Electronic Supplementary Material (ESI) for Polymer Chemistry

Supporting Information

Bis(phosphinimino)methanide Borohydride Complexes of the Rare-Earth Elements as Initiators for the Ring-Opening Polymerization of Trimethylene Carbonate: Combined Experimental and Computational Investigations

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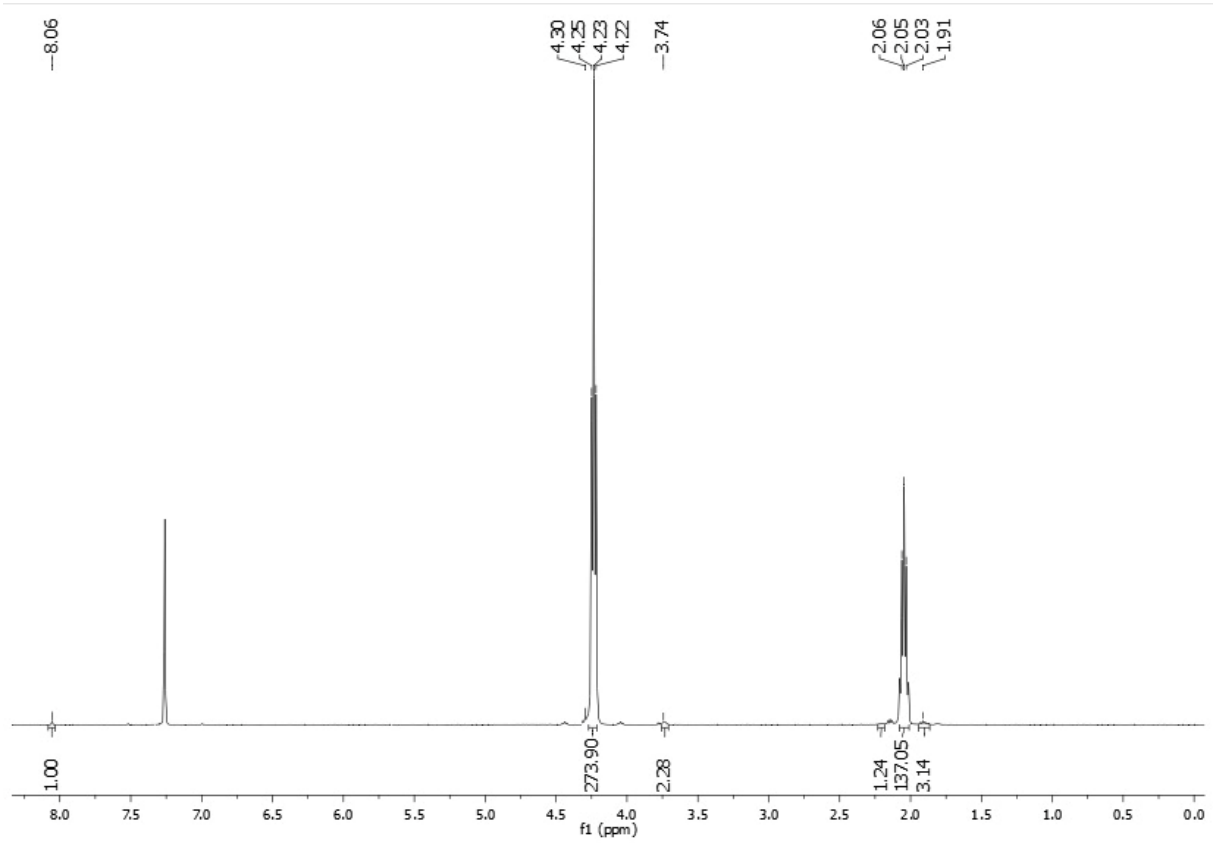

Figure S1. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 °C) of a PTMC sample (Table 1, entry 4).

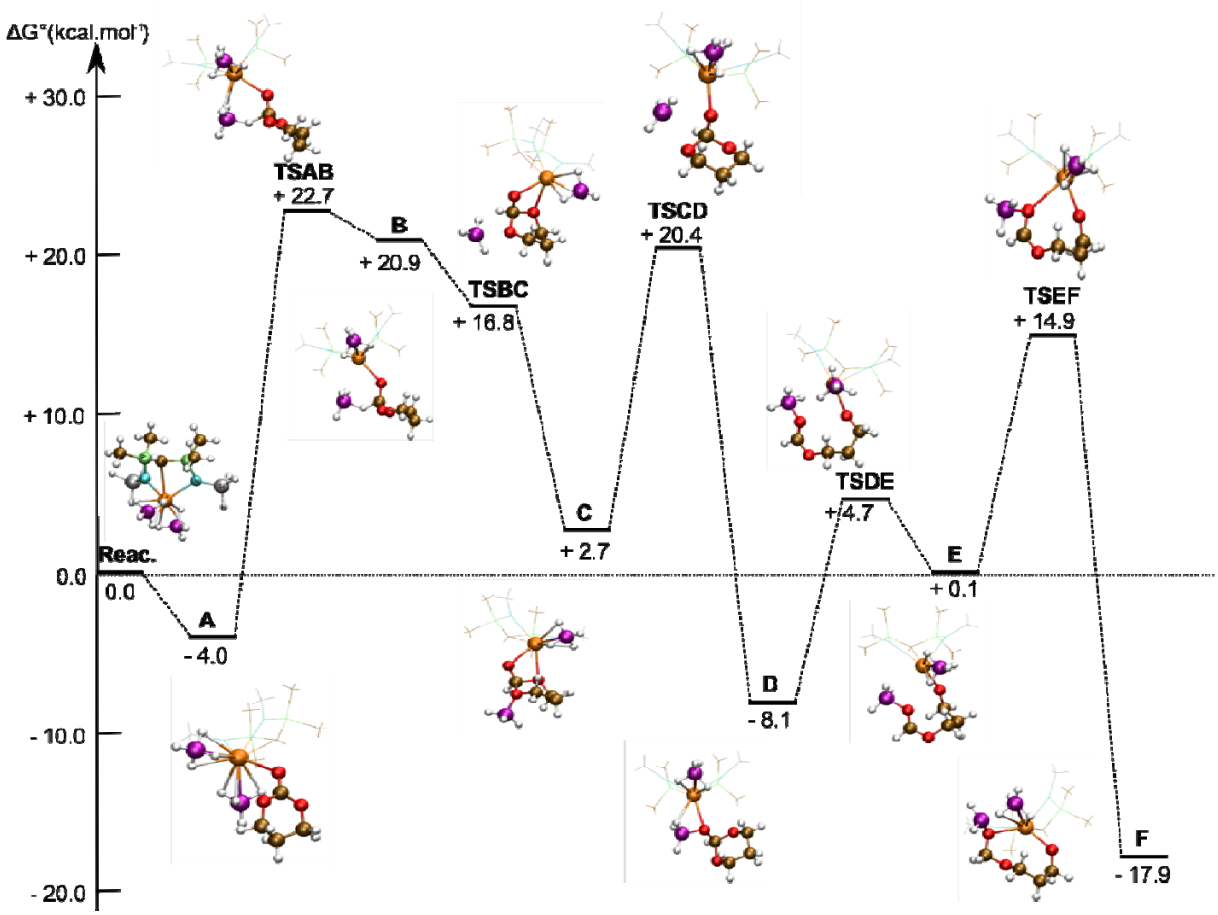

Figure S2. Free energy profile for the formation of an α,ω-dihydroxy telechelic PTMC with complex **1**. Energies are given in kcal.mol^{-1}.

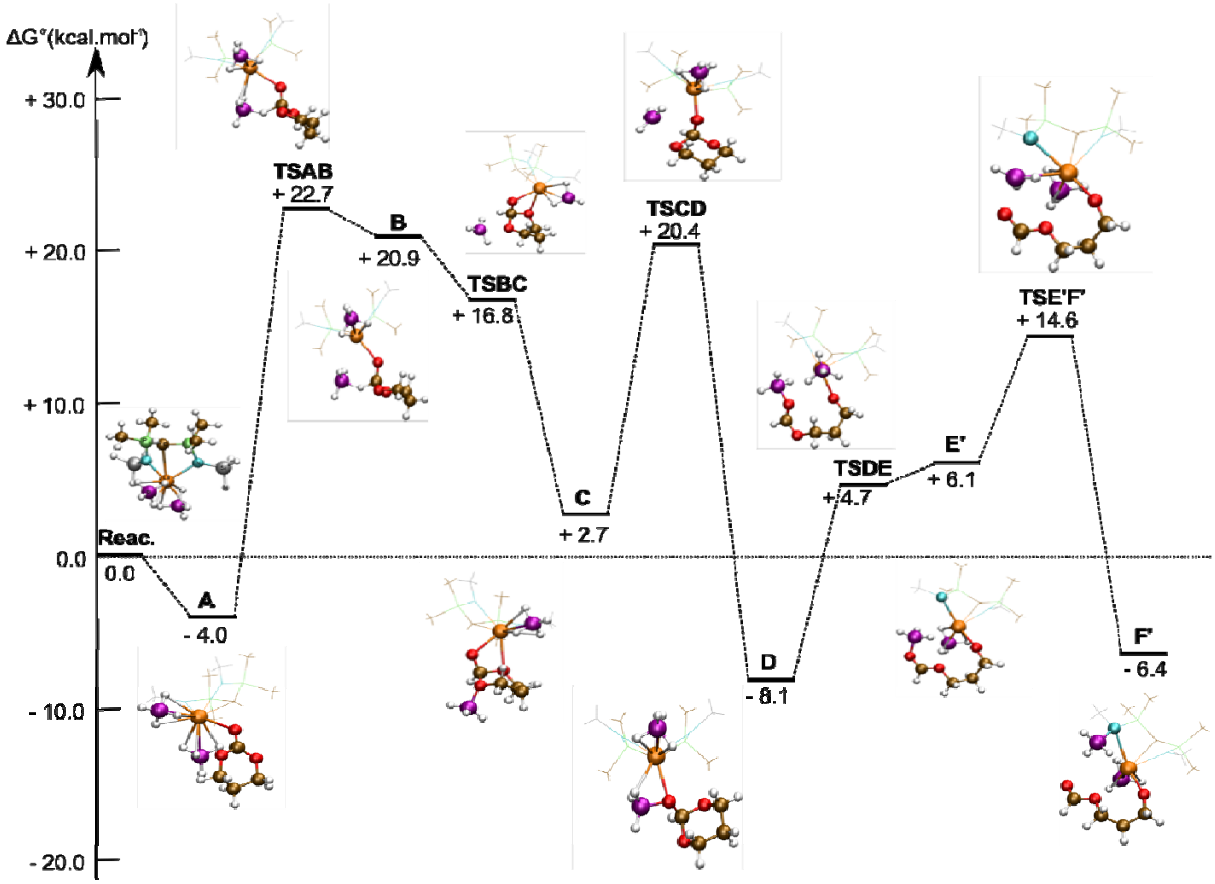

Figure S3. Free energy profile for the formation of an α-hydroxy,ω-formate telechelic PTMC with complex **1.** Energies are given in kcal.mol^{-1}

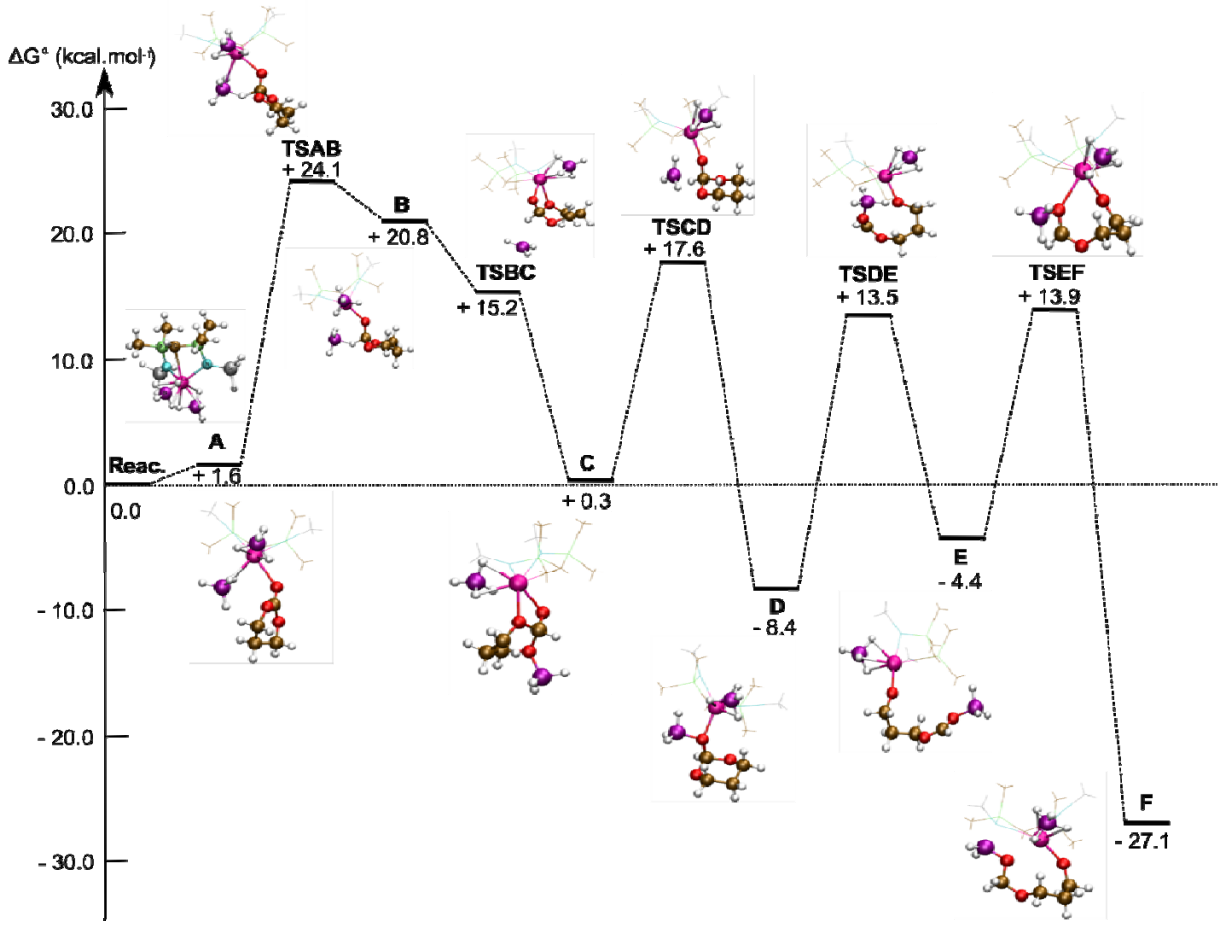

Figure S4. Free energy profile for the formation of an α,ω-dihydroxy telechelic PTMC with complex **3**. Energies are given in kcal.mol^{-1}.

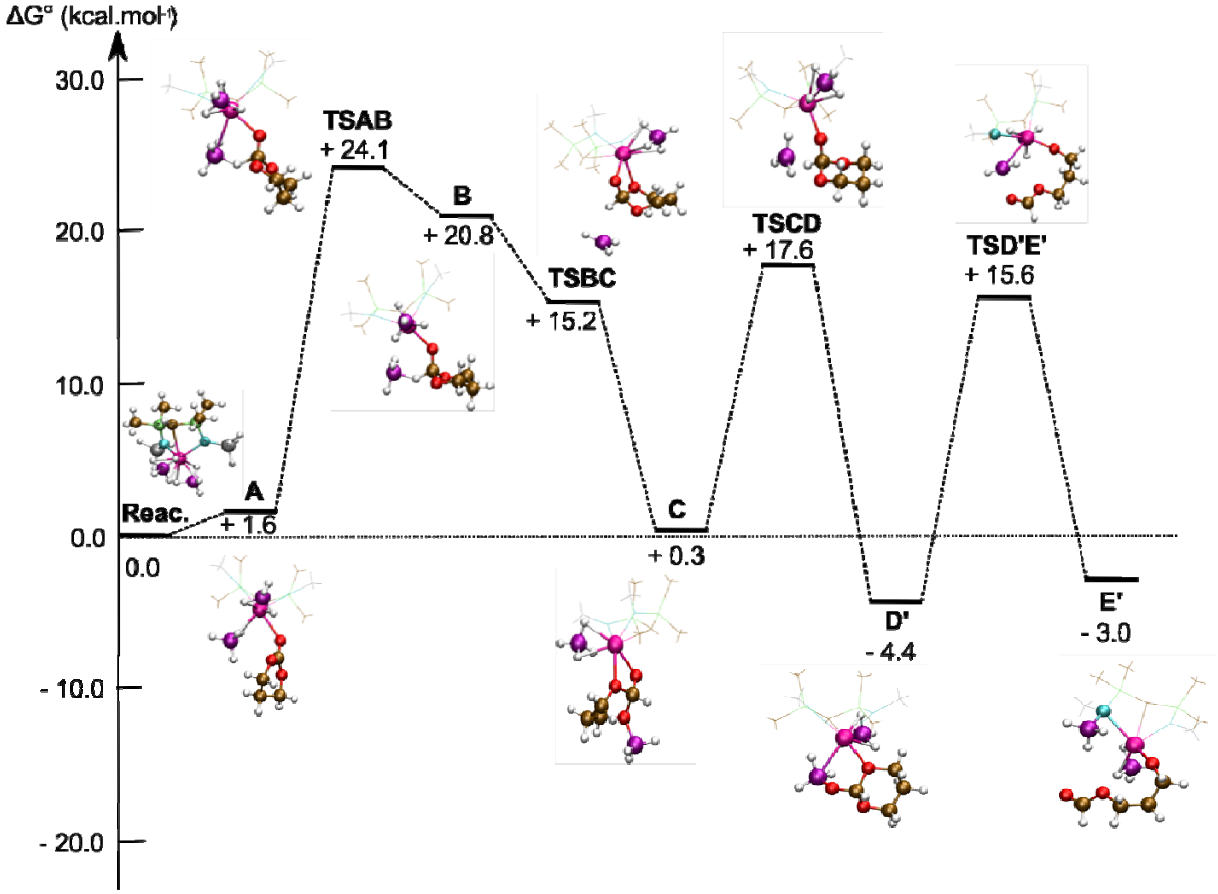

Figure S5 : Free energy profile for the formation of an α-hydroxy,ω-formate telechelic PTMC with complex **1.** Energies are given in kcal.mol^{-1}

Cartesian coordinates of all optimized intermediates:

Reaction between TMC and [{CH(PPh$_2$NSiMe$_3$)$_2$}Y(BH$_4$)$_2$] (2)

All energies in kcal.mol^{-1} are realtive to the origin level, all energies in H are absolute.
Energy of the reactants : - 806.558793 H

A Adduct

C	-10.524271	2.720661	-0.522590
O	-9.292924	1.998515	-0.279254
C	-8.098249	2.515529	-0.486685
O	-7.942518	3.552105	-1.298419
C	-9.102781	4.111687	-1.947976
C	-10.256228	4.141692	-0.970206
O	-7.108441	2.003758	0.025041
Y	-6.828384	1.080911	2.244762
B	-8.290761	3.384281	2.675484
P	-3.795628	1.138957	1.362518
C	-3.460681	2.055614	-0.197777
C	-2.170368	0.354243	1.767547
N	-4.980805	0.010044	1.212468
Si	-4.833935	-1.529170	0.401421
C	-4.400130	2.345001	2.495796
P	-4.635747	2.110533	4.228954
C	-4.962904	3.780065	4.921639
C	-3.173543	1.502732	5.184020
N	-5.915475	1.082823	4.397682
Si	-6.408705	0.333830	5.900463
B	-8.247433	-0.950363	2.419081
H	-5.647850	-0.929743	6.178652
H	-3.767344	-1.478140	-0.663648
H	-4.446671	-2.638803	1.332233
H	-6.122007	-1.885358	-0.258828
H	-6.151045	1.243867	7.072523
H	-7.862615	0.019959	5.853260
H	-4.225975	3.377036	2.202360
H	-8.778711	2.248340	2.550060
H	-7.057959	3.324392	2.529590
H	-8.540336	3.797298	3.787495
H	-4.100040	4.434749	4.773410
H	-5.842883	4.182560	4.414900
H	-5.173048	3.682629	5.989437
H	-2.313958	2.155064	5.010689
H	-3.415864	1.495399	6.251015
H	-2.935828	0.483903	4.872317
H	-1.872189	-0.304852	0.946797
H	-1.406690	1.122107	1.915040
H	-2.276304	-0.242237	2.675649
H	-2.671246	2.796949	-0.048049

H	-3.153967	1.341959	-0.966440
H	-4.387216	2.544352	-0.505700
H	-7.060809	-1.208653	2.659165
H	-8.950232	-1.920325	2.492788
H	-8.279223	-0.435605	1.288750
H	-8.589710	-0.064292	3.214124
H	-8.725684	4.097219	1.786354
H	-11.072780	2.674839	0.420002
H	-11.061804	2.145899	-1.282866
H	-11.151724	4.560256	-1.439721
H	-9.988916	4.766289	-0.112247
H	-9.329199	3.507546	-2.835156
H	-8.789869	5.105744	-2.269272

Energy: 0.6kcal.mol^{-1}
- 806.557809 H

TSAB Nucleophilic attack

C	-10.274260	2.589018	-1.094283
O	-9.666844	2.444593	0.187945
C	-8.378068	2.915408	0.361925
O	-7.998000	4.017015	-0.383358
C	-8.661825	4.343476	-1.608710
C	-10.141692	4.021391	-1.568552
O	-7.462525	2.032957	0.526363
Y	-6.873007	0.929344	2.383440
B	-8.435112	3.340210	2.813002
P	-3.967529	1.214243	1.280020
C	-4.011902	2.159891	-0.294554
C	-2.222355	0.616563	1.402968
N	-5.033164	-0.045590	1.308217
Si	-4.807544	-1.584782	0.507703
C	-4.520922	2.339965	2.513156
P	-4.593710	2.033935	4.250280
C	-4.700059	3.684750	5.050533
C	-3.094124	1.254537	4.995087
N	-5.927755	1.102919	4.525290
Si	-6.351342	0.375541	6.060995
B	-8.259695	-1.091136	2.737172
H	-5.724153	-0.973339	6.246839
H	-4.100084	-1.418426	-0.811654
H	-3.965948	-2.527318	1.317816
H	-6.133159	-2.213319	0.257220
H	-5.873903	1.227935	7.207893
H	-7.831128	0.240794	6.159855
H	-4.447029	3.390864	2.245611
H	-8.910748	2.231010	2.962356
H	-7.225077	3.413595	2.898339
H	-9.065053	4.228695	3.319029

H	-3.776637	4.248197	4.893872
H	-5.545638	4.220619	4.614298
H	-4.873361	3.547990	6.120541
H	-2.201726	1.839272	4.758853
H	-3.218322	1.199144	6.080711
H	-2.993128	0.239996	4.603757
H	-1.990427	-0.012599	0.538333
H	-1.540310	1.470418	1.424456
H	-2.102004	0.025848	2.312767
H	-3.299545	2.988777	-0.266931
H	-3.762602	1.487857	-1.119355
H	-5.030897	2.534680	-0.418439
H	-7.063045	-1.292085	2.994936
H	-8.932199	-2.068421	2.910133
H	-8.310720	-0.684807	1.566417
H	-8.615784	-0.142241	3.454535
H	-8.581997	3.566726	1.507816
H	-11.314093	2.287138	-0.952770
H	-9.809241	1.894648	-1.809816
H	-10.577317	4.146363	-2.565796
H	-10.666053	4.689905	-0.877463
H	-8.178969	3.785150	-2.424264
H	-8.471894	5.408155	-1.767255

Energy: 24.1 kcal.mol^{-1}
- 806.520464 H

B Adduct

C	-10.188401	2.410481	-0.772940
O	-9.937850	2.859300	0.561713
C	-8.602813	3.238615	0.733700
O	-8.248959	4.310368	-0.100629
C	-8.397135	3.964807	-1.481468
C	-9.825848	3.513395	-1.760259
O	-7.737045	2.251626	0.741367
Y	-6.914201	0.991261	2.302094
B	-8.400650	3.578665	3.160868
P	-4.009577	1.301380	1.204321
C	-4.005239	2.313291	-0.329751
C	-2.280732	0.657720	1.320004
N	-5.103195	0.063705	1.156212
Si	-4.881408	-1.443792	0.291414
C	-4.556145	2.384577	2.477931
P	-4.622135	2.018725	4.205679
C	-4.667894	3.639950	5.070160
C	-3.138358	1.170382	4.904396
N	-5.980091	1.115906	4.457149
Si	-6.418893	0.348667	5.969924
B	-8.337474	-1.017114	2.569011

H	-5.691774	-0.945018	6.187518
H	-4.223417	-1.215783	-1.043523
H	-3.995995	-2.397878	1.038346
H	-6.207118	-2.081080	0.068940
H	-6.076806	1.229128	7.142562
H	-7.885073	0.091719	5.979304
H	-4.466288	3.443351	2.248311
H	-8.849264	2.464984	3.281600
H	-7.208826	3.712584	3.065400
H	-9.052374	4.476453	3.610525
H	-3.724334	4.174055	4.932176
H	-5.493079	4.226288	4.661088
H	-4.842542	3.466287	6.134590
H	-2.232609	1.737852	4.677535
H	-3.250975	1.080947	5.989016
H	-3.070557	0.166878	4.479040
H	-2.049594	0.070213	0.426337
H	-1.580277	1.493320	1.396165
H	-2.186641	0.016251	2.197846
H	-3.258587	3.109261	-0.265421
H	-3.779606	1.665670	-1.180456
H	-5.002647	2.741953	-0.448911
H	-7.181335	-1.217722	2.970683
H	-9.037688	-1.981113	2.698849
H	-8.250377	-0.653312	1.386657
H	-8.766080	-0.036012	3.202169
H	-8.684027	3.838260	1.762544
H	-11.251054	2.159779	-0.805542
H	-9.608836	1.497989	-0.969419
H	-9.920228	3.155191	-2.792133
H	-10.508062	4.360305	-1.627616
H	-7.683162	3.169721	-1.740156
H	-8.132911	4.865519	-2.041351

Energy: 21.1 kcal.mol^{-1}
- 806.525151 H

TSBC Trapping by Intracyclic Oxygen

Y	-5.925655	-0.671860	1.183105
N	-3.603123	-0.600110	0.981162
Si	-2.397184	-1.846957	0.724960
O	-7.094500	0.194204	-0.303468
C	-7.590831	1.302077	-0.892813
O	-8.615702	1.902500	-0.105337
C	-9.780403	1.082908	-0.013922
C	-10.303541	0.752584	-1.407072
C	-9.161926	0.173419	-2.233763
O	-8.045768	1.061017	-2.201213
B	-6.810533	4.136433	-2.380934

B	-6.451839	-3.091499	1.435652
N	-6.293438	0.223093	3.298376
Si	-7.049751	-0.408969	4.748168
P	-5.720859	1.767553	3.119471
C	-4.832789	2.313965	4.642722
C	-4.801887	1.797904	1.620702
P	-3.276459	0.999942	1.250497
C	-2.621251	1.844440	-0.245304
C	-7.062479	3.001657	2.896042
C	-1.937175	1.184570	2.507661
H	-5.606681	-2.743812	2.273466
H	-5.993649	-2.808681	0.314655
H	-7.445318	-2.358780	1.597574
H	-6.733147	-4.252581	1.526429
H	-6.832519	2.094401	-1.000975
H	-10.505534	1.656176	0.570761
H	-9.548236	0.158341	0.535940
H	-10.669364	1.669434	-1.883589
H	-11.139407	0.044046	-1.342574
H	-9.434156	0.068997	-3.287010
H	-8.866864	-0.814489	-1.851265
H	-7.702720	-1.705341	4.418372
H	-8.086257	0.535889	5.293314
H	-6.054443	-0.628330	5.851961
H	-7.732443	2.949564	3.758340
H	-6.643321	4.008533	2.818025
H	-7.615518	2.750926	1.985523
H	-4.029049	1.610901	4.869952
H	-4.415793	3.312161	4.488024
H	-5.528048	2.338155	5.487441
H	-2.230397	0.667023	3.422683
H	-1.760512	2.242416	2.716527
H	-1.015176	0.729875	2.130685
H	-2.338814	2.873571	-0.010011
H	-1.747482	1.295418	-0.609062
H	-3.396580	1.836981	-1.016494
H	-5.014426	2.654485	0.986162
H	-3.060411	-3.030982	0.113580
H	-1.725785	-2.262806	2.000515
H	-1.305861	-1.370943	-0.194640
H	-7.855339	4.384270	-2.899623
H	-6.585996	4.534880	-1.271485
H	-5.960844	3.551428	-2.985550

Energy: 16,7 kcal.mol^{-1}
- 806.532256 H

C Adduct

Y	-6.372572	-0.512323	1.639963

N	-4.218811	-0.516047	0.803907
Si	-3.199240	-1.789921	0.157420
O	-7.866694	0.446468	0.481616
C	-8.165562	1.592961	-0.116242
O	-9.500785	1.766486	-0.425127
C	-10.020993	0.759932	-1.296865
C	-9.281426	0.823752	-2.626948
C	-7.786169	0.700375	-2.377976
O	-7.351247	1.670488	-1.395088
B	-6.930895	3.132256	-1.941677
B	-6.926473	-2.922019	1.854311
N	-6.143098	0.259505	3.820710
Si	-6.521223	-0.443343	5.383878
P	-5.482562	1.761533	3.585703
C	-4.133086	2.079765	4.805635
C	-5.064894	1.868165	1.880013
P	-3.745303	1.059266	1.029604
C	-3.512471	1.968426	-0.542571
C	-6.687330	3.114776	3.889300
C	-2.097377	1.112015	1.859763
H	-5.869621	-2.653583	2.445601
H	-6.777146	-2.563612	0.671836
H	-7.805245	-2.181445	2.329779
H	-7.215750	-4.081077	1.941295
H	-7.842673	2.502196	0.400178
H	-11.082849	0.988460	-1.410333
H	-9.921386	-0.228134	-0.829261
H	-9.492466	1.778308	-3.118670
H	-9.606059	0.014482	-3.291217
H	-7.188905	0.902809	-3.268006
H	-7.531319	-0.287886	-1.981918
H	-7.467868	-1.573606	5.180424
H	-7.154921	0.568756	6.297823
H	-5.295802	-0.947221	6.086737
H	-7.078950	3.020596	4.904826
H	-6.207259	4.088990	3.767505
H	-7.508594	3.015741	3.176440
H	-3.375768	1.297859	4.726495
H	-3.680805	3.055275	4.610996
H	-4.546767	2.066295	5.818492
H	-2.134144	0.519344	2.775916
H	-1.826598	2.144875	2.091151
H	-1.343889	0.679743	1.194594
H	-3.078088	2.951930	-0.346060
H	-2.842160	1.391808	-1.184584
H	-4.480545	2.092480	-1.034941
H	-5.392696	2.783337	1.391639
H	-4.068454	-2.895838	-0.330405
H	-2.246899	-2.330112	1.182428
H	-2.361816	-1.287949	-0.985672

H	-6.035710	2.884189	-2.725611
H	-7.899991	3.646594	-2.452373
H	-6.547323	3.709434	-0.941244

Energy: 1.05 kcal.mol^{-1}
- 806.557121 H

TSCD Trapping by Extracyclic Oxygen

O	-8.924718	2.894705	-0.519856
C	-7.578787	2.472816	-0.421554
O	-7.030899	2.189716	-1.691957
C	-7.761145	1.188819	-2.399942
C	-9.220799	1.602765	-2.532399
C	-9.761883	1.922962	-1.145927
O	-7.482122	1.421310	0.432614
Y	-6.657291	0.299219	2.011338
B	-7.827487	-1.870858	2.329376
N	-6.056921	0.985089	4.172665
P	-4.886412	2.113204	3.877490
C	-4.623249	2.148231	2.134419
P	-3.725333	0.968959	1.181878
N	-4.578944	-0.445992	1.271762
Si	-3.976345	-2.013664	0.771918
Si	-6.573103	0.453797	5.760162
C	-5.405128	3.815072	4.339858
C	-3.398280	1.789246	4.922062
C	-1.954847	0.705239	1.642136
C	-3.649007	1.649062	-0.521740
B	-9.116994	2.535380	2.108879
H	-6.734487	-1.872079	2.913049
H	-7.602107	-1.616865	1.134114
H	-8.471943	-0.904099	2.774433
H	-8.418003	-2.905828	2.467241
H	-7.029908	3.354538	-0.069306
H	-10.759550	2.370361	-1.184563
H	-9.812727	1.014054	-0.529233
H	-9.293822	2.493859	-3.166387
H	-9.807223	0.803287	-2.999096
H	-7.272422	1.096517	-3.374853
H	-7.681568	0.226549	-1.878778
H	-6.792800	1.618104	6.685629
H	-5.558522	-0.427999	6.426452
H	-7.851384	-0.293773	5.619156
H	-5.705542	3.822630	5.390232
H	-4.586064	4.519704	4.185550
H	-6.261836	4.093242	3.720537
H	-3.057402	0.765605	4.749585
H	-2.601645	2.494770	4.673916
H	-3.662632	1.894463	5.978484

H	-1.897178	0.278055	2.644698
H	-1.420523	1.658360	1.615496
H	-1.493221	0.010532	0.934054
H	-3.097067	2.592968	-0.533121
H	-3.143491	0.923740	-1.162741
H	-4.669086	1.805066	-0.885713
H	-4.669893	3.142603	1.697437
H	-5.127733	-2.914221	0.494573
H	-3.101839	-2.641514	1.818331
H	-3.135677	-1.904967	-0.471840
H	-8.808220	1.540041	2.723515
H	-8.421146	3.505476	2.182966
H	-10.246412	2.611122	1.726807

Energy: 17.9 kcal.mol^{-1}
- 806.530286 H

D Adduct

Y	-6.718793	0.345908	2.093024
B	-8.837693	2.107612	1.814028
O	-8.842555	2.629451	0.431387
C	-7.655018	2.544514	-0.191382
O	-7.175380	1.136287	-0.189294
O	-7.682451	3.018196	-1.485723
C	-8.590790	2.300009	-2.325506
C	-8.153424	0.843906	-2.396827
C	-8.034744	0.286266	-0.985872
B	-7.618357	-1.912286	2.580373
N	-5.905251	0.900613	4.205104
Si	-6.251936	0.284478	5.809723
P	-4.854156	2.128306	3.871838
C	-3.314798	1.970909	4.881627
C	-4.658285	2.155524	2.114593
P	-3.768759	0.961898	1.161339
C	-3.599534	1.694594	-0.516821
N	-4.675524	-0.411015	1.186642
Si	-4.151203	-1.990124	0.647467
C	-5.515046	3.782591	4.322940
C	-2.023911	0.623312	1.669651
H	-6.411645	-1.843718	2.845618
H	-7.737133	-1.579545	1.385017
H	-8.183650	-1.025337	3.236193
H	-8.076319	-2.999690	2.789646
H	-6.841665	3.071954	0.326303
H	-8.544405	2.790663	-3.300384
H	-9.609668	2.391161	-1.930983
H	-7.184557	0.776386	-2.904806
H	-8.875975	0.247484	-2.965551
H	-7.572707	-0.703726	-0.974707

H	-9.017419	0.225681	-0.503432
H	-6.137634	1.377521	6.838697
H	-5.290779	-0.790015	6.220834
H	-7.636716	-0.259940	5.844688
H	-5.758984	3.785244	5.387955
H	-4.778774	4.562626	4.111836
H	-6.424609	3.954702	3.743724
H	-2.879150	0.982480	4.724427
H	-2.597182	2.744598	4.597453
H	-3.566342	2.079167	5.940828
H	-2.018999	0.147284	2.651835
H	-1.454814	1.555721	1.706379
H	-1.562860	-0.056134	0.946797
H	-2.990374	2.601762	-0.483230
H	-3.125483	0.959438	-1.172013
H	-4.598746	1.922865	-0.892508
H	-4.644045	3.159033	1.694348
H	-5.295445	-2.718088	0.027447
H	-3.593358	-2.822636	1.760521
H	-3.064841	-1.868334	-0.389539
H	-8.908386	0.852399	1.817895
H	-7.735219	2.391424	2.360352
H	-9.745348	2.545021	2.472914

Energy: - 5.4 kcal.mol^{-1}
- 806.567349 H

TSDE Ring Opening

Y	-6.570630	0.181531	1.871802
B	-8.885450	2.610812	2.247873
O	-9.119904	2.637650	0.684906
C	-8.292483	3.207218	-0.043018
O	-7.038296	0.814170	-0.114695
O	-8.293358	3.162438	-1.333389
C	-9.023966	2.090853	-2.009977
C	-8.045717	0.981234	-2.349489
C	-7.633504	0.102691	-1.160004
B	-7.895299	-1.890012	2.192923
N	-5.977857	0.899723	4.075591
Si	-6.560819	0.413543	5.649467
P	-4.819392	2.025344	3.783896
C	-3.310845	1.698348	4.800446
C	-4.571532	2.056729	2.028658
P	-3.611415	0.861479	1.157940
C	-3.625036	1.401609	-0.599479
N	-4.372406	-0.584142	1.393376
Si	-3.643952	-2.140017	1.074621
C	-5.313988	3.731399	4.260831
C	-1.809127	0.759468	1.570487

H	-7.397764	-1.484500	3.255736
H	-6.952710	-2.034783	1.396792
H	-8.587073	-0.962374	1.746944
H	-8.520328	-2.902203	2.343955
H	-7.526000	3.862952	0.374331
H	-9.431844	2.571866	-2.902189
H	-9.840774	1.753282	-1.367534
H	-7.164034	1.429981	-2.823396
H	-8.523389	0.341635	-3.103366
H	-6.951295	-0.671079	-1.554385
H	-8.534693	-0.433689	-0.812099
H	-6.158226	1.407569	6.708770
H	-6.006190	-0.912627	6.073435
H	-8.049907	0.324843	5.644577
H	-5.555035	3.741603	5.326064
H	-4.505020	4.437309	4.058122
H	-6.206722	3.998248	3.690984
H	-2.978050	0.674935	4.615956
H	-2.513635	2.404384	4.551916
H	-3.566709	1.796619	5.859975
H	-1.681956	0.415331	2.597752
H	-1.351771	1.746467	1.454233
H	-1.317813	0.052573	0.894320
H	-3.141305	2.375284	-0.711065
H	-3.097800	0.658103	-1.202944
H	-4.673609	1.452251	-0.902375
H	-4.561142	3.056111	1.596451
H	-4.708316	-3.176688	0.994529
H	-2.663557	-2.538158	2.141018
H	-2.869954	-2.145782	-0.218099
H	-8.497629	1.469661	2.479122
H	-8.043695	3.455893	2.490152
H	-9.956943	2.793320	2.762188

Energy: 3.6 kcal.mol^{-1}
- 806.553188 H

E Adduct

Y	-6.203121	-0.562466	1.495090
N	-5.891595	-0.309350	3.811326
Si	-6.331124	-1.285259	5.197735
O	-7.834971	0.447845	0.759868
C	-9.185969	0.746273	0.638884
C	-9.725335	0.503487	-0.775849
C	-9.263873	1.496619	-1.825067
O	-7.828770	1.370178	-2.059588
C	-7.018314	2.221042	-1.511808
O	-7.372526	3.226470	-0.886333
B	-6.297426	4.271903	-0.302619
B	-6.618687	-3.009724	1.303361

P	-5.223248	1.205781	3.882880
C	-3.952676	1.301020	5.222077
C	-4.709998	1.596821	2.254083
P	-3.425235	0.856318	1.300591
C	-2.058372	0.157634	2.320399
N	-4.131681	-0.336955	0.390147
Si	-3.312971	-1.379018	-0.754411
C	-6.436543	2.508889	4.337133
C	-2.645607	2.162502	0.275571
H	-2.559505	-2.496972	-0.097860
H	-4.325528	-1.960694	-1.681383
H	-2.310793	-0.610002	-1.572198
H	-1.312028	-0.289446	1.657673
H	-2.465404	-0.627359	2.962005
H	-1.589592	0.937473	2.924847
H	-1.990195	1.701455	-0.467119
H	-3.435115	2.729147	-0.224565
H	-2.069844	2.835722	0.915406
H	-5.021169	2.573910	1.888241
H	-7.183792	2.572266	3.543676
H	-5.935620	3.474116	4.444648
H	-6.919564	2.234406	5.277921
H	-3.486912	2.289646	5.212393
H	-3.193229	0.533104	5.066670
H	-4.430059	1.133822	6.192348
H	-7.046636	-0.474279	6.244314
H	-7.229281	-2.384500	4.749196
H	-5.131275	-1.881158	5.875683
H	-5.586698	-2.779434	1.951280
H	-7.547246	-2.413905	1.874868
H	-6.832793	-4.184807	1.196564
H	-6.483005	-2.457244	0.196666
H	-5.964657	1.989487	-1.682159
H	-9.373589	1.799278	0.912898
H	-9.480046	2.528416	-1.538995
H	-10.822092	0.568006	-0.755216
H	-9.708230	1.286819	-2.800266
H	-9.468605	-0.514476	-1.090774
H	-9.785470	0.131021	1.330574
H	-6.613749	5.331019	-0.787420
H	-6.442086	4.224265	0.899843
H	-5.211248	3.869085	-0.687731

Energy: - 0.3 kcal.mol^{-1}
- 806.559221 H

TSEF 2nd H transfer

Y	-6.318102	0.003404	1.329410
N	-5.959449	0.730722	3.593106

Si	-6.742447	0.319612	5.099443
O	-6.515960	0.558327	-0.693855
C	-7.199308	0.102324	-1.815297
C	-8.236691	1.115023	-2.321410
C	-9.085164	1.703913	-1.204787
O	-8.414999	2.902282	-0.699859
C	-7.972467	2.978584	0.513090
O	-7.919217	1.992114	1.349149
B	-9.032773	2.745362	2.227490
B	-7.845037	-1.949857	1.547766
P	-4.604446	1.645929	3.442992
C	-3.291316	1.083821	4.614687
C	-4.151940	1.637020	1.727606
P	-3.244362	0.327066	0.971249
C	-1.505000	0.062144	1.545250
N	-4.176493	-1.016369	1.182123
Si	-3.663481	-2.668450	0.940531
C	-4.870745	3.411722	3.891405
C	-3.056917	0.814016	-0.791528
H	-2.470899	-3.009696	1.791311
H	-4.785832	-3.574291	1.306615
H	-3.253646	-2.954523	-0.478184
H	-1.020739	-0.698068	0.925528
H	-1.504682	-0.276385	2.582434
H	-0.950926	1.001152	1.464002
H	-2.540908	0.016159	-1.331394
H	-4.067786	0.940021	-1.189934
H	-2.488434	1.744095	-0.879822
H	-3.979492	2.624393	1.303776
H	-5.618640	3.832933	3.217131
H	-3.936596	3.974459	3.816800
H	-5.252891	3.461856	4.913585
H	-2.373938	1.661362	4.476077
H	-3.100627	0.023074	4.438132
H	-3.648579	1.206691	5.641489
H	-6.773208	1.487745	6.049560
H	-8.143411	-0.101492	4.819951
H	-6.043482	-0.791017	5.830353
H	-7.128288	-1.805984	2.549197
H	-8.465339	-0.883378	1.396459
H	-8.580342	-2.891842	1.650990
H	-7.082152	-2.051328	0.575423
H	-7.361379	3.868823	0.669974
H	-7.728456	-0.842904	-1.598220
H	-9.245484	1.007296	-0.379471
H	-8.901522	0.625001	-3.044459
H	-10.046432	2.075325	-1.566398
H	-7.752965	1.946103	-2.848664
H	-6.505313	-0.118044	-2.645436
H	-9.261869	3.725059	1.473424

H	-10.019650	2.064513	2.205005
H	-8.547720	3.139008	3.252335

Energy: 15.3 kcal.mol^{-1}
- 806.534448 H

F Product (alcohol termination)

C	-5.021288	4.273487	2.785104
P	-4.717195	2.461692	2.901625
N	-6.096469	1.619435	3.240512
Si	-6.858504	1.550692	4.809552
C	-3.496755	2.286400	4.277353
C	-4.143437	1.967829	1.314013
P	-3.205798	0.516522	0.999517
C	-2.884097	0.514161	-0.812781
C	-1.506827	0.461238	1.732540
N	-4.146776	-0.731877	1.508464
Si	-3.674283	-2.408104	1.676085
H	-4.080475	-2.942453	3.009875
B	-7.596252	-1.797732	2.137157
H	-4.263531	-3.277072	0.610996
H	-2.177761	-2.552306	1.571367
H	-0.989688	-0.444092	1.405109
H	-1.575935	0.453964	2.821691
H	-0.947483	1.342047	1.406100
H	-2.317915	-0.383740	-1.073303
H	-3.855177	0.493865	-1.312046
H	-2.318778	1.401522	-1.110657
H	-4.030887	2.777984	0.598969
H	-5.678725	4.448926	1.930552
H	-4.080359	4.812110	2.646738
H	-5.509942	4.615210	3.700956
H	-2.572843	2.818362	4.037970
H	-3.290643	1.223601	4.423491
H	-3.924225	2.690756	5.199547
H	-6.580013	2.802764	5.603652
H	-8.340634	1.457129	4.643651
H	-6.402461	0.399032	5.650476
H	-6.432141	-2.064478	1.805055
H	-7.525551	-0.926085	3.015823
H	-8.184223	-2.774138	2.514386
H	-8.129197	-1.286831	1.146347
Y	-6.333353	0.204640	1.310896
O	-8.839041	1.410861	1.574460
C	-8.544737	2.802691	1.388886
O	-6.490840	0.390851	-0.731935
C	-6.804164	0.932177	-1.960380
C	-7.027442	2.448390	-1.910033
C	-8.113848	2.868229	-0.935381

O	-7.585664	2.920660	0.403777
H	-8.101303	3.163794	2.318270
H	-7.720175	0.464710	-2.368628
H	-8.947393	2.154005	-0.974125
H	-7.308729	2.801664	-2.911370
H	-8.504117	3.866292	-1.178866
H	-6.097381	2.962111	-1.636866
B	-10.113834	0.967653	1.747525
H	-6.007925	0.728557	-2.700644
H	-9.474104	3.337919	1.149745
H	-10.268766	-0.196173	1.929553
H	-11.010798	1.765817	1.700349

Energy: - 15.2 kcal.mol^{-1}
- 806.582995 H

D' Adduct

B	-5.539028	1.190346	-1.642726
N	-3.263413	-0.412019	1.063458
P	-2.900286	1.055031	1.724700
Y	-5.562619	-0.216654	0.671975
B	-6.081749	-2.627912	0.389985
N	-6.229532	-0.081905	2.943961
P	-5.525949	1.331888	3.421408
C	-6.736276	2.706581	3.595373
O	-7.665018	0.953767	0.227277
C	-8.929839	0.546374	0.775718
C	-9.718035	-0.253823	-0.250035
C	-9.787542	0.542203	-1.546467
O	-8.483180	0.925658	-1.960260
C	-7.839047	1.734978	-1.028729
O	-6.660348	2.154441	-1.453248
C	-4.442884	1.820552	2.122204
C	-1.691360	0.869101	3.110712
C	-2.058103	2.198843	0.559558
Si	-2.102204	-1.678663	0.722446
Si	-6.992272	-1.244769	4.004849
C	-4.794112	1.180211	5.112519
H	-1.883898	-2.577079	1.903246
H	-2.577040	-2.495911	-0.427722
H	-0.757729	-1.096515	0.375553
H	-0.749022	0.480035	2.713432
H	-2.081257	0.159655	3.842907
H	-1.512641	1.836366	3.587085
H	-1.147819	1.718240	0.192989
H	-2.731870	2.389107	-0.278279
H	-1.803161	3.135848	1.061664
H	-4.509378	2.869018	1.841978
H	-7.181157	2.894494	2.616153

H	-6.241953	3.611095	3.959447
H	-7.515028	2.404447	4.299774
H	-4.279873	2.106874	5.379299
H	-4.087667	0.348112	5.130408
H	-5.588859	0.982385	5.837670
H	-7.682016	-0.558377	5.155498
H	-8.026189	-2.003309	3.243366
H	-6.020280	-2.214941	4.602976
H	-5.461922	-2.415225	1.440994
H	-7.098487	-1.913122	0.434793
H	-6.351069	-3.786504	0.241308
H	-5.387084	-2.183011	-0.534518
H	-9.483227	1.451713	1.070825
H	-10.414391	1.440896	-1.410259
H	-10.724429	-0.460107	0.132973
H	-10.210415	-0.043527	-2.365631
H	-9.218045	-1.210867	-0.430002
H	-8.709100	-0.028203	1.677416
H	-8.490139	2.583343	-0.746274
H	-4.925742	1.379794	-2.663126
H	-4.741201	1.347018	-0.687067
H	-5.933716	0.011833	-1.599702

Energy: - 5.0 kcal.mol^{-1}
- 806.566782 H

TSD'E' Trapping by Ligand Nitrogen

B	-4.775403	0.571004	-1.254219
N	-3.670369	-0.101025	0.715088
P	-3.263599	1.212820	1.640479
Y	-6.081481	-0.250182	1.137200
B	-6.686845	-2.641772	0.758683
N	-5.763872	-0.380292	3.497019
P	-5.453394	1.199016	3.838880
C	-6.960652	2.209052	4.142517
O	-7.872846	0.779838	1.087640
C	-9.198421	1.039880	0.805129
C	-9.707777	0.329654	-0.458140
C	-9.182198	0.890743	-1.763093
O	-7.745576	0.721507	-1.806247
C	-7.110138	1.071345	-2.905506
O	-5.897717	1.067657	-2.986641
C	-4.743989	1.847587	2.364116
C	-1.930045	0.759094	2.834218
C	-2.539749	2.577956	0.645557
Si	-2.512708	-1.292223	0.147941
Si	-6.244685	-1.635025	4.614581
C	-4.477420	1.403071	5.397893
H	-1.976523	-2.131763	1.270739

H	-3.174124	-2.180041	-0.845014
H	-1.318614	-0.642539	-0.497996
H	-1.034639	0.457386	2.282866
H	-2.269975	-0.085197	3.437631
H	-1.692920	1.611178	3.475804
H	-1.680688	2.196383	0.089005
H	-3.294806	2.925479	-0.061121
H	-2.228278	3.396379	1.299410
H	-4.934431	2.898968	2.162983
H	-7.597554	2.093091	3.262053
H	-6.699905	3.260469	4.292202
H	-7.476128	1.829434	5.028462
H	-4.223366	2.458886	5.524011
H	-3.563855	0.809022	5.343447
H	-5.067698	1.064833	6.253316
H	-5.662632	-1.391663	5.981915
H	-7.730931	-1.719145	4.797376
H	-5.747573	-2.953174	4.129614
H	-5.465567	-2.499917	0.918144
H	-7.243041	-2.156874	1.756728
H	-6.987020	-3.791822	0.590757
H	-7.013353	-1.925666	-0.199468
H	-9.372657	2.127514	0.683738
H	-9.402391	1.962945	-1.841059
H	-10.802468	0.415053	-0.501153
H	-9.623447	0.373621	-2.624119
H	-9.466901	-0.737577	-0.393196
H	-9.845890	0.718786	1.640537
H	-7.751984	1.368160	-3.753303
H	-3.754572	0.799613	-1.823263
H	-5.322047	1.440840	-0.616517
H	-5.235419	-0.541933	-1.247976

Energy: 15.0 kcal.mol^{-1}
- 806.534880 H

E' Product (formate termination)

B	-4.265621	0.730595	-0.739861
N	-3.525550	0.149597	0.564613
P	-3.181854	1.350124	1.720752
Y	-6.078890	-0.100983	0.962371
B	-6.526128	-2.516258	0.595746
N	-5.711829	-0.387733	3.317715
P	-5.445182	1.157682	3.808697
C	-6.968442	2.137673	4.128680
O	-7.837462	0.940412	0.996637
C	-9.139109	1.368453	0.813907
C	-9.823317	0.749709	-0.407678
C	-9.223438	1.144743	-1.747833

O	-7.974301	0.481879	-1.992884
C	-7.873972	-0.277297	-3.099514
O	-6.866837	-0.844348	-3.416572
C	-4.665828	1.935382	2.436057
C	-1.971088	0.629334	2.898024
C	-2.334557	2.760542	0.916104
Si	-2.413876	-1.189443	0.169161
Si	-6.227186	-1.732605	4.315695
C	-4.539606	1.245752	5.419984
H	-2.129116	-1.998671	1.392109
H	-3.057716	-2.018901	-0.876813
H	-1.107165	-0.646892	-0.331579
H	-1.058171	0.341033	2.370143
H	-2.408028	-0.253420	3.368771
H	-1.730874	1.377690	3.656352
H	-1.458568	2.391570	0.378030
H	-3.023576	3.215173	0.202172
H	-2.036286	3.490805	1.671739
H	-4.885016	2.983827	2.257814
H	-7.572711	2.090892	3.219739
H	-6.718424	3.174267	4.371050
H	-7.514418	1.688340	4.962191
H	-4.297167	2.289489	5.636637
H	-3.622077	0.658038	5.364217
H	-5.165541	0.842721	6.220088
H	-5.763245	-1.544484	5.736476
H	-7.716847	-1.879582	4.371788
H	-5.631764	-2.997943	3.803475
H	-5.330196	-2.312771	0.862220
H	-7.185096	-2.049468	1.539366
H	-6.755816	-3.680005	0.418256
H	-6.799859	-1.826717	-0.394859
H	-9.171617	2.469319	0.703093
H	-9.024640	2.222242	-1.783705
H	-10.873993	1.073135	-0.411680
H	-9.919759	0.903825	-2.563253
H	-9.821574	-0.343309	-0.318895
H	-9.754637	1.128215	1.698949
H	-8.818356	-0.317261	-3.679933
H	-3.519067	1.151753	-1.590845
H	-5.018561	1.631484	-0.355205
H	-4.951789	-0.186429	-1.177588

Energy: - 4.3 $kcal.mol^{-1}$
- 806.565648 H

Reaction between TMC and [{(CH(PPh$_2$NSiMe$_3$)$_2$}La(BH$_4$)$_2$(THF)] (1)

All energies in kcal.mol^{-1} are realtive to the origin level, all energies in H are absolute.

Energy of the reactants : - 799.812763 H

A Adduct

C	-10.505129	2.709909	-1.017846
O	-9.310811	1.935943	-0.756510
C	-8.108541	2.482574	-0.673188
O	-7.891989	3.719849	-1.096605
C	-8.985515	4.538322	-1.564085
C	-10.246615	4.184602	-0.809942
O	-7.174737	1.826327	-0.228297
La	-7.007655	1.015004	2.274420
B	-8.512818	3.292097	2.638352
P	-3.809918	1.082821	1.336586
C	-3.548402	1.961076	-0.259599
C	-2.145925	0.368964	1.720472
N	-4.952875	-0.094746	1.240362
Si	-4.748939	-1.633389	0.444549
C	-4.408027	2.318503	2.447619
P	-4.550956	2.134479	4.198039
C	-4.877375	3.828180	4.837576
C	-3.021628	1.612243	5.100099
N	-5.791228	1.091416	4.487863
Si	-6.196368	0.419002	6.048273
B	-8.527025	-1.165991	2.638211
H	-5.278888	-0.701565	6.446598
H	-4.099306	-1.497151	-0.908786
H	-3.879802	-2.580203	1.222921
H	-6.088489	-2.258322	0.258153
H	-6.103569	1.443893	7.148106
H	-7.591747	-0.099713	5.999229
H	-4.203786	3.337921	2.127898
H	-9.078776	2.468036	1.903436
H	-8.350996	2.746526	3.731341
H	-9.162830	4.306194	2.732049
H	-4.023524	4.484579	4.650017
H	-5.767069	4.212885	4.334407
H	-5.067657	3.769693	5.911764
H	-2.187650	2.268899	4.839665
H	-3.199628	1.662209	6.178595
H	-2.779646	0.581601	4.834211

H	-1.830935	-0.283765	0.900749
H	-1.412708	1.169115	1.849756
H	-2.211370	-0.225677	2.633482
H	-2.788990	2.740489	-0.154868
H	-3.231450	1.237531	-1.014427
H	-4.503477	2.398123	-0.558093
H	-7.344417	-1.366473	2.960603
H	-9.203464	-2.144736	2.806633
H	-8.524406	-0.805634	1.447712
H	-8.936086	-0.203596	3.308140
H	-7.397615	3.533221	2.151488
H	-11.254236	2.311556	-0.331636
H	-10.808304	2.488122	-2.046840
H	-11.093169	4.769970	-1.181731
H	-10.114404	4.400472	0.255768
H	-9.093403	4.378015	-2.643642
H	-8.658998	5.564545	-1.390233

Energy: - 4.0 kcal.mol^{-1}
- 799.819134 H

TSAB Nucleophilic attack

C	-10.416893	2.768610	-1.147249
O	-9.807370	2.586536	0.131432
C	-8.497678	2.996206	0.295087
O	-8.108579	4.135535	-0.382719
C	-8.705363	4.433710	-1.648738
C	-10.200552	4.187127	-1.634673
O	-7.616618	2.082085	0.412398
La	-6.996891	0.820343	2.384301
B	-8.572306	3.415388	2.799157
P	-3.896853	1.143042	1.303244
C	-3.864832	2.106477	-0.262302
C	-2.157840	0.544272	1.497151
N	-4.956553	-0.121676	1.250790
Si	-4.692449	-1.621023	0.390027
C	-4.488211	2.271677	2.518719
P	-4.539073	2.025717	4.267081
C	-4.650646	3.708447	4.999057
C	-3.013016	1.300037	5.013245
N	-5.853012	1.091399	4.617726
Si	-6.257705	0.471210	6.202322
B	-8.374662	-1.449266	2.783322
H	-5.334435	-0.626876	6.645720

H	-4.094935	-1.389423	-0.972751
H	-3.748190	-2.538377	1.111453
H	-6.001668	-2.311192	0.222063
H	-6.182420	1.537640	7.261611
H	-7.649439	-0.058486	6.157039
H	-4.413664	3.316835	2.228445
H	-9.115395	2.337096	2.970433
H	-7.360125	3.417811	2.940864
H	-9.154994	4.350401	3.276397
H	-3.737135	4.274679	4.800651
H	-5.510073	4.216787	4.556712
H	-4.803400	3.618626	6.077032
H	-2.134656	1.882160	4.724200
H	-3.106801	1.296720	6.103134
H	-2.907938	0.268126	4.672000
H	-1.878755	-0.057135	0.626731
H	-1.479056	1.396789	1.582102
H	-2.083267	-0.076756	2.391414
H	-3.139836	2.922219	-0.199439
H	-3.597421	1.439426	-1.085213
H	-4.868509	2.505390	-0.426693
H	-7.170951	-1.578361	3.065066
H	-8.983214	-2.467710	2.968068
H	-8.440998	-1.081342	1.598412
H	-8.813565	-0.515608	3.478924
H	-8.668026	3.615279	1.499561
H	-11.472344	2.532526	-0.996200
H	-10.001221	2.043214	-1.862105
H	-10.614597	4.319430	-2.640205
H	-10.697397	4.893032	-0.960866
H	-8.225365	3.816913	-2.422972
H	-8.456736	5.479791	-1.843685

Energy: 22.7 kcal.mol^{-1}
- 799.776524 H

B Adduct

C	-10.363289	2.693357	-0.936355
O	-10.123233	2.992371	0.441796
C	-8.767948	3.235223	0.684826
O	-8.294193	4.343533	-0.033925
C	-8.422067	4.141881	-1.444645
C	-9.873651	3.847249	-1.802921
O	-7.993176	2.184756	0.653158

La	-7.038732	0.830490	2.306175
B	-8.580028	3.514663	3.136591
P	-3.938846	1.190233	1.216364
C	-3.841064	2.188680	-0.325519
C	-2.217372	0.551680	1.435117
N	-5.019480	-0.053831	1.100617
Si	-4.745618	-1.531548	0.201974
C	-4.537236	2.301254	2.445100
P	-4.579417	2.044060	4.193893
C	-4.643267	3.724011	4.939451
C	-3.060732	1.284538	4.920422
N	-5.907466	1.132804	4.548754
Si	-6.329916	0.527803	6.134779
B	-8.371824	-1.472216	2.683079
H	-5.397106	-0.547937	6.611152
H	-4.088817	-1.258949	-1.125240
H	-3.845319	-2.486278	0.929612
H	-6.057756	-2.192089	-0.042138
H	-6.295356	1.610591	7.178932
H	-7.711654	-0.025691	6.067714
H	-4.461327	3.349142	2.164593
H	-9.125796	2.447811	3.288908
H	-7.375028	3.530282	3.056431
H	-9.125386	4.479450	3.587810
H	-3.717371	4.267508	4.735156
H	-5.492701	4.260757	4.512131
H	-4.785839	3.629779	6.018482
H	-2.174160	1.851633	4.626835
H	-3.145210	1.277403	6.010991
H	-2.977896	0.252276	4.574444
H	-1.930038	-0.030884	0.554608
H	-1.523658	1.387035	1.559689
H	-2.176206	-0.096230	2.312181
H	-3.084402	2.971900	-0.231043
H	-3.585762	1.529857	-1.158816
H	-4.820687	2.637231	-0.504272
H	-7.201411	-1.554631	3.089502
H	-8.971285	-2.499051	2.849160
H	-8.330824	-1.154303	1.482262
H	-8.905661	-0.522868	3.286869
H	-8.859728	3.766021	1.766207
H	-11.441672	2.540903	-1.021919
H	-9.856390	1.756256	-1.204573
H	-9.963553	3.597438	-2.866578

H	-10.484702	4.734903	-1.605993
H	-7.769682	3.315147	-1.760201
H	-8.063031	5.064215	-1.908583

Energy: 20.9 kcal.mol^{-1}
- 799.779451 H

TSBC Trapping by Intracyclic Oxygen

O	-11.633397	3.568447	-1.042543
C	-12.767827	4.310015	-0.399486
O	-13.936936	3.565245	-0.585303
C	-13.781176	2.190793	-0.232968
C	-12.861482	1.494413	-1.256362
C	-12.054302	2.571434	-1.978573
O	-12.386663	4.539938	0.844546
La	-10.169780	3.779601	1.106051
C	-9.475959	6.539940	0.469443
P	-8.023994	5.906432	-0.304378
C	-8.107925	6.459986	-2.056599
H	-11.148015	2.171122	-2.440617
N	-9.608957	5.402251	2.968690
Si	-9.477122	5.207634	4.700246
P	-9.713997	6.855049	2.184819
C	-11.390068	7.596239	2.305971
B	-9.972069	1.223401	1.978386
N	-8.028088	4.258878	-0.166400
Si	-6.754881	3.207276	-0.739433
C	-8.599537	8.113347	2.957764
C	-6.433192	6.599491	0.325864
B	-14.405243	5.891234	-2.744772
H	-6.422707	3.449391	-2.187489
H	-7.212319	1.796547	-0.589416
H	-5.469089	3.378728	0.018156
H	-5.599897	6.206295	-0.263393
H	-6.300984	6.285011	1.363495
H	-6.444061	7.690234	0.262939
H	-8.024812	7.547834	-2.118054
H	-7.295907	5.994569	-2.619999
H	-9.063556	6.136627	-2.475170
H	-10.093109	7.147388	-0.187871
H	-12.091643	6.882072	1.864790
H	-11.433711	8.551174	1.775398
H	-11.634813	7.750462	3.359639

H	-8.655385	9.046782	2.391705
H	-7.572079	7.745355	2.958705
H	-8.910785	8.297492	3.990403
H	-8.106522	5.545319	5.213521
H	-9.768900	3.782783	5.031085
H	-10.438974	6.081985	5.457674
H	-9.295179	2.004568	2.670481
H	-11.148040	1.619121	2.011703
H	-9.574080	1.342643	0.805253
H	-9.874997	0.091092	2.366992
H	-12.921224	5.224131	-1.010096
H	-12.654146	3.053808	-2.759319
H	-14.649990	4.923514	-3.400200
H	-15.194819	6.291735	-1.944303
H	-13.392899	6.500346	-2.942821
H	-13.435114	0.919818	-1.992224
H	-12.190845	0.797373	-0.742296
H	-13.375584	2.111928	0.782002
H	-14.787538	1.767747	-0.225411

Energy: 16.8 kcal.mol^{-1}
-799.785981 H

C Adduct

O	-11.642577	3.648045	-1.208077
C	-12.684658	4.537448	-0.716738
O	-13.958488	3.767179	-0.759409
C	-13.783362	2.353025	-0.540361
C	-13.031240	1.726149	-1.715733
C	-12.046697	2.761098	-2.264785
O	-12.346046	4.904169	0.487649
La	-10.197640	4.014552	0.984772
C	-9.226105	6.717693	0.510172
P	-7.797772	5.982448	-0.218778
C	-7.721025	6.632595	-1.937966
H	-11.131769	2.309969	-2.653745
N	-9.685893	5.512473	2.940851
Si	-9.737210	5.239344	4.669506
P	-9.536301	6.994785	2.222109
C	-11.098911	7.959154	2.268493
B	-10.164629	1.483988	1.921247
N	-7.979132	4.338417	-0.176437
Si	-6.790635	3.185521	-0.743610
C	-8.320442	8.053185	3.127643

C	-6.186250	6.470944	0.536170
B	-15.099046	4.217757	-1.844447
H	-6.319508	3.498972	-2.137549
H	-7.423280	1.835903	-0.749396
H	-5.563267	3.142422	0.119325
H	-5.363582	6.045988	-0.045889
H	-6.135991	6.067944	1.550036
H	-6.093217	7.559154	0.560462
H	-7.522013	7.707020	-1.930172
H	-6.930063	6.114200	-2.484586
H	-8.678383	6.437241	-2.425929
H	-9.736531	7.416229	-0.148572
H	-11.860319	7.381925	1.737626
H	-10.966378	8.935197	1.794493
H	-11.402804	8.095133	3.309061
H	-8.207934	9.009375	2.610176
H	-7.355311	7.546226	3.178712
H	-8.679964	8.232869	4.145284
H	-8.375401	5.306111	5.296759
H	-10.310305	3.884492	4.910225
H	-10.586333	6.256405	5.380862
H	-9.418540	2.232997	2.575788
H	-11.309037	1.965522	1.970452
H	-9.790803	1.546854	0.735819
H	-10.139037	0.358456	2.337483
H	-12.871304	5.328833	-1.455848
H	-12.513803	3.358019	-3.055249
H	-14.720969	3.830981	-2.934216
H	-16.091576	3.655386	-1.443249
H	-15.128188	5.421864	-1.739003
H	-13.723690	1.429879	-2.508501
H	-12.510772	0.829369	-1.363567
H	-13.232757	2.241072	0.397426
H	-14.787282	1.949627	-0.411275

Energy: 2.7 kcal.mol^{-1}
- 799.808425 H

TSCD Trapping by Extracyclic Oxygen

O	-8.944918	2.910882	-0.442744
C	-7.607234	2.430744	-0.353683
O	-6.993343	2.377535	-1.623907
C	-7.694889	1.540986	-2.541395
C	-9.127459	2.037051	-2.692138

C	-9.760458	2.116563	-1.308611
O	-7.584058	1.240506	0.285356
La	-6.816089	0.120336	2.109655
B	-7.937154	-2.271138	2.673084
N	-6.011199	1.076622	4.304904
P	-4.855591	2.172987	3.864267
C	-4.649876	2.091371	2.114804
P	-3.731550	0.898425	1.195141
N	-4.540730	-0.539874	1.289166
Si	-3.913402	-2.072215	0.721651
Si	-6.458126	0.710988	5.956780
C	-5.363681	3.906480	4.215560
C	-3.326190	1.939118	4.874110
C	-1.960877	0.678631	1.681899
C	-3.640492	1.565648	-0.514221
B	-9.389587	2.021246	1.970476
H	-6.694604	-2.327119	2.672068
H	-8.296202	-1.859177	1.557957
H	-8.257923	-1.404126	3.506400
H	-8.427860	-3.337301	2.927374
H	-7.068934	3.226826	0.180506
H	-10.736960	2.607315	-1.330599
H	-9.887484	1.110147	-0.887739
H	-9.120931	3.032400	-3.150706
H	-9.705053	1.365629	-3.338263
H	-7.141432	1.597959	-3.482880
H	-7.680619	0.499761	-2.191289
H	-6.653871	1.957780	6.776568
H	-5.421506	-0.105823	6.671569
H	-7.739738	-0.049962	5.937017
H	-5.637591	3.991543	5.269617
H	-4.548354	4.598291	3.989330
H	-6.233777	4.145133	3.600118
H	-2.983470	0.907674	4.769590
H	-2.545233	2.627422	4.542080
H	-3.551695	2.123977	5.928514
H	-1.908897	0.243052	2.681276
H	-1.447107	1.643264	1.671789
H	-1.472176	0.000068	0.976351
H	-3.054732	2.488860	-0.529900
H	-3.159633	0.820614	-1.152976
H	-4.653943	1.759295	-0.878017
H	-4.699785	3.064034	1.630855
H	-5.054545	-2.963155	0.367618

H	-3.064003	-2.760950	1.748506
H	-3.050277	-1.900248	-0.499843
H	-9.514219	0.827702	2.044620
H	-8.444494	2.554186	2.490349
H	-10.350053	2.670544	1.709808

Energy: 20.4 kcal.mol^{-1}
- 799.780262 H

D Adduct

O	-8.904732	3.172124	-1.010204
C	-7.866249	2.546223	-0.338532
O	-6.976099	1.888320	-1.204128
C	-7.616342	0.931314	-2.057609
C	-8.768650	1.580353	-2.813371
C	-9.677990	2.274379	-1.807439
O	-8.330240	1.617008	0.598001
La	-6.960126	0.288505	2.215896
B	-7.876460	-2.190123	2.669517
N	-5.853803	0.941137	4.373307
P	-4.867164	2.190489	3.930292
C	-4.764198	2.183651	2.167002
P	-3.890663	1.010306	1.170558
N	-4.823237	-0.348313	1.064490
Si	-4.312260	-1.856154	0.337082
Si	-6.094711	0.389072	6.017513
C	-5.550991	3.838750	4.372689
C	-3.266826	2.120648	4.854607
C	-2.186669	0.578336	1.739398
C	-3.637431	1.826394	-0.454142
B	-8.971734	2.169861	1.876685
H	-6.637063	-2.134056	2.741334
H	-8.199667	-1.789807	1.536522
H	-8.328666	-1.366578	3.484632
H	-8.282403	-3.298931	2.884183
H	-7.293941	3.344827	0.148104
H	-10.436126	2.890923	-2.295928
H	-10.184567	1.544949	-1.162599
H	-8.374600	2.320731	-3.518560
H	-9.320698	0.824622	-3.383651
H	-6.835151	0.568932	-2.730574
H	-7.978458	0.081879	-1.462819
H	-6.377235	1.525655	6.961254
H	-4.890336	-0.323520	6.561078

H	-7.255105	-0.544984	6.027676
H	-5.736969	3.868054	5.448786
H	-4.848919	4.630886	4.099582
H	-6.494688	3.972127	3.839279
H	-2.807126	1.140623	4.717175
H	-2.593145	2.901120	4.492026
H	-3.455012	2.271948	5.921708
H	-2.251020	0.026753	2.679279
H	-1.588868	1.482891	1.875585
H	-1.709942	-0.062349	0.991460
H	-3.015174	2.718102	-0.342068
H	-3.147708	1.120315	-1.129198
H	-4.619813	2.088816	-0.855105
H	-4.795937	3.178961	1.729153
H	-5.521171	-2.631178	-0.061566
H	-3.479719	-2.692807	1.261938
H	-3.476424	-1.617897	-0.892585
H	-9.399307	1.169881	2.461573
H	-8.042409	2.647170	2.566727
H	-9.836141	2.982873	1.692761

Energy: - 6.5 kcal.mol^{-1}
- 799.823172 H

TSDE Ring Opening

H	-3.821679	4.387648	4.137704
C	-4.747719	3.824362	4.279205
P	-4.499220	2.045737	3.867719
C	-3.096126	1.532127	4.958646
N	-5.829597	1.128454	4.151828
La	-6.614539	0.451576	1.757903
B	-8.139059	-1.783385	1.705160
P	-3.350645	0.684905	1.303439
C	-1.604825	0.325324	1.808631
C	-3.186359	1.245018	-0.441921
N	-4.319885	-0.637958	1.464231
H	-1.587193	-0.061656	2.828725
Si	-3.832244	-2.287302	1.169397
Si	-6.524024	0.783076	5.708752
H	-5.613983	-0.019452	6.598244
H	-7.775398	-0.002236	5.495024
H	-6.874794	2.022433	6.488500
H	-3.362318	1.705352	6.005380
H	-2.919677	0.463298	4.820238

H	-2.193103	2.096367	4.712833
H	-4.976589	-3.186169	1.483505
H	-2.659195	-2.690486	2.020897
H	-3.407298	-2.533777	-0.253838
H	-1.168784	-0.422805	1.140239
H	-1.016485	1.245226	1.754811
H	-2.747941	0.441310	-1.038390
H	-2.558080	2.137450	-0.508438
H	-4.196900	1.462963	-0.797038
H	-3.964983	2.995113	1.703385
C	-4.158801	2.013362	2.130822
H	-5.074714	3.907529	5.318334
H	-5.529589	4.220895	3.628023
B	-8.716572	2.682270	2.317966
H	-8.862066	1.728057	3.050438
H	-9.360670	3.655599	2.623613
H	-7.495257	-1.687777	2.763534
H	-8.843538	-0.764607	1.608394
H	-8.799220	-2.788259	1.684697
H	-7.323390	-1.752809	0.769926
O	-6.754282	1.111353	-0.405770
H	-7.181119	-0.473806	-1.659503
C	-6.963152	0.611022	-1.678933
H	-6.067149	0.727348	-2.316844
C	-8.119324	1.309222	-2.410451
H	-8.235848	0.869041	-3.408697
H	-7.875985	2.367216	-2.561347
C	-9.452414	1.218759	-1.665254
H	-9.405402	0.549347	-0.804855
H	-10.280948	0.933743	-2.314133
O	-9.861571	2.555362	-1.195289
C	-9.653594	2.907247	0.025386
O	-9.213610	2.153312	0.905103
H	-9.910082	3.948508	0.239441
H	-7.540768	2.956689	2.119098

Energy: 4.7 kcal.mol^{-1}
- 799.805253 H

E Adduct

C	-8.571890	10.043666	1.809839
P	-9.262827	9.015695	0.435897
C	-8.373234	9.624831	-1.058089
N	-10.891839	9.195609	0.332287

La	-11.747694	6.764443	0.100065
O	-11.261994	4.802452	-0.860609
C	-11.057002	3.825642	-1.807456
C	-12.295064	2.941346	-2.026769
C	-8.897916	7.286996	0.519348
P	-9.060414	6.296596	1.967972
C	-8.001656	6.764687	3.413304
Si	-11.754844	10.708055	0.333293
C	-8.422874	4.638838	1.485592
N	-10.660110	6.273707	2.360414
Si	-11.315458	5.725668	3.883003
B	-14.358637	6.551750	0.821569
O	-12.816962	6.265932	-2.867495
C	-12.988399	5.523395	-3.843920
O	-13.388895	4.300929	-3.753423
C	-13.550148	3.697992	-2.414645
B	-12.134559	7.696448	-2.916379
H	-7.371686	4.692504	1.189951
H	-11.069934	4.262701	4.139257
H	-12.784173	5.966750	3.886645
H	-10.708039	6.452972	5.051796
H	-8.084437	6.008666	4.199302
H	-8.329463	7.725066	3.814433
H	-6.960509	6.838053	3.088098
H	-8.533837	3.952570	2.328533
H	-9.036769	4.294998	0.649755
H	-8.098763	6.975492	-0.150056
H	-8.700305	9.034391	-1.916600
H	-7.291870	9.530678	-0.929067
H	-8.633912	10.672274	-1.226835
H	-7.499099	9.865971	1.918284
H	-9.089637	9.784631	2.735804
H	-8.747697	11.102781	1.600584
H	-11.591265	11.473973	1.617499
H	-13.205577	10.418353	0.142694
H	-11.310861	11.639911	-0.762600
H	-13.897321	7.639330	1.195474
H	-14.227589	6.494279	-0.412292
H	-13.649614	5.651342	1.302214
H	-15.508311	6.423104	1.151614
H	-12.816955	5.869817	-4.866690
H	-12.103389	8.076125	-4.062345
H	-12.818069	8.368121	-2.174918
H	-11.017560	7.480530	-2.466232

H	-10.228227	3.149646	-1.527770
H	-10.755710	4.258457	-2.783816
H	-12.532495	2.430266	-1.085268
H	-12.081350	2.167496	-2.775322
H	-14.406942	3.035815	-2.543532
H	-13.789280	4.486940	-1.700122

Energy: 0.1 kcal.mol^{-1}
- 799.812667 H

TSEF 2nd H transfer

C	-8.677779	9.915322	1.701557
P	-9.270200	8.801027	0.351340
C	-8.320099	9.350961	-1.128646
N	-10.896352	8.940253	0.153946
La	-11.742096	6.511489	0.302646
O	-11.324848	4.548328	-0.645686
C	-11.241990	3.482038	-1.520820
C	-12.593206	3.152280	-2.172249
C	-8.869373	7.089958	0.557372
P	-8.961208	6.202167	2.076167
C	-7.850796	6.775046	3.443392
Si	-11.777689	10.437253	-0.013117
C	-8.321320	4.521140	1.685947
N	-10.543396	6.192694	2.537711
Si	-11.117830	5.750155	4.127321
B	-14.334494	6.497122	1.083623
O	-12.125723	6.893484	-2.433319
C	-11.971868	6.225943	-3.525086
O	-12.387826	5.011961	-3.722365
C	-13.284435	4.365432	-2.762792
B	-13.090554	7.903528	-3.263368
H	-7.280674	4.566003	1.353661
H	-10.733684	4.348804	4.520470
H	-12.602413	5.856918	4.141527
H	-10.560831	6.646375	5.198993
H	-7.903185	6.075992	4.283173
H	-8.165726	7.761561	3.787041
H	-6.821721	6.824208	3.077563
H	-8.395496	3.894857	2.578202
H	-8.953349	4.108800	0.896018
H	-8.091729	6.741410	-0.119118
H	-8.560968	8.686680	-1.961302
H	-7.245972	9.320589	-0.929006

H	-8.619040	10.368726	-1.389617
H	-7.604435	9.787601	1.861215
H	-9.224628	9.675638	2.616175
H	-8.888150	10.955416	1.436758
H	-11.708006	11.295045	1.220077
H	-13.206063	10.105496	-0.278968
H	-11.263678	11.289499	-1.141467
H	-13.816423	7.592333	1.345384
H	-14.225966	6.315588	-0.142423
H	-13.656031	5.612952	1.635117
H	-15.482557	6.452156	1.436313
H	-11.217470	6.524016	-4.255708
H	-13.150235	7.297798	-4.358187
H	-14.175401	7.810863	-2.763244
H	-12.531423	8.954805	-3.406146
H	-10.886396	2.568890	-1.012811
H	-10.511336	3.681850	-2.326842
H	-13.278241	2.746601	-1.417464
H	-12.456113	2.381017	-2.940675
H	-14.168250	4.095744	-3.345061
H	-13.565441	5.087935	-1.996913

Energy: 14.9 kcal.mol^{-1}
- 799.789026 H

F Product (alcohol termination)

C	-8.550461	9.718369	1.421455
P	-8.920197	8.457948	0.125009
C	-7.640666	8.739900	-1.168830
N	-10.452951	8.640669	-0.450251
La	-11.530648	6.365462	0.000357
O	-10.902032	4.345643	-0.688866
C	-10.430621	3.933516	-1.933142
C	-11.569235	3.688880	-2.937731
C	-8.725876	6.782793	0.650579
P	-9.124833	6.146978	2.243356
C	-8.166170	6.823888	3.675684
Si	-11.149606	10.127971	-1.043736
C	-8.631903	4.376451	2.180322
N	-10.750491	6.348850	2.447744
Si	-11.572552	6.219097	3.983833
B	-14.451453	6.132068	0.766696
O	-13.348637	7.432431	-1.504844
C	-13.024368	7.105100	-2.830953

O	-12.082909	6.052187	-2.844330
C	-12.666296	4.734989	-2.847314
B	-14.756921	7.509867	-1.058406
H	-7.553857	4.276554	2.027603
H	-11.184061	4.982701	4.749858
H	-13.040426	6.180230	3.734437
H	-11.271469	7.379543	4.890841
H	-8.415117	6.266802	4.583886
H	-8.418059	7.874985	3.825881
H	-7.095864	6.727893	3.475064
H	-8.916849	3.892524	3.117611
H	-9.175601	3.921355	1.347542
H	-7.928382	6.250353	0.137255
H	-7.775407	7.996731	-1.958098
H	-6.637765	8.650603	-0.743759
H	-7.773458	9.738674	-1.592241
H	-7.535182	9.588292	1.803869
H	-9.274306	9.603975	2.231715
H	-8.658341	10.718999	0.994892
H	-10.195338	11.283838	-0.889518
H	-12.403775	10.476695	-0.311794
H	-11.467862	10.040930	-2.505648
H	-13.731847	7.023836	1.187212
H	-15.083606	6.417464	-0.313560
H	-13.836559	5.128187	0.420953
H	-15.342029	5.893457	1.535983
H	-12.524198	7.956719	-3.302493
H	-13.931402	6.833269	-3.386751
H	-15.538522	7.213971	-1.934564
H	-15.013860	8.492891	-0.422972
H	-9.840434	3.006244	-1.844305
H	-9.746012	4.684867	-2.370187
H	-12.042851	2.718058	-2.746009
H	-11.157186	3.655743	-3.954123
H	-13.355340	4.655912	-3.698632
H	-13.250438	4.589354	-1.928729

Energy: - 17.9 kcal.mol^{-1}
- 799.841216 H

E' Adduct

B	-5.075397	0.115158	-2.080336
N	-3.329408	0.019926	1.034536
P	-3.097421	1.383425	1.918348

La	-5.923976	-0.228422	0.967640
B	-7.136492	-2.593752	0.366167
N	-5.816221	-0.474665	3.516719
P	-5.420541	1.052855	3.989035
C	-6.896424	2.087910	4.364797
O	-7.687482	1.127006	0.861139
C	-8.997128	1.516597	0.676885
C	-9.711514	0.740864	-0.442006
C	-9.276496	1.107064	-1.846525
O	-7.856301	0.849396	-2.028979
C	-7.461182	-0.041494	-2.875089
O	-6.272705	-0.357679	-3.009660
C	-4.646678	1.851669	2.622793
C	-1.696077	1.184846	3.111020
C	-2.582799	2.827298	0.894220
Si	-2.081423	-0.958521	0.314185
Si	-6.294529	-1.773212	4.578033
C	-4.477400	1.053958	5.582618
H	-1.045572	-1.399038	1.314133
H	-2.716083	-2.182195	-0.257020
H	-1.326162	-0.259082	-0.781491
H	-0.761295	1.032822	2.564207
H	-1.878887	0.305859	3.732421
H	-1.611227	2.074455	3.740098
H	-1.672956	2.569888	0.346790
H	-3.378491	3.042901	0.177992
H	-2.399363	3.703123	1.522200
H	-4.865850	2.914580	2.548143
H	-7.494685	2.134815	3.452042
H	-6.600563	3.093989	4.674206
H	-7.474481	1.613221	5.161333
H	-4.180341	2.077593	5.825268
H	-3.589824	0.426962	5.482955
H	-5.100125	0.654975	6.388267
H	-5.301033	-1.994661	5.686470
H	-7.617361	-1.532325	5.254233
H	-6.395093	-3.027568	3.781194
H	-5.918809	-2.750983	0.541077
H	-7.609811	-2.066465	1.384669
H	-7.682989	-3.635817	0.113890
H	-7.269499	-1.771265	-0.557571
H	-9.068047	2.598016	0.444785
H	-9.389442	2.178290	-2.035140
H	-10.791047	0.944050	-0.398187

H	-9.834646	0.549786	-2.609483
H	-9.574105	-0.334297	-0.278232
H	-9.590971	1.366771	1.596948
H	-8.209941	-0.528556	-3.509758
H	-4.171805	0.385911	-2.824085
H	-5.444783	1.064222	-1.410938
H	-4.837953	-0.884876	-1.424667

Energy: 6.1 kcal.mol^{-1}
- 799.803097 H

TSE'F' Trapping by Ligand Nitrogen

B	-4.701381	0.564447	-1.295077
N	-3.606449	-0.080224	0.708286
P	-3.254742	1.228052	1.660671
La	-6.210336	-0.380306	1.118663
B	-6.824197	-2.968529	0.639448
N	-5.790633	-0.383516	3.646718
P	-5.415805	1.199411	3.913705
C	-6.897060	2.241015	4.245250
O	-8.133124	0.721372	1.078653
C	-9.432933	1.002554	0.703195
C	-9.814729	0.386470	-0.650211
C	-9.159566	1.029119	-1.854859
O	-7.727173	0.791445	-1.835053
C	-7.061062	1.036984	-2.949994
O	-5.850192	0.995095	-3.020239
C	-4.742242	1.821832	2.411265
C	-1.904759	0.810414	2.850868
C	-2.576080	2.636151	0.692014
Si	-2.401587	-1.209813	0.121220
Si	-6.159452	-1.545736	4.896789
C	-4.393545	1.414019	5.443633
H	-1.765432	-1.986299	1.238566
H	-3.060414	-2.169263	-0.806788
H	-1.276029	-0.525136	-0.605767
H	-0.995774	0.554599	2.298881
H	-2.206711	-0.055364	3.444073
H	-1.705457	1.663138	3.504346
H	-1.702393	2.294858	0.132174
H	-3.339160	2.970647	-0.012369
H	-2.295684	3.453867	1.360525
H	-4.941613	2.874276	2.221815
H	-7.569628	2.132030	3.390731

H	-6.615644	3.289583	4.375194
H	-7.392641	1.879462	5.149562
H	-4.104235	2.463619	5.543146
H	-3.499870	0.791069	5.383200
H	-4.973664	1.114725	6.321577
H	-4.979260	-1.814275	5.789483
H	-7.269671	-1.093677	5.807896
H	-6.566111	-2.824271	4.251060
H	-5.605017	-2.826070	0.826578
H	-7.411855	-2.515878	1.637132
H	-7.108159	-4.120318	0.444754
H	-7.139774	-2.246742	-0.322433
H	-9.606213	2.095104	0.644823
H	-9.315683	2.114726	-1.846424
H	-10.898664	0.489271	-0.799689
H	-9.564966	0.620034	-2.788585
H	-9.591755	-0.687021	-0.637781
H	-10.150570	0.620992	1.450706
H	-7.686826	1.282161	-3.825760
H	-3.682847	0.827018	-1.853424
H	-5.280494	1.418793	-0.666785
H	-5.121023	-0.565481	-1.305712

Energy: 14.6 kcal.mol^{-1}
- 799.789520 H

F' Product (formate termination)

B	-4.183895	0.867999	-0.865082
N	-3.497674	0.238185	0.442276
P	-3.222989	1.395354	1.660528
La	-6.260560	-0.191825	0.785997
B	-6.903473	-2.810426	0.769603
N	-5.687109	-0.433808	3.308105
P	-5.454726	1.124889	3.768826
C	-6.997209	2.064518	4.118027
O	-8.083512	1.020960	1.110666
C	-9.349971	1.486137	0.800911
C	-9.877024	0.912744	-0.517694
C	-8.943681	1.158863	-1.691022
O	-7.810966	0.256766	-1.653844
C	-7.578564	-0.517895	-2.739195
O	-6.666148	-1.290770	-2.788524
C	-4.727449	1.923422	2.376324
C	-2.018848	0.660313	2.836354

C	-2.389370	2.859861	0.937598
Si	-2.338556	-1.043111	0.011499
Si	-6.073185	-1.776457	4.363392
C	-4.516055	1.271637	5.359690
H	-1.961753	-1.829692	1.224708
H	-3.000490	-1.923503	-0.983790
H	-1.082498	-0.464518	-0.568964
H	-1.089658	0.407715	2.319315
H	-2.447257	-0.245012	3.270525
H	-1.809539	1.388884	3.622464
H	-1.492872	2.539622	0.402281
H	-3.073071	3.332458	0.230411
H	-2.126113	3.560088	1.733573
H	-4.959596	2.973883	2.226762
H	-7.628768	1.980481	3.228961
H	-6.770473	3.112369	4.333866
H	-7.501604	1.615427	4.977500
H	-4.276443	2.323843	5.535005
H	-3.596480	0.686846	5.310499
H	-5.124537	0.895049	6.185582
H	-5.448926	-1.582007	5.721880
H	-7.544002	-1.942020	4.598620
H	-5.525082	-3.038253	3.793163
H	-5.671400	-2.650001	0.727525
H	-7.322284	-2.223275	1.781235
H	-7.193674	-3.976595	0.791406
H	-7.390089	-2.230652	-0.208810
H	-9.349413	2.589893	0.715944
H	-8.536439	2.174989	-1.673453
H	-10.846621	1.372751	-0.752727
H	-9.462434	1.012653	-2.646338
H	-10.045733	-0.166809	-0.421677
H	-10.073597	1.238905	1.596810
H	-8.313585	-0.355503	-3.548844
H	-3.395773	1.375456	-1.632285
H	-4.998524	1.720059	-0.490602
H	-4.785397	-0.046734	-1.413975

Energy: - 6.4 kcal.mol^{-1}
- 799.822894 H

Reaction between TMC and [{CH(PPh$_2$NSiMe$_3$)$_2$}Lu(BH$_4$)$_2$] (3)

All energies in kcal.mol^{-1} are realtive to the origin level, all energies in H are absolute.
Energy of the reactants : - 808.191367 H

A Adduct

C	-10.499328	2.720980	-0.526974
O	-9.273499	1.990778	-0.281000
C	-8.075531	2.509475	-0.459773
O	-7.905578	3.562017	-1.247250
C	-9.054314	4.136371	-1.903287
C	-10.222035	4.150061	-0.942235
O	-7.093092	1.985635	0.054354
Lu	-6.818550	1.071062	2.243956
B	-8.296088	3.337022	2.686825
P	-3.811133	1.140239	1.351260
C	-3.485686	2.039339	-0.220946
C	-2.182332	0.361097	1.753921
N	-4.997619	0.009060	1.224603
Si	-4.854115	-1.538188	0.427961
C	-4.415060	2.354585	2.474345
P	-4.649845	2.121819	4.207227
C	-4.990166	3.789516	4.897614
C	-3.186360	1.525997	5.168090
N	-5.922019	1.083042	4.369767
Si	-6.419130	0.342048	5.875659
B	-8.224227	-0.942850	2.422282
H	-5.675770	-0.932087	6.151378
H	-3.783315	-1.497310	-0.633618
H	-4.472184	-2.641255	1.368421
H	-6.139719	-1.897126	-0.235436
H	-6.139470	1.250869	7.043836
H	-7.877959	0.050540	5.840571
H	-4.234446	3.384652	2.178815
H	-8.771405	2.200083	2.531415
H	-7.067692	3.303017	2.508045
H	-8.526620	3.708819	3.816471
H	-4.133875	4.451985	4.746175
H	-5.875012	4.182182	4.391921
H	-5.197313	3.692964	5.965998
H	-2.331072	2.184550	4.997073
H	-3.432009	1.518118	6.234235
H	-2.939043	0.508765	4.858822
H	-1.888016	-0.305998	0.938358
H	-1.418511	1.131127	1.888841
H	-2.281004	-0.226093	2.668819
H	-2.699285	2.786223	-0.083608
H	-3.178512	1.318263	-0.982389
H	-4.415640	2.519955	-0.530939

H	-7.038394	-1.213819	2.645158
H	-8.932948	-1.907925	2.492635
H	-8.270761	-0.418846	1.296997
H	-8.553457	-0.066593	3.232011
H	-8.763323	4.070514	1.831872
H	-11.061257	2.657910	0.406610
H	-11.027272	2.162617	-1.306041
H	-11.109760	4.580271	-1.415955
H	-9.964983	4.755892	-0.067905
H	-9.268885	3.549923	-2.805145
H	-8.734784	5.135831	-2.200809

Energy: 1.6 kcal.mol^{-1}
- 808.188902 H

TSAB Nucleophilic attack

C	-10.261410	2.576536	-1.080595
O	-9.654348	2.419604	0.199502
C	-8.370530	2.902023	0.387045
O	-7.987532	4.001419	-0.361275
C	-8.657420	4.342590	-1.577969
C	-10.136140	4.015320	-1.537100
O	-7.449837	2.022410	0.554286
Lu	-6.853198	0.929790	2.371839
B	-8.420801	3.325918	2.830381
P	-3.970919	1.214656	1.274004
C	-4.000251	2.149452	-0.307112
C	-2.230875	0.604502	1.408060
N	-5.045628	-0.038159	1.308612
Si	-4.827398	-1.581836	0.513545
C	-4.526151	2.349070	2.497344
P	-4.604255	2.044707	4.234155
C	-4.718731	3.695295	5.033781
C	-3.107282	1.270874	4.990447
N	-5.936522	1.107449	4.495669
Si	-6.373019	0.381693	6.028502
B	-8.229259	-1.071716	2.722580
H	-5.773162	-0.979889	6.209093
H	-4.087641	-1.423425	-0.789077
H	-4.018197	-2.536997	1.341121
H	-6.155790	-2.190362	0.231285
H	-5.875609	1.221456	7.176523
H	-7.854951	0.277152	6.133009
H	-4.440527	3.398301	2.227713
H	-8.873952	2.208013	2.979002
H	-7.213572	3.425072	2.896480
H	-9.067209	4.202171	3.335370
H	-3.795443	4.260464	4.882676

H	-5.562388	4.230237	4.593012
H	-4.897914	3.558466	6.102751
H	-2.214379	1.856946	4.759521
H	-3.238566	1.216939	6.075243
H	-3.000636	0.255886	4.601978
H	-1.999266	-0.029976	0.547333
H	-1.542095	1.452898	1.429440
H	-2.118779	0.016639	2.320708
H	-3.281793	2.973063	-0.281917
H	-3.752046	1.470268	-1.126243
H	-5.015366	2.531464	-0.439210
H	-7.037209	-1.282691	2.987466
H	-8.909620	-2.043768	2.890332
H	-8.274943	-0.668754	1.550913
H	-8.587403	-0.123965	3.439244
H	-8.585779	3.545537	1.519776
H	-11.299904	2.267540	-0.943525
H	-9.793057	1.893881	-1.805032
H	-10.575731	4.151861	-2.531059
H	-10.660375	4.672457	-0.835166
H	-8.176938	3.796829	-2.403415
H	-8.471884	5.410174	-1.723768

Energy: 24.1 kcal.mol^{-1}
- 808.152922 H

B Adduct

C	-10.140410	2.382466	-0.777029
O	-9.916137	2.822055	0.564748
C	-8.591507	3.226320	0.760809
O	-8.244862	4.309142	-0.061536
C	-8.369760	3.975692	-1.446540
C	-9.786993	3.502979	-1.747603
O	-7.706376	2.255882	0.776772
Lu	-6.900501	0.993528	2.303035
B	-8.407758	3.580085	3.193931
P	-4.028418	1.302679	1.194053
C	-4.028450	2.305290	-0.345446
C	-2.302157	0.651359	1.304275
N	-5.127947	0.068467	1.160782
Si	-4.916034	-1.441741	0.297224
C	-4.569172	2.391921	2.464185
P	-4.629900	2.025362	4.191446
C	-4.674016	3.644337	5.059823
C	-3.146561	1.175588	4.889573
N	-5.987809	1.120355	4.435582
Si	-6.432855	0.353589	5.946934
B	-8.319494	-0.989282	2.572914
H	-5.738943	-0.960168	6.149747

H	-4.252841	-1.216972	-1.035745
H	-4.038741	-2.401613	1.045967
H	-6.245109	-2.069927	0.070365
H	-6.054308	1.218323	7.120296
H	-7.905322	0.136619	5.972397
H	-4.474099	3.449552	2.232652
H	-8.795712	2.442842	3.309201
H	-7.226653	3.780517	3.100107
H	-9.114839	4.438030	3.637071
H	-3.730275	4.178136	4.922068
H	-5.499108	4.232515	4.653403
H	-4.847413	3.468513	6.124040
H	-2.239956	1.742400	4.664578
H	-3.259947	1.084578	5.973927
H	-3.078613	0.172632	4.463073
H	-2.077925	0.059432	0.411841
H	-1.597230	1.483727	1.373672
H	-2.205864	0.012803	2.183951
H	-3.283197	3.102951	-0.287788
H	-3.804583	1.653842	-1.193563
H	-5.027213	2.731111	-0.462919
H	-7.168155	-1.205307	2.976796
H	-9.032671	-1.943097	2.701740
H	-8.228589	-0.632371	1.388999
H	-8.742090	-0.005518	3.205211
H	-8.702541	3.815023	1.789978
H	-11.197729	2.111831	-0.826005
H	-9.541846	1.483325	-0.976794
H	-9.864271	3.156191	-2.784744
H	-10.485026	4.336198	-1.611094
H	-7.639599	3.196115	-1.707059
H	-8.114664	4.887028	-1.993871

Energy: 20.8 kcal.mol^{-1}
- 808.158153 H

TSBC Trapping by Intracyclic Oxygen

O	-11.522308	3.707740	-0.924292
C	-12.692221	4.367328	-0.256003
O	-13.821520	3.572935	-0.462521
C	-13.587101	2.197635	-0.156687
C	-12.665027	1.583698	-1.226211
C	-11.881511	2.715650	-1.892305
O	-12.301682	4.564794	0.991419
Lu	-10.208304	3.939074	1.073454
C	-9.580209	6.498233	0.402725
P	-8.194897	5.796371	-0.431576
C	-8.412032	6.220602	-2.207788

H	-10.947916	2.366782	-2.340358
N	-9.616361	5.302258	2.849657
Si	-9.388139	5.022261	4.561930
P	-9.712641	6.789718	2.134570
C	-11.348452	7.586561	2.374255
B	-9.935427	1.658704	1.973768
N	-8.238729	4.169837	-0.155272
Si	-6.981863	3.038681	-0.601066
C	-8.504986	7.973410	2.881368
C	-6.539229	6.486812	0.008567
B	-14.458912	6.051504	-2.457336
H	-6.384464	3.385759	-1.939899
H	-7.564270	1.670277	-0.689789
H	-5.841982	3.017550	0.373963
H	-5.774313	6.040149	-0.633605
H	-6.316288	6.228731	1.046046
H	-6.531788	7.572246	-0.116789
H	-8.316221	7.298417	-2.361651
H	-7.654289	5.695531	-2.793950
H	-9.403815	5.886228	-2.518964
H	-10.201179	7.138815	-0.218200
H	-12.097152	6.894714	1.978226
H	-11.396075	8.546566	1.853312
H	-11.516301	7.739594	3.443033
H	-8.557583	8.930493	2.356092
H	-7.495146	7.566711	2.804919
H	-8.746547	8.126329	3.937439
H	-7.966144	5.253536	4.986580
H	-9.760873	3.615481	4.874224
H	-10.230231	5.946341	5.399120
H	-8.949573	2.361233	2.233237
H	-10.929508	2.233059	2.443040
H	-10.063404	1.671782	0.737016
H	-9.824051	0.542799	2.396537
H	-12.893133	5.295690	-0.829545
H	-12.481056	3.198711	-2.672347
H	-13.889811	5.445209	-3.316997
H	-15.542370	5.709644	-2.095876
H	-13.962689	7.044890	-2.009594
H	-13.236952	1.049381	-1.993163
H	-11.981902	0.866046	-0.760834
H	-13.146269	2.111587	0.842465
H	-14.569477	1.721952	-0.134118

Energy: 15.2 kcal.mol^{-1}
- 808.167227 H

C Adduct

O	-11.534165	3.931743	-1.057973

C	-12.623277	4.691907	-0.453843
O	-13.843163	3.863207	-0.564340
C	-13.584456	2.451751	-0.412779
C	-12.799168	1.930671	-1.617562
C	-11.896798	3.052997	-2.137374
O	-12.263787	4.927676	0.779092
Lu	-10.217838	4.129134	0.979413
C	-9.356491	6.636807	0.418739
P	-7.981033	5.847712	-0.354769
C	-8.020303	6.368419	-2.117403
H	-10.958032	2.680665	-2.551394
N	-9.642689	5.389250	2.820457
Si	-9.552589	5.046376	4.537043
P	-9.561394	6.899864	2.149799
C	-11.127831	7.839601	2.321023
B	-10.184487	1.817295	1.827042
N	-8.199300	4.221202	-0.162634
Si	-7.028693	2.991936	-0.594434
C	-8.296230	7.944878	2.999667
C	-6.306951	6.356374	0.233972
B	-15.008460	4.309457	-1.627763
H	-6.312622	3.352067	-1.868881
H	-7.738032	1.698631	-0.802367
H	-5.969481	2.806515	0.450064
H	-5.542154	5.859532	-0.370366
H	-6.186000	6.043591	1.273191
H	-6.188260	7.439537	0.152026
H	-7.802032	7.435702	-2.205526
H	-7.277864	5.793163	-2.675293
H	-9.013780	6.157901	-2.518615
H	-9.875838	7.351905	-0.214411
H	-11.913044	7.242627	1.849605
H	-11.048965	8.818786	1.841391
H	-11.351346	7.967531	3.382834
H	-8.223850	8.913326	2.498128
H	-7.326687	7.444440	2.975829
H	-8.589736	8.098912	4.042339
H	-8.146354	5.143765	5.053377
H	-10.063792	3.669611	4.776427
H	-10.367360	6.019786	5.342990
H	-9.157734	2.431304	2.147718
H	-11.147535	2.466842	2.264618
H	-10.253339	1.865146	0.586809
H	-10.186084	0.689757	2.231286
H	-12.867421	5.554376	-1.087917
H	-12.415140	3.645054	-2.898188
H	-14.611411	4.004459	-2.735967
H	-15.966929	3.671987	-1.258430
H	-15.101975	5.502479	-1.455162
H	-13.474596	1.615195	-2.417718

H	-12.209986	1.062750	-1.304517
H	-13.025242	2.332390	0.518563
H	-14.562602	1.984516	-0.304089

Energy: 0.3 kcal.mol^{-1}
-808.190868 H

TSCD Trapping by Extracyclic Oxygen

O	-8.901979	2.868274	-0.458317
C	-7.550607	2.439314	-0.380947
O	-7.013668	2.190648	-1.662730
C	-7.743895	1.199999	-2.384530
C	-9.200099	1.629052	-2.513282
C	-9.744306	1.921174	-1.120514
O	-7.449164	1.369735	0.437691
Lu	-6.638072	0.290238	2.009288
B	-7.796663	-1.854917	2.355794
N	-6.061681	0.977480	4.144316
P	-4.900204	2.117482	3.857261
C	-4.633131	2.149500	2.115581
P	-3.734222	0.965947	1.170568
N	-4.591580	-0.446133	1.269457
Si	-3.997981	-2.015325	0.762108
Si	-6.576776	0.442335	5.731439
C	-5.437957	3.814770	4.313706
C	-3.414808	1.810738	4.911052
C	-1.966176	0.695525	1.636195
C	-3.651017	1.639626	-0.534829
B	-9.165141	2.568564	2.105198
H	-6.702232	-1.862660	2.934610
H	-7.576616	-1.616724	1.156774
H	-8.433975	-0.882195	2.796897
H	-8.397845	-2.880999	2.501145
H	-7.003063	3.318284	-0.014541
H	-10.736310	2.378912	-1.154028
H	-9.808750	0.997149	-0.530690
H	-9.259284	2.534838	-3.127390
H	-9.793273	0.845473	-2.999090
H	-7.254175	1.117376	-3.358874
H	-7.671000	0.229505	-1.874855
H	-6.760199	1.606280	6.667561
H	-5.575957	-0.467223	6.381517
H	-7.873962	-0.275031	5.597512
H	-5.742208	3.821859	5.362887
H	-4.623527	4.527477	4.160878
H	-6.293057	4.085211	3.690797
H	-3.064149	0.790486	4.742538
H	-2.623664	2.523595	4.666344
H	-3.685665	1.915298	5.965867

H	-1.912376	0.269859	2.639620
H	-1.427063	1.645892	1.609364
H	-1.505716	-0.002389	0.930598
H	-3.090855	2.578604	-0.548294
H	-3.149100	0.908465	-1.173568
H	-4.669674	1.801578	-0.900000
H	-4.671560	3.143333	1.676952
H	-5.151190	-2.899614	0.443002
H	-3.156055	-2.669152	1.817849
H	-3.126963	-1.897267	-0.459705
H	-8.861498	1.538025	2.649755
H	-8.441699	3.515947	2.198681
H	-10.302216	2.694287	1.773203

Energy: 17.6 kcal.mol^{-1}
- 808.163411 H

D Adduct

O	-8.838212	2.998942	-1.016803
C	-7.665798	2.538800	-0.444145
O	-6.911538	1.726880	-1.297607
C	-7.641425	0.617955	-1.840966
C	-8.937693	1.093172	-2.483084
C	-9.692062	1.948633	-1.473970
O	-7.912353	1.835941	0.747145
Lu	-6.770385	0.481743	2.106996
B	-8.014707	-1.619641	2.278245
N	-5.844502	0.802964	4.199001
P	-4.907104	2.137484	3.926908
C	-4.750979	2.244789	2.171294
P	-3.883388	1.082774	1.157603
N	-4.870981	-0.238569	1.030548
Si	-4.409290	-1.770364	0.316158
Si	-6.126815	0.067095	5.763541
C	-5.693367	3.710094	4.454589
C	-3.348636	2.065000	4.918265
C	-2.203651	0.583897	1.739169
C	-3.594062	1.904951	-0.456843
B	-8.544981	2.639242	1.909054
H	-6.864263	-1.727128	2.729723
H	-7.898618	-1.234778	1.101707
H	-8.558946	-0.691356	2.898664
H	-8.631281	-2.642824	2.356571
H	-7.061844	3.427245	-0.232086
H	-10.556872	2.445119	-1.919981
H	-10.036493	1.350788	-0.620543
H	-8.711468	1.694042	-3.371067
H	-9.540535	0.233044	-2.795522
H	-6.968440	0.153953	-2.566197

H	-7.852865	-0.116790	-1.052296
H	-6.436286	1.095226	6.816123
H	-4.924055	-0.687448	6.252057
H	-7.274949	-0.872504	5.648402
H	-5.957011	3.635176	5.512263
H	-5.008335	4.548949	4.305225
H	-6.598766	3.852170	3.859528
H	-2.822744	1.130806	4.715800
H	-2.708239	2.913765	4.665160
H	-3.596699	2.104648	5.983163
H	-2.300335	0.026405	2.672799
H	-1.575581	1.465002	1.892180
H	-1.741203	-0.065844	0.990212
H	-3.010845	2.819906	-0.325306
H	-3.052271	1.215436	-1.108916
H	-4.568496	2.123297	-0.900653
H	-4.777212	3.256664	1.774304
H	-5.626996	-2.469863	-0.179352
H	-3.695077	-2.662021	1.286872
H	-3.472116	-1.562374	-0.843008
H	-8.210203	1.984792	2.924729
H	-8.032625	3.742760	1.969768
H	-9.750285	2.647673	1.853884

Energy: - 4.6 kcal.mol^{-1}
- 808.198755 H

TSDE Ring Opening

Lu	-6.389160	0.000859	1.772681
P	-4.837817	1.915251	3.762457
N	-5.911413	0.697497	3.993850
B	-7.598002	-2.109661	2.107155
Si	-3.512405	-2.332068	1.177872
O	-6.742988	0.684810	-0.191465
C	-7.575732	0.124874	-1.165223
C	-7.842672	1.066146	-2.344726
C	-8.442943	2.401306	-1.944836
O	-7.380544	3.233397	-1.386879
C	-7.274771	3.350481	-0.100046
O	-8.146456	3.134367	0.738927
B	-8.853755	2.068922	1.717373
C	-5.546097	3.584520	4.082183
C	-3.424167	1.807039	4.950743
C	-4.424212	1.901480	2.039752
P	-3.401182	0.674668	1.283949
N	-4.209836	-0.752014	1.445934
Si	-6.508386	0.150676	5.541379
C	-1.657760	0.540468	1.887698
C	-3.229102	1.197905	-0.469559

H	-4.796668	4.363727	3.919021
H	-1.653036	0.195235	2.922932
H	-5.548113	-0.771728	6.235341
H	-7.799638	-0.563363	5.341016
H	-6.738441	1.300542	6.487379
H	-3.795464	1.946024	5.970538
H	-2.973178	0.815516	4.876816
H	-2.677954	2.574170	4.728834
H	-2.681171	-2.372598	-0.077860
H	-4.606002	-3.333718	1.060172
H	-2.592796	-2.742229	2.292752
H	-1.112471	-0.181578	1.272535
H	-1.166720	1.514909	1.821866
H	-2.649711	0.445503	-1.010022
H	-2.731666	2.168676	-0.546255
H	-4.241197	1.247669	-0.879675
H	-4.320769	2.892891	1.602278
H	-5.897397	3.625206	5.115880
H	-6.397590	3.730295	3.414408
H	-7.135903	-2.009814	0.960114
H	-6.640483	-2.007241	2.886510
H	-8.199775	-3.134476	2.261177
H	-8.318837	-1.114659	2.288783
H	-8.555060	-0.151837	-0.736446
H	-7.145385	-0.804385	-1.575881
H	-8.545892	0.578148	-3.032631
H	-6.921691	1.255449	-2.909604
H	-9.240680	2.298142	-1.205321
H	-8.804859	2.969063	-2.804563
H	-6.319963	3.807739	0.178835
H	-9.607939	2.726179	2.384089
H	-9.373254	1.234876	1.020093
H	-7.931665	1.660813	2.417124

Energy: 13.5 kcal.mol^{-1}
- 808.169894 H

E Adduct

C	-9.532360	10.056444	1.304288
P	-10.449818	8.796971	0.313513
C	-10.387804	9.434379	-1.405872
N	-11.995049	8.624982	0.883657
Lu	-12.135190	6.343191	1.241665
O	-12.611104	5.154137	-0.332890
C	-13.214019	4.206487	-1.141396
C	-13.834566	4.842198	-2.392390
C	-9.747532	7.180800	0.257364
P	-9.041495	6.249611	1.570703
C	-7.742564	7.076856	2.591382

Si	-13.081410	9.947599	1.257521
C	-8.149093	4.862796	0.760151
N	-10.299446	5.737203	2.516910
Si	-10.127913	4.928873	4.061721
B	-13.961764	6.244443	2.892373
O	-10.216898	6.280548	-3.605070
C	-10.624945	5.150420	-3.898969
O	-11.848848	4.751739	-3.757070
C	-12.840970	5.664929	-3.178338
B	-8.651541	6.669273	-3.785192
H	-7.321547	5.241850	0.155568
H	-9.004469	3.927307	4.031937
H	-11.394886	4.214006	4.378252
H	-9.812856	5.882552	5.176360
H	-7.313932	6.355828	3.293877
H	-8.189230	7.895021	3.159148
H	-6.953986	7.463434	1.941116
H	-7.770744	4.184282	1.528164
H	-8.856000	4.329477	0.121481
H	-9.332787	6.938623	-0.719904
H	-10.848076	8.698879	-2.067462
H	-9.351754	9.588096	-1.715720
H	-10.941287	10.374732	-1.458322
H	-8.496651	10.125101	0.963321
H	-9.561748	9.775890	2.359140
H	-10.018811	11.029652	1.188837
H	-12.911852	10.459868	2.655745
H	-14.489913	9.495337	1.076544
H	-12.838486	11.117430	0.340809
H	-13.036861	6.955898	3.308162
H	-14.325187	6.717958	1.801352
H	-13.479529	5.125837	2.644830
H	-14.868515	6.176784	3.673011
H	-9.956436	4.390795	-4.312901
H	-8.123576	5.682416	-4.258434
H	-8.670366	7.631541	-4.514213
H	-8.284815	6.921465	-2.656277
H	-14.009693	3.665619	-0.604659
H	-12.481178	3.446107	-1.461691
H	-14.637475	5.524389	-2.086307
H	-14.283863	4.073511	-3.033040
H	-13.294489	6.192813	-4.021536
H	-12.322798	6.370685	-2.528972

Energy: - 4.4 kcal.mol^{-1}
- 808.198296 H

TSEF 2nd H transfer

C	-8.769889	9.939151	1.442209

P	-9.469961	8.735395	0.225501
C	-8.761930	9.285725	-1.381627
N	-11.111085	8.744050	0.252288
Lu	-11.620568	6.431426	0.329902
O	-11.346803	4.587673	-0.520503
C	-11.474602	3.433972	-1.264437
C	-12.851082	3.315328	-1.937952
C	-8.967232	7.048207	0.416975
P	-8.994398	6.177057	1.949548
C	-7.951121	6.842535	3.325666
Si	-12.106193	10.179445	0.334750
C	-8.246711	4.534506	1.595818
N	-10.580944	6.083521	2.386419
Si	-11.165662	5.623457	3.967545
B	-14.003969	6.587976	0.984882
O	-11.715759	6.887167	-2.254749
C	-11.581455	6.152177	-3.307931
O	-12.202864	5.033497	-3.524611
C	-13.276228	4.595600	-2.632070
B	-12.375894	8.015656	-3.198019
H	-7.205089	4.639248	1.280629
H	-10.427426	4.429777	4.514280
H	-12.612090	5.287437	3.874163
H	-10.984546	6.717829	4.980547
H	-7.982496	6.152972	4.174686
H	-8.336718	7.812014	3.645083
H	-6.917623	6.950857	2.986410
H	-8.298350	3.918721	2.496914
H	-8.840458	4.073571	0.803751
H	-8.188848	6.729703	-0.273000
H	-9.121654	8.612357	-2.161265
H	-7.669280	9.278406	-1.347987
H	-9.119419	10.295462	-1.596052
H	-7.679309	9.871385	1.464594
H	-9.178727	9.723592	2.431403
H	-9.065870	10.953087	1.156808
H	-12.267346	10.683342	1.739921
H	-13.452317	9.887151	-0.227776
H	-11.495137	11.314437	-0.445637
H	-13.329451	7.399416	1.628069
H	-13.814761	6.841503	-0.219070
H	-13.532966	5.462211	1.193902
H	-15.169460	6.642674	1.263323
H	-10.708886	6.265703	-3.953872
H	-12.422512	7.389156	-4.284625
H	-13.511038	8.147596	-2.838165
H	-11.622775	8.944679	-3.303737
H	-11.326304	2.533122	-0.644303
H	-10.703617	3.386389	-2.055688
H	-13.620552	3.102539	-1.185830

H	-12.842777	2.478426	-2.647396
H	-14.141109	4.449125	-3.282715
H	-13.490849	5.392347	-1.920662

Energy: 13.9 kcal.mol^{-1}
- 808.169240 H

F Product (alcohol termination)

C	-9.508332	9.616089	1.648867
P	-9.543628	8.727863	0.045123
C	-8.401423	9.674825	-1.035724
N	-11.143393	8.782006	-0.536173
Lu	-11.744624	6.263838	0.173091
O	-11.485789	4.309386	-0.256972
C	-11.431194	3.228531	-1.131303
C	-12.714438	3.059837	-1.953638
C	-9.042494	7.047497	0.155751
P	-9.010647	6.191833	1.695229
C	-7.775331	6.747915	2.957963
Si	-12.300011	10.114247	-0.231158
C	-8.474387	4.477301	1.315940
N	-10.559649	6.313496	2.244728
Si	-11.056471	5.981701	3.890612
B	-14.011249	6.746186	1.050355
O	-11.792532	6.925390	-2.007602
C	-12.150704	6.371431	-3.266671
O	-12.102906	4.991029	-3.252863
C	-13.187602	4.366369	-2.566723
B	-11.287900	8.342884	-2.066132
H	-7.484457	4.473778	0.851983
H	-10.424430	4.731776	4.440702
H	-12.535511	5.838598	3.939127
H	-10.649159	7.092174	4.820146
H	-7.796741	6.059205	3.807941
H	-8.016710	7.750218	3.313679
H	-6.774827	6.742044	2.517435
H	-8.448821	3.901387	2.244214
H	-9.223447	4.054559	0.641992
H	-8.374699	6.711427	-0.632734
H	-8.277301	9.150350	-1.982628
H	-7.439060	9.769440	-0.526677
H	-8.824107	10.663965	-1.228232
H	-8.475933	9.652948	2.002820
H	-10.136535	9.088790	2.368918
H	-9.878577	10.634837	1.516418
H	-12.289015	10.463788	1.223131
H	-13.652066	9.664374	-0.635165
H	-11.893681	11.338304	-0.993845
H	-13.231465	7.645086	1.395011

H	-13.984491	6.696109	-0.189280
H	-13.550348	5.675351	1.467598
H	-15.123180	6.935483	1.457545
H	-11.422873	6.707258	-4.013946
H	-13.153936	6.744473	-3.530364
H	-12.099840	9.083570	-2.600291
H	-10.221133	8.373637	-2.656477
H	-11.249954	2.293074	-0.576163
H	-10.591850	3.352368	-1.833185
H	-13.525856	2.674821	-1.323395
H	-12.531586	2.315854	-2.739668
H	-14.016159	4.194096	-3.269559
H	-13.566276	5.025451	-1.775150

Energy: - 27.1 kcal.mol^{-1}
- 808.234535 H

D' Adduct

B	-5.530724	1.165578	-1.632964
N	-3.287962	-0.414907	1.075657
P	-2.919531	1.060347	1.716091
Lu	-5.555932	-0.216317	0.672642
B	-6.062309	-2.603328	0.374357
N	-6.216175	-0.099685	2.916024
P	-5.544064	1.328825	3.396461
C	-6.777428	2.683767	3.562740
O	-7.641996	0.944295	0.267355
C	-8.908372	0.530389	0.806106
C	-9.701155	-0.241813	-0.237228
C	-9.766694	0.584407	-1.514643
O	-8.460469	0.966996	-1.921899
C	-7.806441	1.749373	-0.975110
O	-6.620495	2.158082	-1.388100
C	-4.465892	1.827146	2.096939
C	-1.711729	0.890106	3.105464
C	-2.071488	2.190009	0.541259
Si	-2.128045	-1.687010	0.750880
Si	-6.958623	-1.277833	3.974299
C	-4.819126	1.194112	5.092037
H	-1.930599	-2.587301	1.933700
H	-2.586002	-2.501884	-0.407724
H	-0.776535	-1.108338	0.425610
H	-0.768866	0.497823	2.712767
H	-2.100517	0.188275	3.845465
H	-1.533493	1.862338	3.571804
H	-1.160116	1.704695	0.183877
H	-2.740932	2.372357	-0.301658
H	-1.817387	3.131993	1.034386
H	-4.529147	2.877860	1.825105

H	-7.220987	2.862241	2.581340
H	-6.299256	3.596997	3.926568
H	-7.554243	2.371457	4.264750
H	-4.322110	2.130023	5.359147
H	-4.098517	0.374513	5.116433
H	-5.614047	0.984868	5.813642
H	-7.648165	-0.604389	5.132792
H	-7.990326	-2.043759	3.217152
H	-5.972650	-2.240387	4.561354
H	-5.457916	-2.402936	1.435522
H	-7.081073	-1.891695	0.409481
H	-6.331025	-3.759388	0.211226
H	-5.353685	-2.154677	-0.537040
H	-9.457635	1.431098	1.121943
H	-10.386927	1.484066	-1.356377
H	-10.708420	-0.451076	0.141709
H	-10.195088	0.021060	-2.346745
H	-9.206712	-1.197163	-0.439461
H	-8.690082	-0.065828	1.694012
H	-8.445409	2.601563	-0.676722
H	-4.955567	1.341869	-2.676862
H	-4.692464	1.297532	-0.712386
H	-5.955608	-0.000562	-1.583621

Energy: - 4.4 kcal.mol^{-1}
- 808.198343 H

TSD'E' Trapping by Ligand Nitrogen

B	-4.781752	0.605649	-1.241053
N	-3.686186	-0.101590	0.716749
P	-3.259132	1.208042	1.639607
Lu	-6.070203	-0.220678	1.142567
B	-6.676682	-2.589700	0.774740
N	-5.783832	-0.364912	3.469644
P	-5.453801	1.207481	3.829703
C	-6.949404	2.232443	4.136348
O	-7.823935	0.832088	1.071207
C	-9.159914	1.042506	0.792539
C	-9.669836	0.255473	-0.424263
C	-9.188508	0.767545	-1.766216
O	-7.747648	0.646354	-1.825979
C	-7.122674	1.149729	-2.870157
O	-5.911046	1.184076	-2.951426
C	-4.733985	1.856213	2.360901
C	-1.929928	0.736811	2.831533
C	-2.518285	2.564897	0.645987
Si	-2.544839	-1.301110	0.134288
Si	-6.293662	-1.621023	4.573795
C	-4.479611	1.382513	5.393006

H	-1.999351	-2.144487	1.249610
H	-3.224932	-2.183580	-0.850580
H	-1.355448	-0.658284	-0.526653
H	-1.038223	0.425796	2.279477
H	-2.278580	-0.104832	3.433570
H	-1.682356	1.584476	3.475033
H	-1.662273	2.174561	0.090913
H	-3.267395	2.921359	-0.062385
H	-2.199135	3.379619	1.300721
H	-4.910284	2.911194	2.167120
H	-7.580656	2.130453	3.250165
H	-6.679117	3.279671	4.296960
H	-7.474857	1.850302	5.015213
H	-4.211054	2.433383	5.529659
H	-3.574153	0.776415	5.336640
H	-5.077266	1.045282	6.243534
H	-5.745862	-1.374671	5.954693
H	-7.783736	-1.702888	4.719516
H	-5.784865	-2.940469	4.104985
H	-5.463840	-2.460362	0.991658
H	-7.275610	-2.091331	1.739786
H	-6.980801	-3.737743	0.605638
H	-6.950772	-1.886969	-0.208137
H	-9.363657	2.117258	0.617531
H	-9.454234	1.824298	-1.896339
H	-10.767397	0.302346	-0.449328
H	-9.620888	0.187764	-2.590677
H	-9.393071	-0.798987	-0.313323
H	-9.789568	0.751624	1.652048
H	-7.773378	1.542930	-3.670898
H	-3.760843	0.842885	-1.806454
H	-5.324865	1.464636	-0.586642
H	-5.246953	-0.504024	-1.256926

Energy: 15.6 kcal.mol^{-1}
- 808.166453 H

E' Product (formate termination)

B	-4.263501	0.721296	-0.723900
N	-3.524487	0.143543	0.585396
P	-3.168990	1.350336	1.730297
Lu	-6.059519	-0.075198	0.975731
B	-6.543867	-2.453080	0.576572
N	-5.723408	-0.371721	3.298187
P	-5.441550	1.167172	3.805482
C	-6.956522	2.158600	4.125451
O	-7.781792	0.979707	0.985302
C	-9.105042	1.344930	0.817545
C	-9.788184	0.675210	-0.377739

C	-9.273345	1.106312	-1.742019
O	-7.990423	0.537738	-2.039688
C	-7.885930	-0.234001	-3.136506
O	-6.855526	-0.731078	-3.494150
C	-4.650077	1.945853	2.441463
C	-1.957375	0.631822	2.908841
C	-2.315230	2.751293	0.915995
Si	-2.418714	-1.199524	0.189795
Si	-6.257980	-1.718413	4.284386
C	-4.542129	1.229528	5.421095
H	-2.130961	-2.006464	1.413843
H	-3.068708	-2.030570	-0.851096
H	-1.112255	-0.662799	-0.317630
H	-1.045003	0.341126	2.381379
H	-2.393464	-0.249529	3.382894
H	-1.716000	1.381742	3.665290
H	-1.438811	2.374966	0.383834
H	-2.999970	3.202347	0.195787
H	-2.016548	3.487210	1.665961
H	-4.857160	2.997930	2.271682
H	-7.552458	2.124787	3.210538
H	-6.699966	3.190843	4.378695
H	-7.513626	1.706786	4.950069
H	-4.289710	2.268616	5.648351
H	-3.630352	0.633034	5.364822
H	-5.175703	0.826272	6.214930
H	-5.808044	-1.536822	5.710347
H	-7.748785	-1.856648	4.324366
H	-5.664375	-2.986054	3.775680
H	-5.344966	-2.278299	0.847647
H	-7.196472	-1.995926	1.528139
H	-6.793976	-3.608028	0.376259
H	-6.805386	-1.744389	-0.403548
H	-9.189653	2.440630	0.688770
H	-9.155639	2.195219	-1.786916
H	-10.858241	0.924921	-0.341848
H	-9.984103	0.812893	-2.527524
H	-9.708500	-0.414662	-0.287147
H	-9.692773	1.095294	1.718527
H	-8.851206	-0.354976	-3.669911
H	-3.515674	1.123118	-1.581826
H	-5.004502	1.633348	-0.345820
H	-4.961278	-0.193613	-1.147622

Energy: - 3.0 kcal.mol^{-1}
- 808.196072 H