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Supplementary material

Grafting of lanthanide complexes on silica surfaces dehydroxylated at 200°C : A theoretical investigation

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c model

G = -1566,825275 kcal.mol^{-1}

O	-0.42384	0.56312	4.07955
Si	-0.49161	0.77596	2.45956
O	0.60650	1.93053	2.01032
Si	1.59307	2.31100	0.74423
O	2.91372	3.03004	1.40787
O	-0.14503	-0.65527	1.70924
Si	-0.53894	-1.51662	0.35481
O	-0.44654	-3.11804	0.67812
O	-2.02158	1.26041	2.06347
Si	-2.79715	2.19760	0.94465
O	-1.78639	3.39852	0.41951
Si	-0.70840	3.72440	-0.79102
O	-1.09926	2.86080	-2.15027
Si	-0.75710	1.41872	-2.88460
O	0.77344	0.93462	-2.49632
Si	1.55603	0.01994	-1.35624
O	2.04624	0.95455	-0.08993
O	0.53202	-1.18214	-0.85681
O	-2.08085	-1.13739	-0.12156
Si	-2.85008	-0.09556	-1.15532
O	-1.85851	0.27220	-2.42233
O	2.93338	-0.61959	-1.98700
O	-4.13337	2.85897	1.61938
O	-3.29912	1.26473	-0.32487
O	0.82057	3.34286	-0.29718
O	-4.18089	-0.80440	-1.81282
O	-0.78229	5.32345	-1.13050
O	-0.83985	1.62140	-4.50659
H	3.63451	3.20051	0.79439
Si	-4.45949	4.27959	2.47302
H	-4.94230	-0.85226	-1.22723
Si	-0.93223	6.23290	-2.54548
Si	-1.88595	1.07597	-5.71605
H	2.79814	-1.28336	-2.66958
Si	0.66098	1.01624	5.29358
Si	-1.52731	-4.29877	1.21288
H	-0.70182	-5.43820	1.70166
H	-2.37753	-3.76779	2.31866
H	-2.39163	-4.74108	0.08031
H	0.22539	0.29906	6.52477
H	2.04926	0.61315	4.92730
H	0.59731	2.49028	5.51074
H	-1.46684	1.76859	-6.96686
H	-1.75368	-0.40065	-5.88118
H	-3.29605	1.42742	-5.38137
H	-0.79773	7.65950	-2.13830
H	0.14502	5.87077	-3.51194
H	-2.26880	6.00088	-3.16601
H	-5.71531	4.03433	3.23617
H	-3.34125	4.59574	3.40859
H	-4.65491	5.40595	1.51524

b model

G = -1648,329387 kcal.mol^{-1}

O	-1.01751	0.59334	3.80022
Si	-0.87547	0.66705	2.17149
O	0.42766	1.62395	1.80109
Si	1.42116	1.94818	0.52567
O	2.75620	2.65381	1.17526
O	-0.62595	-0.87209	1.60831
Si	-0.90558	-1.80104	0.27418
O	-0.95206	-3.37951	0.70968
O	-2.24053	1.24542	1.46279
Si	-2.98214	2.66050	1.00437
O	-1.88574	3.59378	0.14053
Si	-0.85131	3.24161	-1.09332
O	-1.42001	1.85685	-1.82550
Si	-0.91041	0.80543	-2.99684
O	0.63724	0.29587	-2.68985
Si	1.36869	-0.50140	-1.42560
O	1.85442	0.55509	-0.26182
O	0.30583	-1.62788	-0.83934
O	-2.34501	-1.36549	-0.41465
Si	-3.04980	-1.07367	-1.87034
O	-1.96192	-0.47551	-2.97308
O	2.73955	-1.24348	-1.95177
O	-3.40005	3.54796	2.32257
O	-4.31773	2.29847	0.13386
O	0.68834	2.97392	-0.55178
O	-3.73405	-2.41180	-2.53885
O	-0.76583	4.48773	-2.15493
O	-0.94171	1.48377	-4.48751
H	3.47330	2.81310	0.55467
Si	-3.35163	5.18642	2.70754
Si	-3.23779	-3.52345	-3.71217
Si	-1.77144	5.79125	-2.53309
Si	0.22107	1.76535	-5.68172
H	2.59302	-2.04904	-2.45604
Si	-0.17557	1.25961	5.10382
Si	-1.08469	-4.19669	2.18288
H	-1.30047	-5.63088	1.84055
H	0.17419	-4.04294	2.96780
H	-2.24179	-3.67586	2.96641
H	-0.90860	0.83503	6.32962
H	1.22098	0.73616	5.13739
H	-0.15800	2.74761	5.00661
H	1.36615	2.54002	-5.12443
H	0.70735	0.46744	-6.23548
H	-0.46316	2.54871	-6.74809
H	-1.66896	6.83558	-1.47326
H	-1.28022	6.33313	-3.83147
H	-3.18661	5.33982	-2.66852
H	-4.12660	5.34894	3.97043
H	-1.94198	5.62852	2.92032
H	-3.97218	6.00438	1.62353
H	-4.07756	-4.73919	-3.52476
H	-3.46295	-2.95089	-5.07137
H	-1.79517	-3.86059	-3.53723
H	-4.25942	1.49391	-0.41397
O	-4.26629	0.01513	-1.53368
H	-5.00593	-0.01506	-2.14864

ac model

G = -1561,70598 kcal. mol^{-1}

O	-0.63490	1.15370	4.05063
Si	-0.59974	1.15208	2.41521
O	0.50476	2.25746	1.87800
Si	1.56014	2.48703	0.63188
O	2.83716	3.30163	1.26967
O	-0.19632	-0.35504	1.86275
Si	-0.52469	-1.37807	0.60532
O	-0.45682	-2.92106	1.14732
O	-2.11304	1.57096	1.89654
Si	-2.83766	2.33679	0.62026
O	-1.80636	3.48419	0.01746
Si	-0.66585	3.66744	-1.17188
O	-0.99980	2.63036	-2.41622
Si	-0.59046	1.12871	-2.97192
O	0.92379	0.72047	-2.45357
Si	1.64929	-0.03866	-1.17147
O	2.06340	1.03976	0.00427
O	0.60388	-1.18225	-0.58337
O	-2.04247	-1.07372	0.01176
Si	-2.76139	-0.18422	-1.18844
O	-1.70204	0.02196	-2.43617
O	3.06210	-0.73113	-1.64935
O	-4.24837	3.02465	1.11486
O	-3.25883	1.26637	-0.56391
O	0.84341	3.36749	-0.57511
O	-4.06104	-0.98375	-1.80263
O	-0.69446	5.20792	-1.72291
O	-0.57659	1.13061	-4.60811
H	3.56926	3.44645	0.66290
H	-4.18342	3.53434	1.92796
H	-4.87956	-0.84424	-1.31717
Si	-1.86919	6.41172	-1.85940
Si	-1.69217	0.71948	-5.80776
H	2.97687	-1.39293	-2.34186
Si	0.37744	0.56699	5.26960
Si	-1.57573	-4.17429	1.31164
H	-0.85757	-5.28638	1.99460
H	-2.73571	-3.72966	2.13853
H	-2.05272	-4.61868	-0.03008
H	0.22862	1.48742	6.43175
H	-0.05987	-0.80758	5.64890
H	1.79503	0.54191	4.80692
H	-1.20583	1.35081	-7.06651
H	-1.74040	-0.76291	-5.96523
H	-3.04699	1.23874	-5.46129
H	-2.08434	7.05936	-0.53268
H	-1.34330	7.40779	-2.83409
H	-3.15419	5.83627	-2.35389

abc model

G = -1638,091502 kcal. mol^{-1}

O	-1.14410	0.56039	3.67301
Si	-1.17078	1.62300	4.98398
Si	-0.80336	0.64372	2.07626
O	-2.09799	1.08851	1.16084
Si	-2.94552	2.46087	0.74861
O	-4.23332	2.00120	-0.14619
O	0.44007	1.71947	1.84813
Si	1.48786	2.09799	0.63090
O	0.74552	3.04729	-0.50878
Si	-0.74650	3.21624	-1.20163
O	-0.67557	4.46792	-2.26116
Si	-1.15304	6.08640	-2.19747
O	-0.34506	-0.87070	1.58658
Si	-0.46149	-1.83634	0.25218
O	-1.88489	-1.53196	-0.53206
Si	-2.53677	-1.28298	-2.01985
O	-3.86401	-0.31345	-1.74727
O	2.72687	2.91657	1.33693
O	2.07727	0.73307	-0.09948
Si	1.78569	-0.34930	-1.30429
O	3.26346	-0.93441	-1.72901
O	-0.40788	-3.40772	0.71095
Si	-0.50047	-4.21428	2.19283
O	0.79993	-1.57631	-0.78710
O	-1.90935	3.50343	-0.06551
O	-3.44476	3.29307	2.08615
H	-3.06897	4.17626	2.14615
O	-1.15341	1.81951	-2.00343
Si	-0.47177	0.74967	-3.06756
O	-0.37208	1.34557	-4.58887
Si	-1.41914	2.07914	-5.68904
O	1.07171	0.37117	-2.61958
O	-1.43604	-0.60185	-3.06144
O	-3.10832	-2.65132	-2.74867
H	-2.47722	-3.09419	-3.32402
H	3.53740	2.93918	0.81986
H	3.25496	-1.57863	-2.44278
H	-0.57369	-5.66663	1.86685
H	0.71809	-3.93415	3.00576
H	-1.72092	-3.79405	2.93976
H	-0.89568	3.02021	4.54069
H	-2.51741	1.53803	5.61521
H	-0.12534	1.18527	5.95358
H	-0.76206	3.31704	-6.19305
H	-1.65272	1.13064	-6.81662
H	-2.71846	2.41309	-5.03495
H	-0.74569	6.70018	-0.89945
H	-0.46520	6.77331	-3.32653
H	-2.63207	6.18794	-2.36245
H	-4.10098	1.17926	-0.65407
H	-4.56695	-0.43617	-2.39355

bc model

G = -1643,21074 kcal. mol^{-1}

O	0.56793	0.00820	0.26445
Si	0.30719	0.16682	1.87035
O	1.79367	0.17316	2.60142
Si	2.53523	0.83340	3.91970
O	2.31244	-0.10402	5.26510
Si	1.20383	-1.11958	5.95891
O	0.20484	-0.21106	6.93108
Si	-0.46569	1.30117	6.81886
O	0.71433	2.45224	6.65424
Si	1.37020	3.32233	5.40189

O	2.53896	4.28793	6.04120
Si	-0.33208	-0.39396	-1.10566
O	-0.45265	1.57319	2.26622
Si	-1.98810	2.21272	2.32094
O	-2.70359	2.17002	0.83156
O	-0.58618	-1.12506	2.40296
Si	-0.97461	-1.85704	3.82796
O	0.33946	-1.95204	4.83403
O	-1.86928	3.75280	2.85498
O	-2.95177	1.24743	3.30203
Si	-2.65569	0.54212	4.76469
O	-1.42872	1.41206	5.47886
O	-2.18935	-1.03574	4.60536
O	-1.47376	-3.37172	3.42895
O	-4.01160	0.54251	5.68674
Si	-5.41480	1.48278	5.70575
O	1.92930	2.34527	4.20539
O	4.14679	0.92624	3.63986
Si	5.11271	0.73621	2.26576
O	0.24571	4.30690	4.66281
O	1.97388	-2.25939	6.86165
O	-1.29874	1.59775	8.19786
Si	-1.60444	0.71908	9.60886
H	-3.52856	1.67580	0.82117
Si	3.50366	4.20780	7.42696
H	-1.60439	-3.96423	4.17501
H	2.70224	-1.92587	7.39360
H	5.08841	-0.68451	1.81319
H	4.64088	1.63046	1.16951
H	6.49297	1.11705	2.67907
H	-0.44846	0.81478	-1.96868
H	0.41249	-1.46514	-1.82819
H	-1.68612	-0.88811	-0.72212
H	-2.23176	-0.59315	9.28211
H	-0.33320	0.50154	10.36002
H	-2.53806	1.55028	10.41918
H	-6.29297	1.10783	4.55939
H	-6.10200	1.18117	6.99298
H	-5.07511	2.93327	5.63148
H	-1.11400	3.92130	3.44845
H	0.16156	5.17557	5.06875
H	4.64813	5.13337	7.19872
H	2.71581	4.65239	8.61349
H	4.00018	2.81742	7.64137

$La(N(SiMe_3)_2)_3$

G = -937.318437 kcal.mol^{-1}

La	-1.41154	1.70347	4.15118
N	-1.49481	1.38382	1.79055
N	-0.42885	-0.01759	5.47491
Si	-1.20348	2.88115	0.94734
Si	-1.71391	-0.17846	1.02634
Si	1.27886	-0.16220	5.15570
Si	-1.31867	-0.94207	6.66877
C	-0.93477	-0.41696	8.45506
C	-3.17299	-0.63702	6.35924
C	-1.01809	-2.81405	6.54832
C	-2.35994	-1.37521	2.35910
H	1.63608	-2.63263	4.91833
C	-0.09640	-0.90129	0.33784
C	1.79036	-1.76179	4.27374
C	0.26457	2.83496	-0.25619
C	1.73505	1.28509	3.96870
C	-2.70238	3.56922	0.00976
C	-0.75356	4.18570	2.29131
H	-0.57386	5.14424	1.79184
H	0.18390	3.95958	2.82222
H	-1.55761	4.38099	3.01600
H	0.47137	3.83469	-0.65497
H	1.17347	2.46875	0.23179
H	0.05580	2.17915	-1.10792
H	0.30573	-0.28546	-0.47283
H	0.67185	-0.96812	1.11505
H	-0.25832	-1.90981	-0.05972
H	2.85043	-1.73528	3.99694
H	1.20495	-1.91786	3.36243
H	-2.61942	0.43458	-1.24321
H	-3.16993	-1.16988	-0.75216
H	-3.93295	0.27420	-0.06639
C	-2.97879	-0.15277	-0.39127
H	-2.42720	-2.39397	1.96138
H	-3.36512	-1.09199	2.69279
H	-1.69760	-1.41817	3.23335
H	0.01220	-3.07584	6.81193
H	-1.67923	-3.35273	7.23683
H	-1.21132	-3.18420	5.53650
H	-3.43118	0.42921	6.38485
H	-3.77551	-1.12946	7.13069
H	-3.48756	-1.05074	5.39367
H	-1.57704	-0.95219	9.16381
H	-1.09600	0.65607	8.60166
H	0.10479	-0.63459	8.71964
H	2.14841	0.95769	7.23472
H	2.25528	-0.80174	7.37690
H	3.44094	0.07356	6.40260
H	-3.57866	3.64653	0.66070
H	-2.48920	4.56550	-0.39411
H	1.60259	2.27859	4.42342
H	-2.97061	2.91999	-0.82943
H	1.22502	1.24761	2.99485
H	2.80396	1.21671	3.73758
N	-3.10726	3.04287	5.15528
C	2.38313	0.03927	6.68735
Si	-2.45281	4.00919	6.45090
Si	-4.76247	3.12216	4.58199
C	-5.12146	4.69252	3.57196
C	-5.04884	1.62414	3.44155
C	-6.04884	3.04040	5.97823
C	-3.03839	3.51362	8.18584
C	-0.54567	3.73791	6.42546
C	-2.72756	5.87763	6.25388
H	-0.10443	4.32756	7.23679
H	-0.23448	2.70048	6.61798
H	-0.06605	4.10937	5.50715
H	-2.50773	4.08414	8.95667
H	-4.10912	3.70290	8.30979
H	-2.86628	2.44930	8.37342
H	-2.19708	6.43256	7.03598
H	-2.37460	6.23726	5.28207
H	-3.79052	6.12768	6.33622
H	-6.13661	4.66596	3.15940
H	-5.03765	5.59247	4.18950
H	-4.42364	4.79967	2.73504
H	-7.06036	2.97242	5.56169
H	-5.88910	2.16773	6.61937
H	-6.01531	3.93421	6.61045
H	-6.04563	1.67359	2.98916
H	-4.32643	1.58638	2.61632
H	-4.99420	0.68207	3.99964

$La(N(SiMe_3)_2)_3$@**ac-1**

G = -2196.604638 kcal.mol^{-1}

Si	-3.08516	2.24751	0.63709
O	-2.58317	3.68148	0.01102
Si	-1.35327	4.11427	-1.03268
O	-1.79087	5.54696	-1.67789
Si	-1.00493	6.80147	-2.49848
La	-5.34196	-0.15224	-0.87791
O	-3.35347	-1.17607	-1.65173
Si	-2.08372	-0.36988	-1.12379
O	-1.03956	0.24490	-2.26038
Si	-0.29575	1.66499	-2.66069
O	-0.09987	1.75316	-4.28248
Si	0.11652	0.63222	-5.52765
O	-4.76328	2.19529	0.68692
O	-2.46734	1.99830	2.14054
Si	-0.89696	1.80678	2.68424
O	-0.93036	1.65961	4.31054
Si	-1.78681	2.38290	5.57513
O	-2.81826	0.96716	-0.34696
Si	-6.14427	-2.30868	1.69164
C	-4.98118	-0.89561	2.27476
C	-5.15973	-3.90614	1.97747
C	-7.64201	-2.30730	2.85775
N	-6.54636	-1.98084	0.02728
Si	-7.56310	-2.99273	-0.98131
C	-7.17085	-2.57119	-2.79611
N	-6.53155	1.15608	-2.45609
Si	-8.01018	1.85486	-1.83456
C	-9.59273	1.20140	-2.65370
O	-0.04197	3.15207	2.25076
Si	0.96489	3.68265	1.04475
O	1.87939	4.94124	1.57301
O	-0.22349	0.45861	2.03931
Si	0.15531	-0.71672	0.94089
O	1.35941	-0.16297	-0.04840
Si	2.00639	1.26195	-0.58691
O	1.93556	2.42831	0.57954
O	0.07254	4.26443	-0.21643
O	-1.22933	2.95125	-2.19492
O	1.18682	1.76509	-1.93400
O	3.60459	1.05871	-0.91592
C	-9.41679	-2.68976	-0.68671
C	-7.25919	-4.85553	-0.76086
O	-1.17410	-1.13029	0.04664
O	0.69332	-2.03763	1.74105
Si	0.21476	-3.65744	1.81742
Si	-5.91874	1.52034	-4.06747
C	-4.78320	0.10624	-4.63470
C	-7.27715	1.68741	-5.38750
C	-4.90343	3.12791	-4.08997
C	-8.14981	1.39905	0.02392
C	-8.05422	3.75514	-1.92500
H	2.67441	4.68828	2.05174
H	-5.22418	3.04067	0.66901
H	3.82280	0.24867	-1.38603
H	1.20448	-4.33663	2.69959
H	-1.15227	-3.76203	2.40309
H	0.23653	-4.26599	0.45611
H	-2.13280	3.79262	5.22924
H	-3.03135	1.60343	5.83398
H	-0.89954	2.34703	6.77042
H	0.65508	1.39415	-6.68885
H	1.09171	-0.41930	-5.11142
H	-1.18733	0.00381	-5.87985
H	-0.52299	7.80407	-1.50649
H	0.14241	6.26493	-3.28591
H	-2.01504	7.41539	-3.40404
H	-10.48131	1.57384	-2.13122
H	-9.66329	1.51721	-3.69843
H	-9.62402	0.10761	-2.63448
H	-8.94881	4.14775	-1.42805
H	-7.17703	4.20433	-1.44663
H	-8.07476	4.10588	-2.96222
H	-9.11803	1.75804	0.39097
H	-8.13457	0.31737	0.21420
H	-7.38978	1.87607	0.65547
H	-4.54698	3.34739	-5.10308
H	-5.49939	3.98266	-3.75394
H	-4.02411	3.05636	-3.44111
H	-6.81528	1.82872	-6.37154
H	-7.89908	0.78816	-5.43687
H	-7.93303	2.54573	-5.20905
H	-4.30071	0.37879	-5.58032
H	-3.98631	-0.13337	-3.92204
H	-5.35776	-0.80972	-4.80966
H	-7.33096	-2.43173	3.90118
H	-8.20590	-1.37218	2.77842
H	-8.32525	-3.12853	2.61646
H	-4.76097	-1.05514	3.33630
H	-4.00253	-0.90422	1.77504
H	-5.41218	0.11216	2.21367
H	-4.79843	-3.95487	3.01128
H	-5.76424	-4.79870	1.79367
H	-4.29178	-3.94724	1.31127
H	-10.02620	-3.29164	-1.37068
H	-9.70140	-2.95813	0.33613
H	-9.68113	-1.63859	-0.83893
H	-7.82361	-5.41732	-1.51412
H	-6.19990	-5.10425	-0.87738
H	-7.58632	-5.20874	0.22265
H	-7.81580	-3.15020	-3.46664
H	-7.33729	-1.51228	-3.02949
H	-6.13349	-2.82682	-3.04495

TS_{La}

G = -2196.604934 kcal.mol^{-1}

C	-5.52062	-4.15399	1.93426
Si	-6.32131	-2.47558	1.56835
N	-6.58106	-2.15633	-0.12411
Si	-7.34319	-3.09509	-1.37514
C	-6.70935	-4.87480	-1.52100
La	-5.30273	-0.38620	-0.98087
O	-3.33819	-1.43983	-1.72392
Si	-2.08662	-0.60395	-1.17805
O	-1.27165	-1.31114	0.09371
Si	-0.09617	-0.75878	1.12211
O	0.30791	-1.96274	2.15481
Si	-0.01599	-3.61889	2.22874
C	-5.07597	-1.13306	2.14683
C	-7.88674	-2.30687	2.62390
N	-6.45814	1.61700	-1.91607
Si	-5.91207	2.23063	-3.48053
C	-7.22068	2.15833	-4.85505
O	-4.94722	2.09709	0.19436
Si	-3.30013	2.17800	0.24159
O	-2.82624	2.11345	1.81988
Si	-1.32507	1.93267	2.51003
O	-0.38588	3.22981	2.08964
Si	0.74660	3.60297	0.94795
O	0.00925	4.01188	-0.47712
Si	-1.32035	3.82589	-1.43367
O	-1.07200	2.59475	-2.51233
Si	-0.12369	1.25329	-2.71724
O	1.25621	1.40742	-1.82301
Si	1.93788	1.05431	-0.35625
O	3.56131	0.83807	-0.51498
O	-2.84284	0.78075	-0.53292
Si	-8.07147	1.99618	-1.28752
C	-8.18007	1.27405	0.46868
C	-8.38956	3.86397	-1.17792
C	-9.48734	1.21432	-2.28320
C	-9.23438	-3.13148	-1.25403
C	-6.87392	-2.21754	-3.02345
O	-2.66736	3.49418	-0.52130
O	-1.63513	5.21732	-2.23144
Si	-1.03834	6.00518	-3.60004
O	-0.96073	-0.10833	-2.29387
O	0.28754	1.15812	-4.30050
Si	0.24263	-0.06353	-5.46545
O	-1.51090	1.87743	4.13150
Si	-1.21862	2.94639	5.40892
O	-0.62807	0.54376	1.97735
O	1.24393	-0.31734	0.25581
C	-5.28949	4.01902	-3.38102
C	-4.45919	1.14251	-4.06178
O	1.76925	2.33030	0.67616
O	1.59706	4.87207	1.55445
H	2.47677	4.97937	1.18089
H	-5.56625	2.22822	-0.81346
H	3.82196	0.01428	-0.93694
H	0.82000	-4.15532	3.33892
H	-1.46054	-3.84795	2.51926
H	0.35459	-4.27871	0.94295
H	-1.80733	4.28349	5.11035
H	-1.87640	2.34800	6.60399
H	0.24914	3.07204	5.63928
H	0.90189	0.49719	-6.67826
H	0.99155	-1.26278	-4.98716
H	-1.16782	-0.43553	-5.77279
H	-1.47559	5.28583	-4.83049
H	-1.60813	7.38059	-3.57551
H	0.45240	6.06318	-3.55219
H	-10.43936	1.38912	-1.76870
H	-9.57236	1.63236	-3.28966
H	-9.35937	0.13126	-2.37972
H	-9.34740	4.05728	-0.68174
H	-7.60584	4.36797	-0.60334
H	-8.43302	4.32807	-2.16888
H	-9.17090	1.47933	0.88923
H	-8.06010	0.18244	0.47235
H	-7.43741	1.71771	1.13979
H	-4.90883	4.34340	-4.35639
H	-6.09341	4.70346	-3.09307
H	-4.48176	4.13169	-2.65204
H	-6.75957	2.43797	-5.80938
H	-7.64344	1.15523	-4.96954
H	-8.04532	2.85539	-4.67520
H	-4.09964	1.51627	-5.02729
H	-3.59782	1.16731	-3.38587
H	-4.74387	0.09543	-4.22559
H	-7.66437	-2.45673	3.68637
H	-8.34101	-1.31797	2.50802
H	-8.63345	-3.05297	2.33177
H	-4.89044	-1.26007	3.21916
H	-4.08659	-1.22795	1.67575
H	-5.43493	-0.09904	2.04453
H	-5.26150	-4.23493	2.99598
H	-6.19513	-4.98218	1.69476
H	-4.60560	-4.28628	1.34848
H	-9.67831	-3.65890	-2.10573
H	-9.55060	-3.64819	-0.34157
H	-9.65196	-2.12048	-1.22276
H	-7.10676	-5.35585	-2.42191
H	-5.61654	-4.89520	-1.57656
H	-7.01447	-5.47946	-0.66116
H	-7.39301	-2.72243	-3.84566
H	-7.19230	-1.16609	-3.09071
H	-5.80311	-2.29949	-3.26181

$La(N(SiMe_3)_2)_3$@**ac-2**

G = -2196.644843 kcal.mol^{-1}

C	-6.86936	-3.78379	2.68371
Si	-6.93375	-2.03299	1.95098
C	-8.61793	-1.27960	2.40982
N	-6.65899	-1.98076	0.21520
La	-5.32859	-0.37007	-0.87977
O	-4.39683	1.33662	0.30829
Si	-2.86680	1.85027	0.35647
O	-2.25111	1.96141	1.90436
Si	-0.71966	1.50776	2.36898
O	0.38381	2.58486	1.77286
Si	1.06527	3.39656	0.50705
O	-0.01793	3.88573	-0.63396
Si	-1.41940	3.66737	-1.48259
O	-1.23539	2.52859	-2.67369
Si	-0.32541	1.20149	-3.07947
O	1.16562	1.25162	-2.36670
Si	2.10075	1.00099	-1.03430
O	3.58820	0.56694	-1.59533
C	-5.57190	-1.01214	2.79758
Si	-7.16300	-3.20958	-0.91583
C	-9.03219	-3.53387	-0.92182
C	-6.25336	-4.86330	-0.75320
C	-6.70867	-2.55376	-2.67557
O	-1.78167	0.84886	-0.41988
Si	-1.81405	-0.60516	-1.24644
O	-0.78299	-1.56054	-0.33965
Si	0.33141	-0.99069	0.75485
O	1.00257	-2.29528	1.49790
Si	0.71411	-3.95169	1.38523
N	-6.50811	1.84733	-2.04845
Si	-6.10614	1.99196	-3.81547
C	-7.54375	1.32080	-4.83711
O	-3.29196	-1.22715	-1.41939
O	-2.67579	3.30102	-0.46127
O	-1.81191	5.08160	-2.22621
Si	-1.11462	6.61691	-2.24091
Si	-8.12871	2.29403	-1.34894
C	-7.81842	2.67716	0.47137
C	-8.87914	3.82098	-2.17239
C	-9.26769	0.80313	-1.53908
O	-1.10184	-0.21477	-2.70918
O	-0.12324	1.25339	-4.71021
Si	1.18487	0.94641	-5.72807
C	-5.71394	3.78169	-4.25669
C	-4.57466	0.92913	-4.12206
O	-0.34046	-0.04236	1.93391
O	1.54242	-0.18520	-0.03151
O	-0.65656	1.57651	4.01018
Si	-1.70760	2.16226	5.18864
O	2.20963	2.41838	-0.18337
O	1.76866	4.78158	1.05681
H	2.34177	4.65714	1.81895
H	-5.81711	2.40963	-1.53797
H	4.11688	0.07970	-0.95660
H	1.62404	-4.59998	2.37301
H	-0.70471	-4.26738	1.72441
H	1.02622	-4.44981	0.01326
H	-2.07836	3.58181	4.91266
H	-2.94121	1.32524	5.25622
H	-0.97227	2.07824	6.48326
H	2.20391	2.02884	-5.60578
H	1.80582	-0.37338	-5.41362
H	0.63539	0.92774	-7.11494
H	-1.10957	7.20585	-0.87026
H	0.27638	6.56021	-2.77640
H	-1.96781	7.44631	-3.14108
H	-10.25188	1.03287	-1.11646
H	-9.41489	0.52552	-2.58694
H	-8.87708	-0.06686	-0.99904
H	-9.82307	4.07024	-1.67446
H	-8.21695	4.68695	-2.07499
H	-9.09845	3.67421	-3.23380
H	-8.76611	2.91610	0.96597
H	-7.36571	1.84035	1.01160
H	-7.15345	3.53890	0.58799
H	-5.40400	3.84742	-5.30530
H	-6.57853	4.43749	-4.12090
H	-4.88978	4.16766	-3.64767
H	-7.26829	1.35765	-5.89678
H	-7.76797	0.27712	-4.59587
H	-8.45989	1.90539	-4.71682
H	-4.26569	1.04342	-5.16740
H	-3.71677	1.23925	-3.51679
H	-4.73889	-0.14601	-3.97769
H	-8.77992	-1.30825	3.49326
H	-8.68890	-0.23383	2.09201
H	-9.43803	-1.82755	1.93403
H	-5.76362	-0.94859	3.87467
H	-4.59146	-1.48581	2.67053
H	-5.49422	0.01734	2.42837
H	-6.98356	-3.73599	3.77267
H	-7.67120	-4.42310	2.29895
H	-5.91295	-4.27018	2.46816
H	-9.30173	-4.27768	-1.67989
H	-9.35974	-3.91873	0.04983
H	-9.59869	-2.61959	-1.12452
H	-6.50641	-5.53293	-1.58299
H	-5.16925	-4.71002	-0.75838
H	-6.51496	-5.37235	0.17871
H	-7.11210	-3.26323	-3.40640
H	-7.16851	-1.58659	-2.93000
H	-5.62808	-2.52147	-2.87949

$Y(N(SiMe_3)_2)_3$

G = -944.060945 kcal.mol^{-1}

C	-0.66988	-4.55881	0.55526
Si	-1.22995	-2.89952	1.29655
C	0.06868	-2.36763	2.57359
C	-2.85355	-3.22859	2.22916
N	-1.38765	-1.63885	0.07482
Y	0.02508	0.00540	-0.38175
N	2.15874	-0.39615	0.05282
Si	3.19057	0.38843	1.24878
C	2.09713	1.19059	2.57517
Si	-2.69708	-1.60956	-1.08671
C	-2.23423	-0.25662	-2.37406
C	-2.91562	-3.21751	-2.07167
C	-4.38612	-1.13123	-0.37256
Si	2.78074	-1.55387	-1.10486
C	1.36505	-1.85575	-2.37081
N	-0.69112	2.05063	0.07931
Si	-0.05170	3.15823	-1.11583
C	1.16699	4.44844	-0.45010
C	4.26399	-0.93415	-2.11467
C	3.23762	-3.24360	-0.37732
Si	-1.82860	2.54968	1.33003
C	-3.56007	2.91112	0.63214

C	-1.26698	4.11081	2.25751
C	-1.99277	1.15671	2.60746
C	0.92200	2.07086	-2.37086
C	-1.36681	4.08086	-2.12730
C	4.35842	-0.83016	2.12183
C	4.27406	1.74952	0.48051
H	-4.76628	-1.90986	0.29552
H	1.38031	2.73523	-3.11206
H	0.28313	1.39166	-2.95465
H	1.75677	1.51325	-1.92178
H	-0.89540	4.63072	-2.95012
H	-2.10525	3.39496	-2.55400
H	-1.90202	4.80894	-1.50957
H	-3.55558	3.78917	-0.02113
H	-3.94413	2.06705	0.05092
H	-4.26656	3.10718	1.44694
H	-5.12029	-0.99021	-1.17409
H	-4.32405	-0.20225	0.20139
H	-1.27606	4.99807	1.61584
H	-1.94413	4.30697	3.09689
H	-0.25632	3.99440	2.66151
H	-2.77004	1.40624	3.33864
H	-1.05702	1.01127	3.15792
H	-2.26875	0.20826	2.13483
H	-3.61959	-3.66374	1.57868
H	-2.67610	-3.93892	3.04493
H	-3.25985	-2.31045	2.66529
H	1.02640	-2.12927	2.09850
H	0.24245	-3.17596	3.29292
H	-0.26744	-1.49051	3.13668
H	-0.48039	-5.28781	1.35165
H	0.25222	-4.44814	-0.02376
H	-1.43051	-4.98212	-0.10788
H	-1.97508	-3.54127	-2.52877
H	-3.27501	-4.03037	-1.43249
H	-3.65271	-3.07732	-2.87077
H	1.93343	3.98777	0.17924
H	1.66669	4.96678	-1.27664
H	-1.35088	-0.51298	-2.97626
H	0.65094	5.20208	0.15216
H	-2.12335	0.75097	-1.94750
H	-3.05802	-0.17590	-3.09226
H	1.70319	-2.61250	-3.08777
H	0.44684	-2.26567	-1.92585
H	1.12997	-0.96936	-2.97758
H	3.44680	-3.96454	-1.17602
H	4.13002	-3.17454	0.25197
H	2.42671	-3.64226	0.23889
H	4.52012	-1.65683	-2.89803
H	4.05070	0.02655	-2.59425
H	5.14957	-0.80532	-1.48409
H	4.80910	2.30084	1.26242
H	5.02008	1.33386	-0.20422
H	3.67093	2.46855	-0.08256
H	4.90814	-0.31596	2.91860
H	3.80542	-1.65858	2.57588
H	5.09880	-1.25274	1.43442
H	2.71246	1.75324	3.28627
H	1.37619	1.88664	2.13287
H	1.54630	0.43210	3.14172

$Y(N(SiMe_3)_2)_3$@**ac-1**

G = -2203.346895 kcal.mol^{-1}

C	-5.25582	-3.81183	2.03124
Si	-6.13537	-2.17981	1.62745
C	-7.77007	-2.14901	2.59084
N	-6.36527	-1.93848	-0.09936
Y	-5.31518	-0.48091	-1.33720
O	-4.86100	2.76092	0.10658
Si	-3.29659	2.30277	0.05101
O	-2.70534	2.13904	1.58280
Si	-1.21901	2.05993	2.31748
O	-0.25932	3.27981	1.74993
Si	0.93647	3.53987	0.63504
O	0.28176	4.02088	-0.80156
Si	-1.06280	3.79463	-1.73656
O	-0.77863	2.62878	-2.87452
Si	-0.08537	1.13054	-2.88805
O	1.32638	1.15469	-2.03000
Si	1.92363	0.82915	-0.51957
O	3.52705	0.47422	-0.61000
C	-5.02975	-0.76500	2.24903
Si	-7.07708	-3.04679	-1.24118
C	-8.95265	-3.24594	-1.08030
C	-6.28392	-4.76389	-1.32098
C	-6.72441	-2.25140	-2.97585
O	-3.30665	0.79098	-0.70421
Si	-2.28945	-0.51356	-1.20394
O	-1.54836	-1.07772	0.16800
Si	-0.22318	-0.71914	1.09847
O	0.08835	-1.98409	2.08859
Si	0.04614	-3.66483	1.93711
N	-6.41606	1.43153	-1.90187
Si	-5.92983	2.06756	-3.48370
C	-7.30978	2.02968	-4.78920
O	-3.42047	-1.46078	-1.83061
O	-2.34050	3.33855	-0.79773
O	-1.43519	5.18277	-2.51333
Si	-0.84962	6.76829	-2.46403
Si	-8.00709	1.87469	-1.23235
C	-8.03256	1.42304	0.60612
C	-8.35711	3.73543	-1.37367
C	-9.43214	0.94039	-2.07231
O	-1.13104	0.02318	-2.24695
O	0.24595	0.73507	-4.44143
Si	-0.00360	-0.63002	-5.40281
C	-5.24999	3.83311	-3.40566
C	-4.53957	0.95569	-4.17568
O	-0.49984	0.60514	2.03691
O	1.07965	-0.44732	0.11518
O	-1.42123	2.23581	3.93097
Si	-2.62538	2.89725	4.91476
O	1.81458	2.14702	0.46373
O	1.91442	4.77307	1.10880
H	2.54552	4.54708	1.79853
H	-5.41069	2.42171	-0.65601
H	3.75006	-0.26557	-1.18229
H	1.03032	-4.20796	2.91461
H	-1.32223	-4.16138	2.25769
H	0.42240	-4.07359	0.55135
H	-3.05412	4.22639	4.39051
H	-3.79358	1.97304	4.97728
H	-2.02019	3.04966	6.26747
H	0.76453	-0.40213	-6.65843
H	0.50314	-1.85043	-4.70831
H	-1.45425	-0.78702	-5.70819
H	-0.95115	7.31166	-1.07887
H	0.56750	6.80585	-2.92598
H	-1.71323	7.55442	-3.38872
H	-10.37993	1.18771	-1.58029
H	-9.52726	1.19676	-3.13105
H	-9.29441	-0.14300	-1.99688
H	-9.30550	3.96785	-0.87579
H	-7.57223	4.32272	-0.88636
H	-8.44080	4.07202	-2.41181
H	-9.01471	1.65158	1.03519
H	-7.85037	0.35266	0.74845
H	-7.27876	1.98681	1.16458
H	-4.89328	4.14149	-4.39500
H	-6.02223	4.54184	-3.09215
H	-4.41291	3.92275	-2.70797
H	-6.90881	2.37334	-5.74977
H	-7.70591	1.01924	-4.93472
H	-8.14530	2.68655	-4.52906
H	-4.25454	1.36011	-5.15414
H	-3.62682	0.95119	-3.57195
H	-4.84392	-0.08289	-4.36032
H	-7.58554	-2.30264	3.66025
H	-8.29133	-1.19426	2.47326
H	-8.44388	-2.94345	2.25306
H	-4.90951	-0.83596	3.33600
H	-4.02305	-0.81655	1.81878
H	-5.45187	0.22545	2.04376
H	-4.98876	-3.84243	3.09378
H	-5.88909	-4.68074	1.82595
H	-4.33660	-3.91637	1.44655
H	-9.36111	-3.82544	-1.91580
H	-9.19763	-3.77929	-0.15561
H	-9.46058	-2.27796	-1.04866
H	-6.66324	-5.32162	-2.18499
H	-5.19631	-4.68351	-1.41234
H	-6.50645	-5.35034	-0.42454
H	-7.25522	-2.87196	-3.70582
H	-7.13102	-1.24007	-3.13759
H	-5.67075	-2.30122	-3.29384

TS_Y

G = -2203.343674 kcal.mol^{-1}

C	-4.63564	-3.14770	2.10796
Si	-6.12483	-2.01418	1.78783
C	-7.65909	-2.81668	2.57029
N	-6.33078	-1.71067	0.06078
Y	-5.27696	-0.32643	-1.24999
C	-6.71229	-2.22731	-2.80515
Si	-7.09887	-2.85674	-1.01978
C	-6.40039	-4.61477	-0.93365
C	-5.81315	-0.37920	2.69499
C	-8.98565	-2.92819	-0.86277
N	-6.43101	1.45658	-2.16621
Si	-5.85264	2.04568	-3.73857
C	-7.12650	1.89501	-5.13940
O	-5.02394	1.98696	0.02092
Si	-3.37567	2.02911	0.06636
O	-2.88273	1.84953	1.62657
Si	-1.38652	1.63302	2.32656
O	-0.42871	2.91444	1.90387
Si	0.71806	3.29895	0.77170
O	-0.01284	3.82497	-0.61240
Si	-1.34641	3.65294	-1.57046
O	-1.15944	2.39930	-2.62530
Si	-0.23918	1.05730	-2.91512
O	1.16799	1.14625	-2.05160
Si	1.81283	0.72960	-0.58388
O	3.43040	0.46648	-0.72256
O	-3.01733	0.64889	-0.79933
Si	-2.26371	-0.76077	-1.42196
O	-1.50783	-1.49363	-0.13508
Si	-0.27088	-1.05129	0.87607
O	0.10458	-2.31027	1.84877
Si	0.12265	-3.99208	1.68455
O	-3.56112	-1.50808	-1.98824
Si	-8.08745	1.88301	-1.65688
C	-8.30162	1.48282	0.18305
C	-8.45047	3.73499	-1.87584
C	-9.42397	0.92096	-2.60556
O	-2.69489	3.35118	-0.63875
O	-1.60107	5.02781	-2.41286
Si	-1.15211	6.64887	-2.22821
O	-1.09633	-0.29870	-2.50488
O	0.12718	1.00714	-4.50899
Si	0.14971	-0.19213	-5.69792
O	-1.57209	1.57011	3.94707
Si	-2.15069	2.60163	5.15458
O	-0.70860	0.22786	1.81742
O	1.05136	-0.62992	-0.02725
C	-5.26680	3.84707	-3.66571
C	-4.35515	1.00095	-4.27424
O	1.66263	1.97012	0.49379
O	1.64766	4.54735	1.29954
H	2.41237	4.28511	1.82073
H	-5.59571	2.14106	-0.97655
H	3.67905	-0.25339	-1.30958
H	1.01464	-4.50918	2.75969
H	-1.25554	-4.53190	1.85216
H	0.66135	-4.37431	0.34568
H	-3.23043	3.47809	4.61588
H	-2.67871	1.73370	6.24322
H	-1.02387	3.43546	5.66388
H	0.80742	0.41456	-6.88860
H	0.93583	-1.37038	-5.22573
H	-1.24033	-0.61223	-6.03335
H	-2.01302	7.42546	-3.16266
H	-1.38416	7.09133	-0.82282
H	0.28463	6.81648	-2.58795
H	-10.40339	1.12086	-2.15527

H	-9.47594	1.21173	-3.65820
H	-9.25603	-0.15949	-2.56239
H	-9.44141	3.96423	-1.46718
H	-7.71930	4.34941	-1.34025
H	-8.45008	4.04380	-2.92589
H	-9.33534	1.69419	0.47991
H	-8.09922	0.42777	0.39603
H	-7.63843	2.08989	0.80673
H	-4.83799	4.14201	-4.63024
H	-6.08863	4.53258	-3.44061
H	-4.49348	3.98906	-2.90493
H	-6.64952	2.17609	-6.08563
H	-7.49370	0.86886	-5.24286
H	-7.98979	2.55308	-5.00130
H	-4.03536	1.35522	-5.26131
H	-3.49255	1.11928	-3.61156
H	-4.56970	-0.06879	-4.37901
H	-7.51070	-2.92255	3.65106
H	-8.55308	-2.20468	2.41274
H	-7.85507	-3.81643	2.16874
H	-5.66260	-0.57872	3.76233
H	-4.92195	0.14533	2.33606
H	-6.66409	0.30093	2.59453
H	-4.47099	-3.28091	3.18338
H	-4.78183	-4.13713	1.66321
H	-3.72349	-2.72305	1.67604
H	-9.41603	-3.55131	-1.65513
H	-9.28294	-3.35676	0.09895
H	-9.42646	-1.92948	-0.93356
H	-6.84631	-5.24894	-1.70825
H	-5.31608	-4.59980	-1.08115
H	-6.60669	-5.08025	0.03546
H	-7.27773	-2.87446	-3.48487
H	-7.06109	-1.21051	-3.04600
H	-5.65927	-2.34746	-3.09590

$Y(N(SiMe_3)_2)_3$@**ac-2**

G = -2203.390879 kcal.mol^{-1}

N	-4.09111	-1.62417	-0.26738
Y	-2.67644	0.06173	-0.22716
O	-1.18826	-0.17241	-1.70590
Si	0.41489	-0.35260	-1.59833
O	0.95291	-1.87579	-2.02923
Si	2.13241	-2.71463	-1.20472
O	2.23987	-4.20598	-1.88929
Si	1.35440	-4.98223	-3.09507
O	-1.31868	0.13117	1.39891
Si	0.29792	0.06433	1.44503
O	0.87775	-1.19482	2.37194
Si	2.05221	-2.27591	1.89571
O	2.04769	-3.52466	2.96385
Si	1.53685	-3.68561	4.56115
N	-3.01692	2.52311	0.40929
O	1.00737	-0.20031	-0.04170
O	0.96792	1.52233	1.91793
Si	2.36020	2.14874	1.25734
O	2.22359	2.38098	-0.37873
Si	2.53411	1.70043	-1.85874
O	3.88591	0.74844	-1.82246
Si	4.60226	-0.66178	-1.36450
O	5.83095	-0.91388	-2.43331
O	1.24621	0.82607	-2.43775
O	2.80416	2.94615	-2.89523
Si	3.85244	3.16936	-4.19686
O	3.59754	-1.97189	-1.38609
O	1.77504	-2.92873	0.39933
O	5.21277	-0.47978	0.16560
Si	4.48089	-0.23117	1.63053
O	5.62590	-0.06034	2.80299
O	3.53354	-1.54389	1.95696
O	3.65721	1.19403	1.62686
O	2.57544	3.62542	1.94590
Si	3.88762	4.37829	2.69165
H	6.09787	-1.83489	-2.50672
H	-2.12992	2.41584	0.92028
H	6.15668	-0.84758	2.95566
H	5.09724	4.31588	1.82058
H	3.48589	5.79982	2.89830
H	4.17496	3.73907	4.00829
H	3.81692	1.99449	-5.11626
H	3.37256	4.38606	-4.91400
H	5.24425	3.38948	-3.70768
H	2.08166	-4.98546	5.04770
H	2.06642	-2.57151	5.40272
H	0.04707	-3.70416	4.63418
H	1.51611	-4.27886	-4.40151
H	1.90894	-6.36259	-3.19573
H	-0.09210	-5.04436	-2.73285
Si	-4.10162	-3.05673	0.76339
Si	-5.12271	-1.41415	-1.65912
Si	-4.26537	2.66027	1.74014
Si	-2.69750	3.90026	-0.76455
C	-6.97534	-1.41467	-1.25223
C	-4.70533	0.34219	-2.33668
C	-4.79922	-2.59037	-3.10734
C	-4.49172	-4.65104	-0.19306
C	-2.39530	-3.26938	1.55889
C	-5.39524	-2.90241	2.14749
H	-5.36831	-2.27691	-3.99023
H	-3.73576	-2.58859	-3.36786
H	-5.08725	-3.61834	-2.87138
H	-5.38275	0.54200	-3.17424
H	-4.88642	1.16009	-1.62431
H	-3.69471	0.43163	-2.76360
H	-7.57510	-1.18369	-2.13979
H	-7.29203	-2.39658	-0.88491
H	-7.21096	-0.67850	-0.47656
H	-4.42424	-5.50997	0.48444
H	-5.50205	-4.64796	-0.61610
H	-3.77963	-4.81136	-1.00855
H	-5.42557	-3.81729	2.75022
H	-5.16569	-2.06877	2.81901
H	-6.39695	-2.73815	1.73615
H	-2.40906	-4.11908	2.25095
H	-1.62978	-3.47528	0.80262
H	-2.08072	-2.38711	2.12558
C	-2.56758	5.54334	0.16130
C	-1.05775	3.51566	-1.59487
C	-4.07429	4.00510	-2.04836
C	-3.58832	3.71149	3.15239
C	-5.86831	3.37296	1.04966
C	-4.56480	0.91369	2.39011
H	-3.86802	4.86827	-2.69167
H	-4.10538	3.11980	-2.68868
H	-5.06389	4.15147	-1.60867
H	-0.82381	4.30432	-2.31865
H	-0.23202	3.48124	-0.87751
H	-1.07171	2.56532	-2.13694
H	-2.26549	6.32497	-0.54492
H	-3.51458	5.85676	0.61116
H	-1.80771	5.50081	0.94803
H	-6.62988	3.33906	1.83670
H	-5.76558	4.41583	0.73704
H	-6.24564	2.79189	0.20257
H	-4.28288	3.68046	3.99922
H	-2.62662	3.32003	3.50091
H	-3.44949	4.75785	2.86926
H	-5.29207	0.95846	3.20900
H	-4.97729	0.22197	1.64473
H	-3.64376	0.48201	2.79838

$Yb(N(SiMe_3)_2)_3$

G = -945.137877 kcal.mol^{-1}

Yb	-1.31448	1.78471	4.15380
N	-1.49483	1.36472	2.00352
N	-0.54930	0.12662	5.37836
Si	-1.21027	2.84588	1.11469
Si	-1.73097	-0.18340	1.19086
Si	1.17061	-0.03796	5.09544
Si	-1.40789	-0.84699	6.57288
C	-0.97574	-0.34999	8.35744
C	-3.27506	-0.61673	6.33275
C	-1.03635	-2.70451	6.41547
C	-2.42537	-1.43396	2.43529
H	1.59567	-2.50070	4.90305
C	-0.10598	-0.88590	0.49625
C	1.69901	-1.64151	4.23365
C	0.23691	2.77066	-0.11249
C	1.64359	1.41094	3.91957
C	-2.71185	3.52851	0.18007
C	-0.73215	4.16064	2.43501
H	-0.60067	5.12460	1.93139
H	0.23208	3.95826	2.92384
H	-1.51368	4.32973	3.19046
H	0.44153	3.76670	-0.52172
H	1.15419	2.40176	0.35703
H	0.00523	2.11256	-0.95636
H	0.29470	-0.26092	-0.30789
H	0.66328	-0.96187	1.27080
H	-0.26661	-1.88976	0.08633
H	2.74881	-1.58628	3.92370
H	1.09100	-1.83879	3.34650
H	-2.55230	0.51517	-1.09444
H	-3.15760	-1.08115	-0.64858
H	-3.90470	0.36731	0.04122
C	-2.95138	-0.07590	-0.26324
H	-2.47036	-2.43400	1.98999
H	-3.44076	-1.16224	2.74216
H	-1.79769	-1.49303	3.33070
H	0.00106	-2.94086	6.67423
H	-1.67938	-3.27050	7.09941
H	-1.22369	-3.06966	5.40086
H	-3.55578	0.44128	6.35283
H	-3.82716	-1.12738	7.12960
H	-3.60506	-1.04190	5.37897
H	-1.61218	-0.88945	9.06831
H	-1.11878	0.72152	8.52777
H	0.06460	-0.58740	8.60019
H	1.99717	1.07091	7.20150
H	2.13711	-0.68838	7.31954
H	3.31020	0.22264	6.36470
H	-3.59635	3.57858	0.82109
H	-2.50598	4.53655	-0.19780
H	1.54896	2.40134	4.38845
H	-2.95967	2.89677	-0.67793
H	1.11240	1.39419	2.95655
H	2.70506	1.31575	3.66563
N	-2.97821	2.92113	5.03557
C	2.25168	0.16473	6.64314
Si	-2.36177	3.90208	6.34926
Si	-4.65805	3.02569	4.50575
C	-5.01164	4.62766	3.54255
C	-5.04362	1.56102	3.36454
C	-5.89264	2.97467	5.95086
C	-2.94313	3.39033	8.07925
C	-0.45158	3.67360	6.32093
C	-2.67735	5.76530	6.16738
H	-0.02454	4.23698	7.15797
H	-0.12853	2.63363	6.47588
H	0.02386	4.09014	5.42094
H	-2.39238	3.94087	8.85062
H	-4.00761	3.60155	8.21747
H	-2.79177	2.32104	8.25113
H	-2.14667	6.31815	6.95090
H	-2.34214	6.14464	5.19708
H	-3.74285	5.99571	6.26779
H	-6.03234	4.61469	3.14301
H	-4.91877	5.51078	4.18217
H	-4.32607	4.75699	2.69934
H	-6.91656	2.93080	5.56211
H	-5.73745	2.09603	6.58459
H	-5.82310	3.86598	6.58357
H	-6.04857	1.66251	2.93987
H	-4.33152	1.50579	2.53468
H	-5.01009	0.61282	3.91148

$Yb(N(SiMe_3)_2)_3$@**ac-1**

G = -2204.426946 kcal.mol^{-1}

C	-5.23413	-3.77761	2.05230
Si	-6.12768	-2.15515	1.63686
C	-7.78709	-2.16161	2.55933
N	-6.32244	-1.91062	-0.09626
Yb	-5.31528	-0.47653	-1.37233
O	-4.83500	2.85114	-0.00519

Si	-3.30725	2.28991	0.02558
O	-2.74901	2.21939	1.57743
Si	-1.25394	2.05819	2.28270
O	-0.26002	3.26469	1.74732
Si	0.93704	3.52855	0.63465
O	0.29013	4.07634	-0.78176
Si	-1.01075	3.79504	-1.76359
O	-0.59910	2.72752	-2.95892
Si	-0.06758	1.16407	-2.92292
O	1.34554	1.07495	-2.06973
Si	1.91812	0.79360	-0.54131
O	3.52633	0.45382	-0.60589
C	-5.06641	-0.73057	2.30659
Si	-7.04216	-3.03207	-1.22243
C	-8.91727	-3.23503	-1.05734
C	-6.25013	-4.74984	-1.29850
C	-6.70009	-2.24723	-2.96638
O	-3.38441	0.71954	-0.60493
Si	-2.32371	-0.49885	-1.23466
O	-1.53468	-1.15377	0.06598
Si	-0.25524	-0.74845	1.04218
O	0.03275	-1.98711	2.07172
Si	0.05145	-3.67067	1.95399
N	-6.39975	1.43247	-1.92233
Si	-5.92830	2.06939	-3.51031
C	-7.31856	2.02755	-4.80482
O	-3.43670	-1.41851	-1.93025
O	-2.24821	3.15191	-0.88757
O	-1.48463	5.19107	-2.46675
Si	-0.98828	6.80464	-2.36561
Si	-7.98471	1.88461	-1.24128
C	-7.99334	1.44067	0.59879
C	-8.32849	3.74615	-1.38780
C	-9.41970	0.95119	-2.06488
O	-1.21682	0.20016	-2.23274
O	0.21207	0.69720	-4.46577
Si	-0.03482	-0.70972	-5.36424
C	-5.25134	3.83688	-3.44060
C	-4.53816	0.96335	-4.20817
O	-0.59279	0.59207	1.93295
O	1.08217	-0.48156	0.10651
O	-1.42764	2.18021	3.90449
Si	-2.58689	2.85354	4.93268
O	1.78186	2.12202	0.42215
O	1.94541	4.72361	1.14164
H	2.56852	4.46295	1.82630
H	-5.39572	2.45161	-0.73258
H	3.76752	-0.26165	-1.20123
H	0.99973	-4.16288	2.99221
H	-1.31557	-4.20489	2.21413
H	0.51182	-4.09418	0.59847
H	-2.97799	4.21258	4.45791
H	-3.78630	1.97017	4.99271
H	-1.94956	2.94316	6.27638
H	0.79918	-0.57717	-6.59135
H	0.39520	-1.90592	-4.58121
H	-1.47396	-0.83579	-5.73134
H	-1.12403	7.29645	-0.96423
H	0.42572	6.93650	-2.81955
H	-1.89285	7.56989	-3.26830
H	-10.36370	1.20515	-1.56924
H	-9.52247	1.19944	-3.12473
H	-9.28789	-0.13255	-1.98330
H	-9.26739	3.98530	-0.87541
H	-7.53356	4.33327	-0.91716
H	-8.42879	4.07777	-2.42605
H	-8.97273	1.66155	1.03754
H	-7.79957	0.37270	0.74333
H	-7.24032	2.01292	1.14946
H	-4.91051	4.14486	-4.43564
H	-6.01860	4.54590	-3.11626
H	-4.40363	3.92832	-2.75622
H	-6.92613	2.36936	-5.76944
H	-7.71764	1.01793	-4.94713
H	-8.15184	2.68523	-4.53954
H	-4.25687	1.36628	-5.18811
H	-3.62404	0.96025	-3.60643
H	-4.83881	-0.07688	-4.38765
H	-7.62327	-2.28912	3.63553
H	-8.33733	-1.22742	2.41284
H	-8.42784	-2.98379	2.22387
H	-4.96331	-0.81978	3.39377
H	-4.05410	-0.74815	1.88891
H	-5.50906	0.25168	2.10827
H	-4.99215	-3.81006	3.12078
H	-5.84883	-4.65524	1.82897
H	-4.29892	-3.86851	1.49118
H	-9.32594	-3.81302	-1.89366
H	-9.16030	-3.77313	-0.13509
H	-9.43058	-2.27015	-1.02118
H	-6.62845	-5.30997	-2.16120
H	-5.16224	-4.67411	-1.38788
H	-6.47528	-5.33455	-0.40161
H	-7.22641	-2.87709	-3.69111
H	-7.11514	-1.24009	-3.13582
H	-5.64585	-2.29062	-3.28430

TS_{Yb}

G = -2204.421702 kcal.mol^{-1}

C	-5.35971	-3.68242	2.27579
Si	-6.15161	-2.02272	1.80058
C	-7.83676	-1.92226	2.66877
N	-6.27135	-1.79802	0.05830
Yb	-5.24231	-0.36252	-1.19474
O	-4.96838	2.24917	0.17300
Si	-3.33233	2.15752	0.11901
O	-2.75284	1.99811	1.65243
Si	-1.24796	1.81507	2.33414
O	-0.29317	3.07953	1.86113
Si	0.82699	3.44541	0.69830
O	0.07326	3.94242	-0.68304
Si	-1.28615	3.76305	-1.60318
O	-1.09306	2.53765	-2.69227
Si	-0.21245	1.15997	-2.92313
O	1.20797	1.24766	-2.08433
Si	1.88120	0.84735	-0.62484
O	3.49095	0.55517	-0.79109
C	-5.03969	-0.64718	2.48840
Si	-6.97942	-2.93916	-1.06372
C	-8.85046	-3.16546	-0.86973
C	-6.16543	-4.64808	-1.11507
C	-6.65209	-2.17643	-2.81007
O	-3.09755	0.72873	-0.73228
Si	-2.24364	-0.63730	-1.34273
O	-1.46173	-1.31924	-0.04602
Si	-0.18042	-0.89176	0.91616
O	0.21095	-2.16092	1.87071
Si	-0.04872	-3.82900	1.80884
N	-6.39152	1.43404	-1.99764
Si	-5.86182	2.05897	-3.57550
C	-7.17436	1.91897	-4.94232
O	-3.49856	-1.45610	-1.90962
O	-2.60054	3.41622	-0.65087
O	-1.58994	5.15030	-2.40913
Si	-0.97133	6.72384	-2.36035
Si	-8.03714	1.84877	-1.43993
C	-8.18150	1.44850	0.40518
C	-8.42706	3.69505	-1.65597
C	-9.39031	0.85563	-2.33016
O	-1.10004	-0.14821	-2.43255
O	0.12423	1.02083	-4.51812
Si	0.09954	-0.23542	-5.64596
C	-5.29065	3.86436	-3.49208
C	-4.37212	1.03685	-4.17494
O	-0.56905	0.39155	1.87182
O	1.11608	-0.49628	-0.03259
O	-1.39921	1.81578	3.96046
Si	-2.35907	2.62790	5.08948
O	1.76739	2.11082	0.42846
O	1.76286	4.70866	1.17744
H	2.48023	4.47557	1.77425
H	-5.47953	2.20588	-0.70663
H	3.71326	-0.24247	-1.27992
H	0.84871	-4.42855	2.83544
H	-1.47203	-4.13635	2.12664
H	0.29645	-4.35684	0.45616
H	-2.88799	3.89639	4.50993
H	-3.48581	1.74074	5.49575
H	-1.49127	2.92124	6.26469
H	0.75363	0.29449	-6.87474
H	0.86279	-1.40919	-5.12742
H	-1.30560	-0.63591	-5.94021
H	-1.08778	7.27882	-0.98101
H	0.45491	6.72516	-2.79434
H	-1.79965	7.52058	-3.30759
H	-10.36986	1.12099	-1.91565
H	-9.42024	1.05232	-3.40493
H	-9.25720	-0.22147	-2.18758
H	-9.40726	3.91303	-1.21652
H	-7.68773	4.31976	-1.14459
H	-8.46398	4.00189	-2.70571
H	-9.20438	1.64386	0.74647
H	-7.96599	0.39164	0.59343
H	-7.50030	2.05400	1.00988
H	-4.87377	4.16935	-4.45871
H	-6.11488	4.54288	-3.25531
H	-4.51135	4.00933	-2.73825
H	-6.73922	2.25441	-5.89087
H	-7.51030	0.88599	-5.07862
H	-8.05491	2.53932	-4.75001
H	-4.09583	1.40001	-5.17171
H	-3.48671	1.16286	-3.54528
H	-4.57499	-0.03522	-4.27995
H	-7.71587	-2.06023	3.74939
H	-8.31595	-0.95260	2.50562
H	-8.52026	-2.69857	2.31016
H	-4.99825	-0.71049	3.58156
H	-4.00935	-0.74311	2.12773
H	-5.40515	0.35437	2.23812
H	-5.14390	-3.70055	3.35031
H	-6.01597	-4.53153	2.06013
H	-4.41871	-3.83804	1.73905
H	-9.26673	-3.72885	-1.71230
H	-9.07444	-3.72696	0.04343
H	-9.37207	-2.20640	-0.80466
H	-6.55013	-5.22875	-1.96137
H	-5.08100	-4.55583	-1.22823
H	-6.36409	-5.21999	-0.20408
H	-7.19407	-2.79869	-3.53020
H	-7.04398	-1.16061	-2.97542
H	-5.59808	-2.23641	-3.11956

$Yb(N(SiMe_3)_2)_3$@**ac-2**

G = -2204.471133 kcal.mol^{-1}

N	-4.04538	-1.60437	-0.22961
Yb	-2.66077	0.08988	-0.21683
O	-1.19812	-0.12748	-1.69484
Si	0.40355	-0.32665	-1.60230
O	0.92090	-1.85316	-2.04543
Si	2.09299	-2.70956	-1.22783
O	2.17997	-4.19921	-1.91849
Si	1.33421	-4.93492	-3.17691
O	-1.31413	0.15561	1.38974
Si	0.30159	0.07518	1.43926
O	0.87020	-1.19311	2.36041
Si	2.02754	-2.28841	1.87488
O	2.00903	-3.54287	2.93617
Si	1.50609	-3.70852	4.53527
N	-3.02889	2.53145	0.39386
O	1.00928	-0.19052	-0.04876
O	0.98475	1.52434	1.91854
Si	2.38394	2.13741	1.25882
O	2.24505	2.38253	-0.37460
Si	2.54148	1.70617	-1.85906
O	3.88273	0.73908	-1.83370
Si	4.58403	-0.68124	-1.38420
O	5.80703	-0.94014	-2.45796
O	1.24222	0.84849	-2.43895
O	2.82037	2.95464	-2.88969
Si	3.84309	3.16760	-4.21280
O	3.56483	-1.98005	-1.41015
O	1.73847	-2.92958	0.37584
O	5.20061	-0.51545	0.14514
Si	4.47687	-0.27097	1.61455
O	5.62695	-0.12004	2.78490

O	3.51950	-1.57760	1.93677
O	3.66744	1.16225	1.62248
O	2.62408	3.60720	1.95344
Si	3.90649	4.29476	2.80599
H	6.07454	-1.86134	-2.52653
H	-2.14880	2.44148	0.92005
H	6.12738	-0.92375	2.95338
H	5.16513	4.23147	2.00777
H	3.52838	5.71833	3.04167
H	4.09707	3.60119	4.11285
H	3.77692	1.99358	-5.13168
H	3.36102	4.38937	-4.91995
H	5.24697	3.37341	-3.75281
H	2.03089	-5.02212	5.00689
H	2.06173	-2.61158	5.38266
H	0.01693	-3.70065	4.61896
H	1.56196	-4.20803	-4.46060
H	1.87087	-6.32203	-3.28354
H	-0.12696	-4.98035	-2.87721
Si	-4.04644	-3.03631	0.80282
Si	-5.09242	-1.41227	-1.61285
Si	-4.30053	2.67070	1.70480
Si	-2.70565	3.90573	-0.78568
C	-6.94238	-1.41570	-1.19159
C	-4.68150	0.34022	-2.30432
C	-4.78405	-2.59616	-3.05840
C	-4.45161	-4.63154	-0.14691
C	-2.33296	-3.25132	1.58044
C	-5.32557	-2.88391	2.20143
H	-5.35541	-2.28226	-3.93957
H	-3.72278	-2.60562	-3.32677
H	-5.07936	-3.62093	-2.81774
H	-5.36646	0.54541	-3.13391
H	-4.84635	1.16095	-1.59100
H	-3.67389	0.41915	-2.74035
H	-7.55009	-1.19220	-2.07556
H	-7.25323	-2.39696	-0.81764
H	-7.17853	-0.67747	-0.41830
H	-4.37510	-5.48940	0.53097
H	-5.46825	-4.62931	-0.55463
H	-3.75254	-4.79580	-0.97263
H	-5.34873	-3.80073	2.80154
H	-5.09146	-2.05341	2.87510
H	-6.33278	-2.72010	1.80375
H	-2.33866	-4.09738	2.27683
H	-1.57553	-3.46043	0.81722
H	-2.01331	-2.36570	2.13846
C	-2.63215	5.55984	0.12687
C	-1.03765	3.54460	-1.56791
C	-4.05233	3.97694	-2.10309
C	-3.68353	3.78380	3.09735
C	-5.91127	3.31680	0.96838
C	-4.55006	0.93332	2.39587
H	-3.85102	4.84506	-2.74119
H	-4.04876	3.09231	-2.74480
H	-5.05592	4.10065	-1.68856
H	-0.79909	4.32807	-2.29563
H	-0.23025	3.53451	-0.82928
H	-1.02096	2.58748	-2.09749
H	-2.31718	6.33699	-0.57871
H	-3.59934	5.86426	0.53811
H	-1.90028	5.54003	0.94025
H	-6.68528	3.28505	1.74313
H	-5.83184	4.35287	0.62753
H	-6.26004	2.70310	0.13238
H	-4.38506	3.73845	3.93780
H	-2.70860	3.44792	3.46614
H	-3.59219	4.82936	2.79302
H	-5.29221	0.96955	3.20143
H	-4.92310	0.20922	1.66034
H	-3.62040	0.54494	2.82678

$Nd(N(SiMe_3)_2)_3$

G = -939.225261 kcal.mol^{-1}

Nd	-0.13562	-0.77944	-0.45335
N	-0.40812	-0.66443	1.85677
N	1.72093	0.31848	-1.33550
N	-2.07927	-0.76558	-1.73950
Si	-1.70729	0.16837	2.69660
Si	0.81114	-1.63291	2.64507
Si	2.32634	-0.55460	-2.72050
Si	2.49514	1.74383	-0.65969
Si	-2.56898	0.49857	-2.85744
Si	-2.93158	-2.27547	-1.53669
C	4.13776	-1.10344	-2.57228
C	1.27934	-2.16722	-2.84347
C	2.12199	0.34212	-4.37929
C	4.08013	1.33036	0.30627
C	2.96126	3.03316	-1.97627
C	1.27528	2.55989	0.54733
C	-4.41289	0.93981	-2.72339
C	-1.57087	2.06549	-2.45436
C	-2.22886	0.04492	-4.67274
C	-4.59456	-2.14339	-0.63477
C	-3.21790	-3.24095	-3.14619
C	-1.80787	-3.39136	-0.43814
C	2.08973	-0.65372	3.64611
C	0.12560	-3.00872	3.75947
C	1.78364	-2.52518	1.23928
C	-1.09629	1.19184	4.17675
C	-2.53314	1.36142	1.46807
C	-3.04522	-1.01829	3.34187
H	4.41595	-1.75562	-3.40795
H	4.81141	-0.24029	-2.59076
H	4.31936	-1.64798	-1.64018
H	1.62123	-2.73003	-3.71906
H	1.42179	-2.84950	-1.99149
H	0.20623	-1.99139	-3.00990
H	2.39235	-0.31351	-5.21494
H	1.08955	0.67302	-4.52719
H	2.76303	1.22744	-4.42996
H	4.48661	2.22958	0.78344
H	3.89012	0.59203	1.09186
H	4.85592	0.92340	-0.34984
H	1.75438	3.39233	1.07461
H	0.40699	2.96597	0.01644
H	0.92094	1.85249	1.30661
H	3.33333	3.94667	-1.49831
H	3.75186	2.66661	-2.63975
H	2.09959	3.30385	-2.59466
H	-1.77204	2.84726	-3.19536
H	-1.84515	2.46869	-1.47303
H	-0.49054	1.87833	-2.46414
H	-2.46051	0.88962	-5.33173
H	-1.17906	-0.22289	-4.83016
H	-2.83874	-0.80442	-4.99608
H	-4.64340	1.80082	-3.36130
H	-5.05479	0.11323	-3.04677
H	-4.68837	1.19932	-1.69632
H	-5.01526	-3.13777	-0.44651
H	-4.48757	-1.63162	0.32637
H	-5.32144	-1.58164	-1.22934
H	-3.63314	-4.23286	-2.93410
H	-3.92850	-2.72038	-3.79651
H	-2.28796	-3.37503	-3.70786
H	-2.32472	-4.34543	-0.28582
H	-0.85164	-3.65932	-0.91317
H	-1.62891	-2.99314	0.57133
H	2.56275	-3.14011	1.70346
H	1.16801	-3.23414	0.66480
H	2.31680	-1.84849	0.55533
H	2.89579	-1.30886	3.99561
H	2.53639	0.14634	3.04810
H	1.63065	-0.19238	4.52575
H	0.93247	-3.66377	4.10748
H	-0.36317	-2.59241	4.64645
H	-0.60899	-3.62575	3.23225
H	-1.91225	1.80215	4.58058
H	-0.73307	0.55330	4.98905
H	-0.28341	1.86516	3.88714
H	-3.42215	1.81782	1.91746
H	-1.85404	2.17526	1.19037
H	-2.85726	0.84935	0.55402
H	-3.87332	-0.45840	3.79146
H	-3.45675	-1.63398	2.53563
H	-2.64820	-1.69419	4.10567

TS_{Nd}

G = -2198.507445 kcal.mol^{-1}

C	-5.42854	-4.02155	2.05927
Si	-6.21727	-2.34727	1.65059
C	-7.77901	-2.14370	2.70523
N	-6.48531	-2.07961	-0.05260
Nd	-5.25345	-0.39304	-0.98753
O	-4.95695	2.01023	0.08224
Si	-3.31919	2.14768	0.12777
O	-2.81429	2.13333	1.70099
Si	-1.30297	1.93492	2.36737
O	-0.35718	3.21217	1.90498
Si	0.74130	3.59407	0.72568
O	-0.03579	4.00572	-0.67003
Si	-1.37628	3.76618	-1.60470
O	-1.14222	2.48862	-2.62600
Si	-0.17956	1.16242	-2.84213
O	1.21053	1.33186	-1.96560
Si	1.91791	1.00711	-0.50564
O	3.53852	0.78391	-0.67974
C	-4.96249	-0.99547	2.16926
Si	-7.22188	-3.08515	-1.27025
C	-9.10982	-3.17690	-1.13414
C	-6.53171	-4.84664	-1.36564
C	-6.77894	-2.24138	-2.94251
O	-2.81930	0.74385	-0.61336
Si	-2.10210	-0.66316	-1.24736
O	-1.27195	-1.36347	0.01804
Si	-0.09258	-0.78726	1.02973
O	0.32976	-1.97383	2.07545
Si	-0.03467	-3.61654	2.21900
N	-6.43192	1.56778	-1.92259
Si	-5.90579	2.15488	-3.51301
C	-7.22445	2.00726	-4.87099
O	-3.38483	-1.48607	-1.74541
O	-2.71559	3.45885	-0.67086
O	-1.68922	5.12030	-2.46404
Si	-0.80500	6.50239	-2.87339
Si	-8.06773	1.93250	-1.32445
C	-8.16857	1.31630	0.46885
C	-8.44057	3.79291	-1.33463
C	-9.44520	1.05156	-2.28959
O	-0.99506	-0.20797	-2.39750
O	0.20591	1.06262	-4.43083
Si	0.32706	-0.19594	-5.54911
C	-5.33187	3.95853	-3.45449
C	-4.43138	1.08979	-4.07405
O	-0.63382	0.52011	1.87239
O	1.23934	-0.35375	0.14815
O	-1.44209	1.89586	3.99512
Si	-1.98500	2.96019	5.18910
O	1.75165	2.30276	0.50216
O	1.61693	4.91390	1.16752
H	2.38904	4.71780	1.70655
H	-5.54859	2.07497	-0.81590
H	3.79325	-0.07547	-1.02795
H	0.80877	-4.13201	3.33358
H	-1.47853	-3.79822	2.54445
H	0.29487	-4.33443	0.95332
H	-2.74490	4.09257	4.58587
H	-2.86057	2.18932	6.11800
H	-0.79517	3.47167	5.92737
H	1.02064	0.36865	-6.74063
H	1.12575	-1.32172	-4.98026
H	-1.03142	-0.68025	-5.92711
H	-0.70195	7.40376	-1.69038
H	0.55722	6.12493	-3.34925
H	-1.56438	7.17259	-3.96566
H	-10.40537	1.21930	-1.78798
H	-9.53876	1.41741	-3.31524
H	-9.28157	-0.02989	-2.33198
H	-9.40478	3.98585	-0.85081
H	-7.67344	4.35442	-0.79213
H	-8.49724	4.19339	-2.35209
H	-9.16968	1.50841	0.87083
H	-8.00323	0.23333	0.53317
H	-7.44437	1.82362	1.11371
H	-4.94650	4.26753	-4.43270

H	-6.15477	4.63031	-3.19220
H	-4.53408	4.10792	-2.72171
H	-6.77679	2.27876	-5.83404
H	-7.61406	0.98836	-4.95988
H	-8.07005	2.68181	-4.70391
H	-4.09865	1.43943	-5.05811
H	-3.56302	1.17200	-3.41270
H	-4.68215	0.02847	-4.19296
H	-7.55405	-2.27821	3.76925
H	-8.22378	-1.15245	2.57512
H	-8.53404	-2.88713	2.42818
H	-4.77074	-1.06981	3.24546
H	-3.97984	-1.12475	1.69340
H	-5.31284	0.03374	2.00999
H	-5.14593	-4.06492	3.11721
H	-6.11789	-4.85008	1.86800
H	-4.52896	-4.18706	1.45848
H	-9.54386	-3.72889	-1.97525
H	-9.40246	-3.69183	-0.21276
H	-9.55778	-2.17903	-1.11159
H	-6.92210	-5.36723	-2.24748
H	-5.43952	-4.83214	-1.43338
H	-6.80821	-5.43471	-0.48504
H	-7.29301	-2.77597	-3.74881
H	-7.11668	-1.19784	-3.03493
H	-5.70784	-2.31152	-3.18270

$Nd(N(SiMe_3)_2)_3$@**ac-1**

G = -2198.512704 kcal.mol^{-1}

O	-1.59972	1.45530	4.07928
Si	-1.32503	1.49937	2.47236
O	-0.47330	0.17716	1.99746
Si	-0.05267	-0.96011	0.87109
O	1.20596	-0.38675	-0.03466
Si	1.86773	1.04181	-0.54412
O	1.16377	1.48670	-1.97496
Si	-0.24763	1.33642	-2.82481
O	-0.97103	-0.11360	-2.48428
Si	-2.11909	-0.69388	-1.43130
Nd	-5.30902	-0.48948	-1.47522
N	-6.49543	-1.86235	-0.00143
Si	-0.97540	2.25717	5.43357
O	-2.82266	1.50937	1.72783
Si	-3.32225	1.86028	0.20290
O	-4.99405	1.72335	0.13053
O	-0.52559	2.88386	2.05856
Si	0.60483	3.43029	0.98424
O	1.66977	2.23168	0.58325
O	-2.98308	0.68650	-0.89327
O	-2.76565	3.31413	-0.31180
Si	-1.49942	3.76769	-1.30410
O	-1.25240	2.60091	-2.44932
O	-3.31360	-1.57752	-2.00839
O	-1.34227	-1.31809	-0.10064
O	-0.13941	3.97344	-0.39273
O	1.38712	4.65257	1.75343
O	-1.91932	5.18120	-2.00146
Si	-1.71681	5.89831	-3.52113
O	0.43026	-2.31357	1.65014
Si	-0.06955	-3.92982	1.64470
O	3.49379	0.87823	-0.72486
O	0.08180	1.42645	-4.42495
Si	0.41720	0.30387	-5.64288
N	-6.40308	0.49416	-3.26935
H	2.18064	4.97122	1.31318
H	-5.50434	1.90795	0.92861
H	3.77571	0.07455	-1.17131
H	0.85057	-4.64557	2.57198
H	-1.47542	-4.03529	2.12792
H	0.04449	-4.49633	0.26962
H	-1.47426	3.66187	5.45670
H	-1.47671	1.51112	6.62059
H	0.51503	2.24094	5.40021
H	0.96962	1.08199	-6.78657
H	1.42717	-0.68656	-5.16457
H	-0.83163	-0.39953	-6.04797
H	-2.64098	5.26642	-4.50308
H	-2.04849	7.33929	-3.34467
H	-0.30310	5.74680	-3.97320
Si	-5.64802	0.64255	-4.85831
Si	-7.96120	1.23752	-2.94554
Si	-7.07439	-3.25827	-0.89498
Si	-6.60696	-1.81940	1.74958
C	-5.18253	-2.75905	2.58674
C	-6.50394	-0.02577	2.40195
C	-8.24202	-2.51913	2.42470
C	-8.96451	-3.33770	-1.05597
C	-6.38702	-3.11199	-2.67755
C	-6.45758	-4.92672	-0.23006
C	-8.05316	3.06483	-3.46337
C	-9.42270	0.31669	-3.73637
C	-8.25798	1.21863	-1.05869
C	-4.57117	2.20711	-4.95608
C	-4.53324	-0.85921	-5.19464
C	-6.88052	0.70528	-6.30708
H	-10.37453	0.75447	-3.41404
H	-9.38678	0.36382	-4.82847
H	-9.42498	-0.73984	-3.44869
H	-9.01505	3.49820	-3.16570
H	-7.25937	3.64530	-2.98133
H	-7.95475	3.19747	-4.54523
H	-9.28395	1.54660	-0.85683
H	-8.14987	0.22547	-0.60398
H	-7.59165	1.92292	-0.54759
H	-4.09636	2.29940	-5.93969
H	-5.17095	3.10706	-4.78627
H	-3.77520	2.19098	-4.20359
H	-6.32391	0.77503	-7.24907
H	-7.49153	-0.20191	-6.35072
H	-7.55362	1.56697	-6.26101
H	-3.97096	-0.69396	-6.12105
H	-3.80729	-1.06023	-4.39987
H	-5.13397	-1.76489	-5.33116
H	-8.26235	-2.42819	3.51692
H	-9.10543	-1.97642	2.02667
H	-8.36953	-3.57895	2.18256
H	-6.80351	-0.00844	3.45546
H	-5.47875	0.35850	2.36341
H	-7.18416	0.64252	1.86078
H	-5.22917	-2.65592	3.67701
H	-5.21376	-3.82651	2.34819
H	-4.21154	-2.37495	2.25511
H	-9.26169	-4.14403	-1.73635
H	-9.44522	-3.52189	-0.09086
H	-9.36320	-2.39821	-1.45191
H	-6.78283	-5.74150	-0.88712
H	-5.36410	-4.94609	-0.18320
H	-6.84309	-5.14011	0.77231
H	-6.76414	-3.97328	-3.24064
H	-6.73550	-2.22878	-3.23190
H	-5.29186	-3.17220	-2.73355

$Nd(N(SiMe_3)_2)_3$@**ac-2**

G = **-**2198,550396 kcal.mol^{-1}

N	-2.34803	-1.81772	6.75263
Nd	-3.55738	-1.71322	4.77900
O	-5.41146	-2.93618	4.81554
Si	-6.00702	-4.00321	3.76146
O	-6.26170	-5.52123	4.41270
Si	-5.92315	-6.95529	3.64019
O	-6.16168	-8.16653	4.72613
Si	-6.54970	-8.17354	6.36638
O	-2.76677	-2.79724	3.00372
Si	-3.46935	-3.84576	1.99646
O	-2.64303	-5.28768	1.84700
Si	-3.34457	-6.79760	1.83350
O	-2.13776	-7.90829	1.93462
Si	-0.45669	-7.80772	1.88672
N	-3.99598	0.32989	3.05443
O	-4.99448	-4.33132	2.46988
O	-3.74919	-3.15566	0.49470
Si	-5.13929	-3.35097	-0.39475
O	-6.48353	-2.90691	0.46811
Si	-7.71767	-3.53677	1.38063
O	-8.07178	-5.09104	0.94500
Si	-7.71113	-6.69773	0.99331
O	-9.14992	-7.48584	0.83927
O	-7.39348	-3.44971	3.00556
O	-9.03298	-2.59595	1.08601
Si	-10.68258	-2.91007	0.93727
O	-6.98084	-7.18646	2.39075
O	-4.35559	-7.05919	3.11705
O	-6.72383	-7.06790	-0.28450
Si	-5.22371	-6.53081	-0.73474
O	-4.81906	-7.15991	-2.20275
O	-4.13036	-7.02876	0.39746
O	-5.25696	-4.89931	-0.95845
O	-5.03251	-2.32900	-1.67804
Si	-4.92115	-2.56150	-3.34480
H	-9.13664	-8.38931	1.16853
H	-4.23483	-0.37853	2.34991
H	-4.62669	-8.10206	-2.18872
H	-6.13384	-3.25959	-3.86116
H	-4.82990	-1.19838	-3.94411
H	-3.69812	-3.34479	-3.68573
H	-11.15538	-3.80278	2.03534
H	-11.36803	-1.58828	1.03003
H	-10.97200	-3.53485	-0.38586
H	0.04552	-9.21142	1.91594
H	-0.00144	-7.13747	0.63276
H	0.05979	-7.06215	3.07118
H	-7.89822	-7.57484	6.59132
H	-6.55935	-9.60471	6.78492
H	-5.52828	-7.42384	7.15517
Si	-0.82824	-2.67986	6.97505
Si	-3.22029	-1.01866	8.03507
Si	-2.37628	0.96106	2.47436
Si	-5.49433	1.37515	3.15385
C	-2.24757	0.37589	8.87847
C	-4.75999	-0.20273	7.21296
C	-3.93019	-2.16162	9.36983
C	-0.67485	-3.53075	8.66691
C	-0.69930	-4.03468	5.65043
C	0.66649	-1.51973	6.79123
H	-4.57502	-1.59873	10.05449
H	-4.52997	-2.95860	8.91839
H	-3.14206	-2.63051	9.96526
H	-5.29186	0.36563	7.98379
H	-4.52304	0.53288	6.43011
H	-5.49106	-0.92908	6.83007
H	-2.86458	0.89358	9.62142
H	-1.36930	-0.02090	9.39836
H	-1.89524	1.11558	8.15190
H	0.26715	-4.08923	8.71248
H	-0.66856	-2.81358	9.49464
H	-1.49148	-4.23951	8.83538
H	1.60379	-2.06408	6.95299
H	0.70906	-1.07697	5.79071
H	0.62495	-0.70148	7.51780
H	0.27050	-4.53999	5.72159
H	-1.47521	-4.79515	5.79439
H	-0.79173	-3.65403	4.62731
C	-5.91379	2.03925	1.43611
C	-6.89841	0.27722	3.76142
C	-5.22362	2.79549	4.36869
C	-2.22039	0.54085	0.64682
C	-2.19049	2.81505	2.77127
C	-1.03586	0.07296	3.47087
H	-6.20443	3.19176	4.65402
H	-4.72341	2.47737	5.28799
H	-4.64932	3.61636	3.93405
H	-7.83037	0.85382	3.74139
H	-7.05091	-0.60595	3.13502
H	-6.75264	-0.06535	4.79042
H	-6.83331	2.63326	1.48074
H	-5.12437	2.68106	1.03294
H	-6.08524	1.22244	0.72732
H	-1.19320	3.10859	2.42390
H	-2.91824	3.41317	2.21594
H	-2.25746	3.07773	3.83078
H	-1.22175	0.80170	0.28033
H	-2.37220	-0.52950	0.47345
H	-2.95199	1.08993	0.04593
H	-0.05639	0.47978	3.19514
H	-1.13369	0.22169	4.55426

H	-1.00669	-0.99901	3.24439

[La]@**ac-1**
G = -1704,713071 kcal. mol^{-1}

O	-0.44130	1.11614	4.14750
Si	0.64173	0.47922	5.28057
Si	-0.52394	1.18761	2.51936
O	-2.05533	1.75319	2.16569
Si	-2.72746	2.33839	0.78433
O	-2.99961	1.19868	-0.35680
Si	-2.81521	-0.33330	-1.10305
O	-4.32147	-0.74926	-1.40037
O	0.57473	2.26512	1.92478
Si	1.56725	2.51980	0.63080
O	0.76814	3.38284	-0.53756
Si	-0.75197	3.67943	-1.09898
O	-0.78589	5.19627	-1.70633
Si	-1.97418	6.37558	-1.93586
O	-0.28464	-0.29975	1.85695
Si	-0.49311	-1.41004	0.64526
O	-2.00738	-1.29151	-0.00479
O	2.84597	3.37019	1.21391
O	2.07837	1.08796	-0.01781
Si	1.62072	-0.00070	-1.17136
O	3.02322	-0.64943	-1.73332
O	-0.30395	-2.90317	1.28959
Si	-1.27188	-4.28834	1.33197
O	0.65578	-1.17491	-0.51750
O	-1.85587	3.58525	0.15749
O	-4.31938	2.77197	1.09231
O	-1.17283	2.58400	-2.25929
Si	-0.73782	1.10918	-2.88213
O	-0.74688	1.19568	-4.51817
Si	-1.80395	0.63331	-5.71051
O	0.80104	0.74803	-2.39884
O	-1.80214	-0.06073	-2.39686
H	3.56310	3.50690	0.58763
H	-4.53785	3.10576	1.96828
H	2.91807	-1.31708	-2.41741
H	-0.47370	-5.32518	2.04444
H	-2.53442	-4.01260	2.07695
H	-1.58578	-4.74408	-0.05298
H	0.65275	1.41503	6.43919
H	0.15535	-0.86334	5.70866
H	2.00631	0.36656	4.68963
H	-1.37543	1.27971	-6.98255
H	-1.69925	-0.84963	-5.82992
H	-3.20774	1.02034	-5.38589
H	-2.15072	7.15216	-0.67484
H	-1.48534	7.26693	-3.02381
H	-3.26726	5.74138	-2.32599
La	-5.75031	0.91728	-0.44990
N	-6.91466	2.21585	-1.94856
N	-7.04220	0.22353	1.32794
H	-6.71568	2.33405	-2.93936
H	-7.77313	2.73334	-1.77294
H	-6.86663	-0.58302	1.92325
H	-7.94368	0.59388	1.62094

TS_{La}
G = -1704.72287 kcal. mol^{-1}

O	-0.52079	0.36238	3.94250
Si	-0.65303	0.65501	2.33780
O	-2.15670	1.29443	2.04690
Si	-2.85809	2.06671	0.76153
O	-4.41592	2.45139	1.03036
La	-5.62139	0.99349	-0.68294
N	-6.80679	2.27734	-2.15077
Si	0.27115	1.12583	5.22548
O	0.49967	1.74359	1.86977
Si	1.48752	2.10384	0.59785
O	0.70886	3.08072	-0.48772
Si	-0.80864	3.47369	-1.00942
O	-1.22834	2.50776	-2.28408
Si	-0.81394	1.09435	-3.04264
O	0.70735	0.63952	-2.58663
Si	1.50492	-0.23618	-1.43073
O	2.89695	-0.85634	-2.05009
O	-0.46668	-0.77718	1.54370
Si	-0.64604	-1.77048	0.23107
O	-2.14395	-1.58344	-0.44364
Si	-2.89105	-0.45367	-1.40169
O	-4.44296	-0.74527	-1.70444
O	1.97612	0.72546	-0.17592
O	2.78271	2.87395	1.25543
O	0.51700	-1.45121	-0.89634
O	-0.48622	-3.32646	0.71340
Si	-0.44086	-4.12181	2.20025
O	-1.90446	3.31578	0.23471
O	-2.98888	1.00166	-0.52724
O	-0.80562	5.03594	-1.50126
Si	-1.70264	6.40464	-1.08546
O	-1.91590	-0.09941	-2.70332
O	-0.78937	1.33923	-4.66381
Si	-1.90930	1.10700	-5.90396
N	-6.21742	1.12542	1.78217
H	3.49164	3.07296	0.63664
H	-5.23460	1.87108	1.62307
H	2.77787	-1.44483	-2.80136
H	0.79906	-3.75560	2.94413
H	-1.64135	-3.77071	3.01469
H	-0.44149	-5.57982	1.89404
H	-0.09752	2.57041	5.27909
H	-0.18966	0.43482	6.46275
H	1.74710	0.97979	5.07524
H	-1.43218	1.91483	-7.06137
H	-1.96521	-0.33599	-6.27728
H	-3.26387	1.57181	-5.48172
H	-1.47984	6.75521	0.34711
H	-1.21282	7.50419	-1.96335
H	-3.15535	6.16522	-1.32867
H	-6.83270	2.17725	-3.16306
H	-7.34392	3.11449	-1.93560
H	-6.02079	0.38252	2.44868
H	-7.02267	1.62610	2.14999

[La]@**ac-2**
G = -1704,757702 kcal. mol^{-1}

N	-2.33012	-1.19848	6.73207
La	-3.36306	-2.33497	5.01206
O	-2.16720	-3.63997	3.55412
Si	-3.05409	-4.44887	2.47706
O	-4.67053	-4.46187	2.90599
Si	-5.89559	-4.23910	4.02332
O	-7.05587	-3.41738	3.13228
Si	-7.11079	-3.12879	1.50614
O	-8.12032	-1.85926	1.24496
Si	-9.73607	-1.73092	0.76965
N	-4.23841	-0.65464	3.07920
O	-5.38262	-3.38887	5.29376
O	-6.44245	-5.77293	4.37859
Si	-6.44740	-7.08719	3.36200
O	-7.48019	-6.79832	2.10267
Si	-7.76141	-6.09283	0.63744
O	-6.66781	-6.67662	-0.46134
Si	-5.09517	-6.29534	-0.81298
O	-4.10039	-7.07118	0.25166
Si	-3.63051	-7.29948	1.82178
O	-4.93569	-7.46521	2.81810
O	-7.02270	-8.37461	4.20111
Si	-7.51638	-8.58579	5.80084
O	-3.08495	-3.68946	0.98053
Si	-4.38625	-3.32785	0.02850
O	-4.92733	-4.65374	-0.79010
O	-2.63832	-6.05089	2.28691
O	-3.92225	-2.17483	-1.04571
Si	-3.58337	-2.18326	-2.70047
O	-5.61434	-2.64951	0.93701
O	-7.66192	-4.44574	0.67812
O	-9.29805	-6.43589	0.15685
O	-4.71610	-6.76878	-2.34339
O	-2.76144	-8.68968	1.88315
Si	-1.20294	-9.06808	2.40650
H	-9.56322	-7.35023	0.29301
H	-4.70615	-1.22696	2.36947
H	-4.52434	-7.70703	-2.43199
H	-4.83413	-2.40432	-3.48182
H	-3.02300	-0.83662	-3.01064
H	-2.58227	-3.23937	-3.02657
H	-10.59271	-2.66038	1.56106
H	-10.13295	-0.31854	1.03696
H	-9.86687	-2.02766	-0.68576
H	-1.07474	-10.54856	2.28857
H	-0.18592	-8.40155	1.54177
H	-1.01040	-8.65292	3.82672
H	-8.70337	-7.73236	6.09911
H	-7.88142	-10.02494	5.93415
H	-6.40572	-8.25452	6.74055
H	-1.33446	-1.00702	6.82597
H	-2.75008	-0.89054	7.60695
H	-3.50431	-0.14836	2.58793
H	-4.91964	0.04366	3.36997

[La]@**c-1**
G = -1709,828719 kcal. mol^{-1}

O	-0.36281	0.83707	4.11266
Si	0.83558	1.03769	5.28995
Si	-0.44267	1.04338	2.49519
O	-1.92435	1.73807	2.17101
Si	-2.55962	2.46336	0.83791
O	-2.89908	1.40488	-0.36783
Si	-2.81788	-0.08420	-1.21470
O	-4.34805	-0.35941	-1.55481
O	0.74781	2.07210	1.98977
Si	1.74778	2.33980	0.70330
O	1.01037	3.33203	-0.40076
Si	-0.47762	3.76979	-0.95612
O	-0.40229	5.32192	-1.46222
Si	-1.14648	6.22477	-2.68218
O	-0.31484	-0.40488	1.72896
Si	-0.59380	-1.43128	0.46159
O	-2.09394	-1.17351	-0.18402
O	3.08560	3.05729	1.33146
O	2.15360	0.91897	-0.03769
Si	1.62708	-0.06510	-1.25391
O	2.98305	-0.78054	-1.84852
O	-0.50804	-2.97158	1.00844
Si	-1.61158	-4.24979	1.08168
O	0.57449	-1.20763	-0.68578
O	-1.59139	3.67316	0.28511
O	-4.09667	3.00826	1.19089
Si	-4.74538	3.78920	2.57643
O	-0.96355	2.78489	-2.19236
Si	-0.63061	1.31906	-2.89600
O	-0.63203	1.51265	-4.52343
Si	-1.62187	0.93898	-5.76686
O	0.87618	0.82256	-2.43338
O	-1.77471	0.19925	-2.48287
H	3.80853	3.18579	0.71022
La	-5.62899	1.39050	-0.54396
H	2.82679	-1.47687	-2.49310
H	-0.89879	-5.37029	1.75694
H	-2.81167	-3.85373	1.87423
H	-2.02060	-4.65720	-0.29352
H	0.33349	0.34986	6.51185
H	2.11515	0.42032	4.83710
H	1.03427	2.49018	5.56101
H	-1.14414	1.60186	-7.01276
H	-1.48841	-0.54135	-5.89231
H	-3.04514	1.30202	-5.50666
H	-0.96377	7.65640	-2.31469
H	-0.48952	5.94072	-3.99014
H	-2.59937	5.89299	-2.75851
H	-6.07351	4.30775	2.15513
H	-4.86197	2.81337	3.69076
H	-3.83219	4.90876	2.94325
N	-6.60610	2.91546	-1.96089
N	-6.99055	0.81956	1.22922
H	-6.89167	0.01290	1.84165
H	-7.85504	1.27737	1.51033
H	-7.41505	3.49818	-1.75586
H	-6.36179	3.10894	-2.92936

[La]@**abc-1**,
G = -1781,165567 kcal. mol^{-1}

O	0.19364	0.63862	0.18037
Si	-0.59604	0.05542	-1.12404

O	-2.02257	-0.70333	-0.71851
La	-2.80039	-3.24326	-0.16308
N	-1.45952	-3.88200	1.60178
Si	0.13761	1.99559	1.18597
O	-0.93134	1.29359	-2.16870
Si	-1.28742	1.49468	-3.77020
O	-2.89271	1.19981	-4.05625
Si	-4.04595	0.21249	-3.39275
O	-3.57500	-1.38003	-3.58256
Si	-3.16393	-2.26443	-4.93530
O	-2.66336	-3.76123	-4.47547
Si	-2.08349	-4.47936	-3.07486
O	-1.13345	-5.73959	-3.57104
H	-0.85314	-5.68101	-4.48908
O	0.38059	-1.08297	-1.81957
Si	0.29503	-2.47334	-2.71430
O	-1.09644	-3.28055	-2.29309
O	-0.91751	3.06162	-4.10253
O	-0.37017	0.48396	-4.70729
Si	-0.39753	-1.02316	-5.37162
O	-1.94320	-1.48712	-5.75983
O	1.62604	-3.38062	-2.42341
Si	2.99566	-3.19810	-1.44851
O	0.25306	-2.14605	-4.33695
Si	-3.61360	-0.12001	-0.36178
O	-4.30917	-1.44906	0.18391
O	-4.23128	0.52198	-1.78461
O	-3.46171	1.16921	0.67165
O	-5.44270	0.52895	-4.19294
Si	-7.07515	0.37002	-3.79002
O	0.51991	-0.91450	-6.73367
O	-3.14442	-4.79399	-1.92373
O	-4.44885	-2.38900	-5.94799
Si	-4.65926	-2.20744	-7.61288
N	-5.00522	-4.66581	0.44457
H	-3.71267	2.00867	0.27388
H	-0.97901	3.30507	-5.03087
H	0.70782	-1.75293	-7.16508
H	3.75682	-1.98247	-1.85856
H	2.59948	-3.09417	-0.01533
H	3.82246	-4.41773	-1.66846
H	-0.44887	1.59804	2.49583
H	1.54515	2.45014	1.37515
H	-0.66744	3.08350	0.56081
H	-4.42024	-0.79246	-8.01746
H	-3.72533	-3.10727	-8.35340
H	-6.06911	-2.59323	-7.90090
H	-7.50529	1.53616	-2.96504
H	-7.82836	0.35047	-5.07529
H	-7.31083	-0.89654	-3.03727
H	-5.09571	-5.25303	-0.38210
H	-5.82388	-4.06629	0.50148
H	-5.00127	-5.26752	1.26209
H	-1.33415	-3.38925	2.48342
H	-0.86523	-4.70638	1.65559

[La]@**bc-1**

G = -1786,283861 kcal. mol^{-1}

O	0.14519	0.60798	0.20467
Si	-0.64451	0.00403	-1.16155
Si	-0.07523	0.64636	1.82196
O	-0.76967	-0.76883	2.32169
Si	-0.94879	-1.65380	3.70749
O	-1.29531	-3.18130	3.20751
O	1.40736	0.87980	2.51336
Si	2.10852	1.51712	3.87164
O	3.64994	1.94353	3.52649
Si	4.61263	1.91620	2.13713
O	-1.04398	1.91780	2.29769
Si	-2.76150	2.14619	2.30873
O	-3.38878	1.10940	3.46969
Si	-2.84042	0.45706	4.88093
O	-4.08845	0.24653	5.92467
Si	-5.54363	1.06135	6.18686
O	2.14589	0.41516	5.10319
Si	1.21613	-0.78737	5.76645
O	2.17653	-1.86639	6.55416
O	1.20602	2.83289	4.34409
Si	0.96802	3.68139	5.83074
O	-0.01199	4.85703	5.36987
O	0.12541	-0.11377	6.82017
Si	-0.71261	1.32259	6.87882
O	-1.64122	1.30670	8.23089
Si	-1.66835	0.36581	9.63231
O	0.44794	-1.65934	4.59609
O	0.33635	2.58659	6.93071
O	-1.66743	1.46246	5.51758
O	2.45496	4.09790	6.41278
Si	3.21859	3.95408	7.90520
O	-3.35398	1.59484	0.86003
O	-2.85807	3.70827	2.62255
O	-2.18567	-1.04235	4.62502
H	-3.89151	0.80125	0.94512
H	-1.25927	-3.84932	3.89845
H	2.81230	-1.47268	7.15892
H	4.80491	0.51077	1.67539
H	3.98476	2.72813	1.05603
H	5.92175	2.50781	2.53168
H	-1.16890	1.15135	-1.95317
H	0.37188	-0.74133	-1.95858
H	-1.75354	-0.91190	-0.77013
H	-2.00228	-1.04965	9.30385
H	-0.34449	0.42537	10.32021
H	-2.72168	0.95205	10.50786
H	-6.54215	0.65702	5.15464
H	-6.01776	0.65562	7.53962
H	-5.33687	2.53843	6.13758
La	-0.65385	4.46046	3.13686
H	-2.30079	6.70001	4.70556
H	4.50578	4.69849	7.79974
H	2.38026	4.54382	8.99094
H	3.49640	2.52015	8.21897
N	-2.33726	6.47888	3.71412
N	0.56651	5.46730	1.45859
H	-3.24093	6.05509	3.51425
H	-2.27416	7.34999	3.19685
H	0.34560	5.47516	0.46509
H	1.43967	5.98116	1.55441

[La]@**b-1**

G = -1791,402492 kcal.mol^{-1}

O	0.09460	0.72485	0.23535
Si	0.69287	2.23885	0.69215
Si	-0.64146	0.12139	-1.09409
O	0.34855	-1.02578	-1.75861
Si	0.32347	-2.39352	-2.69096
O	0.32931	-2.03126	-4.30313
Si	-0.31548	-0.92249	-5.35611
O	0.63339	-0.80723	-6.69522
O	-2.06957	-0.63822	-0.70150
Si	-3.68700	-0.10495	-0.41331
O	-3.60852	1.15284	0.65261
O	-0.93828	1.35393	-2.15560
Si	-1.27508	1.57102	-3.76038
O	-0.32532	0.58554	-4.69208
La	-2.85107	-3.22833	-0.25390
N	-5.08629	-4.63785	0.25084
N	-1.58704	-3.89411	1.55624
Si	-2.02065	-4.41751	-3.15131
O	-3.11217	-4.76995	-2.03857
O	-1.06882	-3.23119	-2.32763
O	-4.39002	-1.46110	0.05673
O	-2.86908	1.25683	-4.08044
Si	-4.03000	0.25423	-3.45425
O	-5.40635	0.56259	-4.29185
Si	-7.04926	0.38105	-3.94698
O	-0.91843	3.14701	-4.06161
O	-3.53568	-1.33208	-3.64624
Si	-3.08771	-2.19422	-5.00239
O	-4.34371	-2.30656	-6.05199
Si	-4.50666	-2.08278	-7.71756
O	-4.26028	0.54324	-1.85023
O	-2.60365	-3.69768	-4.54726
O	-1.84680	-1.40235	-5.77877
O	-1.00588	-5.61915	-3.65081
O	1.65589	-3.28584	-2.36451
Si	2.98631	-3.10069	-1.33810
Si	-0.75015	-6.40910	-5.11464
Si	-4.47392	2.58881	0.82630
H	-1.01471	3.41760	-4.97941
H	0.85655	-1.64842	-7.10447
H	3.74846	-1.87163	-1.70482
H	2.53646	-3.01740	0.08069
H	3.83492	-4.30810	-1.54063
H	1.23463	2.06826	2.06925
H	1.78041	2.66016	-0.23792
H	-0.40015	3.25198	0.69050
H	-4.24678	-0.66031	-8.08073
H	-3.56020	-2.97237	-8.45389
H	-5.91142	-2.44973	-8.05194
H	-7.52565	1.54253	-3.14148
H	-7.75651	0.34654	-5.25788
H	-7.29318	-0.88723	-3.19945
H	-5.16418	-5.21496	-0.58394
H	-5.89079	-4.01775	0.28706
H	-5.12339	-5.24681	1.06208
H	-1.49129	-3.40955	2.44610
H	-1.00147	-4.72357	1.62548
H	-4.16553	3.10909	2.18901
H	-4.04657	3.58171	-0.20196
H	-5.94107	2.33879	0.70186
H	0.21147	-7.51459	-4.84060
H	-2.02804	-6.96952	-5.64588
H	-0.16305	-5.47599	-6.12276

[La]@**bc-3**

G = -1786.239237 kcal.mol^{-1}

O	1.52840	0.79172	0.94731
Si	2.24364	-0.03894	-0.31165
O	2.80087	-1.50888	0.20417
Si	4.23886	-2.24143	-0.22328
O	4.37363	-3.48661	0.84297
Si	1.85518	0.68534	2.61778
O	1.03828	-0.15022	-1.44150
Si	1.14947	-0.58853	-3.04542
O	-0.39720	-0.81262	-3.54548
Si	-1.15259	-0.88245	-5.05160
O	3.49760	0.77160	-0.99304
Si	4.48525	1.98180	-0.27611
O	4.02086	2.17432	1.28155
La	2.43129	3.77029	0.78170
N	2.56977	5.78106	1.87878
O	1.98015	-2.01232	-3.15734
Si	3.53948	-2.56434	-3.27570
O	4.41538	-1.48328	-4.16916
Si	5.41048	-0.18243	-3.92093
O	4.52231	1.19892	-3.79551
Si	2.99890	1.77704	-4.11674
O	1.84970	0.58546	-3.95794
O	3.56436	-4.04005	-4.00469
O	4.18392	-2.79937	-1.77889
O	4.01276	3.39216	-0.98109
O	6.02791	1.42609	-0.55572
Si	6.44404	-0.13544	-0.93710
O	6.31725	-0.42274	-2.56008
N	0.56259	3.33602	-1.12347
O	5.53299	-1.22110	-0.07063
O	8.01842	-0.36138	-0.52532
Si	9.15445	0.61060	0.25755
O	6.41839	-0.07151	-5.21182
Si	8.08060	-0.23879	-5.43620
O	2.69170	3.06003	-3.13542
O	2.87785	2.22908	-5.69889
Si	3.18590	3.68609	-6.48438
H	5.17795	-4.00645	0.75450
H	3.43846	-4.01577	-4.95780
H	-2.38351	-1.70409	-4.87699
H	-1.52230	0.49520	-5.49028
H	-0.25649	-1.51092	-6.06632
H	1.79866	2.11580	3.08941
H	0.69876	-0.02299	3.23963
H	3.14053	0.04185	2.96452
H	8.52952	-1.60362	-5.03241
H	8.32674	-0.03502	-6.89220
H	8.82035	0.78951	-4.64789
H	8.67466	0.98914	1.61856
H	10.39383	-0.21105	0.36757

H	9.43171	1.83908	-0.54233
H	1.14306	3.25668	-1.97426
H	3.32995	3.19288	-2.34826
H	2.01312	4.60139	-6.34518
H	4.40402	4.35179	-5.93600
H	3.39078	3.36126	-7.92537
H	-0.18419	3.99343	-1.33462
H	0.12474	2.42217	-1.00986
H	3.36579	6.09722	2.42883
H	1.90754	6.55382	1.88295

[La]@**bc monografted to bc-1**
G = -1786.220801 kcal. mol^{-1}

O	0.77299	-0.12272	-0.03194
Si	0.65553	-0.02439	-1.71366
Si	0.27756	0.82848	1.20966
O	-1.30930	0.51547	1.53303
Si	-2.43154	0.59601	2.74980
O	-3.22775	2.04608	2.68493
Si	-2.90667	3.65362	2.45754
O	-4.25938	4.41189	1.90612
O	1.22617	0.45654	2.50814
Si	2.16030	1.11222	3.70822
O	1.85748	0.59339	5.20158
La	3.65120	-0.89057	5.77654
N	3.70893	-3.09886	5.17179
O	0.47875	2.41345	0.77965
Si	-0.12615	3.92546	1.04320
O	-1.76047	3.89490	1.29461
O	2.28583	2.75507	3.49154
Si	1.23107	4.00518	3.77155
O	1.99565	5.24325	4.52359
Si	3.20523	5.35809	5.69598
O	3.72834	0.44814	3.50694
N	5.43459	-0.24846	7.06465
O	0.63236	4.60622	2.35383
O	0.20102	4.78359	-0.32095
O	-0.00091	3.36808	4.68020
Si	-1.52143	3.80383	5.18982
O	-1.44365	5.02944	6.27611
Si	-2.23643	6.50991	6.44970
O	-2.19683	2.46717	5.87296
Si	-1.79241	0.84069	5.78900
O	-0.40281	0.47459	6.55768
O	-2.42069	4.32824	3.89500
O	-3.05484	0.02572	6.46448
Si	-4.27171	0.46382	7.54234
O	-1.64059	0.41510	4.18213
O	-3.57058	-0.55765	2.51155
Si	-3.62597	-2.23642	2.66830
H	-0.27556	5.61550	-0.39675
H	-5.07933	4.09513	2.29639
H	-4.04085	-2.80438	1.35316
H	-2.28942	-2.77579	3.05509
H	-4.63697	-2.57876	3.70861
H	0.65859	-1.42463	-2.22447
H	-0.60253	0.66751	-2.11801
H	1.83706	0.71216	-2.24940
H	-1.88215	7.42359	5.32532
H	-3.71450	6.30686	6.48990
H	-1.76631	7.08426	7.74167
H	4.54247	5.30250	5.03706
H	3.02336	6.67183	6.37352
H	3.08368	4.24765	6.68569
H	0.42019	0.60027	6.01503
H	-4.93125	-0.80211	7.97392
H	-3.70651	1.17047	8.72943
H	-5.27376	1.34306	6.86916
H	4.44463	-3.76448	5.40073
H	3.02960	-3.61553	4.61773
H	5.64552	0.66991	7.44804
H	6.20470	-0.85119	7.34847
H	4.07612	0.36849	2.61357

[La]@**bc monografted rear**
G = -1786.236977 kcal. mol^{-1}

O	-6.89914	2.38517	-1.46237
Si	-6.91108	3.56505	-0.38924
O	-5.36430	4.14312	0.01324
Si	-4.15174	3.37795	0.80720
O	-4.18303	3.71531	2.43369
Si	-4.78248	2.82258	3.69507
O	-3.92554	1.41218	3.86526
Si	-4.08136	-0.19247	3.52166
O	-3.09797	-1.04877	4.52319
La	-6.89301	0.35180	-2.52728
N	-5.39958	0.13531	-4.27324
O	-4.40573	1.73436	0.67639
Si	-3.81211	0.22151	0.49264
O	-3.60910	-0.52433	1.95848
O	-5.00446	-0.62615	-0.32787
Si	-5.80966	-2.02863	0.04962
O	-4.87431	-3.36089	-0.08765
O	-6.55094	-2.02427	1.52003
Si	-6.93111	-0.88564	2.67670
O	-8.21700	-1.44984	3.51127
Si	-8.59071	-1.70142	5.14211
O	-6.93810	-1.94426	-1.18652
O	-7.25158	0.52079	1.86985
Si	-7.54727	2.09137	2.36922
O	-6.38982	2.50699	3.48116
O	-5.64956	-0.70196	3.71232
O	-2.43017	0.19049	-0.37637
Si	-0.87022	-0.42831	-0.15048
O	-7.59019	3.10457	1.09447
O	-8.98617	2.13959	3.16675
Si	-10.48688	2.79727	2.75894
O	-2.68675	3.82005	0.21918
Si	-2.21497	4.61796	-1.19688
N	-9.00664	-0.31370	-3.20752
O	-7.76498	4.88982	-0.90223
H	-7.65590	5.65992	-0.33667
O	-4.53600	3.63078	5.10779
H	-11.42659	2.38128	3.83891
H	-2.82497	3.96780	-2.39213
H	-0.73010	4.50597	-1.25440
H	-7.70033	-2.53133	-1.19134
Si	-4.45969	-4.66350	0.91859
H	-4.59171	0.71978	-4.47482
H	-5.46984	-0.52022	-5.04847
H	-9.23977	-0.87631	-4.02290
H	-9.89083	0.05306	-2.86183
H	-0.07844	0.00142	-1.33500
H	-10.07004	-1.85815	5.21031
H	-8.15030	-0.54055	5.96584
H	-7.92181	-2.94795	5.61649
H	-0.28159	0.12720	1.10142
H	-0.92339	-1.91657	-0.07300
H	-2.73238	-0.52944	5.24572
H	-4.87638	4.53009	5.12285
H	-10.40436	4.28614	2.70620
H	-2.61722	6.05243	-1.13240
H	-10.95682	2.26879	1.44511
H	-3.43595	-5.44484	0.17278
H	-3.90671	-4.16278	2.20699
H	-5.67026	-5.49970	1.16502

[La]@**bc TS to bc-1**
G = -1786.223552 kcal. mol^{-1}

O	-7.13387	-1.46863	-1.45715
Si	-6.51686	-2.37461	-2.68754
O	-7.42643	-3.71053	-3.00881
Si	-7.34515	-5.35414	-2.82236
O	-6.59006	-5.64995	-1.37251
Si	-6.08859	-7.06438	-0.62883
O	-5.30101	-6.71231	0.75764
Si	-4.10656	-5.77378	1.50193
O	-2.67803	-6.11825	0.65844
Si	-2.30524	-5.92298	-0.92709
O	-2.49108	-7.34431	-1.76043
Si	-3.77635	-7.96844	-2.60213
O	-3.43365	-9.50952	-3.06490
La	-5.44459	-2.36752	0.62006
N	-4.40018	-0.45772	1.33551
N	-7.80646	-2.32920	0.98289
O	-5.01565	-2.85191	-2.05173
Si	-3.75475	-3.73157	-2.73432
O	-3.39013	-4.82716	-1.56781
O	-4.46688	-4.21323	1.51357
O	-6.27886	-1.48980	-4.04097
O	-2.50295	-2.72963	-3.04679
Si	-1.64391	-2.25798	-4.42958
O	-4.30180	-4.43721	-4.12077
Si	-4.91992	-5.90821	-4.60224
O	-6.48266	-6.02738	-4.07008
O	-8.86416	-5.95627	-2.84969
Si	-9.73216	-6.96004	-3.89942
O	-3.98610	-7.13848	-4.02032
O	-4.89754	-5.96418	-6.24405
O	-5.15229	-7.92360	-1.68941
O	-7.39185	-8.01061	-0.29784
Si	-8.26729	-8.30444	1.11482
O	-0.75663	-5.42318	-1.12032
Si	0.37215	-4.72593	-0.06980
O	-3.90945	-6.38140	3.02925
H	-3.65218	-7.30779	3.04913
Si	-6.81465	0.02594	-4.57717
H	-3.52357	-0.38301	1.84577
H	-8.33221	-3.17470	1.19534
H	-4.76445	0.48893	1.25450
H	-8.34049	-1.56368	1.38909
H	-7.70261	-1.89361	-0.71407
H	-0.50688	-1.42972	-3.94299
H	-11.06787	-7.15645	-3.27054
H	-9.03563	-8.26834	-4.05592
H	-9.88153	-6.29821	-5.22787
H	-1.14008	-3.46215	-5.14974
H	-2.52703	-1.45630	-5.32322
H	-4.37160	-6.68613	-6.60104
H	-3.16432	-10.09628	-2.35226
H	-0.23053	-3.56500	0.64677
H	-7.47198	-9.15882	2.04442
H	1.50213	-4.26858	-0.92643
H	0.85017	-5.74163	0.91147
H	-8.62525	-7.02245	1.78981
H	-9.50409	-9.02370	0.69828
H	-6.38620	0.13294	-5.99903
H	-8.29957	0.11126	-4.47401
H	-6.17941	1.10190	-3.76371

[La]@**bc monografted to bc-3**
G = -1786.215727 kcal. mol^{-1}

O	0.61113	-0.38369	0.54313
Si	1.86285	-0.48810	-0.50264
O	2.74778	0.89418	-0.61566
Si	3.75211	1.85778	0.30810
La	2.85409	4.68171	1.42516
N	4.29268	6.24022	2.32487
Si	0.39813	-0.56811	2.21068
O	2.84790	-1.74267	-0.04737
Si	4.19794	-2.46216	-0.66526
O	5.52843	-1.47809	-0.57540
Si	5.97721	0.10295	-0.75197
O	5.55134	0.63399	-2.27115
Si	5.72583	0.18814	-3.85114
O	4.67534	1.12629	-4.72844
Si	3.32288	2.02591	-4.40161
O	2.83850	2.72345	-5.81035
Si	2.93304	2.28940	-7.44197
O	1.22613	-0.78026	-2.00697
Si	1.56946	-0.41428	-3.57848
O	2.14411	1.13596	-3.68409
O	4.42855	-3.80938	0.24758
O	3.95287	-2.88841	-2.24941
Si	4.01934	-2.35315	-3.80104
O	5.37281	-1.41811	-4.05419
O	0.20026	-0.54684	-4.46969
Si	-1.41969	-0.84000	-4.08593
O	2.69067	-1.45228	-4.21182
O	5.24212	1.09521	0.34083
O	3.21748	2.36222	1.72876
O	3.86394	3.31750	-0.56675
O	7.60483	0.16616	-0.54781
Si	8.61391	1.13557	0.39898
O	4.09167	-3.70290	-4.73910
O	3.64406	3.27253	-3.33183
O	7.24328	0.45872	-4.40536

Si	8.46653	-0.52281	-5.03442
N	0.79994	5.53200	0.82700
H	5.18210	-4.34868	-0.00919
H	3.89603	-3.55621	-5.66909
H	-1.57579	-2.21040	-3.51886
H	-1.91511	0.17561	-3.11273
H	-2.17087	-0.72912	-5.36831
H	-0.21238	0.68839	2.73096
H	-0.54027	-1.70794	2.42423
H	1.69709	-0.83736	2.88736
H	8.78194	-1.63467	-4.09293
H	8.04488	-1.07913	-6.35368
H	9.65471	0.35832	-5.21058
H	8.40962	0.83740	1.84567
H	10.00833	0.79372	-0.00128
H	8.34900	2.58009	0.13440
H	3.80245	3.26869	-1.54343
H	3.93585	4.07913	-3.76935
H	1.85368	3.03854	-8.14353
H	4.26553	2.68356	-7.98471
H	2.73264	0.82030	-7.60465
H	0.52281	6.51156	0.84137
H	-0.01920	5.01781	0.51063
H	5.20170	6.08082	2.75318
H	4.13321	7.24423	2.38051

[La]@**bc TS to bc-3**
G = -1786.201778 kcal. mol^{-1}

O	0.53972	-0.31832	0.41473
Si	-0.03095	0.78382	1.48939
O	-0.02179	2.27223	0.75960
Si	-0.55068	3.79974	1.09139
O	-0.39809	4.62490	-0.32395
Si	1.56429	-0.27131	-0.92389
O	-1.57419	0.33455	1.88323
Si	-2.58163	0.47192	3.19443
O	-3.74840	-0.67798	3.06105
Si	-4.04946	-1.91205	1.95385
O	0.84642	0.81447	2.87739
Si	2.26068	1.34561	3.58790
O	3.63210	0.66834	2.98711
La	3.86289	-0.64939	5.37584
N	4.05611	-1.75253	7.37557
O	-3.34124	1.94345	3.18824
Si	-3.12087	3.54934	2.86201
O	-2.50103	4.29650	4.21006
Si	-1.45359	3.82752	5.41231
O	-1.98593	2.45752	6.14974
Si	-1.54586	0.84179	6.13492
O	-1.73134	0.26134	4.58260
O	-4.56000	4.23676	2.45088
O	-2.13757	3.79147	1.56200
O	2.18783	0.84246	5.17831
O	2.31699	3.01123	3.46257
Si	1.12611	4.13627	3.68840
O	0.03774	3.50094	4.76418
N	3.75479	-1.82932	3.18789
O	0.36748	4.51702	2.27014
O	1.79254	5.52626	4.26065
Si	3.34423	5.93749	4.77199
O	-1.37015	5.04982	6.50395
Si	-2.05693	6.58551	6.61370
O	-0.02947	0.56010	6.66250
O	-2.56892	0.06846	7.16751
Si	-4.18888	0.21844	7.58010
H	-0.74491	5.52158	-0.30381
H	-5.29226	3.99482	3.02544
H	-4.26470	-1.35325	0.58718
H	-2.91600	-2.88329	1.92728
H	-5.28793	-2.59827	2.42111
H	2.54077	-1.39057	-0.77539
H	0.75067	-0.48689	-2.15559
H	2.28769	1.02857	-1.00409
H	-1.73672	7.39727	5.40370
H	-3.53786	6.48116	6.77108
H	-1.46501	7.22260	7.82424
H	4.29363	5.93243	3.62078
H	3.24966	7.30957	5.34596
H	3.82602	4.98701	5.81920
H	0.71815	0.76733	6.05302
H	-4.73751	-1.15893	7.74579
H	-4.31270	0.96068	8.86987
H	-4.95731	0.93722	6.51990
H	4.51583	-2.30452	2.71766
H	2.91099	-2.32993	2.91167
H	3.59593	-1.47557	8.24180
H	4.47518	-2.65916	7.57425
H	3.65802	-0.59547	2.83802

[La]@**abc-2**
G = -1781,186924 kcal. mol^{-1}

O	-0.52790	5.09694	-2.95823
Si	-0.21194	6.44431	-3.83769
O	0.71494	7.47282	-2.92833
Si	1.80634	8.66222	-3.30086
O	3.06624	7.99663	-4.15304
Si	4.79578	7.85738	-3.92393
N	5.60850	9.36009	-3.74235
O	-1.60344	7.22509	-4.27931
Si	-2.08179	8.09472	-5.61059
O	-1.11493	9.42647	-5.81435
Si	0.49276	9.78837	-5.81046
O	1.35173	8.67999	-6.70163
Si	1.36072	8.36791	-8.41144
O	-0.08842	7.59615	-8.72962
Si	-1.12262	6.45723	-8.12490
O	-2.11928	5.96980	-9.33631
Si	-2.14866	6.28741	-10.99263
O	0.65281	6.07011	-5.22751
Si	0.61307	4.69527	-6.25306
O	2.15539	4.48838	-6.63119
La	3.16777	6.60486	-6.40611
O	5.17026	7.05801	-5.27433
O	-3.59145	8.70146	-5.36955
O	-2.07605	7.11465	-6.93664
O	2.31826	9.40396	-1.93499
Si	2.32621	8.97742	-0.29414
O	1.09413	9.81230	-4.27123
O	0.68804	11.26033	-6.53390
Si	0.40099	12.85396	-6.02002
O	-0.36748	5.10791	-7.53222
O	2.65487	7.42976	-8.53729
O	1.36521	9.81634	-9.20236
N	4.84335	5.41338	-8.11968
O	-0.14653	3.49465	-5.37739
Si	-0.17511	1.81405	-5.62647
O	4.82905	7.05476	-2.45943
H	-1.41216	1.31730	-4.96054
H	1.02618	1.19542	-4.99624
H	-0.20769	1.51013	-7.08536
H	1.17745	9.65688	0.37211
H	2.22720	7.50298	-0.12326
H	3.60770	9.48895	0.27036
H	-0.84575	5.92271	-11.62230
H	-3.23764	5.43952	-11.55689
H	-2.44719	7.72722	-11.24541
H	0.17620	13.65325	-7.25643
H	1.60382	13.35482	-5.29550
H	-0.79592	12.90390	-5.13422
H	-0.56326	4.31304	-3.52894
H	-4.30028	8.05777	-5.45905
H	1.11875	10.55748	-8.63333
H	4.62396	4.42437	-8.20069
H	5.84307	5.50999	-7.97121
H	4.59860	5.85594	-9.00291
H	5.71915	6.94414	-2.11065
H	5.33448	9.98427	-2.99712
H	5.88286	9.85825	-4.57643

[La]@**bc-2**
G = -1786,303784 kcal.mol^{-1}

O	0.38638	-0.26946	0.20217
Si	0.12092	-0.09975	1.81085
O	1.53555	0.07558	2.65191
Si	2.16543	-0.59002	4.03600
O	3.71208	-0.07402	4.25502
O	-0.70836	-1.42425	2.43365
Si	-0.82519	-3.04769	1.89944
O	-2.36867	-3.41014	2.12359
La	-3.16374	-1.97616	3.82238
O	-2.45517	-3.27460	5.63182
Si	-1.08215	-2.65978	6.18780
O	0.30797	-3.33937	5.55715
Si	1.18750	-3.56424	4.17933
O	2.19209	-4.84474	4.40758
Si	2.19200	-6.42679	3.82676
O	-0.81730	1.24127	2.06957
Si	-1.72293	1.65787	3.39670
O	-2.21050	3.21629	3.26948
Si	-2.11283	4.38074	2.04273
N	-4.93506	-3.96789	4.04661
O	-3.02225	0.62887	3.50445
Si	-4.76510	0.79505	3.53525
O	-5.15835	-0.74809	3.80195
O	-1.18121	-1.05338	5.56514
Si	-0.22525	0.30083	5.76260
O	1.34187	-0.05908	5.37072
O	-0.82138	1.48346	4.77368
O	-0.27354	0.82440	7.31198
Si	0.85465	1.49537	8.37698
O	2.13653	-2.23706	3.89369
O	0.25407	-3.89520	2.84535
O	-0.26908	-3.08209	0.32399
Si	-0.85502	-4.02151	-0.96801
O	-5.02944	1.44990	2.02320
N	-5.34753	1.89348	4.72138
O	-0.86356	-2.58538	7.81825
Si	0.09981	-3.46146	8.89107
H	0.14682	-3.86874	-2.06047
H	-2.18204	-3.51103	-1.41486
H	-0.96059	-5.45009	-0.55545
H	-0.77123	5.03108	2.08696
H	-2.34612	3.76649	0.70691
H	-3.17229	5.38448	2.34659
H	0.85942	-7.06696	4.03326
H	2.53848	-6.44792	2.37497
H	3.23228	-7.15933	4.60328
H	1.82060	0.45099	8.82244
H	0.07465	2.00134	9.54135
H	1.58415	2.61901	7.72096
H	0.33017	-1.20052	-0.06745
H	4.35312	-0.46061	3.65134
H	-4.90312	-4.60643	3.25695
H	-5.90107	-3.69392	4.19855
H	-4.60463	-4.47341	4.86555
H	-5.94641	1.70538	1.88165
H	-5.01829	2.84858	4.70603
H	-5.47205	1.55185	5.66346
H	-0.34786	-3.08279	10.26185
H	-0.08670	-4.92863	8.68608
H	1.53716	-3.10658	8.71110

[La]@**b-2**
G = -1791,422124 kcal.mol^{-1}

O	0.31067	-0.25645	0.20297
Si	0.06295	-0.08695	1.81439
O	1.48540	0.10731	2.63823
Si	2.13570	-0.55715	4.01347
O	3.67838	-0.02475	4.22031
O	-0.74360	-1.41815	2.45125
Si	-0.85741	-3.04178	1.91808
O	-2.39445	-3.41709	2.16539
La	-3.17918	-2.00805	3.88631
O	-2.42642	-3.30697	5.67698
Si	-1.05377	-2.67336	6.21189
O	0.33680	-3.32980	5.55915
Si	1.19464	-3.54295	4.16573
O	2.21757	-4.81188	4.37447
Si	2.23869	-6.38615	3.77254
O	-0.88777	1.24472	2.08177
Si	-1.79390	1.63903	3.41554
O	-2.30672	3.19150	3.29317
Si	-1.85676	4.48842	2.29945
N	-4.95394	-3.99348	4.12693
O	-3.08347	0.60070	3.52280
Si	-4.83149	0.74340	3.59948
O	-5.18676	-0.79982	3.90431

O	-1.18840	-1.06807	5.59020
Si	-0.24773	0.29956	5.76937
O	1.31857	-0.03891	5.35740
O	-0.87810	1.46743	4.78449
O	-0.28219	0.83081	7.31635
Si	0.86281	1.47875	8.37804
O	2.12254	-2.20370	3.86594
O	0.24157	-3.88191	2.84785
O	-0.32601	-3.07227	0.33424
Si	-0.93538	-4.00806	-0.95009
O	-5.20274	1.34466	2.09374
Si	-6.62832	2.00520	1.49075
N	-5.37278	1.86989	4.77799
O	-0.80976	-2.59265	7.83828
Si	0.16876	-3.46708	8.89925
H	0.04216	-3.84406	-2.06267
H	-2.27423	-3.50165	-1.36489
H	-1.02461	-5.43917	-0.54268
H	-0.39302	4.74485	2.42173
H	-2.21405	4.19745	0.88254
H	-2.62780	5.66345	2.79489
H	0.92223	-7.05448	3.99232
H	2.56155	-6.38150	2.31520
H	3.30563	-7.10766	4.52266
H	1.83454	0.42571	8.78884
H	0.09996	1.96294	9.56273
H	1.58323	2.61447	7.73276
H	0.25758	-1.18805	-0.06553
H	4.31944	-0.40644	3.61353
H	-4.94570	-4.62859	3.33388
H	-5.91191	-3.69767	4.28981
H	-4.62833	-4.51161	4.93975
H	-5.07231	2.83219	4.70932
H	-5.43096	1.56120	5.73771
H	-0.26380	-3.09072	10.27540
H	-0.01579	-4.93448	8.69460
H	1.60256	-3.10721	8.70194
H	-6.57607	1.86822	0.00602
H	-7.82793	1.29086	2.02040
H	-6.71706	3.45403	1.84724

La]@**c-1 TS NH2 transfer**

G = -1709.794417 kcal. mol^{-1}

O	-2.69902	-2.99473	-1.58936
Si	-1.92194	-1.68152	-0.97851
O	-0.61594	-1.35473	-1.91722
Si	0.82432	-0.47091	-1.64148
O	1.90707	-1.46827	-2.38956
Si	1.57844	-2.95415	-3.14660
Si	-4.15397	-3.21534	-2.40973
O	-2.99262	-0.40814	-0.97361
Si	-3.19390	1.21726	-1.04632
O	-1.94714	2.00096	-1.80329
Si	-0.32601	2.29998	-1.82979
O	0.21107	2.76278	-0.33116
Si	0.27784	2.66602	1.31130
O	1.35902	1.47960	1.76635
La	3.92114	1.14152	0.81814
N	3.16808	0.75495	-1.38738
O	-1.53236	-2.05317	0.59702
Si	-1.45374	-1.35443	2.09198
O	0.09886	-0.89671	2.49139
Si	1.27337	-0.23552	1.53790
O	0.68454	-0.34482	-0.00120
O	-4.58604	1.47063	-1.88808
O	-3.34205	1.85159	0.48124
Si	-2.62440	1.58922	1.94661
O	-1.18557	2.40770	2.01031
O	-1.96679	-2.43014	3.21771
Si	-2.06986	-4.11555	3.25165
O	-2.44477	-0.03224	2.18202
O	0.50705	0.98936	-2.39273
O	-0.04193	3.56576	-2.83764
Si	0.34176	3.67564	-4.47709
O	-3.52832	2.24356	3.15541
O	2.80823	-0.65371	1.74629
N	6.18327	1.12711	1.23255
O	0.94597	4.06222	1.86908
Si	0.31321	5.43913	2.62531
H	-4.80329	2.39619	-2.03288
H	-4.26292	1.69423	3.44462
H	-3.25493	-4.56889	2.46727
H	-0.82839	-4.72915	2.69716
H	-2.23430	-4.49507	4.68343
H	-4.18135	-4.64419	-2.83524
H	-5.30848	-2.93683	-1.50591
H	-4.22698	-2.32836	-3.60747
H	-0.87815	5.93969	1.88113
H	-0.05331	5.12038	4.03421
H	1.40242	6.45610	2.59530
H	-0.49517	2.73992	-5.28251
H	0.07055	5.08472	-4.87963
H	1.78752	3.36321	-4.68047
H	2.90710	-3.42506	-3.63877
H	1.02845	-3.94433	-2.17868
H	0.65478	-2.77795	-4.30255
H	3.59158	0.01499	-1.94555
H	2.92749	1.48472	-2.05574
H	6.93514	1.26642	0.56039
H	6.63996	0.85210	2.09981

La]@**c-1 Intermediate NH2 transfer**

G = -1709.818628 kcal.mol^{-1}

O	1.87655	-0.95539	-2.21201
Si	2.71542	-1.28889	-0.86183
O	2.96211	0.02494	0.13496
Si	2.16423	1.25564	0.88318
O	0.81977	0.70518	1.69430
Si	0.46044	-0.41290	2.84860
O	-1.11338	-0.06736	3.33785
Si	-2.41267	-0.25522	2.33941
O	-1.85113	-0.72962	0.85899
La	-2.47969	0.89364	-1.02276
N	-1.40533	0.49959	-3.22554
Si	0.35748	-0.17375	-2.68106
O	0.35519	-1.05369	-4.12453
Si	1.53804	-2.13121	-4.66172
O	-0.35851	-0.59018	-1.13019
Si	-1.43225	-1.72811	-0.49472
O	-2.76154	-1.57246	-1.36451
O	0.95034	1.40811	-2.58039
Si	0.61110	2.57090	-1.44853
O	0.92089	4.05154	-2.12378
Si	2.16102	5.16272	-1.90347
O	2.03567	-2.49178	0.08166
Si	0.76128	-2.96844	0.98925
O	0.49366	-1.96364	2.28164
O	-0.64861	-3.05471	0.06769
O	1.01535	-4.47983	1.56694
Si	2.31173	-5.55857	1.46325
O	4.20777	-1.87429	-1.27561
O	-0.95077	2.47498	-0.94699
O	1.67441	2.42922	-0.15852
O	3.18285	1.90140	2.01928
O	1.43283	-0.33969	4.16254
Si	1.97637	0.86819	5.21229
N	-3.58397	-1.16768	3.17679
O	-3.14373	1.18337	1.79598
Si	-3.83293	2.43373	2.73698
H	1.48399	0.52025	6.57841
H	4.11385	1.77687	1.81066
H	1.99805	6.19682	-2.96791
H	2.54946	-5.95078	0.04438
H	-5.20463	2.03180	3.16059
H	4.39323	-1.74334	-2.21052
H	1.64479	-3.35027	-3.80703
H	3.50223	4.51960	-2.03902
H	2.05900	5.81738	-0.56438
H	3.46509	0.86451	5.20360
H	-2.97510	2.72601	3.91542
H	-3.91204	3.60700	1.81955
H	1.44513	2.20237	4.81393
H	1.06938	-2.55686	-6.01898
H	2.88298	-1.49972	-4.82154
H	3.54469	-4.94954	2.04015
H	1.91302	-6.75299	2.26148
H	-4.43957	-1.44610	2.71902
H	-3.25220	-1.86945	3.82355
H	-1.20407	1.25462	-3.87859
H	-1.82010	-0.24976	-3.77837

La]@**c-1 TS Si-O activation**

G = -1709.814615 kcal.mol^{-1}

O	-2.52470	-3.13797	-2.03098
Si	-3.77287	-4.16730	-1.55290
Si	-1.66041	-1.97946	-1.24971
O	-2.17507	-1.98709	0.32865
Si	-1.79457	-1.35208	1.80537
O	-2.27261	0.22967	1.90236
Si	-2.56473	1.68049	1.15699
O	-3.79830	2.43875	1.94113
O	-0.04086	-2.28394	-1.42679
Si	1.00003	-0.93380	-1.60339
O	2.06124	1.14708	-1.82995
La	3.49317	0.64130	-0.02961
N	5.77982	0.73825	-0.22003
O	-1.96471	-0.51058	-1.96463
Si	-2.06561	1.13447	-1.80628
O	-2.94474	1.44001	-0.43247
O	0.72727	-0.52701	-3.18591
Si	0.28382	-1.45708	-4.52243
O	0.55655	-0.15444	-0.15651
Si	0.95140	-0.39955	1.49011
O	2.52261	-0.73324	1.57721
N	2.67216	-1.50751	-1.37668
O	-0.61960	1.91549	-1.75828
Si	0.96972	2.31531	-1.50646
O	1.26961	3.71604	-2.32106
Si	0.41716	4.62395	-3.45921
O	-2.83968	1.73921	-3.13054
O	1.26317	2.66880	0.13621
Si	0.34749	2.55433	1.52778
O	0.85817	3.74287	2.53572
Si	0.08740	4.92950	3.46004
O	0.66057	1.08618	2.21103
O	-1.27046	2.71217	1.23462
O	-0.15831	-1.47169	2.10226
O	-2.60060	-2.21255	2.94432
Si	-2.13049	-2.99316	4.36708
H	-3.63158	1.25402	-3.38049
H	-4.47915	1.84575	2.27217
H	-3.38534	-3.49868	4.99240
H	-1.22044	-4.13294	4.05536
H	-1.45154	-2.03542	5.28739
H	-3.30762	-5.09381	-0.48033
H	-4.94444	-3.38016	-1.06679
H	-4.15618	-4.94507	-2.76540
H	-0.65778	5.86900	2.57401
H	-0.84581	4.29992	4.43859
H	1.17028	5.65553	4.18187
H	0.10274	3.80079	-4.66269
H	-0.84167	5.15895	-2.86421
H	1.31427	5.75299	-3.84055
H	0.33940	-0.54085	-5.69643
H	1.27575	-2.56279	-4.70849
H	-1.08100	-2.03423	-4.38715
H	2.70613	-2.36118	-0.82426
H	3.12010	-1.68580	-2.27198
H	6.32133	1.16711	-0.96792
H	6.46269	0.32623	0.41299

[La]@**c-2**

G = -1709,833421 kcal. mol^{-1}

O	0.72343	0.54361	3.53800
Si	-0.28830	0.47000	2.25574
O	-1.86773	0.54456	2.81585
Si	-3.20989	0.38226	1.87297
O	-4.00228	1.81731	1.42632
Si	-4.92819	2.84430	2.44800
Si	1.10921	1.70036	4.71004
O	-2.77607	-0.05787	0.34048
Si	-2.10952	-0.68801	-1.09780
La	-3.92815	1.73545	-1.30318
N	-6.11739	2.35656	-1.62880
N	-4.31864	-0.57115	2.74907
O	-3.34443	-0.51907	-2.09871
O	-0.94631	0.47039	-1.49444

Si	-0.26572	0.79490	-2.99644
O	-0.39889	2.41615	-3.23913
Si	-0.85020	3.55952	-2.08029
O	-2.39183	3.35455	-1.63217
O	-0.58517	5.03706	-2.76988
Si	0.61149	6.19946	-2.57763
O	0.26337	3.43124	-0.82821
Si	0.99688	2.45930	0.26991
O	1.96941	1.31336	-0.42962
Si	2.06664	0.00315	-1.42402
O	1.30846	0.29283	-2.87746
O	-0.15202	1.75005	1.22882
O	1.94384	3.35871	1.28367
O	3.67591	-0.23482	-1.67458
O	1.42154	-1.36640	-0.73582
Si	0.18051	-1.93665	0.18243
O	-1.25579	-2.04845	-0.68918
O	0.56754	-3.45292	0.66706
Si	-0.26794	-4.91652	0.74456
O	-0.05439	-0.98640	1.51702
O	-0.99265	-0.04006	-4.20803
Si	-2.45056	0.21585	-5.02626
H	0.71665	1.14263	6.03733
H	2.78948	3.62117	0.90770
H	0.40817	7.20724	-3.65839
H	-0.51985	-5.44203	-0.62807
H	-6.30826	2.29821	2.56556
H	3.89155	-1.03394	-2.16430
H	-2.11565	0.68047	-6.40459
H	1.97543	5.60200	-2.70518
H	0.49154	6.86784	-1.24685
H	2.58030	1.92595	4.67143
H	-4.26874	2.91688	3.78021
H	-4.93791	4.17136	1.77644
H	0.37392	2.97209	4.45737
H	-3.21389	-1.05579	-5.07847
H	-3.25905	1.29565	-4.36875
H	0.60412	-5.85692	1.50245
H	-1.56584	-4.73903	1.46206
H	-5.20276	-0.84186	2.34462
H	-3.95389	-1.26718	3.38299
H	-6.47336	3.30000	-1.76679
H	-6.91898	1.73796	-1.73305

La]@**c-2 TS NH2 transfer**
G = -1709.801087 kcal. mol^{-1}

O	0.97242	-0.14633	-2.71531
Si	1.74377	-0.46886	-1.30211
O	1.95361	0.88579	-0.36685
Si	1.17233	2.15010	0.35808
O	-0.13980	1.63490	1.22610
Si	-0.55844	0.54038	2.38357
O	-2.13513	0.88792	2.83617
Si	-3.41785	0.67521	1.80920
O	-2.76302	0.35891	0.32055
La	-3.56550	1.84199	-1.76562
N	-2.76151	1.57921	-3.91503
Si	-0.49826	0.63128	-3.12636
O	-0.77712	-0.15240	-4.55845
Si	0.19858	-1.31979	-5.30366
O	-1.37282	0.29749	-1.72399
Si	-2.47724	-0.73954	-0.95659
O	-3.82503	-0.62653	-1.79935
O	-0.08024	2.23390	-3.14768
Si	-0.41112	3.42780	-2.01456
O	-0.03182	4.86658	-2.73967
Si	1.20566	5.97463	-2.49248
O	0.98054	-1.63047	-0.39083
Si	-0.30459	-2.04100	0.54568
O	-0.49999	-1.01850	1.83061
O	-1.71509	-2.07104	-0.36829
O	-0.10011	-3.55813	1.12568
Si	1.13748	-4.70202	1.00600
O	3.22683	-1.11052	-1.64559
O	-1.96441	3.37624	-1.53125
O	0.67208	3.26085	-0.74522
O	2.21888	2.84633	1.43358
O	0.39071	0.61714	3.71558
Si	0.83903	1.81739	4.81589
N	-4.48722	-0.43706	2.54261
O	-4.27679	2.06756	1.41254
Si	-5.18823	3.06269	2.44978
H	0.24483	1.46644	6.13973
H	3.13722	2.83753	1.14775
H	1.07935	6.99994	-3.56965
H	1.33392	-5.10628	-0.41606
H	-6.58578	2.54402	2.52542
H	3.54862	-0.86108	-2.51689
H	0.31137	-2.55304	-4.47271
H	2.54659	5.32203	-2.58625
H	1.07264	6.63859	-1.16096
H	2.32475	1.81869	4.91856
H	-4.57460	3.10932	3.80493
H	-5.19253	4.41461	1.82075
H	0.34096	3.15333	4.38024
H	-0.50173	-1.64800	-6.58067
H	1.55611	-0.78355	-5.61405
H	2.40809	-4.15457	1.56238
H	0.69064	-5.87388	1.81152
H	-5.30845	-0.75164	2.04623
H	-4.08470	-1.16936	3.11057
H	-2.32391	2.28552	-4.50038
H	-2.97639	0.78608	-4.51327

La]@**c-2 Intermediate NH2 transfer**
G = -1709.80611 kcal. mol^{-1}

O	1.87655	-0.95539	-2.21201
Si	2.71542	-1.28889	-0.86183
O	2.96211	0.02494	0.13496
Si	2.16423	1.25564	0.88318
O	0.81977	0.70518	1.69430
Si	0.46044	-0.41290	2.84860
O	-1.11338	-0.06736	3.33785
Si	-2.41267	-0.25522	2.33941
O	-1.85113	-0.72962	0.85899
La	-2.47969	0.89364	-1.02276
N	-1.40533	0.49959	-3.22554
Si	0.35748	-0.17375	-2.68106
O	0.35519	-1.05369	-4.12453
Si	1.53804	-2.13121	-4.66172
O	-0.35851	-0.59018	-1.13019
Si	-1.43225	-1.72811	-0.49472
O	-2.76154	-1.57246	-1.36451
O	0.95034	1.40811	-2.58039
Si	0.61110	2.57090	-1.44853
O	0.92089	4.05154	-2.12378
Si	2.16102	5.16272	-1.90347
O	2.03567	-2.49178	0.08166
Si	0.76128	-2.96844	0.98925
O	0.49366	-1.96364	2.28164
O	-0.64861	-3.05471	0.06769
O	1.01535	-4.47983	1.56694
Si	2.31173	-5.55857	1.46325
O	4.20777	-1.87429	-1.27561
O	-0.95077	2.47498	-0.94699
O	1.67441	2.42922	-0.15852
O	3.18285	1.90140	2.01928
O	1.43283	-0.33969	4.16254
Si	1.97637	0.86819	5.21229
N	-3.58397	-1.16768	3.17679
O	-3.14373	1.18337	1.79598
Si	-3.83293	2.43373	2.73698
H	1.48399	0.52025	6.57841
H	4.11385	1.77687	1.81066
H	1.99805	6.19682	-2.96791
H	2.54946	-5.95078	0.04438
H	-5.20463	2.03180	3.16059
H	4.39323	-1.74334	-2.21052
H	1.64479	-3.35027	-3.80703
H	3.50223	4.51960	-2.03902
H	2.05900	5.81738	-0.56438
H	3.46509	0.86451	5.20360
H	-2.97510	2.72601	3.91542
H	-3.91204	3.60700	1.81955
H	1.44513	2.20237	4.81393
H	1.06938	-2.55686	-6.01898
H	2.88298	-1.49972	-4.82154
H	3.54469	-4.94954	2.04015
H	1.91302	-6.75299	2.26148
H	-4.43957	-1.44610	2.71902
H	-3.25220	-1.86945	3.82355
H	-1.20407	1.25462	-3.87859
H	-1.82010	-0.24976	-3.77837

La]@**c-2 TS Si-O activation**
G = -1709.803267 kcal. mol^{-1}

O	2.21254	-0.60238	-2.60826
Si	0.76531	0.17412	-2.78007
O	-0.21032	-0.09779	-1.35485
Si	-1.07210	-1.59550	-1.30090
O	-0.22864	-2.16328	-2.76664
Si	0.18343	-3.70020	-3.31147
Si	2.83908	-0.94719	-1.09996
O	2.14295	-2.22099	-0.31842
Si	0.86599	-2.72421	0.61457
O	-0.56779	-2.75934	-0.22373
O	2.74058	0.38236	-0.12392
Si	2.08083	1.56518	0.82691
O	1.29163	2.76652	0.01538
Si	0.49084	2.89889	-1.45760
O	-1.12172	2.68911	-1.29369
La	-2.43470	0.95502	-0.78981
O	-3.03654	1.20435	1.77931
Si	-3.65195	2.39196	2.84550
O	4.42068	-1.34751	-1.35390
O	0.96395	0.99563	1.91353
Si	0.58601	-0.35148	2.79410
O	-1.00371	-0.11573	3.27634
Si	-2.26110	-0.30541	2.20423
O	-1.71961	-0.67866	0.73143
O	3.33317	2.21069	1.69842
O	1.51280	-0.48504	4.14283
Si	1.71587	0.45583	5.52793
O	0.79113	-1.74756	1.94395
O	1.16709	1.76978	-2.46311
N	-0.11545	0.30258	-4.23192
O	0.85711	4.40282	-2.05152
Si	1.78227	5.65978	-1.43375
O	-2.55634	-1.12644	-1.75228
O	1.15382	-4.25750	1.12308
Si	2.40997	-5.36343	0.92604
N	-3.49736	-1.17140	3.03704
H	0.79433	-0.03968	6.59347
H	4.19149	2.04434	1.29726
H	1.70876	6.76908	-2.43079
H	2.71769	-5.56040	-0.52055
H	-4.73449	3.11029	2.10611
H	4.70843	-1.16775	-2.25403
H	1.31264	-4.27271	-2.52334
H	3.20907	5.25165	-1.26010
H	1.24269	6.13871	-0.12567
H	3.12821	0.28648	5.97204
H	-4.19481	1.75027	4.07072
H	-2.56406	3.36857	3.13387
H	1.42815	1.89250	5.24830
H	-0.99102	-4.62069	-3.25357
H	0.61898	-3.53944	-4.73288
H	3.63270	-4.89637	1.64199
H	1.93301	-6.64531	1.51937
H	-4.36246	-1.28682	2.52336
H	-3.21594	-2.07289	3.40383
H	-0.31389	-0.54449	-4.74768
H	0.18096	1.07392	-4.81884

[La]@**c-3**
G = -1709,875361 kcal. mol^{-1}

O	-5.29826	0.65572	0.69198
Si	-5.68557	1.62578	1.92448
O	-7.22572	1.45489	2.48906
Si	-8.43809	0.35918	2.08179
La	-3.27722	0.37757	-0.33531
O	-2.72005	1.70010	-2.16530
Si	-2.52128	3.18654	-1.58349
O	-0.95417	3.52236	-1.07658
Si	-0.25251	2.94723	0.29992
O	1.37862	3.03903	0.17678

Si	2.42152	3.35809	-1.11827
O	-2.23897	-1.62880	-0.23991
Si	-1.10631	-2.36112	0.66423
O	-0.25810	-1.15480	1.54400
Si	-0.69349	0.37956	1.86789
O	-2.34849	0.48289	2.22163
Si	-3.05939	1.33207	3.51939
O	-2.70360	0.59560	4.94744
O	-3.38399	3.07273	-0.09252
Si	-4.32187	4.13906	0.82462
O	-3.24586	4.80008	1.91304
Si	-1.93909	4.16712	2.69668
O	-0.71090	3.76912	1.65170
O	-1.82697	-3.37786	1.77002
Si	-1.15820	-4.69411	2.57798
O	-5.50383	3.25363	1.55249
O	-4.67197	1.34427	3.24966
N	-5.06529	5.35515	-0.12159
O	-2.99429	4.48370	-2.46823
Si	-4.33028	4.74838	-3.47184
N	0.17430	-3.23211	-0.11004
O	-0.71321	1.32056	0.46602
O	0.23132	1.04516	3.03430
Si	1.46653	0.46163	4.04616
O	-2.35841	2.81890	3.57053
O	-1.42189	5.35048	3.71388
H	2.64743	0.08275	3.21980
H	-3.32988	-0.09029	5.19987
H	-8.83923	0.51893	0.65220
H	2.27313	4.77415	-1.55930
H	-0.99544	-5.86036	1.65810
H	-0.64047	5.12724	4.22806
H	-4.75052	6.16658	-3.29500
H	-9.59864	0.66939	2.96503
H	-7.98895	-1.04545	2.31833
H	1.80950	1.59064	4.95372
H	0.16019	-4.35754	3.19367
H	-2.12489	-5.05809	3.65696
H	0.97810	-0.70897	4.82581
H	-3.90266	4.53026	-4.88527
H	-5.45279	3.82379	-3.14242
H	3.79840	3.12179	-0.60020
H	2.13532	2.43340	-2.25307
H	-0.10092	-3.88912	-0.82868
H	0.94875	-2.66844	-0.43564
H	-6.05476	5.49025	0.03199
H	-4.58026	6.23404	-0.23386

La]@b**c-1 TS NH2 transfer**
G = -1786.240007 kcal. mol^{-1}

O	-0.26899	0.57273	0.03953
Si	-0.72364	-0.56293	-1.12811
Si	-0.28340	0.59272	1.67852
O	1.25660	0.92899	2.20094
Si	2.01215	1.60262	3.50456
O	2.15207	0.54146	4.76165
Si	1.32524	-0.67094	5.54990
O	2.39400	-1.67176	6.30282
O	-1.22228	1.81429	2.27178
Si	-2.90081	2.25767	2.39398
O	-3.87221	2.00255	1.07196
O	-0.79539	-0.88433	2.21385
Si	-0.92300	-1.69615	3.65125
O	0.51912	-1.61227	4.46920
La	-0.86299	4.39026	2.91887
N	-1.33653	6.99578	3.50314
N	-1.87947	4.03224	0.77452
Si	1.01901	3.79456	5.49264
O	0.07898	5.01868	5.08860
O	1.12270	2.93735	3.97825
O	-2.90181	3.57079	3.35782
O	-2.13163	-1.09187	4.60071
Si	-2.80901	0.41752	4.80490
O	-3.97412	0.22905	5.95184
Si	-5.48506	0.94669	6.17262
O	-1.23429	-3.25527	3.22840
O	-1.59449	1.43123	5.36131
Si	-0.59300	1.41560	6.68168
O	-1.43407	1.45017	8.08948
Si	-1.48554	0.46987	9.46045
O	-3.43916	0.96405	3.39405
O	0.41208	2.72001	6.61920
O	0.31845	0.01707	6.67271
O	2.57069	4.12155	5.96351
Si	3.36296	4.04428	7.44686
O	3.50519	2.09412	3.03801
Si	5.05358	1.42352	3.11096
H	-4.48506	1.28198	1.26618
H	-1.38649	-3.85016	3.96848
H	2.84715	-1.27838	7.05430
H	5.03113	0.00504	2.64956
H	5.90854	2.24498	2.20889
H	5.57309	1.49300	4.50767
H	-0.66170	0.14671	-2.43702
H	0.23204	-1.70828	-1.12405
H	-2.10850	-1.05203	-0.87368
H	-1.80865	-0.93882	9.09416
H	-0.17238	0.51345	10.17149
H	-2.55103	1.03031	10.33826
H	-6.43980	0.47036	5.12849
H	-5.95838	0.51231	7.51834
H	-5.38398	2.43356	6.12346
H	4.67384	4.73157	7.26486
H	2.57432	4.73316	8.51093
H	3.59897	2.62421	7.84544
H	-1.52350	3.50480	-0.02046
H	-2.75797	4.43339	0.45261
H	-2.31503	7.20887	3.67977
H	-0.86208	6.94381	4.40689
H	-0.95078	7.78031	2.98589

La]@b**c-1 Intermediate NH2 transfer**
G = -1786.252901 kcal. mol^{-1}

O	0.16288	-1.21032	-4.04893
Si	0.18933	-2.55010	-5.07737
Si	0.08213	-1.07243	-2.40984
O	1.60858	-0.67474	-1.86549
Si	2.42549	-0.08143	-0.56786
O	2.61666	-1.19236	0.63614
Si	1.83033	-2.45480	1.39418
O	2.93816	-3.43361	2.11686
O	-0.89618	0.18324	-1.99931
Si	-2.69546	0.55299	-1.80150
O	-3.96644	0.10135	-2.80524
O	-0.38298	-2.53782	-1.80856
Si	-0.47002	-3.41321	-0.40019
O	1.03555	-3.38151	0.29735
La	-0.67824	2.41970	-0.80140
N	-0.80688	5.14390	-0.73958
N	-2.24204	2.03367	-2.91984
Si	1.44018	2.03758	1.53911
O	0.35025	3.16527	1.19955
O	1.56487	1.24245	-0.00134
O	-2.67781	1.57444	-0.46477
O	-1.62483	-2.81352	0.62042
Si	-2.27786	-1.26517	0.63149
O	-3.42491	-1.27840	1.81416
Si	-4.77888	-0.32435	2.13173
O	-0.81467	-4.98300	-0.76036
O	-0.97948	-0.27945	1.14016
Si	-0.08698	-0.40844	2.54504
O	-1.02684	-0.42381	3.88694
Si	-1.25759	-1.51390	5.15532
O	-2.85232	-0.94652	-0.85040
O	0.95448	0.87465	2.62923
O	0.80973	-1.81249	2.53443
O	2.94662	2.53040	1.99259
Si	3.82589	2.38096	3.42433
O	3.90212	0.43870	-1.05971
Si	5.44693	-0.24433	-1.07087
H	-4.37526	-0.69859	-2.45267
H	-1.70922	-5.23721	-0.51469
H	3.37436	-3.04645	2.88138
H	5.39503	-1.65400	-1.55552
H	6.26618	0.58857	-1.99580
H	6.03026	-0.20104	0.30171
H	0.47954	-2.01678	-6.43958
H	1.25888	-3.50746	-4.67035
H	-1.13559	-3.23463	-5.07441
H	-1.53044	-2.88513	4.64116
H	-0.04462	-1.53436	6.02732
H	-2.42396	-1.00991	5.93353
H	-5.66244	-0.24081	0.93235
H	-5.50890	-1.00949	3.23896
H	-4.37871	1.04298	2.56991
H	5.05553	3.20544	3.24858
H	3.03599	2.88751	4.58465
H	4.20663	0.95694	3.65975
H	-1.93608	1.72282	-3.83958
H	-3.09204	2.57202	-3.07637
H	-1.73662	5.54258	-0.63491
H	-0.33728	5.22068	0.16406
H	-0.30740	5.73751	-1.39613

La]@b**c-1 TS Si-O activation**
G = -1786.251405 kcal. mol^{-1}

O	0.70772	-1.89985	-3.96348
Si	0.47815	-1.51895	-2.38341
O	-0.04764	-2.85415	-1.58143
Si	-0.62605	-3.30486	-0.08151
O	-1.37369	-4.76654	-0.21576
Si	0.60769	-3.33978	-4.84058
O	1.92460	-0.97296	-1.77529
Si	2.63612	-0.45875	-0.37110
O	4.23965	-0.23754	-0.63163
Si	5.15120	0.46005	-1.86733
O	-0.56443	-0.22700	-2.25579
La	-0.53085	1.86281	-0.66751
O	-2.60822	0.62341	-0.74287
Si	-2.33453	-0.05869	-2.39033
O	-2.78978	-1.53338	-1.55896
Si	-2.56400	-0.94314	0.02323
O	-0.93650	0.33046	1.09108
Si	-0.12940	0.07927	2.50495
O	0.47906	-1.46330	2.69613
Si	1.49581	-2.43841	1.84796
O	0.68377	-3.53979	0.90970
O	2.48076	-1.51594	0.86767
O	1.88415	0.99909	-0.01665
Si	1.81441	2.04750	1.37815
O	3.33747	2.51610	1.77697
Si	4.26498	2.33811	3.18087
O	2.42654	-3.26787	2.92316
O	-3.00243	-0.47835	-3.87390
N	-2.05267	1.72550	-2.88371
O	-1.56646	-2.15057	0.62165
N	-1.99195	3.86652	0.39196
O	0.78407	3.14960	0.81227
O	1.19571	1.10978	2.60513
O	-3.82506	-0.94040	1.09301
Si	-5.03121	0.20899	1.31657
O	-1.11040	0.36220	3.80249
Si	-1.29805	-0.43037	5.27858
H	-3.33135	-1.38466	-3.83042
H	-2.24356	-4.71217	-0.62450
H	2.62196	-4.16854	2.64802
H	5.50916	-0.58245	-2.87176
H	4.38010	1.55317	-2.53336
H	6.38364	1.01578	-1.24271
H	0.92722	-2.98603	-6.25252
H	1.59406	-4.33386	-4.32690
H	-0.77081	-3.90465	-4.75794
H	-1.88319	-1.78787	5.08188
H	0.00732	-0.53947	5.99465
H	-2.23690	0.40825	6.08087
H	-5.83291	0.40642	0.07123
H	-5.91309	-0.30269	2.40357
H	-4.45903	1.52744	1.73403
H	5.56660	3.00831	2.89924
H	3.59072	3.00786	4.33144
H	4.48631	0.89640	3.48551
H	-1.73721	1.75795	-3.85136
H	-2.93750	2.22960	-2.86610
H	-2.74820	3.49148	0.96004
H	-1.25704	4.18837	1.02354
H	-2.36036	4.67361	-0.10256

$OPPh_3$
G = -1110,983597 kcal. mol^{-1}

P	0.00000	0.00000	0.00000
O	0.00000	0.00000	1.60000
O	1.50849	0.00000	-0.53333
O	-0.75425	-1.30640	-0.53333
O	-0.75425	1.30640	-0.53333
H	2.10561	0.00000	0.20556
H	0.44783	0.77567	1.91667
H	-0.30641	-2.08207	-0.21667

$OPPh_3$@[La]@**ac-1**
G = -2815,712139 kcal. mol^{-1}

C	-6.683995	-2.937384	-1.713655
C	-8.015854	-2.670991	-2.067897
C	-8.937556	-3.719342	-2.183837
C	-8.528200	-5.032196	-1.958956
C	-7.204515	-5.298641	-1.611586
C	-6.288640	-4.253906	-1.487019
P	-8.478212	-0.945241	-2.370578
C	-8.048556	-0.551610	-4.087045
C	-7.708034	0.771945	-4.400817
C	-7.401787	1.106570	-5.718720
C	-7.436577	0.136339	-6.719740
C	-7.766382	-1.181947	-6.405661
C	-8.066959	-1.529613	-5.090643
C	-10.280322	-0.807059	-2.204112
C	-10.788279	-0.458575	-0.945315
C	-12.163888	-0.351466	-0.757687
C	-13.035688	-0.590967	-1.819796
C	-12.533062	-0.930389	-3.075377
C	-11.157369	-1.034791	-3.271641
O	-7.796904	-0.004692	-1.383462
La	-5.964906	1.447908	-0.598202
O	-3.171662	1.618204	-0.270015
Si	-2.463474	2.720742	0.750304
O	-1.336724	3.614483	-0.059888
Si	-0.301148	3.514135	-1.344926
O	-0.144079	4.990201	-2.036597
Si	-0.894391	5.790131	-3.318290
N	-6.667856	1.937311	1.573501
N	-6.237714	3.173704	-2.145055
Si	-3.017460	-0.002171	-0.793314
O	-1.990687	-0.016190	-2.108774
Si	-0.788203	0.837652	-2.842362
O	-0.930209	0.678816	-4.471517
Si	-2.148913	0.059464	-5.458697
O	-4.521976	-0.428386	-1.091504
O	-2.258252	-0.848673	0.427113
Si	-0.758366	-1.315038	0.929991
O	-0.168382	-0.246329	2.047516
Si	-0.282153	1.343749	2.476374
O	-0.151765	1.480859	4.102452
Si	1.079173	1.979869	5.145957
O	-3.668535	3.694288	1.273610
H	-3.380254	4.381915	1.878310
O	-1.756674	1.946236	2.030336
O	0.296117	-1.416359	-0.339799
Si	1.425616	-0.492385	-1.121925
O	0.698650	0.261514	-2.405640
O	-0.854087	-2.801096	1.621133
Si	-2.138457	-3.753213	2.154364
O	2.111466	0.612194	-0.107172
Si	1.879659	2.168664	0.407996
O	3.315035	2.834488	0.856712
O	2.670553	-1.433918	-1.645209
O	1.191050	3.038104	-0.822613
O	0.931500	2.211456	1.757669
O	-0.895798	2.445797	-2.462359
H	3.986918	2.844432	0.168626
H	2.404669	-2.199671	-2.162520
H	-1.535933	-4.879656	2.922247
H	-3.055397	-2.968698	3.031443
H	-2.898378	-4.293089	0.987909
H	0.627445	1.621054	6.520161
H	2.354275	1.275137	4.826268
H	1.271824	3.454991	5.041550
H	-1.718793	0.317980	-6.862807
H	-2.303100	-1.408630	-5.241244
H	-3.444880	0.748708	-5.192608
H	-0.542389	7.231408	-3.180406
H	-0.380586	5.263465	-4.616302
H	-2.374987	5.615768	-3.253521
H	-6.621139	1.330113	2.388729
H	-7.194189	2.756915	1.868563
H	-6.728038	4.049682	-1.975167
H	-5.732139	3.304489	-3.018371
H	-10.768840	-1.275795	-4.257241
H	-13.211187	-1.103943	-3.906001
H	-14.108433	-0.504583	-1.670953
H	-12.554778	-0.075642	0.217436
H	-10.102448	-0.257686	-0.127412
H	-9.974031	-3.511506	-2.434379
H	-9.245138	-5.843726	-2.045548
H	-6.887842	-6.322350	-1.431195
H	-5.259561	-4.459961	-1.207493
H	-5.961780	-2.129352	-1.601126
H	-8.298278	-2.562529	-4.844110
H	-7.778706	-1.942181	-7.181471
H	-7.197627	0.405156	-7.745089
H	-7.131431	2.130492	-5.960483
H	-7.647918	1.533095	-3.622069

$OPPh_3$@[La]@**ac-2**
G = -2815,77005 kcal. mol^{-1}

Si	-6.41507	-7.22057	7.05378
Si	-6.26309	-5.69735	-0.17692
O	-5.26383	-6.70582	0.66573
Si	-5.99651	-6.17645	4.22618
Si	-4.11066	-6.93308	1.83083
O	-7.31883	-5.87857	3.27740
O	-6.52366	-6.34161	-1.67299
O	-7.70222	-5.57522	0.63719
O	-7.70300	-3.36390	2.18970
Si	-6.62020	-2.14358	2.45897
O	-5.54669	-2.00135	1.20633
O	-5.88604	-2.30488	3.93239
O	-3.24923	-3.38003	0.54406
O	-4.34192	-4.08575	2.81266
Si	-2.91047	-4.22221	1.95664
O	-3.54067	-2.90032	5.19523
Si	-4.74808	-3.48478	4.32105
O	-5.52846	-4.79703	5.01887
La	-1.23272	-2.74700	4.82659
O	-1.16111	-0.60087	6.07590
P	-1.97304	0.39163	6.91974
C	-0.84197	1.58311	7.68983
C	-1.22406	2.34692	8.80066
C	-0.33096	3.25902	9.35668
C	0.94589	3.40673	8.81365
C	1.33241	2.64108	7.71464
C	0.44147	1.72998	7.15105
O	-6.45534	-7.26830	5.37284
O	-4.78539	-6.88001	3.34236
O	-1.60238	-3.67798	2.70802
O	-2.85710	-5.86723	1.62340
O	-3.50172	-8.45070	1.62435
Si	-1.93756	-9.00959	1.35459
Si	-4.75181	-2.89012	0.05408
O	-4.55524	-1.89343	-1.24172
Si	-4.71871	-2.11029	-2.90245
O	-7.46708	-0.72524	2.52747
Si	-9.06594	-0.34525	2.15293
Si	-8.07807	-4.96630	2.13131
O	-9.70893	-5.04008	2.36717
O	-5.65616	-4.18935	-0.43101
N	0.10187	-4.22845	5.99745
N	0.37949	-1.59118	2.92015
C	-3.18649	1.30154	5.93809
C	-3.14018	2.69602	5.81087
C	-4.07472	3.34872	5.00968
C	-5.05065	2.61546	4.33635
C	-5.09986	1.22580	4.45845
C	-4.17001	0.56397	5.25661
C	-2.85633	-0.45104	8.25830
C	-4.14613	-0.07308	8.64993
C	-4.77919	-0.74287	9.69549
C	-4.13204	-1.79037	10.34770
C	-2.84662	-2.17034	9.96021
C	-2.20704	-1.50264	8.92082
H	-10.03710	-5.92889	2.53197
H	1.38042	-1.76010	2.95561
H	-6.53572	-7.30323	-1.67838
H	-6.15645	-2.25282	-3.27526
H	-4.15732	-0.88349	-3.54089
H	-3.95674	-3.30752	-3.36509
H	-9.99822	-0.94574	3.15071
H	-9.15944	1.14367	2.21940
H	-9.42096	-0.80754	0.77988
H	-2.02773	-10.49838	1.31262
H	-1.40798	-8.50714	0.05216
H	-1.02213	-8.59615	2.45920
H	-7.32767	-6.16202	7.58022
H	-6.88692	-8.55669	7.52174
H	-5.02926	-6.97745	7.55277
H	0.50929	-4.14257	6.92514
H	0.27433	-5.18835	5.70604
H	0.24369	-0.62927	2.62386
H	-0.01534	-2.19820	2.19936
H	-2.37870	3.26884	6.33137
H	-4.03702	4.42981	4.91028
H	-5.77683	3.12709	3.71081
H	-5.85940	0.65286	3.93524
H	-4.21123	-0.52066	5.33973
H	-4.66227	0.72746	8.12857
H	-5.78391	-0.45409	9.98957
H	-4.63199	-2.31749	11.15525
H	-2.34517	-2.99193	10.46297
H	-1.20793	-1.80307	8.61780
H	-2.21111	2.22151	9.23768
H	-0.62833	3.84834	10.21919
H	1.64226	4.11532	9.25315
H	2.32953	2.74991	7.29789
H	0.73538	1.11943	6.30275

$OPPh_3$@[La]@**c-1**
G = -2820,835638 kcal. mol^{-1}

O	-6.93695	-2.95579	-4.42646
O	-5.99392	-1.12662	-2.68486
Si	-5.69623	-1.86870	-1.23818
Si	-6.51811	-4.55118	-4.53665
Si	-5.98982	-4.91102	-1.53178
Si	-2.76300	-4.97832	-2.22831
Si	-3.36825	-4.69608	-5.19429
O	-2.04047	-3.50289	-2.03664
H	-1.06919	-2.38664	1.18517
Si	-0.92669	-1.04608	0.54615
O	-1.53100	-1.06627	-1.02760
Si	-2.63258	-1.96160	-1.84558
O	-2.85066	-1.24584	-3.31621
Si	-3.20536	-1.60695	-4.89302
O	-4.82767	-1.37936	-5.13268
Si	-6.24041	-1.46065	-4.28767
O	-7.21662	-0.31765	-4.95979
La	-4.10946	-6.78358	0.36820
O	-2.19814	-6.17078	-1.25437
Si	-0.94854	-7.51109	-1.44948
O	-6.58570	-5.26971	-3.04786
O	-6.44312	-3.34404	-1.15903
O	-4.30535	-4.84655	-1.63066
O	-6.25614	-6.02835	-0.41964
O	-7.59833	-5.29981	-5.51890
Si	-8.56359	-6.67148	-5.35175
O	-5.01364	-4.68278	-5.19877
O	-2.77359	-3.15331	-5.26787
O	-2.85851	-5.55148	-6.49109
Si	-1.51189	-5.47971	-7.50904
O	-2.79482	-5.42655	-3.81738
O	-6.31852	-0.91129	-0.05429
Si	-7.26855	-1.22145	1.30034
O	-4.06114	-1.99274	-1.00524
O	-5.29113	-8.66417	1.43512
P	-6.10417	-9.27048	2.57809
N	-3.50885	-5.68350	2.31124
N	-2.34190	-8.51245	-0.38328
O	-2.33904	-0.65084	-5.91296

H	-2.47725	0.29331	-5.79289
H	-8.11363	-0.30263	-4.61376
H	-9.21310	-6.88967	-6.67545
H	-7.73710	-7.86043	-4.98987
H	-9.60773	-6.44981	-4.30826
H	-1.43973	-6.79864	-8.19924
H	-1.69754	-4.39085	-8.51105
H	-0.26899	-5.24243	-6.72014
H	-7.32814	0.05157	2.07380
H	-8.64715	-1.62572	0.89356
H	-6.66266	-2.29548	2.14189
H	0.51233	-0.66833	0.45956
H	-1.66881	-0.02617	1.34347
H	0.03927	-7.72045	-0.32656
H	-1.01342	-8.59789	-2.50137
H	-0.11333	-6.52342	-2.27472
H	-2.69191	-9.24731	-0.99771
H	-1.83862	-9.01876	0.34456
H	-2.56421	-5.58222	2.67621
H	-4.08541	-5.02165	2.82590
C	-6.82142	-10.85174	2.05222
C	-5.06644	-9.58632	4.03032
C	-7.45342	-8.17949	3.09632
C	-8.05392	-11.31383	2.52931
C	-8.54561	-12.54635	2.10373
C	-7.81538	-13.31565	1.19887
C	-6.59174	-12.85359	0.71390
C	-6.09323	-11.62493	1.13781
H	-8.63507	-10.70743	3.21813
H	-9.50423	-12.90050	2.47167
H	-8.20413	-14.27353	0.86489
H	-6.02774	-13.44814	0.00113
H	-5.14800	-11.25322	0.75375
C	-7.98295	-8.24333	4.39318
C	-9.04075	-7.41203	4.75244
C	-9.56225	-6.50845	3.82609
C	-9.02527	-6.43290	2.54181
C	-7.97270	-7.26674	2.16753
H	-7.56027	-8.92706	5.12474
H	-9.44851	-7.46078	5.75807
H	-10.38257	-5.85523	4.11062
H	-9.41841	-5.71928	1.82393
H	-7.54809	-7.17899	1.16989
C	-5.16499	-10.76829	4.77484
C	-4.34924	-10.95778	5.88909
C	-3.43255	-9.97452	6.25718
C	-3.32862	-8.79949	5.51185
C	-4.14134	-8.59645	4.39934
H	-5.86703	-11.54342	4.48090
H	-4.42516	-11.87682	6.46310
H	-2.79426	-10.12600	7.12331
H	-2.60938	-8.03635	5.79531
H	-4.04252	-7.67945	3.81494

$OPPh_3$@[La]@**abc-1**,
G = -2892,154332 kcal. mol^{-1}

C	0.84552	4.64574	4.54357
C	-0.52493	4.82905	4.78614
C	-0.94206	5.38928	5.99825
C	0.00009	5.76382	6.95593
C	1.35883	5.58001	6.70952
C	1.78154	5.02078	5.50222
P	-1.70408	4.24908	3.52877
C	-3.37173	4.68476	4.09145
C	-3.91710	5.95450	3.85521
C	-5.20147	6.25252	4.30255
C	-5.94933	5.28450	4.97429
C	-5.41282	4.01849	5.20330
C	-4.12281	3.71414	4.76959
O	-1.55605	2.74747	3.31263
La	-2.49884	0.51864	2.64000
Si	-4.86448	-0.45541	4.78269
O	-6.25830	0.24809	5.37060
N	-0.34148	0.21151	4.34917
N	-3.46907	1.69800	0.83950
O	-3.55064	0.44570	4.79766
O	-5.07001	-0.79555	3.11504
Si	-6.38581	-1.32293	2.25364
O	-5.87588	-1.83902	0.77067
Si	-4.48688	-2.41313	0.07333
O	-4.47470	-4.07757	0.11085
Si	-4.85229	-5.26934	1.19880
O	-5.14649	-6.67140	0.38360
Si	-1.53459	-2.28646	1.04945
O	-0.89095	-2.58913	-0.44950
O	-3.18505	-1.84412	0.90737
O	-0.90799	-1.05412	1.84542
O	-7.50238	-0.14972	2.01431
Si	-8.88329	0.42456	2.78872
O	-7.09984	-2.56761	3.09230
Si	-6.77580	-4.16148	3.38228
O	-8.20787	-4.81880	3.86005
O	-5.63941	-4.32193	4.57755
Si	-4.33508	-3.46292	5.12849
O	-3.76970	-4.27622	6.44178
Si	-3.15474	-3.78383	7.93111
O	-6.24564	-4.93103	2.01574
O	-3.59439	-5.48269	2.25887
Si	-2.43927	-4.52123	2.97471
O	-1.51818	-3.77478	1.84157
O	-3.17791	-3.37531	3.93335
O	-1.49145	-5.50237	3.89249
Si	-1.39352	-7.17210	4.09926
O	-4.46423	-1.97143	-1.50698
Si	-5.53412	-1.14125	-2.51204
O	-4.76692	-1.93730	5.57631
C	-1.35421	5.18635	2.01830
C	-0.75458	6.45294	2.04869
C	-0.52901	7.14219	0.85903
C	-0.89422	6.56770	-0.35825
C	-1.48732	5.30570	-0.38756
C	-1.72306	4.60675	0.79500
H	-2.59056	-5.00209	8.57861
H	-6.84756	-1.84767	-2.57368
H	-0.93911	-3.51536	-0.70363
H	-6.79794	-0.36720	5.87733
H	-8.22338	-5.78037	3.85844
H	-4.59686	-6.79852	-0.39495
H	-5.73329	0.25568	-2.03053
H	-4.90618	-1.12782	-3.86438
H	-8.67656	1.86393	3.11587
H	-10.02623	0.28915	1.83841
H	-9.17170	-0.34939	4.03006
H	-2.68517	-7.72238	4.60204
H	-1.03283	-7.83639	2.81107
H	-0.31602	-7.40671	5.10259
H	-4.24269	-3.21749	8.78147
H	-2.07912	-2.76379	7.75096
H	0.24105	-0.45018	3.84433
H	-0.62006	-0.19984	5.23389
H	0.18840	1.05292	4.54577
H	-4.25335	2.34640	0.86736
H	-3.34044	1.46183	-0.14262
H	-3.34822	6.70207	3.30917
H	-5.62347	7.23566	4.11401
H	-6.95615	5.51646	5.31093
H	-5.99501	3.25177	5.70560
H	-3.72383	2.71673	4.94654
H	-0.45247	6.89480	2.99438
H	-0.06109	8.12237	0.88267
H	-0.71212	7.10433	-1.28557
H	-1.76772	4.85793	-1.33696
H	-2.19253	3.61634	0.77342
H	-2.00072	5.52882	6.19512
H	-0.33028	6.19676	7.89577
H	2.09080	5.87203	7.45741
H	2.84085	4.87805	5.30836
H	1.17757	4.21369	3.60306

$OPPh_3$@[La]@**bc-1**
G = -2897,27464 kcal. mol^{-1}

C	-1.57600	4.58098	0.79566
C	-1.18834	5.13063	2.02778
C	-0.44310	6.31607	2.07031
C	-0.08704	6.95361	0.88327
C	-0.46824	6.40791	-0.34180
C	-1.20915	5.22627	-0.38305
P	-1.69237	4.25238	3.52992
O	-1.47151	2.74524	3.42209
La	-2.54978	0.59343	2.70316
O	-0.95966	-0.91950	1.80990
Si	-1.60306	-2.14371	1.01540
O	-1.52888	-3.64654	1.77416
Si	-2.42136	-4.43989	2.89961
O	-1.43954	-5.40116	3.80354
Si	-1.22124	-7.06938	3.90706
C	-0.69975	4.92314	4.89750
C	0.63389	4.50225	5.00828
C	1.43370	4.98000	6.04200
C	0.90914	5.87888	6.97200
C	-0.41510	6.29935	6.86702
C	-1.22067	5.82360	5.83299
C	-3.42766	4.66301	3.85526
C	-3.99261	5.86504	3.40764
C	-5.33048	6.14559	3.67569
C	-6.11039	5.22544	4.37658
C	-5.55271	4.02580	4.81700
C	-4.21135	3.74246	4.56581
Si	-4.97480	-0.47657	4.81516
O	-4.80800	-1.97949	5.55977
Si	-4.34230	-3.48147	5.07660
O	-3.19325	-3.33269	3.87643
N	-0.45636	0.12380	4.46225
N	-3.57375	1.86241	0.99343
O	-3.65421	0.41922	4.80635
O	-6.32685	0.19321	5.51134
Si	-7.20988	-0.23093	6.88016
O	-5.29038	-0.76016	3.16750
Si	-6.54511	-1.36668	2.28280
O	-7.19972	-2.68337	3.05563
Si	-6.77690	-4.25601	3.33137
O	-6.21452	-4.97243	1.94760
Si	-4.81108	-5.22204	1.11913
O	-3.54229	-5.42998	2.16881
O	-5.96612	-1.80677	0.79725
Si	-4.55211	-2.30901	0.09897
O	-4.53235	-1.81723	-1.46704
Si	-5.59940	-0.94861	-2.44121
O	-7.73587	-0.25863	2.07199
Si	-9.41379	-0.29230	2.23713
O	-4.47563	-3.97144	0.08378
O	-3.26901	-1.72520	0.95833
O	-5.05342	-6.59951	0.24715
O	-1.02495	-2.39960	-0.51831
O	-8.16505	-4.99818	3.81242
O	-5.61968	-4.36935	4.51049
O	-3.74729	-4.31673	6.36274
Si	-2.99428	-3.86857	7.80060
H	-2.33158	-5.09234	8.33459
H	-6.89943	-1.67177	-2.56558
H	-1.08974	-3.31587	-0.80302
H	-8.09696	-5.95346	3.89946
H	-4.47010	-6.69739	-0.51078
H	-5.83204	0.41479	-1.88412
H	-4.95110	-0.84702	-3.78003
H	-9.89830	1.05718	1.82781
H	-10.00700	-1.33313	1.34723
H	-9.79784	-0.55990	3.65296
H	-2.46281	-7.73661	4.39420
H	-0.83916	-7.63050	2.57662
H	-0.11233	-7.28650	4.87962
H	-4.00469	-3.37247	8.77990
H	-1.97097	-2.80759	7.55861
H	0.14827	-0.49350	3.92823
H	-0.75149	-0.35185	5.30835
H	0.05867	0.95479	4.72972
H	-4.36306	2.49792	1.09131
H	-3.48287	1.68681	-0.00552
H	-3.39481	6.57151	2.83821
H	-5.76714	7.07606	3.32403
H	-7.15738	5.44074	4.57166
H	-6.15825	3.29515	5.34437
H	-3.79604	2.79593	4.90638
H	-0.13447	6.73630	3.02331
H	0.49353	7.87123	0.91635
H	-0.18500	6.90388	-1.26638
H	-1.50350	4.80197	-1.33903

H	-2.16520	3.65671	0.77225
H	-2.25508	6.14601	5.75924
H	-0.82587	6.99431	7.59379
H	1.53363	6.24904	7.78029
H	2.46553	4.65040	6.12402
H	1.04003	3.79982	4.28557
H	-8.21903	0.85191	7.07754
H	-7.91007	-1.53435	6.69188
H	-6.32846	-0.30432	8.08427

$OPPh_3$@[La]@**b-1**
G = -2902,397165 kcal. mol^{-1}

C	-0.95295	5.03949	1.23220
C	-0.67069	5.31060	2.58200
C	0.22947	6.32756	2.92140
C	0.84260	7.07667	1.91805
C	0.56236	6.80998	0.57916
C	-0.33157	5.79325	0.23954
P	-1.48840	4.27708	3.82862
O	-1.28430	2.78830	3.55158
La	-2.28595	0.90803	2.21119
O	-1.73333	-1.08139	1.10480
Si	-2.44447	-2.38775	0.50558
O	-2.09875	-3.79082	1.37305
Si	-2.63298	-4.45603	2.77492
O	-1.37638	-5.17617	3.55719
Si	-1.01675	-6.77783	3.93942
C	-0.79486	4.69608	5.45309
C	0.18251	3.84873	5.98865
C	0.74864	4.13462	7.22874
C	0.34315	5.26487	7.93736
C	-0.63541	6.10794	7.41042
C	-1.20862	5.82428	6.17303
C	-3.24068	4.73577	3.84328
C	-3.67388	6.00688	3.44185
C	-5.02976	6.32370	3.48881
C	-5.95506	5.37287	3.92024
C	-5.52788	4.10342	4.30889
C	-4.17206	3.78262	4.27964
Si	-5.03829	-0.33785	4.36898
O	-4.72635	-1.67491	5.34680
Si	-4.19257	-3.21275	5.11116
O	-3.28707	-3.25297	3.71676
N	0.42025	0.47053	2.03768
N	-3.12380	2.34937	0.58022
O	-3.71965	0.48278	3.96901
O	-5.80085	-0.86647	2.97398
Si	-7.07201	-1.78382	2.49249
O	-7.39347	-2.98411	3.59619
Si	-6.80519	-4.45407	4.05704
O	-6.45177	-5.40595	2.74776
Si	-5.22307	-5.70015	1.68326
O	-3.77123	-5.63078	2.48314
O	-6.12735	0.56627	5.25200
O	-6.73180	-2.44856	1.01612
Si	-5.46081	-3.01904	0.12364
O	-5.84424	-2.91806	-1.47166
Si	-6.06304	-1.66483	-2.57294
O	-8.42976	-0.86929	2.34092
Si	-10.05570	-1.13590	2.69130
O	-5.23918	-4.63799	0.41527
O	-4.10969	-2.16451	0.50504
O	-5.45056	-7.22021	1.08637
O	-1.98810	-2.74521	-1.05617
O	-8.01516	-5.15570	4.92723
O	-5.44685	-4.28533	4.99275
O	-3.30286	-3.69998	6.40862
Si	-2.32667	-2.89014	7.51395
H	-1.46019	-3.92026	8.15586
H	-7.52293	-1.50129	-2.83787
Si	-1.08679	-3.99971	-1.70719
Si	-6.73784	0.35316	6.80298
H	-7.85827	-6.07803	5.14959
H	-5.33984	-7.27081	0.13230
H	-5.50121	-0.38484	-2.05131
H	-5.36926	-2.04719	-3.83682
H	-10.81442	-0.04070	2.02008
H	-10.50691	-2.45756	2.16540
H	-10.28668	-1.07387	4.16417
H	-2.07134	-7.36645	4.81435
H	-0.87597	-7.59577	2.69844
H	0.28476	-6.74778	4.66793
H	-3.16309	-2.21988	8.55204
H	-1.47162	-1.87300	6.83091
H	0.28641	-0.40527	1.53074
H	0.94700	0.27651	2.88353
H	0.98464	1.09405	1.46885
H	-3.92981	2.95940	0.70094
H	-3.02323	2.21672	-0.42408
H	-2.95886	6.73872	3.07589
H	-5.36454	7.30805	3.17393
H	-7.01303	5.61926	3.94342
H	-6.24079	3.34838	4.62555
H	-3.85562	2.78239	4.56772
H	0.45598	6.53223	3.96369
H	1.54140	7.86474	2.18393
H	1.04201	7.39432	-0.20145
H	-0.54850	5.58527	-0.80460
H	-1.64702	4.23798	0.96034
H	-1.98760	6.47023	5.77720
H	-0.96115	6.98105	7.96842
H	0.78317	5.48498	8.90597
H	1.50182	3.47161	7.64469
H	0.47820	2.96281	5.43523
H	-7.65485	1.50646	7.05200
H	-7.50444	-0.92107	6.92300
H	-5.64482	0.37645	7.82204
H	-0.91698	-3.69786	-3.15984
H	0.26279	-4.08838	-1.06831
H	-1.78399	-5.31230	-1.55738

$OPPh_3$@[La]@**bc-3**
G = -2897,210275 kcal. mol^{-1}

O	1.263337	0.167168	1.761896
Si	2.300428	0.093217	0.492336
O	2.859057	1.566635	0.053078
Si	4.028665	2.701486	0.463879
La	3.416102	5.828461	0.997656
N	5.190151	7.313479	0.770786
Si	1.211217	-0.588603	3.268523
O	3.543970	-0.924205	0.915117
Si	4.777955	-1.737250	0.184198
O	6.020397	-0.724584	-0.233526
Si	6.175027	0.861124	-0.692459
O	5.399298	1.068716	-2.155506
Si	5.371535	0.320270	-3.628117
O	4.091511	0.960776	-4.466152
Si	2.733371	1.824375	-4.068177
O	1.935435	2.167390	-5.466698
Si	1.879487	1.454906	-6.997771
O	1.473622	-0.548339	-0.798200
Si	1.447656	-0.505707	-2.445621
O	1.795456	1.018726	-2.984602
O	5.285855	-2.845619	1.289478
O	4.242285	-2.517456	-1.179672
Si	3.997744	-2.280252	-2.788114
O	5.182737	-1.318789	-3.450919
O	-0.046880	-0.935750	-2.968680
Si	-1.524960	-1.210139	-2.202408
O	2.531613	-1.572899	-3.095281
O	5.502995	1.891534	0.392940
O	3.817335	3.559101	1.790688
O	3.956351	3.871648	-0.752541
O	7.785060	1.150068	-0.844452
Si	8.777305	2.408140	-0.306657
O	4.052307	-3.778540	-3.468446
O	3.104312	3.276183	-3.337267
O	6.738741	0.586418	-4.490883
Si	8.011797	-0.383351	-5.029740
N	1.515266	6.530429	-0.182184
H	6.004517	-3.409844	0.989561
H	3.750380	-3.814833	-4.380695
H	-1.431330	-2.393834	-1.299405
H	-1.942281	-0.008872	-1.422082
H	-2.510352	-1.477103	-3.288684
H	0.019054	-0.034421	3.971653
H	1.056537	-2.064154	3.105184
H	2.445335	-0.294631	4.051731
H	8.551245	-1.214643	-3.916073
H	7.542619	-1.266113	-6.138573
H	9.060390	0.547201	-5.533926
H	8.916354	2.356623	1.177665
H	10.105771	2.184219	-0.945995
H	8.227037	3.729721	-0.723882
H	3.678984	3.616404	-1.652921
H	3.133461	4.028876	-3.936151
H	0.665153	1.996060	-7.670292
H	3.099294	1.826401	-7.772358
H	1.784604	-0.029739	-6.884223
H	1.348193	7.481656	-0.505230
H	0.776721	5.964359	-0.593570
H	6.127763	7.227007	1.155975
H	5.196820	8.165201	0.213709
O	2.566704	6.273969	3.285604
P	1.672273	5.958011	4.477253
C	1.320715	7.482462	5.399169
C	0.084713	5.244883	3.967916
C	2.464341	4.786700	5.611370
C	0.145088	7.666552	6.137144
C	-0.058155	8.854641	6.836443
C	0.903990	9.863072	6.794323
C	2.070034	9.687819	6.049352
C	2.281514	8.501405	5.351485
H	-0.617673	6.892935	6.152089
H	-0.972747	8.996470	7.405167
H	0.740493	10.790669	7.335936
H	2.813966	10.478088	6.006321
H	3.177854	8.364361	4.753611
C	2.331627	4.891011	7.001923
C	2.946946	3.955122	7.830834
C	3.701346	2.922751	7.274867
C	3.842421	2.824799	5.890539
C	3.226683	3.750114	5.049931
H	1.762419	5.707417	7.437828
H	2.845566	4.039468	8.909184
H	4.186162	2.197132	7.922437
H	4.438390	2.027160	5.456688
H	3.353631	3.665737	3.970384
C	-0.640596	4.390147	4.809095
C	-1.872785	3.888670	4.395667
C	-2.377621	4.227751	3.140648
C	-1.649100	5.064821	2.296739
C	-0.419106	5.579301	2.702847
H	-0.236647	4.102276	5.776144
H	-2.431102	3.223070	5.047794
H	-3.334972	3.828998	2.816445
H	-2.033811	5.316546	1.312569
H	0.154267	6.207019	2.019444

$OPPh_3$@[La]@**abc-2**
G = -2892,181062 kcal. mol^{-1}

Si	0.17396	7.49139	-9.42080
O	-0.41095	6.72559	-8.02672
Si	-0.78200	7.40212	-6.53223
O	-2.05414	6.41860	-5.91406
Si	-3.06357	5.30064	-6.65006
O	-2.29113	4.56351	-7.90114
La	-0.89925	6.63913	-3.34831
N	1.01172	7.81769	-1.90816
Si	-2.94694	9.22664	-3.48870
O	-3.89977	10.15592	-2.49042
H	-3.62908	10.08624	-1.56934
O	-1.43818	8.94279	-3.04328
O	-3.20322	9.91069	-4.98865
Si	-2.90136	9.63257	-6.58647
O	-2.88255	11.07641	-7.37562
Si	-2.97809	12.66955	-6.83601
O	-3.60390	7.63078	-3.57264
Si	-5.15857	7.09772	-3.83087
O	-5.13321	5.44398	-3.80537
Si	-3.97995	4.26722	-3.95014
O	-4.67835	2.85328	-3.49306
Si	-4.45034	1.23635	-3.91961
O	-5.70537	7.63912	-5.29754
Si	-5.18042	7.52006	-6.86203
O	-6.53467	7.65184	-7.78976
O	-4.11587	8.72044	-7.25720

O	-4.45558	6.04903	-7.13999
O	-6.18485	7.60158	-2.65720
Si	-7.23393	8.91073	-2.44967
O	0.31489	7.36224	-5.38399
Si	-2.44521	4.67110	-1.28119
O	-1.91019	3.10803	-0.98522
O	-2.65456	4.63215	-3.02326
O	-1.40130	5.88225	-1.13754
O	-1.44937	8.89463	-6.87568
N	-3.93177	4.86304	-0.42586
O	-3.44466	4.14917	-5.51957
O	0.72615	4.76800	-3.56926
P	2.04029	4.14364	-4.02537
H	-1.97538	2.89788	-0.04791
H	0.74011	6.41083	-10.27970
H	1.24051	8.47309	-9.06890
H	-0.93517	8.17611	-10.14441
H	-5.30505	0.90812	-5.09756
H	-3.01966	0.96443	-4.24221
H	-4.87342	0.42026	-2.74607
H	-1.90028	12.96216	-5.84575
H	-2.79449	13.52717	-8.04295
H	-4.31185	12.94240	-6.22537
H	-7.05844	9.92675	-3.52199
H	-6.95352	9.50200	-1.10949
H	-8.62997	8.38113	-2.46820
H	-1.52941	5.09986	-8.18196
H	-6.36083	7.81183	-8.72191
H	1.99183	7.78025	-2.16761
H	0.91264	7.51227	-0.94424
H	0.68584	8.77965	-1.97667
H	-4.67084	4.19094	-0.58255
H	-4.30427	5.79923	-0.34638
C	3.43423	5.29841	-3.88134
C	2.39481	2.67243	-3.02574
C	1.96391	3.60566	-5.75421
C	3.08867	3.61829	-6.58798
C	2.98974	3.14234	-7.89394
C	1.77042	2.66432	-8.37251
C	0.64494	2.66132	-7.54804
C	0.73994	3.12644	-6.23923
H	4.03389	4.01313	-6.22571
H	3.86257	3.15596	-8.54053
H	1.69451	2.30103	-9.39365
H	-0.31235	2.31355	-7.92331
H	-0.13684	3.12994	-5.59864
C	3.41604	1.77416	-3.36647
C	3.64851	0.65375	-2.57431
C	2.85489	0.41846	-1.45030
C	1.82656	1.29976	-1.12275
C	1.59071	2.42908	-1.90595
H	4.01966	1.93949	-4.25525
H	4.44029	-0.04114	-2.83920
H	3.03308	-0.46054	-0.83693
H	1.19615	1.10690	-0.25977
H	0.77407	3.10459	-1.66859
C	4.57949	5.00878	-3.13008
C	5.60176	5.95162	-3.02741
C	5.48129	7.18399	-3.66714
C	4.33566	7.47894	-4.40877
C	3.30874	6.54369	-4.52191
H	4.67184	4.05427	-2.62086
H	6.48872	5.72330	-2.44325
H	6.27872	7.91764	-3.58512
H	4.23714	8.44141	-4.90301
H	2.40431	6.79184	-5.07939

$OPPh_3$@[La]@**bc-2**

G = -2897,300122 kcal. mol^{-1}

Si	0.48971	7.70089	-9.25764
O	-0.67749	7.16650	-8.15510
Si	-1.00736	7.67933	-6.58760
O	-2.25048	6.61541	-6.04549
Si	-3.31405	5.64099	-6.90846
O	-2.57792	5.02507	-8.24096
La	-0.95857	6.44801	-3.56986
N	0.99662	7.58200	-2.13267
Si	-3.09000	9.05261	-3.23062
O	-3.90854	9.88852	-2.05478
Si	-3.54375	10.09287	-0.42666
O	-1.58224	8.63297	-2.88998
O	-3.31359	9.96352	-4.61284
Si	-3.09480	9.92548	-6.24742
O	-3.04215	11.47397	-6.80232
Si	-3.14293	12.96744	-6.03164
O	-3.87358	7.55880	-3.49919
Si	-5.41728	7.07026	-3.84091
O	-5.38312	5.42090	-3.99970
Si	-4.21358	4.30171	-4.33649
O	-4.85797	2.83017	-4.00440
Si	-4.42607	1.24408	-4.39272
O	-5.95640	7.76930	-5.24375
Si	-5.41557	7.90934	-6.80073
O	-6.76855	8.16038	-7.70582
O	-4.38230	9.18384	-6.98781
O	-4.66080	6.51718	-7.30304
O	-6.46977	7.45848	-2.64341
Si	-7.93876	8.29387	-2.62465
O	0.13827	7.51498	-5.49677
Si	-2.43326	4.17645	-1.78379
O	-2.11371	2.54059	-1.96670
O	-2.84850	4.59164	-3.43402
O	-1.21885	5.19973	-1.52989
O	-1.69490	9.18939	-6.72711
N	-3.74429	4.32020	-0.67354
O	-3.75323	4.38053	-5.92920
O	0.70628	4.70036	-4.12374
P	2.07203	4.03250	-4.21254
H	-2.06577	2.08296	-1.12177
H	-0.05487	7.43562	-10.62039
H	1.75339	6.92898	-9.06840
H	0.75473	9.15723	-9.07891
H	-5.35695	0.75380	-5.45178
H	-3.02189	1.16918	-4.88580
H	-4.59371	0.41659	-3.16456
H	-2.05950	13.11550	-5.01534
H	-2.97252	13.99767	-7.09719
H	-4.47299	13.13993	-5.37692
H	-7.77635	9.66360	-3.18862
H	-8.34466	8.37536	-1.19207
H	-8.96875	7.54122	-3.39862
H	-1.84925	5.60632	-8.51663
H	-6.59346	8.43648	-8.61014
H	1.93109	7.67630	-2.51734
H	1.06742	7.21357	-1.18911
H	0.56587	8.50426	-2.08438
H	-4.59913	3.81259	-0.85646
H	-3.93495	5.24006	-0.30101
H	-4.73981	10.72374	0.20366
H	-3.26644	8.78338	0.23843
H	-2.36200	10.99044	-0.25238
C	3.40935	5.26209	-4.22007
C	2.33744	2.91508	-2.81026
C	2.21293	3.06344	-5.73789
C	3.43048	2.89555	-6.40854
C	3.48356	2.12368	-7.56758
C	2.32430	1.52899	-8.06402
C	1.10786	1.70473	-7.40411
C	1.04832	2.46857	-6.24174
H	4.33016	3.38077	-6.03978
H	4.42805	1.99762	-8.08912
H	2.36703	0.93432	-8.97225
H	0.20199	1.25332	-7.79769
H	0.10157	2.61858	-5.73152
C	3.28051	1.87924	-2.85779
C	3.48507	1.07331	-1.74058
C	2.74414	1.29302	-0.57905
C	1.78973	2.30836	-0.53943
C	1.57629	3.12201	-1.65147
H	3.84078	1.68886	-3.76968
H	4.21463	0.26947	-1.78002
H	2.90350	0.66268	0.29157
H	1.20024	2.46831	0.35897
H	0.80280	3.88793	-1.62576
C	4.64686	5.03633	-3.60381
C	5.63807	6.01522	-3.65410
C	5.39454	7.22206	-4.30857
C	4.15791	7.45333	-4.91225
C	3.16107	6.47920	-4.87549
H	4.83291	4.10753	-3.07200
H	6.59589	5.83785	-3.17320
H	6.16677	7.98578	-4.34197
H	3.96158	8.39673	-5.41382
H	2.18944	6.68158	-5.32692

$OPPh_3$@[La]@**b-2**

G = -2902,419094 kcal. mol^{-1}

Si	1.24675	7.57720	-7.84215
O	-0.32546	7.35643	-7.27842
Si	-1.10298	7.86750	-5.92124
O	-1.56359	6.51868	-5.08031
Si	-2.49459	6.23430	-3.72436
O	-3.19477	7.74670	-3.27500
Si	-4.71619	8.38634	-3.58026
O	-5.84362	7.19261	-3.66734
La	-1.45642	7.82997	-1.06222
N	0.69342	6.76276	0.09435
Si	0.20922	9.38660	-3.52158
O	1.40153	10.52311	-3.70585
Si	2.70265	10.90527	-2.71071
O	0.44585	8.25336	-2.41797
O	-0.09783	8.86883	-5.08092
O	-1.21975	10.16707	-2.98359
Si	-2.14669	11.40886	-3.57108
O	-3.47637	11.53871	-2.59188
Si	-4.26948	10.56555	-1.51500
O	-5.31810	11.51498	-0.68106
Si	-6.93595	11.35857	-0.22535
O	-2.62201	11.10783	-5.13067
Si	-3.45105	9.91636	-5.92311
O	-4.11821	10.64939	-7.23835
O	-2.46278	8.68628	-6.41244
O	-4.65791	9.28859	-4.96568
O	-1.33592	12.83511	-3.55048
Si	-1.03397	14.01241	-4.72587
O	-1.72633	5.77402	-2.41281
Si	-2.18061	10.39952	0.79759
O	-3.20239	10.34671	2.12135
Si	-3.14394	11.27232	3.52055
O	-3.19832	9.80069	-0.50640
O	-0.98242	9.33644	0.73274
O	-3.79106	5.30515	-4.25829
Si	-3.80966	4.10330	-5.45401
N	-1.74153	12.05317	0.58362
O	-5.11159	9.37044	-2.30673
O	-2.75471	6.42113	0.51805
P	-3.24333	5.10329	1.11138
H	-5.05972	3.32020	-5.23093
H	-2.61988	3.21418	-5.31872
H	-3.83983	4.71877	-6.81147
H	-7.82087	11.52954	-1.41391
H	-7.18194	10.02667	0.40075
H	-7.19801	12.44157	0.76437
H	2.24262	7.07980	-6.84774
H	1.35256	6.78022	-9.09873
H	1.50562	9.01674	-8.13770
H	-0.33788	13.41818	-5.90158
H	-0.16036	15.02802	-4.07133
H	-2.31316	14.64905	-5.15590
H	-5.41410	6.34337	-3.87033
H	-4.44675	10.04077	-7.90644
H	0.75142	5.79263	0.38531
H	0.92296	7.36004	0.88407
H	1.37520	6.92982	-0.64274
H	-2.46625	12.75435	0.51366
H	-0.97313	12.25633	-0.04048
H	-4.08467	10.63629	4.49271
H	-1.77375	11.29835	4.11609
H	-3.59691	12.67372	3.26449
H	3.29966	12.15970	-3.25460
H	2.26068	11.13449	-1.30226
H	3.72801	9.81880	-2.73496
C	-1.95803	3.82101	1.08974
C	-3.76022	5.36406	2.82951
C	-4.66801	4.45086	0.20155
C	-1.59195	3.10371	2.23533
C	-0.58372	2.14328	2.16196

C	0.06331	1.90176	0.95130
C	-0.29520	2.62134	-0.18997
C	-1.30438	3.58056	-0.13123
H	-2.08572	3.29716	3.18290
H	-0.30160	1.58915	3.05270
H	0.85000	1.15407	0.89708
H	0.21072	2.43730	-1.13363
H	-1.56521	4.15309	-1.02284
C	-4.91445	3.07613	0.09790
C	-6.04209	2.62254	-0.58346
C	-6.91693	3.53543	-1.17149
C	-6.66857	4.90508	-1.07959
C	-5.54935	5.36491	-0.39059
H	-4.22043	2.36117	0.53141
H	-6.22969	1.55574	-0.66570
H	-7.79022	3.17842	-1.71032
H	-7.33327	5.61897	-1.55574
H	-5.35172	6.43051	-0.32493
C	-4.56627	4.44251	3.51158
C	-4.92022	4.67780	4.83738
C	-4.48119	5.83546	5.48122
C	-3.69443	6.76166	4.79870
C	-3.33176	6.53189	3.47259
H	-4.92915	3.55164	3.00576
H	-5.54644	3.96374	5.36453
H	-4.76311	6.01977	6.51418
H	-3.36728	7.67044	5.29485
H	-2.73944	7.26051	2.92695

$OPPh_3$@[La]@**c-2**

G = -2820,847058 kcal. mol^{-1}

O	0.63055	0.05242	3.43423
Si	0.94829	0.95311	4.82406
Si	-0.30482	0.24977	2.10249
O	0.06008	-1.01620	1.10255
Si	-0.18147	-1.66382	-0.39530
O	-0.01274	-3.29589	-0.29708
Si	-1.07499	-4.58985	-0.47440
O	-1.90346	0.16692	2.54477
Si	-3.25177	0.59832	1.67809
N	-4.38377	-0.66879	1.91667
O	-0.07608	1.71676	1.38250
Si	1.03721	2.45099	0.40486
O	2.11076	3.18607	1.42665
O	-3.91299	2.04243	2.14144
La	-4.07187	2.67215	-1.61100
O	-2.27964	4.06875	-1.29359
Si	-0.72926	4.13995	-1.71860
O	0.35752	3.58826	-0.56007
O	-2.80306	0.93737	0.10127
Si	-2.38887	0.11045	-1.33133
O	-1.73944	-1.37138	-0.93845
Si	-4.93627	2.46407	3.41417
O	-3.67735	0.33144	-2.24795
O	-1.09049	1.03300	-1.85737
Si	-0.32353	1.61846	-3.20842
O	-0.98103	1.09946	-4.62383
Si	-0.43063	0.05499	-5.82969
N	-6.16227	3.24151	-0.75987
O	-0.41963	3.25758	-3.13243
O	1.23687	1.04933	-3.10361
Si	1.83727	0.27666	-1.76414
O	0.97364	-1.10953	-1.43611
O	-0.22135	5.68012	-2.08240
Si	0.83124	6.72567	-1.30702
O	1.84714	1.28591	-0.45824
O	3.37516	-0.15550	-2.17096
H	0.54068	0.13363	6.00310
H	2.68530	3.82608	0.99634
H	0.81954	8.00372	-2.07840
H	-1.57820	-4.67045	-1.87702
H	-6.30380	1.90533	3.19717
H	3.74505	-0.85220	-1.62106
H	-0.03379	-1.26092	-5.24960
H	2.22667	6.18403	-1.29197
H	0.40501	6.99414	0.10011
H	2.41298	1.22142	4.88400
H	-4.39418	1.96423	4.71218
H	-5.00091	3.95291	3.43165
H	0.18772	2.23616	4.81541
H	-1.57032	-0.13369	-6.77194
H	0.72615	0.65892	-6.55321
H	-0.30127	-5.81954	-0.14203
H	-2.23165	-4.45681	0.46198
H	-5.26433	-0.64151	1.42259
H	-4.02448	-1.60995	1.98964
H	-6.39766	4.04525	-0.18188
H	-7.00121	2.66574	-0.79255
O	-4.49663	3.20473	-3.92738
P	-5.22751	3.30008	-5.26556
C	-6.42603	4.65974	-5.24050
C	-4.04288	3.59141	-6.60226
C	-6.13060	1.76912	-5.61647
C	-4.33437	3.27785	-7.93651
C	-3.39796	3.54672	-8.93169
C	-2.16832	4.11509	-8.59755
C	-1.86965	4.40983	-7.26786
C	-2.80305	4.15016	-6.26673
H	-5.27842	2.80626	-8.19635
H	-3.62311	3.30088	-9.96549
H	-1.43704	4.31771	-9.37505
H	-0.90629	4.83514	-7.00320
H	-2.56301	4.35489	-5.22832
C	-7.29548	1.76353	-6.39522
C	-7.94765	0.56148	-6.65970
C	-7.44775	-0.63174	-6.13852
C	-6.29732	-0.62503	-5.35040
C	-5.63114	0.57018	-5.08673
H	-7.70322	2.69575	-6.77709
H	-8.85209	0.55887	-7.26133
H	-7.96213	-1.56741	-6.33973
H	-5.91431	-1.55075	-4.93131
H	-4.74594	0.56373	-4.45441
C	-6.69706	5.44211	-6.36978
C	-7.64640	6.45975	-6.29791
C	-8.31736	6.70429	-5.10067
C	-8.03771	5.93480	-3.97124
C	-7.09528	4.91128	-4.03284
H	-6.15714	5.27118	-7.29681
H	-7.85211	7.06826	-7.17383
H	-9.05254	7.50237	-5.04519
H	-8.55049	6.13430	-3.03471
H	-6.86865	4.32851	-3.13963

$OPPh_3$@[La]@**c-3**

G = -2820,892243 kcal. mol^{-1}

O	-5.51482	0.57004	1.15242
La	-3.65232	-0.28986	0.05546
O	-0.31684	1.03395	0.87503
Si	-0.73690	0.49073	2.38716
O	0.01488	1.34701	3.56704
Si	0.72337	0.93688	5.04920
Si	-5.73902	1.85076	2.09205
O	-4.71216	1.81265	3.43909
Si	-3.07780	1.87416	3.58666
O	-2.46153	3.37524	3.31200
Si	-1.91486	4.38295	2.11016
O	-1.46117	5.82269	2.76841
O	-7.27373	1.97971	2.70590
Si	-7.85251	2.40597	4.22341
O	-5.43213	3.30508	1.30641
Si	-4.25897	3.80571	0.26194
N	-5.01574	4.65867	-1.01742
O	-2.55125	0.57992	-1.82104
Si	-2.39551	2.16522	-1.63421
O	-2.82874	3.15314	-2.88659
Si	-3.95931	2.92508	-4.11660
O	-2.37747	-1.98426	0.89700
Si	-1.08407	-2.44615	1.75108
N	0.27267	-3.14806	0.92283
O	-2.40744	0.79261	2.46413
O	-3.42251	2.44913	-0.28424
O	-0.88444	2.71521	-1.17280
Si	-0.08896	2.57371	0.26754
O	-0.60432	3.68396	1.37578
O	1.51340	2.82841	0.01246
Si	2.44640	2.99469	-1.38315
O	-0.40649	-1.10128	2.54299
O	-1.54259	-3.54705	2.92930
Si	-0.53703	-4.66455	3.68577
O	-2.66159	1.44809	5.12895
O	-3.11666	4.74344	1.03911
H	2.15523	0.58859	4.80861
H	-3.32281	0.89752	5.55991
H	-9.33580	2.51979	4.09692
H	2.06815	4.23407	-2.12226
H	-0.23705	-5.82219	2.78849
H	-0.69341	5.76717	3.34504
H	-4.44817	4.27663	-4.51611
H	-7.28996	3.71242	4.67794
H	-7.52788	1.35134	5.23167
H	0.64143	2.14556	5.91491
H	0.73881	-4.05351	4.16121
H	-1.30333	-5.17139	4.86696
H	0.02743	-0.21573	5.68512
H	-3.29668	2.27650	-5.28762
H	-5.10589	2.08273	-3.66653
H	3.86216	3.09076	-0.92542
H	2.28255	1.80623	-2.27104
H	0.05588	-3.83021	0.20735
H	0.94492	-2.48069	0.56632
H	-5.91266	5.06823	-0.79544
H	-4.44388	5.29264	-1.55820
O	-5.15985	-1.84328	-1.02390
P	-6.33042	-2.82816	-0.92259
C	-6.15299	-4.10084	-2.20070
C	-6.37248	-3.64206	0.69361
C	-7.91878	-1.99322	-1.15716
C	-6.70015	-5.38190	-2.05515
C	-6.55211	-6.31951	-3.07474
C	-5.85225	-5.98578	-4.23412
C	-5.29637	-4.71465	-4.37617
C	-5.44494	-3.77018	-3.36347
H	-7.22509	-5.65220	-1.14300
H	-6.97364	-7.31380	-2.95876
H	-5.73284	-6.72116	-5.02485
H	-4.74180	-4.45858	-5.27421
H	-5.00325	-2.78295	-3.46055
C	-7.57895	-4.07032	1.26428
C	-7.57141	-4.70459	2.50443
C	-6.36798	-4.89656	3.18353
C	-5.16815	-4.45904	2.62375
C	-5.16367	-3.83887	1.37602
H	-8.52099	-3.89201	0.75285
H	-8.50724	-5.03328	2.94728
H	-6.36771	-5.37934	4.15695
H	-4.22805	-4.58122	3.15256
H	-4.22067	-3.49173	0.95954
C	-8.91839	-2.51185	-1.98936
C	-10.12860	-1.83391	-2.12308
C	-10.33905	-0.64050	-1.43377
C	-9.34093	-0.12027	-0.60897
C	-8.12863	-0.78991	-0.46436
H	-8.75091	-3.43452	-2.53743
H	-10.90266	-2.23493	-2.77112
H	-11.28244	-0.11235	-1.54232
H	-9.50099	0.81082	-0.07336
H	-7.35094	-0.37099	0.17337