902003	0.014676405	-0.191487393
C	-1.113994925	-1.828749104	-0.66054666
H	-2.16000401	-1.586909907	-0.898073029
H	-0.650234788	-2.219485087	-1.578426715
H	-1.120039472	-2.641918966	0.077253836

Table 4. Cartesian coordinates for geometry optimized structures of $Me_3Si(CH_2Ph)$ with constraints on the Si-CH_2-Ph angle.

$Me_3Si(CH_2Ph)$

-680.256216632838 Hartrees

atom	x	y	z
Si	0.059624391	0.395324875	-0.153480779
C	0.434029194	0.875704515	1.664995331
C	1.619450548	0.16116719	2.266352374
C	2.914375112	0.693830274	2.164403791
C	4.01751007	0.014635523	2.682008458
C	3.851490457	-1.216554008	3.317095976
C	2.570543811	-1.75763696	3.431417495
C	1.469542206	-1.076167133	2.912622428
H	0.588877569	1.961802669	1.695642132
H	-0.470496913	0.676281617	2.253855518
H	3.056845987	1.655405304	1.676613051

H	5.008758531	0.451237292	2.591730232
H	2.425750136	-2.712677831	3.929633653
H	0.47585369	-1.506445915	3.013537461
H	4.709432702	-1.746101544	3.721508346
C	-1.43005235	1.416469557	-0.726951323
H	-1.69392367	1.185824964	-1.765265546
H	-2.313099533	1.216039406	-0.10985959
H	-1.223634954	2.491263495	-0.670130037
C	1.55876522	0.78013691	-1.241690759
H	1.371950666	0.492095202	-2.282434892
H	1.798644958	1.849392197	-1.233761234
H	2.446386426	0.238017119	-0.899383319
C	-0.346413857	-1.450008467	-0.259784065
H	-0.543472854	-1.74862121	-1.295668297
H	0.483675876	-2.060470318	0.110856141
H	-1.234657686	-1.702352895	0.330502271

Si–CH_2–Ph angle fixed at 85˚

-680.225805636943 Hartrees

atom	x	y	z
Si	0.002693199	-0.005831844	-0.026408866
C	0.00514875	-0.004563865	1.970566387
C	1.529129786	4.4538E-06	1.835343287
C	2.261973033	1.202570634	1.840709735
C	3.652034291	1.209477128	1.74223507
C	4.361170154	0.009645799	1.6735908
C	3.659389922	-1.195150675	1.727891989

C	2.269196254	-1.197991815	1.826830786
H	-0.404960336	0.904165555	2.40826383
H	-0.400362675	-0.915616887	2.407736985
H	1.729880683	2.147110926	1.919411778
H	4.183265235	2.15761781	1.735695607
H	4.196393794	-2.139894685	1.709990216
H	1.743042126	-2.146619109	1.895185731
H	5.444682599	0.013397941	1.598757711
C	0.778404657	1.536863479	-0.805486319
H	0.4314152	1.582774689	-1.844910732
H	0.447147551	2.458364465	-0.314561455
H	1.869803598	1.527815792	-0.81071727
C	0.749041415	-1.567166985	-0.797538383
H	0.399770287	-1.613535768	-1.836151286
H	1.84039579	-1.578180972	-0.804750209
H	0.401624116	-2.47932979	-0.300278553
C	-1.822211331	0.010119596	-0.593747983
H	-1.91745383	0.008281877	-1.686321872
H	-2.360640137	-0.866321037	-0.214341367
H	-2.343851742	0.898585917	-0.218904001

Si–CH_2–Ph angle fixed at 90˚

-680.236172366940 Hartrees

atom	x	y	z
Si	0.004234782	0.005767076	-0.02058677
C	0.002864172	0.007812824	1.953187398
C	1.529069636	0.000218734	1.954255077
C	2.266503138	1.197367259	1.989750187

C	3.660616791	1.192959388	1.984826747
C	4.362489759	-0.013026921	1.974184875
C	3.64941321	-1.212282576	1.987511163
C	2.255194469	-1.203658337	1.992301994
H	-0.428716168	0.913805828	2.379443891
H	-0.437504367	-0.893955738	2.379469402
H	1.737083187	2.146357906	2.018882689
H	4.199492794	2.136685954	2.002154438
H	4.179360998	-2.161003961	2.007252097
H	1.717045639	-2.147590322	2.024426897
H	5.448660186	-0.018093893	1.971250834
C	0.816757742	1.546627427	-0.763171947
H	0.544433599	1.588981482	-1.824670766
H	0.450357628	2.468831751	-0.298860597
H	1.906345007	1.541916657	-0.693139207
C	0.791375228	-1.553040163	-0.753356417
H	0.518793238	-1.598560016	-1.814635479
H	1.880903583	-1.56566155	-0.683269772
H	0.409668558	-2.465758999	-0.282570938
C	-1.806906904	0.019265264	-0.617162458
H	-1.878630698	0.017089326	-1.711349644
H	-2.351612478	-0.858165839	-0.249516782
H	-2.336889443	0.907546624	-0.254128314

Si–CH_2–Ph angle fixed at 95˚

-680.244130021708 Hartrees

atom	x	y	z
Si	0.020735814	-0.285940458	0.016021389
C	0.099249292	-0.70890009	1.924067423
C	1.509571202	-0.17095011	2.121287287
C	1.733655436	1.16404366	2.499259094
C	3.024830255	1.666971688	2.655853011
C	4.131961345	0.840885045	2.45873972
C	3.928788517	-0.496676904	2.117813916
C	2.63590568	-0.996211291	1.962636902
H	-0.648712273	-0.162276207	2.501682159
H	0.022837725	-1.781911754	2.110950257
H	0.882098849	1.817757386	2.671202129
H	3.164658379	2.705915734	2.942857873
H	4.779569536	-1.159143419	1.981380398
H	2.49571115	-2.045077782	1.713385855
H	5.138385228	1.230974198	2.580510813
C	0.216676451	1.56853074	-0.308918009
H	-0.015818339	1.761915836	-1.362979366
H	-0.480047258	2.164202181	0.291467106
H	1.227531233	1.933850499	-0.114179619
C	1.318731065	-1.248835349	-0.969501935
H	1.112482844	-1.116828711	-2.038289476
H	2.339563963	-0.909922688	-0.779491339
H	1.274398233	-2.323661868	-0.760894426
C	-1.685237956	-0.796631701	-0.655642802

H	-1.780539793	-0.581793065	-1.726496668
H	-1.861966997	-1.869620879	-0.517978576
H	-2.491804815	-0.263112679	-0.139618755

Si–CH_2–Ph angle fixed at 100°

-680.249861441379 Hartrees

atom	x	y	z
Si	0.020436081	-0.286141426	0.038389298
C	0.118780237	-0.708296818	1.931399408
C	1.508612103	-0.18546375	2.246197652
C	1.708684587	1.13826892	2.671496726
C	2.988451767	1.633247442	2.921552416
C	4.104910129	0.811139953	2.766220206
C	3.923272278	-0.514096022	2.369754882
C	2.641856994	-1.006112862	2.121173414
H	-0.658602601	-0.184969094	2.494494768
H	0.030490534	-1.784537726	2.102187139
H	0.848082335	1.788843029	2.807280858
H	3.111671769	2.663329607	3.245513362
H	4.781426257	-1.171924128	2.259512322
H	2.516379579	-2.044434533	1.823928373
H	5.102209793	1.195711776	2.959454324
C	0.206735741	1.574241023	-0.254714166
H	0.042454146	1.790071481	-1.316932306
H	-0.532054515	2.150950997	0.31314426
H	1.199774566	1.943804316	0.013472973
C	1.34911894	-1.219982248	-0.934149394
H	1.199008829	-1.048664584	-2.006525124

H	2.361024646	-0.89364618	-0.681276907
H	1.291557172	-2.301259363	-0.765408989
C	-1.677979245	-0.820984481	-0.624738334
H	-1.779917092	-0.600149814	-1.693436746
H	-1.835847962	-1.897727504	-0.494360373
H	-2.491289075	-0.304178844	-0.102573646

Si–CH_2–Ph angle fixed at 105°

-680.253633604587 Hartrees

atom	x	y	z
Si	0.008176858	-0.266336125	0.062767865
C	0.126702564	-0.681919103	1.945277118
C	1.493426742	-0.188101035	2.370307579
C	1.681155618	1.126166293	2.827905472
C	2.947582421	1.5976283	3.173739825
C	4.060658488	0.761588514	3.079003613
C	3.889576682	-0.552624636	2.642605009
C	2.621698918	-1.020790455	2.297622162
H	-0.674593836	-0.175915976	2.493371786
H	0.020856507	-1.760709533	2.098832896
H	0.821977513	1.7870106	2.914647492
H	3.063161264	2.620231072	3.523401461
H	4.745155377	-1.219501187	2.574800605
H	2.502687713	-2.049951082	1.967309222
H	5.047517973	1.127605376	3.347675314
C	0.150306166	1.601051443	-0.209966647
H	0.039651468	1.831993586	-1.275806187
H	-0.631806941	2.149847775	0.326866217

H	1.118333263	1.99064693	0.118072207
C	1.377376369	-1.153818601	-0.895908084
H	1.278557696	-0.944425895	-1.967357582
H	2.373973274	-0.830232775	-0.582141539
H	1.321674723	-2.240840759	-0.768280462
C	-1.674739095	-0.855228443	-0.587474253
H	-1.78839213	-0.639628597	-1.655933133
H	-1.798305444	-1.936081521	-0.454447247
H	-2.500282755	-0.361876278	-0.062195559

Si–CH_2–Ph angle fixed at 110˚

-680.255699280803 Hartrees

atom	x	y	z
Si	0.0115241	0.320689256	0.082014186
C	0.176614668	0.71880358	1.956336167
C	1.479495721	0.168976077	2.488647986
C	2.655783709	0.934931936	2.459245527
C	3.869684098	0.412237024	2.905466233
C	3.936409917	-0.89186759	3.397455632
C	2.774636993	-1.663345316	3.442614503
C	1.562427159	-1.137525969	2.995567791
H	0.124141378	1.805291251	2.092657118
H	-0.678358546	0.28320005	2.486433343
H	2.616848233	1.954934302	2.084168568
H	4.764691002	1.028109336	2.87234496
H	2.809863812	-2.677782115	3.831202308
H	0.663574867	-1.747820727	3.042608504
H	4.880978769	-1.30014869	3.745637632

C	-1.633999605	1.030782746	-0.536117108
H	-1.779274161	0.827883673	-1.603151053
H	-2.483959343	0.59509661	0.000987592
H	-1.677672931	2.117072142	-0.39807697
C	1.437820101	1.112721293	-0.876433212
H	1.352629294	0.888227264	-1.945853499
H	1.440472085	2.20338296	-0.768927555
H	2.408517502	0.74102899	-0.53359593
C	0.031181284	-1.55258069	-0.184796264
H	-0.060132902	-1.790205995	-1.250851745
H	0.961611874	-1.999827716	0.178896711
H	-0.800020387	-2.043683455	0.333778781

Si–CH_2–Ph angle fixed at 120˚

-680.255397980286 Hartrees

atom	x	y	z
Si	0.004239082	0.003313299	-0.001012583
C	0.005122285	0.009858209	1.910854043
C	1.31062793	0.003675867	2.663826721
C	1.948198961	1.202922427	3.018360898
C	3.171581491	1.198710672	3.688537996
C	3.788621555	-0.008307762	4.019244719
C	3.167719862	-1.209292511	3.674147663
C	1.944318307	-1.201649044	3.004207439
H	-0.585456614	0.88733217	2.210135909
H	-0.596103317	-0.858718445	2.214918574
H	1.474843528	2.150200803	2.770510716

H	3.642112397	2.141336956	3.955714271
H	3.635315745	-2.15653611	3.929848136
H	1.467785371	-2.144360512	2.745349344
H	4.740638814	-0.012976093	4.542490272
C	-1.806830835	0.021135601	-0.554570591
H	-1.884628784	0.015515426	-1.647652464
H	-2.349464525	-0.854458149	-0.18078759
H	-2.328114413	0.913932485	-0.191518317
C	0.89834635	1.53814915	-0.652974783
H	0.9300008	1.545388409	-1.748355524
H	0.401210527	2.460113098	-0.331045208
H	1.930998627	1.574523226	-0.289565213
C	0.863923882	-1.556192633	-0.641101104
H	0.895134083	-1.572795318	-1.736404349
H	1.895723541	-1.612580327	-0.277723128
H	0.346438688	-2.464326292	-0.311911814

Si–CH_2–Ph angle fixed at 125˚

-680.253819089395 Hartrees

atom	x	y	z
Si	0.006688846	0.000734846	-0.003241052
C	0.006284042	0.000654843	1.905541756
C	1.239891001	-0.000173751	2.769712732
C	1.835999905	1.201621773	3.182058508
C	2.988219645	1.202548955	3.968150978
C	3.574585001	-0.001894268	4.358572956
C	2.995363757	-1.205539683	3.955025131
C	1.843248215	-1.202888216	3.16890523

H	-0.611635325	0.869847373	2.177544957
H	-0.61278804	-0.867862843	2.17718753
H	1.385297472	2.146868981	2.888330191
H	3.427057784	2.147161686	4.278674407
H	3.439871366	-2.150816069	4.255293769
H	1.398187874	-2.147514696	2.864792971
H	4.470820816	-0.002555393	4.972498024
C	-1.811445587	0.004945405	-0.530686113
H	-1.901957504	0.004275419	-1.622789495
H	-2.340931092	-0.87779011	-0.155176987
H	-2.336579489	0.891012137	-0.156841429
C	0.878468386	1.54681412	-0.658977827
H	0.897237454	1.563253875	-1.75452768
H	0.378274358	2.462263811	-0.323525982
H	1.915353197	1.588998088	-0.307967472
C	0.871811508	-1.549179175	-0.659240681
H	0.891290429	-1.565574996	-1.754784364
H	1.908228122	-1.596150642	-0.307564341
H	0.367293771	-2.462513896	-0.324403604

Si–CH_2–Ph angle fixed at 130°

-680.251302263762 Hartrees

atom	x	y	z
Si	0.010492084	0.001724724	-0.005574518
C	0.005971288	0.002367095	1.901223934
C	1.157622409	0.000332362	2.872238901
C	1.716400063	1.20133922	3.33546718
C	2.786258178	1.201281565	4.230185487

C	3.326824909	-0.003790925	4.680395772
C	2.785039134	-1.206829216	4.226166823
C	1.715361926	-1.202810333	3.331296581
H	-0.631857421	0.868433554	2.140629795
H	-0.635009735	-0.861314029	2.140995389
H	1.300627182	2.147053476	2.995240502
H	3.196642489	2.145582198	4.578342314
H	3.194395538	-2.15268313	4.571299122
H	1.298745755	-2.146969211	2.987793582
H	4.158692916	-0.005346547	5.379092051
C	-1.814929535	-0.002205935	-0.506507611
H	-1.918551883	-0.003059155	-1.597494966
H	-2.335972758	-0.887419962	-0.125155636
H	-2.339144834	0.881475	-0.126083319
C	0.865183529	1.551285653	-0.676345849
H	0.858528009	1.57261009	-1.771984713
H	0.372591133	2.465099954	-0.325458163
H	1.910092307	1.593161723	-0.349745289
C	0.871321058	-1.545150036	-0.674358592
H	0.865164114	-1.567552147	-1.769970093
H	1.916245187	-1.582490424	-0.347253738
H	0.382133094	-2.460535899	-0.322687133

Si–CH_2–Ph angle fixed at 135˚

-680.248015880363 Hartrees

atom	x	y	z
Si	0.019443899	-0.001082713	-0.008636552
C	0.015258957	-0.003491722	1.897206762

C	1.07785259	-0.001004858	2.964488151
C	1.578042434	1.202118269	3.485000373
C	2.553573522	1.206279422	4.481343064
C	3.057901268	0.003644971	4.977428598
C	2.575538192	-1.201607004	4.465751572
C	1.599514373	-1.202021713	3.469401619
H	-0.645965823	0.854590236	2.105474277
H	-0.639398177	-0.867345634	2.102879073
H	1.18941948	2.145906461	3.109460658
H	2.918480899	2.152106672	4.872987427
H	2.957763148	-2.145801433	4.844883374
H	1.227743426	-2.147815496	3.08153863
H	3.81580262	0.005451516	5.755703555
C	-1.812873612	0.008133193	-0.483569999
H	-1.929989871	0.008968698	-1.573071966
H	-2.335180822	-0.873802155	-0.096495157
H	-2.326270496	0.895134151	-0.096125592
C	0.872432905	1.543583505	-0.69244525
H	0.836055754	1.571148317	-1.787446787
H	0.399096541	2.460444	-0.32345276
H	1.926275404	1.573159748	-0.394558317
C	0.857947563	-1.552470215	-0.695383283
H	0.821424567	-1.577622627	-1.790426903
H	1.91143584	-1.592411405	-0.397343073
H	0.375960596	-2.465580424	-0.328123259

Si–CH_2–Ph angle fixed at 140°

-680.243870535419 Hartrees

atom	x	y	z
Si	0.005668141	0.000670111	-0.002272315
C	0.006320957	0.003894856	1.902755473
C	0.975044803	0.001871795	3.056447282
C	1.429489644	1.2028578	3.622121506
C	2.307589479	1.202183705	4.705646819
C	2.758857039	-0.002969606	5.244940264
C	2.322734963	-1.20570407	4.687967531
C	1.4445761	-1.201486859	3.604661936
H	-0.665671354	0.862914841	2.077882785
H	-0.670432419	-0.851210426	2.079702963
H	1.081030683	2.148500104	3.213171404
H	2.637694686	2.146295064	5.131015757
H	2.664908823	-2.151737528	5.099287405
H	1.108015923	-2.14532887	3.18183484
H	3.440205083	-0.004885874	6.09102619
C	-1.832109923	0.013440018	-0.453656749
H	-1.959896153	0.009072736	-1.541968894
H	-2.353195066	-0.864845347	-0.056874405
H	-2.338590992	0.904147631	-0.065726607
C	0.85301976	1.540180878	-0.70412034
H	0.797041598	1.567287146	-1.798299821
H	0.390881944	2.459402614	-0.327093186
H	1.912238061	1.564840229	-0.425405544
C	0.829702425	-1.555350444	-0.695933058

H	0.774337421	-1.586811009	-1.790033049
H	1.888229868	-1.59514154	-0.416092052
H	0.352961759	-2.46544591	-0.314995444

Si–CH_2–Ph angle fixed at 145°

-680.238981914559 Hartrees

atom	x	y	z
Si	0.011181464	0.000684854	-0.003671186
C	0.012162046	0.003846389	1.901010903
C	0.877261048	0.001707424	3.135167266
C	1.27887524	1.202778364	3.739206002
C	2.050959355	1.202106276	4.900679544
C	2.447619622	-0.003025169	5.48148798
C	2.064503818	-1.205814409	4.886751546
C	1.292663331	-1.201711003	3.725214904
H	-0.67386635	0.859927029	2.042360937
H	-0.680619372	-0.846606786	2.044439318
H	0.971917295	2.148345173	3.298270418
H	2.341199181	2.146318749	5.354027393
H	2.365393167	-2.151867125	5.329202626
H	0.996829833	-2.145494431	3.272994894
H	3.046125378	-0.00489338	6.388086928
C	-1.830001757	0.012703776	-0.439604487
H	-1.963566404	0.009285336	-1.527253925
H	-2.348132151	-0.866441455	-0.04095557
H	-2.33477568	0.902781857	-0.048147551
C	0.849613299	1.541103764	-0.714018747
H	0.777768154	1.571915411	-1.807214676

H	0.394136899	2.459574863	-0.327240557
H	1.912782176	1.56359753	-0.450528666
C	0.827576379	-1.55504953	-0.706670914
H	0.755914682	-1.589595458	-1.799767468
H	1.890227936	-1.59184131	-0.442495567
H	0.358555336	-2.465120501	-0.316230403

Si–CH_2–Ph angle fixed at 150°

-680.233404812394 Hartrees

atom	x	y	z
Si	0.004526311	-0.000207168	-0.001016375
C	0.005258788	-0.000192722	1.903530508
C	0.759959194	-1.76264E-05	3.20954974
C	1.098677362	1.20190489	3.84923024
C	1.757231724	1.203111083	5.078437317
C	2.102947101	-0.000763789	5.693189426
C	1.783895836	-1.204273057	5.063338587
C	1.125339461	-1.202173088	3.834214929
H	-0.697246934	0.849032892	2.011381087
H	-0.695783728	-0.850825171	2.010992193
H	0.831190033	2.146739243	3.381741207
H	1.998689993	2.148165707	5.557848187
H	2.046383292	-2.149671598	5.530885647
H	0.87880138	-2.146728061	3.35478933
H	2.612734888	-0.001102874	6.652447694
C	-1.838866249	0.004146868	-0.426109737
H	-1.974617018	0.003048794	-1.513546716
H	-2.351795089	-0.878642561	-0.02897615

H	-2.346873773	0.890866889	-0.031391184
C	0.828047356	1.545756754	-0.716715573
H	0.739686296	1.5800276	-1.80861006
H	0.375581067	2.461548012	-0.320081202
H	1.894791777	1.570605724	-0.468795149
C	0.820534291	-1.550850897	-0.71529425
H	0.732643463	-1.58550519	-1.807203318
H	1.887004971	-1.580961516	-0.46673464
H	0.3631319	-2.464037862	-0.318273888