Electronic Supplementary Material (ESI) for Dalton Transactions

DFT study of the Ring Opening Polymerization of ε-caprolactone by grafted lanthanide complexes : 2- Effect of the initiator ligand

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4 Polymerization of ε-Caprolactone

4.1 Catalyst of type X-La@c-1 : (NMe_2)La@c-1 and (CH_3)La@c-1

(NMe_2)La@c-1

63

O	0.689901	0.531227	3.561518
Si	1.094229	1.689950	4.725193
Si	-0.310288	0.466961	2.269726
O	-0.080958	-0.990120	1.531324
Si	0.160676	-1.935247	0.194362
O	0.541610	-3.454158	0.675806
Si	-0.295980	-4.917438	0.734780
O	-1.894131	0.551763	2.814462
Si	-3.233809	0.394159	1.867034
N	-4.352233	-0.544295	2.748029
O	-0.155110	1.747282	1.246641
Si	0.995478	2.459813	0.292816
O	1.948970	3.343235	1.314580
O	-4.013315	1.836391	1.417111
La	-3.930190	1.752883	-1.325401
O	-2.384754	3.374234	-1.624569
Si	-0.838331	3.577346	-2.054922
O	0.262870	3.447777	-0.791652
O	-2.806115	-0.059944	0.338046
Si	-2.123637	-0.680170	-1.096609
O	-1.268925	-2.040215	-0.687459
Si	-4.872994	2.900769	2.456620
O	-3.347271	-0.514444	-2.110578
O	-0.959219	0.483310	-1.480279
Si	-0.269883	0.809571	-2.977895
O	-1.010163	-0.002842	-4.197749
Si	-2.477483	0.278042	-4.989224
N	-6.112783	2.346753	-1.715510
O	-0.375155	2.434274	-3.209451
O	1.295963	0.281723	-2.862892
Si	2.055948	0.000782	-1.408393
O	1.410291	-1.363467	-0.711330
O	-0.564064	5.055458	-2.740569
Si	0.641752	6.207921	-2.546306
O	1.960677	1.318250	-0.423507
O	3.664757	-0.240115	-1.659049
H	0.704059	1.141386	6.056970
H	2.793942	3.608363	0.938951
H	0.452710	7.214109	-3.631180
H	-0.540635	-5.430109	-0.644011
H	-6.272996	2.413085	2.598850
H	3.878934	-1.040077	-2.148042
H	-2.159314	0.779249	-6.358747
H	2.001245	5.598552	-2.664840

H	0.520759	6.881758	-1.218338
H	2.567067	1.902050	4.677565
H	-4.188873	2.946791	3.777096
H	-4.843708	4.227278	1.784094
H	0.369097	2.967238	4.471222
H	-3.251588	-0.985322	-5.063917
H	-3.273129	1.349083	-4.298030
H	0.570796	-5.865762	1.488878
H	-1.597699	-4.745140	1.446559
H	-5.236459	-0.811657	2.341473
H	-3.992269	-1.242898	3.382012
C	-6.640006	3.672237	-1.961439
C	-7.146566	1.336271	-1.793925
H	-7.946419	1.484712	-1.046337
H	-7.636483	1.305496	-2.783169
H	-6.729208	0.331233	-1.620911
H	-7.410022	3.963860	-1.225007
H	-5.841964	4.425418	-1.909860
H	-7.104348	3.761692	-2.959266

D

81

C	3.685163	7.996196	10.184230
C	2.557228	8.253190	11.164895
C	2.379291	9.709733	11.595324
C	2.010410	10.674751	10.468712
C	3.058268	10.762207	9.341716
C	3.022354	9.597456	8.399372
O	3.352365	8.365034	8.816593
La	2.901568	7.086469	6.385844
O	2.696102	9.671992	7.222437
O	2.612247	4.406005	5.916560
Si	2.146172	4.324614	7.554786
O	3.035036	5.475507	8.220774
Si	3.434915	3.472943	4.788335
O	3.507101	4.483713	3.482560
Si	4.275740	4.322085	1.989324
O	2.584859	2.075756	4.503543
Si	0.975615	1.746185	4.736027
O	0.755802	1.165592	6.269167
Si	0.898689	1.618247	7.850453
O	2.132834	2.735042	8.050147
O	0.506567	0.542037	3.729185
Si	0.144836	0.400981	2.087692
O	0.157735	3.154946	4.464309
Si	-1.311029	3.821929	4.829539
O	-1.235297	5.450156	5.002203
Si	-0.685150	6.915161	5.620190
O	-1.028100	6.887894	7.283300
Si	-0.664720	5.618387	8.257148
O	-0.254681	6.177092	9.759016
Si	-0.908712	5.712299	11.251405
O	-1.908767	3.059149	6.179728
Si	-1.886777	3.003729	7.829014
O	-1.914775	4.539631	8.460209
O	-2.294006	3.465303	3.548107
O	-3.252496	2.282396	8.403373
O	-0.564385	2.160563	8.392222
O	1.293821	0.303838	8.753425
Si	2.714064	-0.231123	9.483059
N	5.015516	2.964571	5.219079
O	0.528199	4.755874	7.493892
O	-1.716922	8.058837	5.002352

Si	-2.832152	8.017703	3.754436
O	0.866329	7.242135	5.346172
H	1.004121	-0.683788	1.529456
H	-3.088001	4.005986	3.501207
H	-3.435955	9.379176	3.664369
H	3.051828	0.627071	10.656556
H	5.722101	4.671599	2.114746
H	-3.255066	1.323728	8.328535
H	-2.360278	6.041740	11.319338
H	-3.916770	7.022410	4.026839
H	-2.184190	7.674672	2.451977
H	-1.290567	0.025136	1.949895
H	4.144305	2.926795	1.475166
H	3.609316	5.273311	1.056015
H	0.415189	1.679665	1.369120
H	-0.688772	4.259324	11.498516
H	-0.168952	6.509212	12.275151
H	2.458223	-1.628000	9.934673
H	3.848509	-0.214820	8.511407
H	5.714293	3.662463	5.429782
H	5.108590	2.146606	5.804035
H	4.064870	10.840414	9.774046
H	2.888956	11.646779	8.725093
H	1.896447	11.681629	10.883982
H	1.037136	10.408160	10.038731
H	1.601037	9.757693	12.365172
H	3.305048	10.059123	12.074743
H	2.775365	7.645281	12.051498
H	1.632409	7.846588	10.739187
H	3.876710	6.927374	10.082647
H	4.611562	8.513733	10.460166
N	4.872457	7.519457	5.273747
C	4.959991	8.141194	3.972167
C	6.177678	7.186967	5.793953
H	5.446366	7.491451	3.222089
H	3.959562	8.381048	3.585068
H	5.532241	9.086655	3.991768
H	6.734997	6.488532	5.140941
H	6.826237	8.073834	5.922329
H	6.097655	6.705301	6.780959

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81

C	3.830507	7.983635	10.069829
C	3.630821	9.033973	11.151469
C	4.261688	10.394381	10.849403
C	3.796506	11.057533	9.550247
C	4.142113	10.256863	8.278455
C	3.151502	9.162046	8.000189
O	2.939510	8.192382	8.955879
La	2.177817	6.737330	6.791427
O	2.189654	9.277678	7.216726
O	2.374425	4.086945	6.483811
Si	1.455266	3.937979	7.911147
O	1.939982	5.246461	8.696879
Si	3.362736	3.722396	5.199174
O	3.318702	5.252893	4.500096
Si	3.779291	5.776122	2.943225
O	2.726473	2.476391	4.324750
Si	1.197176	1.823881	4.515731
O	1.079377	1.156667	6.018269
Si	0.675410	1.156628	7.621506
O	1.545379	2.357131	8.418385

O	1.012090	0.608128	3.436098
Si	0.850521	0.474775	1.760763
O	0.170329	3.086237	4.265705
Si	-1.450511	3.389608	4.411306
O	-1.709522	4.973569	4.739937
Si	-1.349081	6.352542	5.635713
O	-1.934169	6.038929	7.195634
Si	-1.504459	4.719041	8.079734
O	-1.319422	5.114173	9.662452
Si	-0.958324	6.554002	10.465028
O	-2.107056	2.367589	5.541091
Si	-2.281188	2.064819	7.151208
O	-2.592608	3.469975	7.986702
O	-2.105428	3.001685	2.942985
O	-3.576314	1.052800	7.272085
O	-0.955348	1.301041	7.813802
O	1.130119	-0.272982	8.288310
Si	2.370629	-0.724357	9.335584
N	4.989996	3.312082	5.502054
O	-0.122828	4.094976	7.374909
O	-2.326321	7.541244	5.024608
Si	-3.648494	7.511449	3.993389
O	0.207063	6.778640	5.649904
H	1.950728	-0.408279	1.274072
H	-3.067052	3.004389	2.923649
H	-4.248437	8.877592	4.019814
H	2.137529	-0.159583	10.696610
H	5.262091	5.924596	2.888372
H	-3.661720	0.621876	8.127565
H	-2.225695	7.127324	11.006772
H	-4.670169	6.515014	4.438733
H	-3.228021	7.185878	2.596650
H	-0.467565	-0.151734	1.463523
H	3.322995	4.788274	1.927129
H	3.118910	7.094373	2.744496
H	0.951124	1.811854	1.108113
H	-0.038694	6.225116	11.590215
H	-0.321029	7.544321	9.550093
H	2.352584	-2.213346	9.392651
H	3.691872	-0.255791	8.819437
H	5.610797	3.957225	5.966351
H	5.225087	2.345957	5.674118
H	5.153582	9.844114	8.359884
H	4.120966	10.904706	7.400583
H	4.280701	12.036944	9.467177
H	2.717285	11.251957	9.580807
H	4.057949	11.071825	11.687051
H	5.354463	10.278620	10.811245
H	4.061946	8.637484	12.079349
H	2.553327	9.136948	11.329636
H	3.556960	6.989507	10.428400
H	4.866108	7.953587	9.714661
N	4.387809	7.839247	6.587217
C	4.786941	8.746537	5.534928
C	5.533373	7.135976	7.114610
H	5.211527	8.223057	4.659017
H	3.924846	9.328356	5.187701
H	5.562264	9.465642	5.862430
H	6.088657	6.576234	6.337201
H	6.280282	7.808888	7.582590
H	5.234329	6.407967	7.884044

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81

C	4.789364	7.338905	9.565100
C	3.981144	8.029761	10.660876
C	4.359490	9.493636	10.897231
C	4.011710	10.441873	9.751054
C	4.571898	10.022683	8.390990
C	3.827185	8.840808	7.757967
O	4.358102	7.526810	8.212325
La	2.116358	6.764833	6.932923
O	2.500464	8.855119	7.934692
O	2.274548	4.082960	6.793516
Si	1.171869	4.027809	8.094282
O	1.554253	5.385898	8.849563
Si	3.409371	3.665964	5.665048
O	3.542336	5.203880	4.961991
Si	4.232820	5.589062	3.445994
O	2.833422	2.467178	4.691387
Si	1.278828	1.841472	4.767545
O	1.036949	1.212644	6.271426
Si	0.441764	1.240572	7.816466
O	1.198081	2.470393	8.682224
O	1.166614	0.608619	3.698022
Si	1.126170	0.443738	2.017639
O	0.300169	3.116268	4.410176
Si	-1.325599	3.435620	4.372954
O	-1.590150	5.033364	4.626410
Si	-1.373491	6.405390	5.575398
O	-2.139023	6.079604	7.046152
Si	-1.760428	4.783734	7.988654
O	-1.670282	5.191654	9.572148
Si	-1.202939	6.579913	10.420005
O	-2.124334	2.447013	5.437025
Si	-2.453635	2.134153	7.022240
O	-2.841707	3.533053	7.834644
O	-1.819659	3.020693	2.849221
O	-3.756939	1.125887	7.002181
O	-1.201491	1.359272	7.803257
O	0.833619	-0.168692	8.561136
Si	1.945788	-0.581171	9.758328
N	4.966334	3.186124	6.169416
O	-0.337111	4.141606	7.377337
O	-2.266098	7.593144	4.845857
Si	-3.516713	7.551944	3.727464
O	0.166577	6.851082	5.788248
H	2.223083	-0.493769	1.637387
H	-2.773720	2.950241	2.749168
H	-4.143685	8.906059	3.729076
H	1.555000	0.019429	11.066444
H	5.707304	5.747686	3.596502
H	-3.963138	0.728745	7.853440
H	-2.432477	7.152894	11.044838
H	-4.544266	6.528676	4.088871
H	-2.991496	7.255269	2.360067
H	-0.190063	-0.134885	1.630198
H	3.921923	4.511960	2.468888
H	3.617961	6.881833	3.035351
H	1.334812	1.760581	1.349457
H	-0.245875	6.172795	11.483897
H	-0.595159	7.594786	9.513808
H	1.928546	-2.068165	9.853481
H	3.315968	-0.117399	9.384031
H	5.530743	3.787925	6.750172
H	5.128788	2.206645	6.352812

H	5.645266	9.802646	8.453338
H	4.466432	10.866258	7.698930
H	4.388759	11.442982	9.993251
H	2.924358	10.522810	9.651734
H	3.867415	9.847127	11.811627
H	5.440681	9.544564	11.096019
H	4.171034	7.468045	11.584640
H	2.912783	7.927153	10.445499
H	4.742177	6.254595	9.706816
H	5.846789	7.635681	9.642287
N	4.073429	8.670757	6.273842
C	3.455129	9.737053	5.479244
C	5.473534	8.503811	5.885233
H	3.401870	9.422718	4.431776
H	2.447592	9.933487	5.848473
H	4.030526	10.675408	5.517011
H	5.524807	8.221567	4.828828
H	6.051900	9.432734	6.006978
H	5.933810	7.718510	6.484473

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81

C	1.515029	9.879458	6.269764
N	2.792609	9.163832	6.414983
C	3.745781	9.570911	5.386772
C	3.269798	9.119694	7.786728
O	2.418467	8.610627	8.582017
La	2.301237	6.517507	7.227907
O	0.627799	6.663174	5.701283
Si	-0.904893	6.377683	5.282475
O	-1.540482	7.642118	4.416504
Si	-3.118141	8.171176	4.186199
C	4.200804	10.212565	8.267592
C	4.582040	10.109160	9.743427
C	5.750746	9.171916	10.047810
C	5.571434	7.706020	9.642486
C	5.622536	7.429613	8.134992
O	4.440543	7.665476	7.410392
O	2.226872	3.866957	7.132880
Si	3.538806	3.282037	6.306673
N	4.846446	2.594967	7.161621
Si	0.940025	3.908825	8.255299
O	-0.409312	4.117880	7.288635
Si	-1.861307	4.880417	7.618471
O	-2.989744	3.718892	7.255449
Si	-2.570022	2.260054	6.569284
O	-1.545707	1.426853	7.589132
Si	0.059728	1.183259	7.870474
O	0.213899	-0.241044	8.671706
Si	1.064741	-0.721816	10.044455
O	1.304362	5.245451	9.053855
O	4.030870	4.782560	5.701572
Si	5.327595	5.105185	4.633582
O	0.753832	2.365314	8.848929
O	3.048913	2.162463	5.201124
Si	1.463897	1.648791	5.001458
O	0.654707	2.963674	4.432139
Si	-0.916025	3.396665	4.133702
O	-1.176815	3.001693	2.549292
O	0.904646	1.095071	6.450147
O	1.464425	0.385174	3.961846
Si	1.686138	0.171468	2.300981
O	-1.133985	5.007224	4.343679

O	-1.929973	2.473299	5.066292
O	-1.928843	6.193195	6.621659
O	-2.044310	5.310791	9.187578
Si	-1.596504	6.648377	10.124621
O	-3.927295	1.352606	6.344553
H	2.775794	-0.832837	2.124971
H	-2.059865	3.206176	2.227704
H	-3.592479	8.943614	5.373572
H	0.506664	-0.069108	11.263852
H	6.562300	5.374953	5.422714
H	-4.305201	0.999507	7.155349
H	-2.858656	7.322485	10.554121
H	-4.048283	7.029336	3.934795
H	-3.101160	9.068864	2.993166
H	0.419419	-0.350242	1.717216
H	5.528050	3.932449	3.738479
H	4.936411	6.309626	3.852098
H	2.072519	1.455562	1.648860
H	-0.859645	6.157393	11.319230
H	-0.772246	7.609811	9.339950
H	0.908210	-2.200680	10.139245
H	2.512987	-0.378283	9.911335
H	5.293702	3.093309	7.916472
H	4.842703	1.595997	7.309269
H	5.083341	10.274352	7.623387
H	3.636054	11.143316	8.104841
H	4.845597	11.111227	10.102289
H	3.695274	9.795980	10.305113
H	5.946941	9.214982	11.126558
H	6.659644	9.557115	9.561690
H	6.387686	7.130604	10.100153
H	4.637777	7.306139	10.059454
H	5.893951	6.370172	7.988667
H	6.454548	8.011802	7.700310
H	1.046993	9.580606	5.329415
H	0.845654	9.614988	7.087882
H	1.662138	10.970635	6.268442
H	3.324205	9.332203	4.405735
H	3.952842	10.651612	5.411461
H	4.674638	9.016961	5.520811

F

81

C	0.434992	11.152100	8.260123
N	1.886595	11.139395	8.133635
C	2.531632	12.423969	8.348088
C	2.530951	9.997267	7.843598
O	1.885351	8.921885	7.746878
La	2.290302	6.534068	7.123441
O	1.028269	6.492078	5.216171
Si	-0.462294	6.138623	4.715499
O	-1.018977	7.226677	3.591357
Si	-2.544913	7.853379	3.290892
C	4.027436	9.970014	7.650150
C	4.776327	9.610525	8.948515
C	6.227577	9.166038	8.703364
C	6.447838	7.675435	8.408337
C	5.835471	7.102573	7.124852
O	4.457286	6.922654	7.197706
O	2.307358	3.827124	6.985581
Si	3.558472	2.805883	6.522471
N	4.627728	2.302958	7.765248
Si	0.954800	3.876100	8.023248

O	-0.341732	4.096386	6.986787
Si	-1.743025	4.998509	7.097250
O	-2.951159	3.925989	6.733084
Si	-2.604417	2.344990	6.333423
O	-1.780880	1.646469	7.607341
Si	-0.243499	1.162855	7.961727
O	-0.350872	-0.052692	9.061948
Si	0.513573	-0.439866	10.454218
O	1.237782	5.216557	8.856740
O	4.362683	3.762318	5.437205
Si	5.761911	3.514230	4.528430
O	0.696470	2.364288	8.669367
O	2.949703	1.412907	5.866411
Si	1.425844	1.049310	5.311487
O	0.870462	2.401808	4.545904
Si	-0.583062	2.987801	4.008984
O	-0.717701	2.463437	2.445890
O	0.480307	0.598497	6.589249
O	1.509400	-0.253800	4.323273
Si	2.024645	-0.555784	2.746033
O	-0.646804	4.627142	4.015658
O	-1.796744	2.286217	4.900541
O	-1.589158	6.212757	5.990549
O	-2.039980	5.596767	8.596783
Si	-1.466527	6.850631	9.561351
O	-4.008190	1.510474	6.110183
H	3.042167	-1.646117	2.807448
H	-1.354600	2.957877	1.921891
H	-2.929054	8.847410	4.339717
H	0.216959	0.537035	11.542168
H	6.969537	3.765648	5.370855
H	-4.375096	1.147705	6.921802
H	-2.638084	7.721819	9.885588
H	-3.582863	6.780318	3.229417
H	-2.473892	8.546992	1.970182
H	0.854778	-1.005916	1.941084
H	5.808383	2.121605	3.994682
H	5.725484	4.492885	3.405345
H	2.632347	0.664364	2.140295
H	-0.896021	6.299768	10.818452
H	-0.458347	7.683094	8.839913
H	0.072651	-1.803928	10.861397
H	1.982607	-0.448534	10.180127
H	5.090579	3.002765	8.327239
H	4.360330	1.497879	8.313650
H	4.208052	9.174615	6.923384
H	4.412408	10.903795	7.231268
H	4.765401	10.478881	9.619976
H	4.236180	8.811221	9.468733
H	6.813582	9.414421	9.597037
H	6.659612	9.768394	7.891018
H	7.533006	7.507803	8.363889
H	6.078097	7.078816	9.253781
H	6.329786	6.138950	6.918966
H	6.102785	7.763939	6.278791
H	0.022997	11.948368	7.631955
H	0.036048	10.191565	7.942373
H	0.145785	11.339367	9.300219
H	2.313437	13.110195	7.521446
H	2.148362	12.867238	9.272894
H	3.609280	12.317133	8.447910

(CH_3)La@c-1

58

O	0.703953	0.559762	3.510869
Si	1.106155	1.697727	4.696023
Si	-0.325465	0.495477	2.243281
O	-0.091914	-0.945635	1.477228
Si	0.114694	-1.896819	0.137308
O	0.473813	-3.422769	0.613267
Si	-0.387479	-4.872698	0.668688
O	-1.898869	0.537877	2.830286
Si	-3.241669	0.385427	1.890423
N	-4.330766	-0.623347	2.724993
O	-0.229610	1.798503	1.238777
Si	0.925644	2.488272	0.268864
O	1.837377	3.440783	1.266730
O	-4.063536	1.828298	1.509256
La	-4.000256	1.812796	-1.210413
O	-2.454225	3.379774	-1.679511
Si	-0.909224	3.566707	-2.130127
O	0.205643	3.407421	-0.881850
O	-2.811053	0.031556	0.331807
Si	-2.136173	-0.583161	-1.118678
O	-1.337678	-1.979925	-0.715225
Si	-4.905931	2.841253	2.618212
O	-3.366513	-0.350050	-2.117524
O	-0.911384	0.506155	-1.494759
Si	-0.252960	0.824043	-3.010195
O	-0.913344	-0.093942	-4.195568
Si	-2.289841	0.052851	-5.169474
C	-6.420885	2.450454	-1.526147
O	-0.474525	2.428307	-3.299680
O	1.345117	0.411302	-2.855353
Si	2.045556	0.047227	-1.390845
O	1.362079	-1.345425	-0.784826
O	-0.629833	5.048770	-2.802258
Si	0.599156	6.180507	-2.627887
O	1.926448	1.319108	-0.348080
O	3.660413	-0.201718	-1.590445
H	0.759934	1.104779	6.020720
H	2.682904	3.710081	0.895353
H	0.408380	7.191961	-3.707115
H	-0.658012	-5.368204	-0.711398
H	-6.291940	2.324523	2.784676
H	3.885720	-1.008417	-2.063104
H	-1.821855	0.324775	-6.560545
H	1.944981	5.546606	-2.770600
H	0.512415	6.851885	-1.296062
H	2.571532	1.948467	4.619935
H	-4.175014	2.845973	3.913477
H	-4.914623	4.189203	1.989482
H	0.343477	2.962121	4.491734
H	-3.040892	-1.228405	-5.124673
H	-3.149662	1.191658	-4.725661
H	0.472034	-5.841908	1.404106
H	-1.677276	-4.684659	1.398282
H	-5.219752	-0.879968	2.322115
H	-3.955188	-1.341940	3.326625
H	-6.675388	2.506990	-2.598444
H	-7.126003	1.720983	-1.094464
H	-6.696878	3.431085	-1.107029

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76

C	5.204114	8.304884	9.454031

C	4.878709	7.117577	10.345645
C	3.870002	7.417723	11.456762
C	2.489773	7.856606	10.967194
C	2.511670	9.118495	10.078431
C	2.955918	8.812980	8.677494
O	4.218849	8.512262	8.410671
La	2.579623	7.084205	5.840243
O	2.171470	8.801740	7.727661
O	1.704456	4.343776	5.988711
Si	2.004334	4.616933	7.644539
O	3.326873	5.525410	7.644109
Si	2.890337	3.712748	4.978164
O	3.343048	5.113264	4.156710
Si	4.460931	5.209001	2.851773
O	2.156359	2.580405	4.021243
Si	1.059608	1.515588	4.695146
O	1.522362	1.359088	6.288205
Si	1.099536	1.746875	7.840803
O	1.906350	3.115675	8.363383
O	1.229176	0.063352	3.958020
Si	0.182781	-0.934645	3.081672
O	-0.487710	2.030102	4.507804
Si	-1.557579	3.287175	4.678629
O	-0.826695	4.745133	4.475163
Si	-0.913222	6.310614	5.071150
O	-1.466570	6.203444	6.655840
Si	-0.921900	5.713692	8.125938
O	-1.308964	6.831799	9.272712
Si	-2.618242	7.882724	9.431925
O	-2.241710	3.154285	6.182762
Si	-1.882559	2.851495	7.754543
O	-1.614403	4.272724	8.563940
O	-2.707781	3.042207	3.523106
O	-3.177057	2.059699	8.393003
O	-0.536287	1.895568	7.938576
O	1.574324	0.516271	8.820470
Si	2.564207	0.428830	10.181214
N	4.306536	3.055772	5.681351
O	0.729348	5.570097	8.155220
O	-2.150821	7.042630	4.232629
Si	-2.158346	8.532541	3.451203
O	0.482915	7.111233	4.944266
H	0.974803	-2.147533	2.730440
H	-3.123496	3.857950	3.226217
H	-3.544922	8.724255	2.931346
H	2.050833	1.319230	11.263778
H	5.791451	5.614062	3.378293
H	-3.008795	1.647358	9.245151
H	-3.901829	7.194280	9.110038
H	-1.197948	8.550399	2.307598
H	-1.829003	9.644755	4.393216
H	-0.991378	-1.315622	3.918144
H	4.537611	3.862443	2.219144
H	3.924904	6.210564	1.894642
H	-0.272941	-0.245300	1.840584
H	-2.624858	8.327336	10.856543
H	-2.439117	9.067346	8.542551
H	2.532731	-0.990503	10.633418
H	3.963532	0.819103	9.835929
H	4.757314	3.621576	6.390342
H	4.278229	2.080312	5.945140
H	3.164405	9.881827	10.520805
H	1.508465	9.538018	9.989685

H	1.855590	8.078236	11.831841
H	1.995564	7.045937	10.420552
H	3.753266	6.524606	12.080865
H	4.281346	8.198042	12.113689
H	5.821074	6.787214	10.799517
H	4.526406	6.302969	9.700213
H	6.119526	8.132665	8.886809
H	5.322398	9.237354	10.019472
C	4.287098	8.371656	4.485306
H	4.261986	9.405471	4.876044
H	5.331467	8.040104	4.595207
H	4.095526	8.462477	3.405698

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76

C	3.701795	7.840917	10.215016
C	3.686032	8.960318	11.243672
C	4.517538	10.192701	10.878088
C	4.199738	10.826412	9.518943
C	4.529926	9.907834	8.325177
C	3.414109	8.936760	8.033677
O	2.893789	8.188249	9.071407
La	2.120824	6.696288	6.975982
O	2.556716	9.141487	7.142036
O	2.377421	4.037613	6.749722
Si	1.254985	3.910412	8.024362
O	1.593680	5.257055	8.830727
Si	3.340650	3.769798	5.419051
O	3.147446	5.308615	4.745160
Si	3.309973	5.850527	3.129923
O	2.785802	2.488392	4.543606
Si	1.263473	1.797395	4.648954
O	1.067807	1.150869	6.150463
Si	0.522204	1.131322	7.712768
O	1.301126	2.344797	8.582591
O	1.175501	0.566347	3.575126
Si	1.120064	0.411994	1.894212
O	0.239316	3.040702	4.313942
Si	-1.385630	3.356397	4.348410
O	-1.641756	4.947792	4.645154
Si	-1.353309	6.311919	5.588457
O	-2.063227	5.977237	7.089740
Si	-1.668435	4.656197	7.986771
O	-1.531466	5.034960	9.576970
Si	-1.048466	6.419334	10.414725
O	-2.132604	2.342816	5.427587
Si	-2.400881	2.015833	7.020819
O	-2.758673	3.413175	7.850245
O	-1.941233	2.968839	2.839310
O	-3.701181	1.004128	7.048895
O	-1.121757	1.238550	7.755075
O	0.939156	-0.292890	8.413174
Si	2.180724	-0.754619	9.455886
N	5.004851	3.521827	5.669442
O	-0.263025	4.020899	7.323855
O	-2.268078	7.515739	4.914290
Si	-3.565079	7.502032	3.850007
O	0.197000	6.734503	5.746260
H	2.228549	-0.503347	1.495032
H	-2.899534	2.924899	2.769630
H	-4.167121	8.867035	3.883112
H	1.925555	-0.231510	10.829402
H	4.608461	5.367141	2.581022

H	-3.828362	0.548515	7.886230
H	-2.260495	6.990928	11.074237
H	-4.595240	6.496303	4.251799
H	-3.105427	7.200923	2.460187
H	-0.190736	-0.185882	1.517010
H	2.171672	5.352083	2.314729
H	3.297876	7.337310	3.217947
H	1.297165	1.737381	1.233527
H	-0.059566	6.023578	11.454218
H	-0.470217	7.445947	9.499369
H	2.186270	-2.244670	9.471549
H	3.497394	-0.249350	8.963825
H	5.572342	4.253918	6.070838
H	5.346477	2.593751	5.868106
H	5.468933	9.387666	8.525517
H	4.662447	10.483393	7.406519
H	4.801894	11.735457	9.411624
H	3.151596	11.146200	9.472515
H	4.386414	10.946947	11.662964
H	5.583046	9.922155	10.892642
H	4.054381	8.547126	12.191054
H	2.639810	9.242376	11.414840
H	3.231701	6.936438	10.605750
H	4.712184	7.586409	9.875182
C	4.770623	7.154812	7.076538
H	5.661793	7.690322	7.408707
H	4.882819	6.125940	7.472134
H	4.851296	7.102109	5.977909

H

76

C	2.584079	9.204454	9.486656
C	1.733483	9.951200	8.468440
C	2.526443	10.752402	7.434324
C	3.620728	9.973466	6.694912
C	4.785314	9.538400	7.588925
C	4.620031	8.190109	8.310502
O	3.238246	8.073744	8.902784
La	2.677288	5.992192	7.547308
O	4.669258	7.133386	7.455795
O	2.537232	3.463987	6.818006
Si	1.623270	3.188105	8.234958
O	2.297440	4.247031	9.225985
Si	3.438550	3.295628	5.436261
O	3.687096	4.955201	5.205756
Si	4.706328	5.708901	4.044320
O	2.548195	2.504743	4.297060
Si	0.943930	2.052305	4.488720
O	0.823354	1.060369	5.800826
Si	0.430200	0.703100	7.368188
O	1.459115	1.544178	8.403981
O	0.490626	1.185506	3.177642
Si	0.296007	1.489264	1.526741
O	0.121536	3.470739	4.656837
Si	-1.448795	3.921613	4.933172
O	-1.499969	5.398403	5.644146
Si	-0.920873	6.472673	6.799763
O	-1.416638	5.852335	8.295943
Si	-1.133285	4.303270	8.776421
O	-0.769698	4.230249	10.373180
Si	0.085716	5.210149	11.452519
O	-2.231535	2.752086	5.812311
Si	-2.375768	2.098098	7.319316

O	-2.409455	3.284222	8.486382
O	-2.166009	3.982701	3.444320
O	-3.812916	1.293229	7.308768
O	-1.161072	1.010889	7.662780
O	0.688450	-0.893782	7.636105
Si	1.885987	-1.772817	8.434002
N	4.963708	2.539398	5.497000
O	0.089842	3.711838	7.793363
O	-1.779861	7.872116	6.585104
Si	-3.262147	8.187168	5.860839
O	0.672981	6.733179	6.761277
H	1.254171	0.612601	0.791703
H	-3.127106	4.013570	3.468013
H	-3.698798	9.532217	6.337778
H	1.822465	-1.525648	9.903303
H	6.110280	5.703478	4.535752
H	-3.955344	0.724780	8.071315
H	-0.899762	5.736447	12.444066
H	-4.284690	7.166753	6.241888
H	-3.124845	8.213510	4.373251
H	-1.101198	1.136855	1.151259
H	4.593165	4.957855	2.762951
H	4.191916	7.095521	3.893944
H	0.577855	2.919581	1.214232
H	1.105859	4.382534	12.147735
H	0.720966	6.366221	10.753858
H	1.615298	-3.208911	8.143790
H	3.239005	-1.401654	7.920423
H	5.676658	2.854417	6.138007
H	5.022573	1.551010	5.301062
H	5.005317	10.333255	8.314030
H	5.694224	9.412459	6.990759
H	4.014577	10.615099	5.897876
H	3.193610	9.099974	6.183869
H	1.821787	11.165814	6.702869
H	2.994601	11.616545	7.927931
H	1.062530	10.627799	9.013814
H	1.089835	9.218956	7.964403
H	1.955311	8.806857	10.290557
H	3.333001	9.857843	9.952059
C	5.610870	8.042934	9.461408
H	6.631455	8.105286	9.072317
H	5.483639	8.823275	10.219114
H	5.479592	7.064861	9.931987

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76

Si	3.389911	3.468594	5.407511
O	2.523837	3.607892	6.811969
Si	1.600901	3.320066	8.208664
O	0.033265	3.733693	7.780640
O	-1.583129	5.340783	5.614890
O	-2.236553	2.672670	5.849383
O	-1.090952	1.002575	7.727114
Si	0.511801	0.765636	7.423948
O	0.868010	1.102670	5.843503
H	3.419096	-1.179446	8.001583
Si	0.326369	1.402958	1.564089
H	-1.060888	0.992991	1.209635
Si	2.089612	-1.615861	8.525437
O	0.842884	-0.813130	7.724442
Si	-2.348428	2.035156	7.366155
O	-3.749617	1.167844	7.371028

O	-2.434684	3.239428	8.511941
Si	-1.192435	4.308180	8.770829
O	-0.812685	4.282201	10.364392
O	-1.531180	5.836751	8.258301
Si	-0.004429	5.334486	11.413820
Si	-3.318363	8.149178	5.738757
O	-1.859662	7.831133	6.507326
Si	-1.014771	6.429812	6.760355
O	0.582771	6.682896	6.739779
La	2.609811	6.200030	7.609188
O	3.541715	5.125391	5.116750
Si	4.427700	5.883786	3.864981
O	2.213231	4.425694	9.195912
O	1.519356	1.672480	8.423489
O	2.533766	2.585616	4.308611
Si	0.954702	2.061931	4.505644
O	0.063829	3.442188	4.622168
Si	-1.510010	3.850067	4.933670
O	-2.268705	3.866207	3.463810
N	4.959978	2.802331	5.447957
O	0.552330	1.136420	3.216613
O	3.154593	8.010590	8.885097
C	5.204083	7.929559	7.983932
C	5.890480	7.555709	9.269624
C	5.273197	9.380308	7.574417
C	4.139588	9.921984	6.689356
C	3.138847	10.824642	7.426610
C	2.119236	10.150304	8.350505
C	2.687802	9.217257	9.420542
O	4.935062	7.042033	7.136728
H	1.307712	0.549862	0.831638
H	-3.229116	3.854142	3.515303
H	-3.751671	9.507501	6.180108
H	2.020498	-1.356587	9.992633
H	5.876277	5.909609	4.207832
H	-3.850498	0.584507	8.128935
H	-1.012263	5.824409	12.402031
H	-4.363136	7.148033	6.110655
H	-3.142629	8.147781	4.254918
H	4.207872	5.137838	2.594397
H	3.887449	7.266913	3.763497
H	0.550546	2.837052	1.222938
H	1.060482	4.576221	12.122039
H	0.562531	6.505587	10.685190
H	1.896339	-3.068373	8.254291
H	5.671786	3.192547	6.047312
H	5.066087	1.807604	5.313211
H	5.400234	10.003798	8.464668
H	6.229899	9.440587	7.032289
H	4.585763	10.510155	5.879625
H	3.626434	9.088676	6.193742
H	2.582215	11.398572	6.675172
H	3.710602	11.567954	8.001548
H	1.539130	10.940064	8.846958
H	1.397709	9.575451	7.753984
H	1.902240	9.012080	10.165285
H	3.497234	9.731131	9.971523
H	6.973263	7.669734	9.122535
H	5.589122	8.210737	10.088311
H	5.689752	6.515725	9.532598

Si	3.041323	4.008032	5.326813
O	2.129011	4.109036	6.701060
Si	1.347452	3.778197	8.173026
O	-0.281006	3.848138	7.807133
O	-2.091990	5.017936	5.519705
O	-2.307718	2.302148	5.979475
O	-0.871941	0.989495	7.938312
Si	0.742534	1.013711	7.607642
O	1.013198	1.261524	5.992462
H	3.961037	-0.314852	8.176541
Si	0.317095	1.115636	1.731360
H	-0.996701	0.451586	1.504608
Si	2.760989	-0.942492	8.808904
O	1.351451	-0.452812	8.028364
Si	-2.298068	1.753959	7.534028
O	-3.515840	0.645116	7.610972
O	-2.609578	2.991327	8.603323
Si	-1.584998	4.289558	8.758577
O	-1.218126	4.465348	10.346760
O	-2.182565	5.684008	8.119480
Si	-0.655811	5.744123	11.299013
Si	-4.233750	7.532620	5.450187
O	-2.751442	7.490128	6.233967
Si	-1.709374	6.253871	6.596175
O	-0.169274	6.737581	6.577710
La	1.967886	6.715758	7.346806
O	2.893625	5.634275	4.863273
Si	3.444891	6.353350	3.416629
O	1.805935	5.034839	9.058175
O	1.592298	2.162271	8.497290
O	2.382373	2.889807	4.308799
Si	0.920466	2.113541	4.584051
O	-0.196346	3.321450	4.608189
Si	-1.804851	3.506450	4.955410
O	-2.592045	3.285711	3.516397
N	4.711948	3.679410	5.451470
O	0.683762	1.032170	3.377197
O	2.338211	8.696040	8.224283
C	5.601933	6.976194	7.998955
C	6.997271	6.423288	8.039719
C	5.329351	8.272470	8.706260
C	5.397598	9.454304	7.710769
C	4.804224	10.755131	8.275921
C	3.293184	10.948096	8.090564
C	2.357969	9.964918	8.801433
O	4.712181	6.388572	7.377571
H	1.387455	0.378508	0.997407
H	-3.542264	3.163948	3.602261
H	-4.851781	8.855038	5.762581
H	2.713573	-0.579001	10.254891
H	4.877408	6.741187	3.568698
H	-3.513262	0.112505	8.411692
H	-1.760987	6.130506	12.226623
H	-5.139624	6.440793	5.920813
H	-4.054101	7.414050	3.971146
H	3.278010	5.407068	2.280911
H	2.610783	7.573783	3.230360
H	0.272432	2.532325	1.267886
H	0.509355	5.260234	12.088499
H	-0.280939	6.923199	10.467692
H	2.835032	-2.423422	8.658669
H	5.230901	4.267801	6.089858
H	5.005531	2.713494	5.483459

H	4.316435	8.228899	9.115601
H	6.052320	8.429727	9.513810
H	6.445372	9.617633	7.428719
H	4.862096	9.185508	6.792805
H	5.308336	11.596399	7.783953
H	5.060189	10.839112	9.341625
H	3.043909	11.958051	8.444176
H	3.051589	10.930838	7.018627
H	1.344278	10.396465	8.791530
H	2.652550	9.900766	9.865369
H	7.728746	7.212817	7.838138
H	7.200232	6.060399	9.055030
H	7.125247	5.602327	7.333368

4.2 Catalysts of (alkyl or dialkylamido)(X_2)La@**c**-2

- (CH3)(NMe2)La@c-2

$(CH_3)(NMe_2)$La@**c**-2

64

C	3.253302	7.326164	10.707679
N	2.651975	6.550371	9.647263
C	3.414370	6.642036	8.419965
La	0.803185	5.195884	9.757543
O	0.490493	4.071847	11.841159
Si	-0.871452	4.617522	12.456917
O	-2.143736	3.544114	12.488000
Si	-3.696489	3.473518	13.046466
O	-3.806141	4.162425	14.545584
Si	-4.181220	5.602398	15.268290
O	-4.821828	5.347333	16.761157
O	-2.818314	6.534351	15.370490
Si	-1.365390	6.781877	14.620364
O	-0.294957	7.294327	15.748099
Si	1.272049	6.834281	16.183497
O	-1.538180	7.958900	13.465987
Si	-2.686751	8.750312	12.585414
O	-2.664493	8.159976	11.023969
Si	-2.345329	6.682474	10.377292
O	-1.305907	5.833833	11.321492
O	-2.333372	10.343351	12.508515
Si	-3.054510	11.760385	13.084670
O	-4.183281	8.538954	13.253721
Si	-5.494415	7.524583	13.224426
O	-6.877687	8.383856	13.446167
O	-5.581259	6.807894	11.739336
Si	-5.073676	5.455650	10.940475
O	-6.207803	4.963296	9.874932
Si	-7.538930	3.920776	9.927671
O	-3.726195	5.854061	10.043299
O	-4.729713	4.254882	12.014390
O	-5.360498	6.396990	14.426452
O	-0.810947	5.384109	13.932793
O	-4.160330	1.907462	13.146086
Si	-3.376436	0.434021	12.869887
O	-1.428255	6.807540	8.983723
Si	-1.826145	7.455662	7.442196
C	0.577877	3.662790	7.757975
H	-8.239206	4.042464	11.239081
H	-7.221236	8.350985	14.344018
H	-4.277275	4.823379	17.355937
H	-4.366212	-0.625663	13.211873
H	-2.979523	0.322896	11.436741

H	-2.174802	0.317038	13.745201
H	-7.077610	2.518006	9.722858
H	-8.441246	4.334324	8.817725
H	1.720147	7.817445	17.209045
H	1.259016	5.459926	16.762977
H	2.176035	6.879244	14.998303
H	-4.360664	11.980366	12.399916
H	-3.260451	11.670823	14.559292
H	-2.109546	12.865085	12.762103
H	-0.522940	7.793310	6.810145
H	-2.553179	6.422324	6.658245
H	-2.664467	8.669800	7.639054
H	4.452044	6.279096	8.533055
H	2.954483	6.034444	7.624536
H	3.479681	7.676252	8.035748
H	4.282395	6.999032	10.943190
H	3.311208	8.402489	10.463793
H	2.668970	7.237878	11.634025
H	1.441322	2.981108	7.675128
H	-0.311594	3.014818	7.806127
H	0.523084	4.190300	6.791217

D

82

C	3.665165	7.187307	11.387790
N	2.380556	7.337287	10.748351
La	0.379455	6.343506	11.355514
O	0.042992	7.659885	13.805032
Si	-0.468760	9.228827	13.945607
O	0.583656	10.129541	14.841955
Si	1.659644	9.977133	16.088707
O	2.871645	11.048578	15.846171
Si	3.732003	12.115572	16.832338
C	2.434459	8.295807	9.669430
O	0.669823	5.082580	7.972111
C	0.714947	4.000184	8.739110
O	0.669652	4.163770	9.954329
C	-1.718014	7.069804	10.097774
Si	-0.112828	6.135245	14.579358
O	-1.610476	6.125789	15.313492
Si	-2.340542	6.437578	16.757466
O	-3.571766	5.376894	16.985274
Si	-4.093149	4.018087	16.129619
O	0.083188	5.111786	13.378855
C	0.721966	5.019292	6.529707
C	-0.516263	4.393290	5.907379
C	-0.535885	2.864274	5.930351
C	-0.465924	2.242574	7.325380
C	0.792142	2.626348	8.128161
O	1.022194	6.058566	15.796172
Si	1.977501	6.965215	16.784547
O	1.262135	7.160722	18.264802
Si	-0.253685	7.217546	18.926534
O	-1.276352	6.287001	18.014408
O	3.411085	6.201060	17.015267
Si	4.085529	4.783618	16.398505
O	2.274629	8.445122	16.109371
O	-1.979140	9.301874	14.614652
Si	-2.704435	9.457465	16.095348
O	-4.136573	10.228228	15.895337
Si	-5.753060	9.747525	15.949408
O	-0.518815	9.781999	12.400307
Si	-1.304197	11.067347	11.627434

O	-1.756535	10.378959	17.083671
Si	-0.573296	10.217369	18.231719
O	-0.791771	8.775230	19.014500
O	-2.978910	7.968058	16.760354
O	-0.638788	11.457537	19.310040
O	0.917178	10.310229	17.531477
O	-0.224613	6.675020	20.480263
H	-1.339247	11.383396	19.964857
H	0.014470	5.748788	20.578547
H	-5.235088	3.456050	16.906009
H	-4.550129	4.404128	14.763132
H	-2.999080	3.008398	16.033454
H	-5.980677	8.569283	15.062734
H	-6.143035	9.409914	17.349323
H	-6.549710	10.910578	15.466404
H	5.456156	4.690387	16.976945
H	3.279932	3.598645	16.816103
H	4.164929	4.841112	14.910194
H	2.872246	13.277445	17.199539
H	4.205125	11.422295	18.065717
H	4.897629	12.577950	16.027174
H	-0.629771	11.245023	10.312042
H	-2.744914	10.741665	11.433402
H	-1.168948	12.308547	12.445221
H	0.812720	6.068225	6.245013
H	1.640676	4.504220	6.223686
H	-0.563489	4.735111	4.866307
H	-1.399969	4.807832	6.408183
H	-1.443464	2.510364	5.428521
H	0.308458	2.490807	5.333623
H	-1.359096	2.503068	7.906844
H	-0.473281	1.151816	7.228027
H	0.936956	1.940189	8.964134
H	1.680412	2.559376	7.486196
H	3.135799	7.999564	8.865491
H	1.445078	8.413415	9.200259
H	2.747882	9.302449	10.003756
H	4.447551	6.823524	10.694204
H	4.043580	8.132599	11.819334
H	3.606878	6.461256	12.211116
H	-2.511029	7.445451	10.764050
H	-1.536558	7.865302	9.356469
H	-2.171381	6.231971	9.540403

$TS_{D\rightarrow E}$

82

C	2.725940	6.323765	11.097181
N	1.464837	6.545978	10.423127
La	-0.617488	5.735690	11.410198
O	-0.432147	7.227578	13.702643
Si	-0.645431	8.872925	13.724443
O	0.665211	9.628947	14.377651
Si	1.834408	9.355044	15.520038
O	3.198432	10.119803	15.041687
Si	4.276831	11.197239	15.771052
C	1.531952	7.717510	9.581251
O	-0.120614	5.024862	8.644276
C	0.981045	4.551160	9.300969
O	0.698068	3.879018	10.317055
C	-2.791627	6.495370	10.362594
Si	-0.800416	5.832476	14.646315
O	-2.165013	6.201516	15.523834
Si	-2.640069	6.757715	17.003045

O	-4.006419	5.982591	17.468933
Si	-4.900857	4.708928	16.808938
O	-0.966906	4.717717	13.522885
C	-0.036115	5.594237	7.323880
C	0.145341	4.526090	6.254259
C	1.571984	3.988588	6.118854
C	2.165498	3.389228	7.395694
C	2.278016	4.394421	8.559626
O	0.444980	5.611534	15.726977
Si	1.668127	6.403400	16.499911
O	1.198706	6.863854	18.018518
Si	-0.182453	7.279515	18.830947
O	-1.467119	6.496555	18.138348
O	2.959900	5.405984	16.649236
Si	3.311057	3.851243	16.092009
O	2.124224	7.734167	15.628517
O	-2.017879	9.287854	14.541748
Si	-2.514962	9.720026	16.063562
O	-3.792484	10.732454	15.913732
Si	-5.411561	10.682178	16.391235
O	-0.812217	9.274210	12.136986
Si	-1.633656	10.539971	11.358557
O	-1.293402	10.520308	16.833546
Si	-0.024373	10.218961	17.856085
O	-0.405752	8.914377	18.799039
O	-2.971914	8.380833	16.918389
O	0.285260	11.528164	18.800714
O	1.352333	9.956324	16.984428
O	-0.057927	6.884275	20.422775
H	-0.297727	11.624517	19.559535
H	0.020067	5.942792	20.602562
H	-6.007512	4.443896	17.771284
H	-5.458981	5.101882	15.483053
H	-4.046619	3.494921	16.664759
H	-6.090922	9.493694	15.799012
H	-5.508903	10.633785	17.879223
H	-6.032866	11.935762	15.879481
H	4.705440	3.560610	16.530213
H	2.370910	2.862335	16.694969
H	3.221528	3.795724	14.604287
H	3.610965	12.512082	15.997841
H	4.769287	10.643331	17.065190
H	5.409822	11.355435	14.816289
H	-1.157956	10.533724	9.947575
H	-3.102671	10.305852	11.415128
H	-1.291081	11.836416	12.012072
H	-0.993776	6.104411	7.202873
H	0.758410	6.346437	7.290161
H	-0.162849	4.963145	5.296052
H	-0.559018	3.711481	6.464538
H	1.591591	3.232494	5.325075
H	2.226041	4.804239	5.778757
H	1.584665	2.516460	7.718934
H	3.173088	3.020839	7.172793
H	2.999863	4.043546	9.298645
H	2.631583	5.361221	8.185614
H	2.287076	7.625452	8.773656
H	0.563011	7.915621	9.103819
H	1.801288	8.628593	10.143780
H	3.575615	6.229270	10.394193
H	2.988978	7.143352	11.788538
H	2.688974	5.397086	11.684758
H	-3.499650	6.926214	11.088210

H	-2.662231	7.250633	9.569992
H	-3.319116	5.648881	9.891510

E

82

C	2.880639	5.801834	11.414875
N	1.913666	6.466147	10.538221
La	-0.652676	5.809540	11.393800
O	-0.445633	7.081841	13.775467
Si	-0.680258	8.693906	13.556100
O	0.640407	9.531212	14.073957
Si	1.791281	9.251000	15.246156
O	3.179814	9.952943	14.744740
Si	4.298853	11.012698	15.443014
C	2.443992	7.750193	10.082019
O	0.318944	6.440356	8.937762
C	1.376506	5.549761	9.459396
O	0.797913	4.508118	10.076714
C	-2.916710	6.081520	10.291609
Si	-0.818030	5.633720	14.623422
O	-2.195964	5.947467	15.504509
Si	-2.658413	6.687385	16.905628
O	-4.044574	6.005400	17.447424
Si	-4.960902	4.671487	16.955393
O	-0.964725	4.589870	13.433306
C	-0.175717	6.301166	7.605571
C	-0.363723	4.881574	7.073837
C	0.909320	4.245847	6.511070
C	1.992664	3.953664	7.548208
C	2.407388	5.160109	8.391518
O	0.437913	5.424008	15.699643
Si	1.636318	6.336591	16.379296
O	1.173826	6.891910	17.868054
Si	-0.191820	7.342742	18.687362
O	-1.490573	6.526848	18.064558
O	2.980563	5.418741	16.564751
Si	3.341797	3.789783	16.299592
O	2.014729	7.623916	15.405612
O	-2.059617	9.251642	14.258981
Si	-2.548869	9.653877	15.799710
O	-3.849941	10.633847	15.665720
Si	-5.469826	10.546926	16.141210
O	-0.846019	8.754418	11.902160
Si	-1.539376	9.949849	10.888988
O	-1.327048	10.476396	16.542549
Si	-0.045512	10.227270	17.563462
O	-0.414307	8.975264	18.578226
O	-2.952717	8.298918	16.648098
O	0.279267	11.583616	18.431973
O	1.316623	9.918196	16.681864
O	-0.037258	7.029884	20.294204
H	-0.267322	11.703706	19.214165
H	0.002395	6.097627	20.526784
H	-6.072958	4.554778	17.940285
H	-5.508027	4.899218	15.587308
H	-4.126748	3.435330	16.975386
H	-6.117154	9.342198	15.546781
H	-5.564130	10.495473	17.628940
H	-6.116784	11.786400	15.628233
H	4.751994	3.603082	16.742685
H	2.434289	2.920566	17.103927
H	3.211198	3.459559	14.851391
H	3.683197	12.359383	15.616043

H	4.758998	10.484504	16.759178
H	5.441030	11.088138	14.489498
H	-1.060384	9.642593	9.515893
H	-3.021599	9.870744	10.974181
H	-1.055252	11.288503	11.331358
H	-1.140712	6.815703	7.631687
H	0.478492	6.863797	6.920884
H	-1.106696	4.945810	6.268110
H	-0.800350	4.252569	7.856805
H	0.648090	3.312170	5.997560
H	1.316846	4.913729	5.737197
H	1.649327	3.172566	8.234545
H	2.878535	3.563003	7.032346
H	3.329455	4.905916	8.926806
H	2.641543	6.026757	7.760025
H	3.404769	7.640533	9.554733
H	1.725885	8.228613	9.416865
H	2.611734	8.398059	10.948394
H	3.872680	5.702896	10.945772
H	3.004304	6.390274	12.329819
H	2.518513	4.804759	11.670785
H	-3.727045	6.213172	11.027264
H	-2.990080	6.931861	9.594839
H	-3.185204	5.187538	9.704257

$TS_{E \rightarrow F}$

82

C	-3.311611	5.700693	9.985682
La	-1.034230	5.534908	11.081710
N	2.004038	4.765592	11.105457
C	2.136761	3.455311	11.744101
O	0.330719	4.066008	9.733344
C	1.421134	4.743350	9.799677
C	2.338945	4.737451	8.592707
C	1.631190	4.776877	7.236234
C	1.412287	6.176787	6.659244
C	0.502391	7.107817	7.462332
C	1.011046	7.482736	8.856587
O	0.803085	6.519234	9.858556
Si	-0.950105	5.416325	14.305728
O	-1.167451	4.348562	13.147483
O	-0.828702	6.880829	13.408363
Si	-1.240256	8.473763	13.308443
O	-2.545684	8.854587	14.238050
Si	-2.843562	9.219830	15.833505
O	-2.984959	7.840521	16.720941
Si	-2.527521	6.254836	16.861443
O	-1.198915	6.161622	17.846135
Si	0.131028	7.044009	18.280327
O	-0.252780	8.657753	18.262381
Si	-0.190978	9.966218	17.252668
O	-1.607734	10.148163	16.424262
O	-2.210866	5.615772	15.373549
O	0.451977	5.321570	15.196757
Si	1.679661	6.290468	15.709673
O	1.410619	6.775883	17.271952
O	-3.743638	5.420700	17.571662
Si	-4.749014	4.159618	17.059924
O	3.090970	5.460894	15.636258
Si	4.228460	4.972354	16.786857
O	1.815008	7.621032	14.729794
Si	1.395960	9.213076	14.674038
O	2.642718	10.060194	14.037350

Si	2.787285	11.430011	13.060786
O	1.068883	9.774689	16.193222
O	0.055890	9.417646	13.700487
O	-0.012124	11.350540	18.122202
O	0.618922	6.589693	19.784732
O	-1.635446	8.616447	11.706735
Si	-2.710715	9.668921	10.897315
O	-4.241638	10.064146	15.873925
Si	-4.848036	11.337717	16.805880
C	3.175034	5.604252	11.305259
H	2.460354	11.080155	11.647989
H	-3.939586	2.939688	16.778097
H	-5.687138	3.903312	18.188946
H	-0.098539	6.346627	20.377438
H	0.745314	11.362197	18.714787
H	-5.509102	4.565201	15.842806
H	-6.327615	11.312296	16.636949
H	-4.487908	11.149430	18.240966
H	-4.295730	12.629240	16.305572
H	4.834530	6.162914	17.450442
H	3.589836	4.090348	17.805412
H	5.273214	4.218894	16.037727
H	1.873799	12.508814	13.538616
H	4.205482	11.872982	13.163388
H	-2.517646	11.052015	11.420822
H	-2.338719	9.599818	9.458742
H	-4.111444	9.218814	11.112009
H	0.500883	8.403289	9.180380
H	2.083513	7.739482	8.790853
H	0.381138	8.039047	6.891803
H	-0.502119	6.672907	7.557023
H	0.998464	6.070928	5.648185
H	2.389043	6.667589	6.533151
H	0.676004	4.248195	7.329505
H	2.232124	4.207314	6.517367
H	2.885147	3.787013	8.690160
H	3.092564	5.526735	8.673789
H	4.092199	5.177594	10.867203
H	2.988468	6.588542	10.874313
H	3.341714	5.726007	12.379396
H	3.007476	2.896094	11.362592
H	2.264036	3.597856	12.820400
H	1.236599	2.866187	11.576608
H	-4.122146	5.987769	10.675264
H	-3.360244	6.410394	9.143051
H	-3.612465	4.725256	9.566542

F

82

C	-2.836064	5.626083	10.373645
La	-0.495598	5.739017	11.356981
N	1.732205	2.107061	9.293397
C	0.925449	1.054196	9.894616
O	0.536631	3.690580	10.353966
C	1.493133	3.396325	9.595363
C	2.342774	4.502070	9.017689
C	1.757172	5.061434	7.706390
C	2.354554	6.423230	7.315743
C	1.681741	7.665392	7.917324
C	1.722301	7.831416	9.442104
O	0.848713	6.986247	10.113253
Si	-0.404392	6.048319	14.609358
O	-0.292543	4.846959	13.576556

O	-0.651063	7.404388	13.574653
Si	-1.421178	8.870943	13.564266
O	-2.747671	8.861565	14.546975
Si	-3.198246	9.224291	16.098945
O	-3.053501	7.890953	17.058205
Si	-2.179014	6.485840	17.154847
O	-0.881648	6.721042	18.157022
Si	0.171015	7.917801	18.602594
O	-0.611204	9.379195	18.558036
Si	-0.855448	10.653725	17.531516
O	-2.258387	10.456150	16.684361
O	-1.705516	6.010409	15.650498
O	0.944672	6.366567	15.530556
Si	1.918402	7.572817	16.073250
O	1.501420	7.971742	17.628399
O	-3.122376	5.328456	17.832751
Si	-3.868774	3.941522	17.221572
O	3.485142	7.091501	16.049235
Si	4.551995	6.504385	17.216752
O	1.789517	8.900830	15.092768
Si	0.924881	10.304284	15.003061
O	1.864997	11.497437	14.391360
Si	2.351861	11.969748	12.846630
O	0.441393	10.778789	16.508382
O	-0.390802	10.083363	14.014579
O	-1.047768	12.050863	18.379009
O	0.729717	7.612384	20.121298
O	-1.883984	9.074528	12.001855
Si	-3.155100	9.889207	11.231926
O	-4.760491	9.710298	16.064666
Si	-5.633027	10.966423	16.780412
C	2.753593	1.647903	8.368686
H	2.577805	10.777920	11.978444
H	-2.844346	2.912075	16.882331
H	-4.754254	3.437419	18.309778
H	0.059880	7.285910	20.729470
H	-0.254432	12.364557	18.823098
H	-4.680882	4.270974	16.014569
H	-7.071679	10.664272	16.536908
H	-5.361921	11.023380	18.246110
H	-5.270837	12.266537	16.145165
H	5.001458	7.614863	18.105537
H	3.907102	5.432871	18.030321
H	5.718399	5.947009	16.474157
H	1.309284	12.847673	12.240100
H	3.621705	12.731412	13.013596
H	-3.274890	11.269507	11.788508
H	-2.799300	9.950098	9.787941
H	-4.431306	9.147899	11.428459
H	1.480497	8.884098	9.667532
H	2.765824	7.684004	9.784870
H	2.162474	8.546676	7.469485
H	0.628473	7.695749	7.607155
H	2.301551	6.515808	6.223533
H	3.426955	6.431986	7.560285
H	0.670626	5.158858	7.808907
H	1.929696	4.337837	6.898710
H	3.382855	4.195358	8.873960
H	2.322637	5.300597	9.762867
H	3.189051	2.476217	7.814558
H	3.549948	1.116245	8.903089
H	2.304368	0.956918	7.647332
H	0.286433	0.583831	9.138586

H	1.583473	0.290849	10.322522
H	0.302827	1.482262	10.677135
H	-3.628457	5.736243	11.131880
H	-3.036250	6.387027	9.603192
H	-3.018983	4.650533	9.891018

G

82

C	2.722618	5.787418	2.717979
La	3.168655	4.543967	4.885562
Si	5.516867	5.866696	7.468619
O	5.301122	7.503413	7.772067
Si	4.963035	8.555007	8.979208
O	6.345687	9.216902	9.606150
Si	7.944848	8.825259	9.768332
O	8.804618	10.221091	9.613206
O	8.184793	8.167015	11.269213
Si	7.353369	7.318590	12.421758
O	7.808029	7.789341	13.931212
O	7.641832	5.701697	12.214662
Si	7.964627	4.629614	10.997881
O	8.806323	5.376286	9.788656
Si	8.522956	6.128403	8.340197
O	9.804781	5.846392	7.355475
Si	9.934633	5.216966	5.792744
O	5.735037	7.639802	12.337167
Si	4.365396	7.051217	11.620806
O	3.082063	7.341346	12.601593
Si	2.939952	7.876983	14.197737
O	8.436109	7.766057	8.597621
O	7.148952	5.553494	7.647570
O	6.561598	3.986679	10.401397
Si	4.968726	4.380608	10.173653
O	4.063574	3.013843	10.274966
Si	3.378182	2.140901	11.543079
O	8.880397	3.436746	11.648264
Si	9.324465	1.876654	11.185537
O	4.716150	5.049830	8.700042
O	4.489294	5.421808	11.379223
O	4.091460	7.817641	10.181813
O	4.027086	9.778707	8.388473
Si	4.354874	11.422593	8.161528
O	4.951677	5.440766	6.040899
O	1.379623	6.750844	6.653911
C	0.482993	5.774689	6.596865
C	-0.903875	5.958661	7.145746
C	-0.949060	6.204207	8.666394
C	-0.592186	7.631565	9.080323
C	0.811921	8.080396	8.679751
C	1.088619	8.073010	7.187548
O	0.847111	4.716995	6.083072
N	3.416492	2.297727	4.450263
C	4.182564	1.305098	5.165364
C	2.780180	1.739061	3.278114
H	8.743409	7.678385	14.125117
H	3.728954	7.005354	15.114804
H	3.399239	9.291082	14.312077
H	2.073772	0.924254	3.523962
H	9.456901	1.784089	9.702141
H	9.643672	10.110064	9.156354
H	11.376505	5.320748	5.428436
H	9.507141	3.788065	5.770704
H	9.108525	6.012223	4.839353

H	10.634192	1.591146	11.836561
H	8.298148	0.904614	11.662758
H	4.562099	12.098824	9.474028
H	5.549009	11.608292	7.289033
H	3.144833	11.982641	7.491339
H	1.489064	7.786440	14.530186
H	3.230989	0.735290	11.070723
H	4.249819	2.187105	12.753543
H	2.035203	2.704910	11.871328
H	2.001293	8.626402	6.967618
H	0.265205	8.506000	6.607347
H	0.973296	9.109605	9.019984
H	1.580653	7.482553	9.181773
H	-0.696958	7.721396	10.167239
H	-1.328609	8.321200	8.643268
H	-0.293726	5.483523	9.171035
H	-1.966911	5.978199	9.001308
H	-1.446775	5.048794	6.884376
H	-1.385611	6.794440	6.620122
H	2.983502	6.856626	2.770363
H	1.665264	5.741902	2.405518
H	3.299788	5.376215	1.873880
H	3.503197	1.323721	2.551742
H	2.204891	2.508412	2.738540
H	4.656831	1.744664	6.053209
H	3.559671	0.461254	5.516500
H	4.990486	0.865186	4.551421

$TS_{G\rightarrow H}$

82

C	1.400947	5.334305	4.712046
La	3.319710	4.416429	6.325084
Si	5.763939	6.339594	7.287093
O	5.646462	7.911832	7.815048
Si	5.300636	8.796355	9.157767
O	6.704331	9.273299	9.899458
Si	8.269800	8.764047	10.031557
O	9.203811	10.117759	10.087742
O	8.441213	7.875255	11.420190
Si	7.528722	6.937596	12.432878
O	7.974137	7.161341	13.999950
O	7.721057	5.347789	12.005194
Si	8.006258	4.422004	10.668200
O	8.879693	5.273455	9.557827
Si	8.736617	6.263292	8.238151
O	10.047162	6.039204	7.279727
Si	10.245018	5.527388	5.681083
O	5.937006	7.370481	12.363723
Si	4.545780	6.977611	11.559389
O	3.263829	7.215210	12.547227
Si	3.072590	7.809167	14.118106
O	8.733443	7.842695	8.736791
O	7.367593	5.899882	7.393734
O	6.565720	3.918822	10.009197
Si	5.029509	4.490677	9.804668
O	3.988226	3.236861	9.563992
Si	2.998881	2.323660	10.601046
O	8.859843	3.108305	11.143043
Si	8.951796	1.498960	10.640076
O	4.909993	5.360750	8.407151
O	4.573830	5.375831	11.122648
O	4.380234	7.906301	10.206439
O	4.437427	10.124990	8.734959

Si	4.803786	11.769668	8.613023
O	5.043097	5.986847	5.910988
O	1.493665	6.610302	7.319153
C	0.782031	5.502678	6.944459
C	-0.685773	5.644475	6.613165
C	-1.468062	6.321494	7.754921
C	-1.399593	7.850801	7.716649
C	-0.004692	8.447483	7.917727
C	1.060981	7.931977	6.960492
O	1.209731	4.450002	7.508013
N	3.806447	2.366314	5.398650
C	4.999951	2.036487	4.651786
C	2.905743	1.238266	5.481772
H	8.893417	6.957304	14.195133
H	3.750004	6.908690	15.094663
H	3.629816	9.188591	14.221935
H	3.358239	0.368419	5.992842
H	8.981547	1.418183	9.150525
H	10.101124	9.991643	9.765441
H	11.714190	5.523591	5.431094
H	9.693812	4.152571	5.504748
H	9.569069	6.472573	4.746497
H	10.213649	0.950482	11.210839
H	7.780519	0.738930	11.165166
H	5.021640	12.349821	9.969425
H	6.014991	11.976156	7.767725
H	3.618987	12.407759	7.971497
H	1.604549	7.829460	14.372771
H	2.428591	1.231717	9.766687
H	3.827750	1.755051	11.703816
H	1.918214	3.180834	11.161270
H	1.965276	8.539699	7.033186
H	0.726003	7.947159	5.916779
H	-0.060028	9.537152	7.800189
H	0.348664	8.262875	8.939608
H	-2.070436	8.259353	8.482001
H	-1.797771	8.191843	6.750106
H	-1.119434	5.941164	8.722930
H	-2.517582	6.018370	7.665589
H	-1.047289	4.628298	6.443255
H	-0.836421	6.204541	5.686301
H	1.041997	6.339917	4.475736
H	0.638460	4.610512	4.403164
H	2.254908	5.184097	4.017272
H	2.573869	0.884538	4.488320
H	1.997224	1.500207	6.044828
H	5.674014	2.902142	4.589107
H	5.574985	1.212461	5.112671
H	4.777170	1.724560	3.614760

H

82

C	-0.737662	4.104355	5.658399
La	3.172615	4.540446	6.838495
Si	5.438052	6.752622	7.613258
O	5.347799	8.245529	8.338836
Si	5.155649	8.906950	9.836374
O	6.632298	9.206180	10.525128
Si	8.193365	8.675511	10.504160
O	9.151149	10.001372	10.682919
O	8.424905	7.614155	11.757675
Si	7.539599	6.580388	12.697059
O	8.076237	6.596152	14.250942

O	7.663939	5.051544	12.066724
Si	7.792514	4.274571	10.617050
O	8.474130	5.261847	9.493042
Si	8.438677	6.449744	8.342971
O	9.728499	6.246457	7.353517
Si	9.897424	6.046624	5.683501
O	5.958609	7.049137	12.774731
Si	4.497596	6.810490	12.040178
O	3.296467	6.966659	13.135940
Si	3.170005	7.627393	14.688001
O	8.579990	7.925588	9.080296
O	7.053992	6.369893	7.449983
O	6.273792	3.787949	10.121947
Si	4.823459	4.561813	9.997116
O	3.651031	3.490383	9.496681
Si	2.699981	2.359665	10.370721
O	8.717628	2.942830	10.824658
Si	8.672302	1.343955	10.280310
O	4.807624	5.621553	8.744855
O	4.408827	5.263249	11.427037
O	4.288065	7.878207	10.802100
O	4.317654	10.307939	9.723417
Si	4.729765	11.929266	9.491353
O	4.534093	6.478788	6.335636
O	1.209011	5.562981	5.518361
C	0.184931	5.010861	6.469599
C	-0.598989	6.151041	7.145655
C	0.233618	7.339310	7.633271
C	0.459145	8.417286	6.567069
C	1.336987	8.002508	5.385085
C	0.924682	6.702298	4.705746
O	0.941314	4.310014	7.353369
N	3.977114	2.732822	5.659740
C	5.317133	2.728017	5.113454
C	3.269012	1.517492	5.326885
H	9.010299	6.396182	14.362042
H	3.909541	6.775193	15.662153
H	3.715121	9.015610	14.704730
H	3.768827	0.613578	5.722261
H	8.425969	1.303198	8.809638
H	10.027770	9.910893	10.297859
H	11.363778	5.988409	5.424484
H	9.251160	4.775095	5.247833
H	9.294097	7.201812	4.958765
H	10.002873	0.755757	10.598441
H	7.597210	0.597637	10.996225
H	5.136997	12.534874	10.791772
H	5.840402	12.051929	8.502685
H	3.506500	12.605171	8.974596
H	1.716558	7.640747	15.013090
H	2.204563	1.385822	9.364104
H	3.571773	1.692291	11.378813
H	1.580313	3.077039	11.035392
H	1.494385	6.563306	3.780358
H	-0.139535	6.702928	4.434844
H	1.326451	8.800293	4.630178
H	2.381549	7.892811	5.703680
H	0.905947	9.301666	7.037659
H	-0.524279	8.736969	6.192404
H	1.192804	6.983627	8.034625
H	-0.280905	7.803414	8.483000
H	-1.101948	5.668853	7.990620
H	-1.395002	6.514912	6.481951

H	-1.258182	4.648699	4.862957
H	-1.489055	3.664542	6.321004
H	-0.151602	3.296394	5.213406
H	3.170539	1.369235	4.235527
H	2.252574	1.531766	5.742507
H	5.843399	3.663174	5.354780
H	5.934504	1.899636	5.507726
H	5.327168	2.633058	4.011909

$TS_{E \rightarrow I}$

82

C	-3.571841	-0.432906	8.287067
N	-3.373183	0.089101	9.618856
C	-4.416836	-0.348578	10.519564
La	-1.589557	1.373609	10.310712
O	0.287277	0.595888	9.196773
C	1.465258	-0.120991	9.433614
C	2.258230	0.412726	10.628914
C	2.974501	1.750565	10.420334
C	2.132128	2.934343	9.922399
C	1.752963	2.861064	8.436283
C	0.332413	2.466635	8.100714
C	0.115231	1.841403	6.747635
O	-2.306717	3.344668	12.121432
Si	-3.516907	4.425439	11.791134
O	-4.808422	4.209864	12.794806
Si	-5.375947	4.756834	14.253701
O	-4.887953	6.320126	14.494496
Si	-3.650299	7.156319	15.196315
O	-2.434997	7.446130	14.107171
Si	-1.793224	6.811280	12.725995
O	-0.537924	5.793000	13.076585
Si	0.008808	4.861672	14.334113
O	-0.491567	3.304828	14.145051
Si	-1.664763	2.392756	13.399936
O	-1.170133	1.091947	12.622642
O	-2.964276	5.976833	11.896167
O	-1.263916	8.055475	11.804221
Si	-0.077514	8.254773	10.619493
O	-2.896226	2.160454	14.493640
Si	-3.546179	2.814084	15.862830
O	-4.089097	1.619397	16.843056
Si	-4.119913	-0.066588	16.724187
O	-2.415583	3.688040	16.698605
Si	-1.816931	5.226764	16.805883
O	-3.029207	6.307761	16.474388
O	-4.822178	3.796039	15.475178
O	-0.553744	5.466875	15.770574
O	-1.214710	5.481867	18.316030
O	-7.008754	4.695459	14.194003
Si	-8.267920	5.584166	14.886626
O	-4.309621	8.574440	15.704801
O	-0.631475	3.015882	8.695033
O	1.645165	4.930235	14.323598
Si	2.832930	5.046824	15.518631
O	-3.935517	4.052407	10.244583
Si	-5.278411	4.383755	9.261143
H	-1.775187	5.162040	19.029238
H	-4.939635	-0.487556	15.551420
H	2.570204	4.072154	16.616438
H	-3.673961	9.237755	15.989237
H	-4.744846	-0.554799	17.985834
H	-2.733794	-0.601704	16.598002

H	-9.478199	4.717892	14.821883
H	-7.950922	5.920829	16.304941
H	-8.489435	6.833273	14.102975
H	2.869213	6.433919	16.065843
H	4.126890	4.730502	14.850243
H	-0.436650	9.488960	9.866291
H	1.256360	8.420890	11.265829
H	-0.054089	7.079798	9.700491
H	-4.817290	4.230390	7.854278
H	-6.367828	3.413995	9.563001
H	-5.748153	5.778344	9.505709
H	1.221981	-1.181147	9.615658
H	2.106279	-0.113917	8.532273
H	3.011210	-0.335960	10.911777
H	1.572064	0.489548	11.484135
H	3.435334	2.038430	11.373588
H	3.808976	1.606851	9.718324
H	1.226520	3.055272	10.529809
H	2.712519	3.848948	10.087509
H	1.849838	3.857555	7.978356
H	2.449725	2.216672	7.890504
H	0.794835	1.005192	6.577084
H	0.314793	2.606713	5.985181
H	-0.918657	1.512207	6.635351
H	-4.519809	-0.091622	7.830734
H	-2.760545	-0.113848	7.617549
H	-3.589284	-1.538333	8.260749
H	-5.419748	0.002910	10.214656
H	-4.476930	-1.449922	10.597470
H	-4.244261	0.029896	11.537933

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82			
C	-3.079335	-1.265689	8.708303
N	-3.091976	-0.403187	9.866559
C	-4.325681	-0.533088	10.607996
La	-1.322926	0.852262	10.659708
O	0.513164	-0.097854	9.894712
C	1.744198	-0.709131	9.677646
C	2.946178	0.135632	10.117273
C	3.332036	1.338989	9.245635
C	2.307619	2.481990	9.162477
C	1.242440	2.261967	8.061660
C	0.065620	3.171043	8.272629
C	0.018120	4.486503	7.554020
O	-2.383722	3.085531	12.174299
Si	-3.580901	4.148214	11.752185
O	-4.859903	4.054529	12.794650
Si	-5.454497	4.768648	14.163558
O	-4.966005	6.350090	14.237431
Si	-3.732520	7.242343	14.873189
O	-2.512604	7.410152	13.763248
Si	-1.860163	6.633931	12.457210
O	-0.570603	5.715438	12.938041
Si	-0.083458	4.883460	14.286333
O	-0.633123	3.337024	14.244408
Si	-1.769835	2.316238	13.579978
O	-1.200756	0.938038	13.025430
O	-3.000667	5.696607	11.716860
O	-1.354728	7.738830	11.355714
Si	-0.058536	8.813369	11.265151
O	-3.027119	2.214906	14.667328
Si	-3.660749	2.999785	15.971598

O	-4.202352	1.909873	17.068992
Si	-4.381983	0.229012	17.044504
O	-2.524187	3.944491	16.720120
Si	-1.921818	5.484322	16.689992
O	-3.120960	6.539144	16.240718
O	-4.931108	3.953630	15.499528
O	-0.645147	5.633147	15.653867
O	-1.352565	5.874769	18.184794
O	-7.087764	4.711393	14.085736
Si	-8.344059	5.760086	14.502514
O	-4.389288	8.706267	15.238313
O	-0.842692	2.856769	9.046520
O	1.555665	4.916532	14.282152
Si	2.742436	4.636495	15.450120
O	-4.067928	3.700818	10.251006
Si	-5.495947	3.878196	9.363187
H	-1.864751	5.505241	18.910237
H	-5.205368	-0.190026	15.873577
H	2.241669	3.704711	16.501588
H	-3.803767	9.303739	15.712633
H	-5.079628	-0.126776	18.312676
H	-3.045991	-0.431123	16.993900
H	-9.590901	4.944552	14.485988
H	-8.121008	6.329662	15.863080
H	-8.440241	6.860057	13.499846
H	3.140756	5.934840	16.066996
H	3.909082	4.034448	14.743707
H	-0.546191	10.028580	10.553499
H	0.427552	9.176172	12.628464
H	1.048370	8.183904	10.486571
H	-5.126128	3.706775	7.930228
H	-6.479628	2.835790	9.769996
H	-6.071523	5.237589	9.583347
H	1.790897	-1.665849	10.223927
H	1.866769	-0.967057	8.608172
H	3.820695	-0.528466	10.162378
H	2.764541	0.473396	11.147018
H	4.264352	1.753753	9.649213
H	3.575464	0.995850	8.229856
H	1.816472	2.594998	10.136379
H	2.825656	3.428918	8.966308
H	1.692556	2.432565	7.077739
H	0.879717	1.232760	8.136572
H	-0.109021	4.301994	6.480135
H	0.970945	5.014862	7.668743
H	-0.804933	5.100779	7.920005
H	-3.878247	-1.016667	7.984719
H	-2.123307	-1.184798	8.173407
H	-3.213679	-2.332692	8.968290
H	-5.212793	-0.237001	10.017730
H	-4.509903	-1.566835	10.956421
H	-4.317061	0.104324	11.505080

- (CH3 or NMe2)(BH4)La@c-2

(NMe_2)(BH_4)La@**c**-2

65

O	3.040881	6.959213	11.088640
Si	2.357267	6.512474	9.633828
O	6.883568	10.176909	9.296529
Si	0.835638	3.874403	9.194667
O	3.444803	6.836165	8.436318

H	0.499995	4.159600	7.769780
Si	3.780731	7.975500	7.290355
O	4.852266	9.074341	7.920568
Si	5.307281	9.756705	9.355217
O	4.388224	11.083638	9.692125
Si	2.990158	11.859538	9.262974
O	2.458671	11.275541	7.810109
Si	1.503811	10.085366	7.169289
O	2.409073	8.755547	6.796470
O	4.452822	7.194223	6.010928
O	0.957828	7.342553	9.371926
Si	0.016002	8.695070	9.524514
O	-1.553379	8.236718	9.497650
Si	-2.869542	8.490909	10.531226
O	2.065658	4.910375	9.722370
Si	8.150240	9.955858	8.197304
Si	3.868341	8.284821	11.596801
O	4.361679	8.054762	13.177032
Si	5.262131	6.760047	13.880740
O	2.893128	9.591768	11.819031
Si	1.460572	10.508677	11.584648
O	1.837229	11.646219	10.433982
La	2.799356	9.990738	14.460755
B	2.212019	8.224221	16.416279
N	4.344477	11.522560	15.122985
C	4.436079	12.835303	14.514399
C	5.292891	11.368991	16.207541
O	1.184081	11.014152	13.073957
O	5.117253	8.652693	10.595491
O	3.302560	13.456472	9.094784
Si	2.686769	14.874782	9.776268
O	0.329077	9.468621	10.953440
O	0.309320	9.707169	8.250866
O	0.851945	10.574096	5.741407
H	4.275895	7.601872	5.157875
H	0.212806	11.289735	5.805606
H	-4.036489	7.838934	9.874280
H	-2.606819	7.865224	11.858637
H	-3.119446	9.952349	10.692759
H	-0.371258	4.055264	10.050790
H	1.369139	2.491872	9.336030
H	3.418240	15.996991	9.125391
H	1.225048	14.985419	9.498076
H	2.926393	14.887897	11.247828
H	8.391356	8.499970	7.981841
H	7.821535	10.615976	6.901139
H	9.346594	10.592809	8.813437
H	6.065738	7.371624	14.970122
H	4.308724	5.744769	14.394750
H	6.137738	6.192940	12.817286
H	5.141048	12.117719	17.004025
H	5.196604	10.379512	16.673056
H	6.337071	11.471615	15.864464
H	4.255397	13.646881	15.240661
H	5.426471	13.019928	14.063798
H	3.690986	12.951345	13.714406
H	3.434848	8.218581	16.198739
H	1.915579	7.472839	17.303293
H	1.900971	9.399216	16.698990
H	1.632540	7.924150	15.361161

C	2.943458	5.333070	12.175371
N	1.700820	5.690294	11.525320
C	0.571677	5.532582	12.413298
La	1.712777	6.298222	9.318535
O	0.193297	9.224979	10.666114
C	-0.887580	10.099030	11.066207
C	-1.615658	10.730418	9.889876
C	-0.918893	11.952607	9.289005
C	0.481937	11.686841	8.737752
C	1.473282	11.131920	9.780802
C	1.273716	9.664097	10.039155
O	2.086435	8.824588	9.656271
B	-0.709013	6.662984	8.099346
Si	4.083622	4.657878	7.815837
O	5.450409	3.950069	8.441977
Si	6.036872	2.557227	9.103789
O	7.163393	2.921184	10.237788
Si	7.893407	4.349931	10.757904
O	3.812531	6.162102	8.275851
O	2.707754	3.847720	8.437299
Si	1.744886	2.521503	8.170224
O	1.638824	2.202103	6.552195
Si	2.389374	1.300279	5.382465
O	2.961963	-0.099073	6.044413
Si	4.349006	-0.709226	6.714178
O	4.446205	-2.331861	6.467678
O	0.280537	2.964621	8.759068
Si	-1.319920	2.506793	8.427519
O	4.092468	4.400887	6.171201
Si	4.704190	3.371993	5.034634
O	3.614953	2.171322	4.693191
O	2.313074	1.195898	8.969747
Si	3.726264	0.518003	9.498889
O	4.818851	1.710869	9.831512
O	4.334460	-0.509137	8.351274
O	3.411016	-0.324583	10.864487
Si	3.777663	-1.880731	11.410436
O	5.642569	0.056874	6.022194
Si	6.654108	1.325996	6.315510
O	8.119184	0.874374	5.718117
O	6.123219	2.696551	5.549605
O	6.754487	1.624525	7.940542
O	4.991761	4.205618	3.651960
Si	4.902148	5.841207	3.241936
O	1.291397	0.903602	4.234833
Si	0.876334	1.516002	2.717627
H	4.643770	-2.592376	5.563239
H	8.788476	1.564791	5.724496
H	5.348567	5.935103	1.822933
H	3.500254	6.334797	3.368395
H	5.805621	6.647567	4.113450
H	0.801459	3.005520	2.755226
H	1.883391	1.084453	1.705111
H	-0.458033	0.943225	2.384317
H	8.919457	3.951220	11.762409
H	8.549201	5.046958	9.612411
H	6.886955	5.252148	11.388242
H	3.015095	-2.892447	10.623868
H	5.241651	-2.141865	11.294241
H	3.361678	-1.925622	12.840564
H	-2.148558	3.045073	9.539590
H	-1.753131	3.070033	7.119991
H	-1.406778	1.016556	8.396118

H	-1.547269	9.427815	11.616993
H	-0.501926	10.849981	11.766579
H	-2.608186	11.028366	10.249083
H	-1.780445	9.954243	9.132468
H	-1.543864	12.359192	8.486024
H	-0.856048	12.738649	10.055140
H	0.432919	10.998652	7.885148
H	0.898189	12.624071	8.353548
H	2.500204	11.235831	9.426835
H	1.381582	11.691939	10.720426
H	-0.010837	7.691029	8.094589
H	-0.038676	5.767968	7.560308
H	-0.912211	6.342323	9.275019
H	-1.737895	6.841733	7.500547
H	0.646668	6.177792	13.308111
H	-0.364097	5.791762	11.901742
H	0.465958	4.495368	12.778901
H	3.156393	5.964147	13.057663
H	2.957150	4.283865	12.520365
H	3.795441	5.452299	11.489102

$TS_{D\rightarrow E}$

83

C	2.585176	6.245831	11.321143
N	1.400832	6.533374	10.536581
C	0.215897	6.017926	11.186703
La	1.628743	6.793443	8.135057
O	0.292478	8.895315	9.503312
C	-0.954443	9.156328	10.180307
C	-1.093636	10.623578	10.558112
C	-0.306124	11.043472	11.801287
C	1.200578	10.781622	11.739136
C	1.569599	9.291304	11.594270
C	1.482622	8.820022	10.170996
O	2.471447	8.792009	9.402404
B	-0.571677	6.812325	6.568110
Si	3.995786	4.904300	7.030026
O	5.371031	4.427544	7.828876
Si	5.942491	3.268759	8.858357
O	7.046084	3.934792	9.869470
Si	7.730814	5.471121	10.017814
O	3.676578	6.469229	7.059873
O	2.637434	4.281330	7.883576
Si	1.671212	2.927274	7.940997
O	1.598586	2.194164	6.465921
Si	2.352294	0.999190	5.596405
O	2.922092	-0.153540	6.631257
Si	4.306363	-0.548973	7.451621
O	4.414928	-2.175276	7.662461
O	0.197876	3.524000	8.351947
Si	-1.396660	3.038880	8.010837
O	3.999192	4.191151	5.531219
Si	4.650550	2.911439	4.713047
O	3.581251	1.645175	4.698227
O	2.213147	1.871073	9.084159
Si	3.637933	1.391976	9.781961
O	4.700922	2.655414	9.762122
O	4.269306	0.095727	8.970635
O	3.326297	0.966138	11.329405
Si	3.705458	-0.368351	12.295606
O	5.604082	0.005720	6.587688
Si	6.600679	1.319488	6.528754
O	8.075494	0.738511	6.090703

O	6.065990	2.423621	5.414869
O	6.675279	2.052003	8.011810
O	4.954235	3.351110	3.165511
Si	4.777603	4.794694	2.302110
O	1.253706	0.303588	4.604248
Si	0.942869	0.348342	2.944256
H	4.678336	-2.668831	6.880161
H	8.729925	1.410037	5.877296
H	5.261636	4.507350	0.922430
H	3.344692	5.205405	2.268773
H	5.605027	5.869888	2.921552
H	0.859954	1.759117	2.467535
H	2.018618	-0.375621	2.206817
H	-0.363733	-0.339365	2.747983
H	8.712290	5.380156	11.135205
H	8.429313	5.851298	8.755352
H	6.680603	6.479623	10.340255
H	2.972436	-1.573575	11.812842
H	5.175203	-0.621120	12.277660
H	3.262363	-0.016730	13.674051
H	-2.270898	3.838082	8.911456
H	-1.718327	3.299885	6.582705
H	-1.537459	1.584932	8.317760
H	-1.708645	8.867796	9.445881
H	-1.050107	8.497216	11.049008
H	-2.159712	10.819524	10.728326
H	-0.802346	11.227444	9.689711
H	-0.475243	12.111366	11.982963
H	-0.716755	10.517456	12.675017
H	1.658699	11.354257	10.923260
H	1.657188	11.149009	12.664864
H	2.603380	9.122196	11.899508
H	0.929650	8.681536	12.241146
H	-0.001202	7.917269	6.608035
H	0.253738	5.982641	6.159102
H	-0.874179	6.511740	7.734298
H	-1.541787	6.850637	5.861000
H	0.036320	6.485390	12.175654
H	-0.676345	6.186628	10.571184
H	0.276757	4.931766	11.369560
H	2.514615	6.643127	12.350864
H	2.778222	5.164289	11.417107
H	3.471692	6.700670	10.860284

E
83

C	3.219482	6.474770	11.161898
N	1.796122	6.475082	10.807090
C	1.050606	5.607736	11.721171
La	1.503029	6.757174	8.081596
O	-0.087957	7.499831	10.085594
C	-1.214401	8.375342	10.202382
C	-0.960489	9.865801	9.992390
C	-0.436491	10.598947	11.229427
C	0.970639	10.196934	11.667214
C	1.155795	8.698285	11.912001
C	1.240776	7.871609	10.624969
O	1.950548	8.442983	9.638574
B	-0.395395	7.318408	6.246575
Si	4.043811	5.106603	6.967584
O	5.405831	4.626770	7.795273
Si	5.836128	3.443752	8.867793
O	6.932436	4.042161	9.927059

Si	7.944148	5.395794	9.942072
O	3.628823	6.642948	7.041636
O	2.725376	4.376271	7.791323
Si	1.590114	3.193185	7.930701
O	1.333663	2.374468	6.528228
Si	2.148876	1.200015	5.669896
O	2.690697	0.062350	6.733829
Si	4.047562	-0.360301	7.585503
O	4.082795	-1.978792	7.863707
O	0.253735	4.119692	8.285170
Si	-1.420437	3.752955	8.131110
O	4.099424	4.426296	5.451994
Si	4.586072	3.021651	4.729956
O	3.398928	1.870037	4.829597
O	1.989043	2.174833	9.161637
Si	3.432662	1.693578	9.841870
O	4.517241	2.934131	9.732777
O	4.011202	0.347706	9.077957
O	3.136674	1.355439	11.413212
Si	3.526808	0.075467	12.450298
O	5.377424	0.101951	6.718496
Si	6.428270	1.371338	6.617196
O	7.883504	0.712328	6.229245
O	5.960370	2.443822	5.445826
O	6.503768	2.156925	8.072428
O	4.888909	3.307755	3.147943
Si	4.878040	4.704238	2.190641
O	1.089556	0.504759	4.639921
Si	0.869207	0.497847	2.962801
H	4.383809	-2.512835	7.122632
H	8.550420	1.339896	5.935703
H	5.300019	4.266559	0.830410
H	3.506368	5.285290	2.144154
H	5.843883	5.703956	2.730650
H	0.786822	1.894636	2.447625
H	1.998169	-0.223724	2.307896
H	-0.411838	-0.220963	2.718935
H	8.880294	5.201086	11.084347
H	8.708261	5.486534	8.663398
H	7.138626	6.634146	10.142084
H	2.771780	-1.146813	12.053358
H	4.993613	-0.189764	12.412988
H	3.116673	0.515188	13.813218
H	-2.127684	4.715695	9.014352
H	-1.829884	3.899776	6.711543
H	-1.624852	2.353789	8.604318
H	-1.907252	8.006726	9.440627
H	-1.685228	8.214029	11.184090
H	-1.924372	10.307250	9.707896
H	-0.287939	10.006097	9.139167
H	-0.453584	11.679088	11.038966
H	-1.138786	10.425997	12.058752
H	1.698420	10.502081	10.908049
H	1.221206	10.736628	12.588677
H	2.104456	8.547854	12.439502
H	0.368308	8.300236	12.564569
H	0.149322	8.341284	6.698115
H	0.485335	6.616366	5.731852
H	-0.857170	6.693309	7.219144
H	-1.262954	7.597215	5.464581
H	1.169384	5.916865	12.771018
H	-0.007635	5.622679	11.462870
H	1.424404	4.583532	11.630235

H	3.385058	6.747995	12.215807
H	3.625231	5.470432	11.010541
H	3.756723	7.183214	10.529696

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83

B	-3.453634	5.674549	10.216430
La	-0.941353	5.490065	11.162026
O	-0.649257	6.830505	13.474421
Si	-1.109843	8.405799	13.309790
O	-1.503189	8.452475	11.700828
Si	-2.622996	9.443479	10.855806
O	0.199741	4.183458	9.414410
C	1.330587	4.696663	9.704074
C	2.407440	4.784241	8.646222
C	1.890003	5.057015	7.232625
C	1.756340	6.535727	6.865301
C	0.779164	7.364339	7.703018
C	1.182767	7.582839	9.163638
O	0.896029	6.522443	10.041862
Si	-0.712354	5.369494	14.374913
O	0.703074	5.320819	15.247388
Si	1.886778	6.354816	15.744294
O	1.962543	7.665614	14.732601
Si	1.505024	9.246155	14.645590
O	0.161566	9.395854	13.665791
O	-0.895953	4.298699	13.208351
N	1.708293	4.461369	11.081891
C	2.903527	5.141955	11.572270
C	1.714584	3.037525	11.449589
O	-1.970884	5.512089	15.449496
Si	-2.312958	6.200863	16.911113
O	-3.504389	5.357769	17.648922
Si	-4.564142	4.138295	17.142073
O	-2.426283	8.786847	14.220747
Si	-2.728964	9.147758	15.817403
O	-4.157968	9.935334	15.872840
Si	-4.742019	11.312328	16.661823
O	-2.806355	7.767848	16.709810
O	-1.523236	10.126077	16.390898
Si	-0.098381	10.003507	17.215831
O	0.043919	11.409245	18.056821
O	-0.983492	6.179182	17.898665
Si	0.318077	7.114456	18.305494
O	0.829178	6.710745	19.816296
O	-0.115030	8.714511	18.252349
O	1.599956	6.862374	17.294887
O	1.161662	9.828278	16.153094
O	3.327721	5.577225	15.685485
Si	4.503848	5.186897	16.835271
O	2.732527	10.107088	13.991498
Si	2.859677	11.517983	13.071936
H	2.534437	11.218910	11.647208
H	-3.802505	2.887947	16.860541
H	-5.505656	3.921053	18.276256
H	0.124461	6.452603	20.417888
H	0.792187	11.447729	18.659816
H	-5.310427	4.573062	15.927047
H	-6.218890	11.303744	16.471701
H	-4.406611	11.257069	18.113982
H	-4.149811	12.534942	16.046927
H	5.046148	6.427660	17.460609
H	3.926814	4.296767	17.883019

H	5.582192	4.474849	16.093316
H	1.933613	12.564923	13.593944
H	4.272735	11.973229	13.189840
H	-2.466876	10.839245	11.360410
H	-2.231659	9.362924	9.424456
H	-4.004262	8.950310	11.082931
H	0.655816	8.470093	9.545260
H	2.259530	7.825077	9.206279
H	0.695251	8.355710	7.237305
H	-0.225696	6.922833	7.671158
H	1.452199	6.597417	5.812676
H	2.748341	7.009176	6.918532
H	0.927212	4.547981	7.113737
H	2.580224	4.592253	6.518675
H	2.888175	3.794325	8.673917
H	3.177386	5.504008	8.940522
H	3.828546	4.715769	11.155285
H	2.840561	6.200441	11.321160
H	2.947372	5.038472	12.659529
H	2.622228	2.529565	11.088061
H	1.672213	2.957440	12.537726
H	0.840990	2.539391	11.030150
H	-2.980333	4.530853	10.097512
H	-4.573893	5.734967	9.790611
H	-3.405100	5.965988	11.422824
H	-2.694069	6.451210	9.610478

F

83

B	-3.046277	6.023787	9.967362
La	-0.650922	5.812735	11.225525
O	-0.692472	7.446104	13.466207
Si	-1.403557	8.944785	13.529698
O	-1.934923	9.209496	12.002728
Si	-3.328702	9.903753	11.322146
O	0.204607	3.691142	10.265565
C	1.247076	3.257623	9.713072
C	2.353443	4.226570	9.376142
C	2.114843	4.923484	8.021930
C	2.934892	6.212155	7.849320
C	2.311913	7.502452	8.402312
C	2.138409	7.621414	9.920231
O	1.096191	6.848602	10.430026
Si	-0.370624	6.076748	14.451869
O	1.045942	6.346065	15.274604
Si	2.088769	7.506723	15.790660
O	1.934184	8.864700	14.857033
Si	1.084886	10.278444	14.846063
O	-0.301763	10.102892	13.950914
O	-0.337359	4.902641	13.373001
N	1.347159	1.951672	9.412683
C	2.461838	1.349041	8.701763
C	0.284664	1.029634	9.791087
O	-1.592627	5.997490	15.578267
Si	-1.956636	6.474503	17.115046
O	-2.884693	5.334385	17.839553
Si	-3.694281	3.963161	17.274025
O	-2.667656	8.950076	14.591650
Si	-2.986936	9.269455	16.185503
O	-4.536167	9.782634	16.291171
Si	-5.330408	11.021891	17.119512
O	-2.793272	7.903246	17.088571
O	-1.975157	10.461118	16.732655

Si	-0.517945	10.606363	17.493615
O	-0.625063	11.984274	18.386284
O	-0.588473	6.661042	18.028529
Si	0.515687	7.824972	18.434711
O	1.163418	7.472684	19.906886
O	-0.235541	9.302251	18.472662
O	1.783391	7.871671	17.379500
O	0.712876	10.728748	16.391844
O	3.630269	6.968972	15.655017
Si	4.845089	6.582716	16.760456
O	2.007790	11.451707	14.172680
Si	1.902433	12.392054	12.775507
H	1.828328	11.521721	11.566131
H	-2.711030	2.918348	16.866073
H	-4.515249	3.469875	18.416088
H	0.527473	7.149929	20.552254
H	0.189597	12.243569	18.826839
H	-4.575332	4.313087	16.122786
H	-6.787868	10.742538	16.987859
H	-4.935797	11.024124	18.558107
H	-5.004244	12.339013	16.500392
H	5.249802	7.793418	17.532115
H	4.382441	5.515863	17.694899
H	5.996190	6.086857	15.953385
H	0.701738	13.275479	12.836620
H	3.141837	13.217953	12.735316
H	-3.579661	11.222663	11.977252
H	-3.033135	10.101531	9.878168
H	-4.497588	9.005325	11.516776
H	1.963140	8.683019	10.156896
H	3.091321	7.352756	10.411677
H	2.949215	8.337316	8.078938
H	1.331631	7.665791	7.933988
H	3.102245	6.363421	6.775553
H	3.933932	6.070086	8.286789
H	1.049160	5.156910	7.916274
H	2.356489	4.222390	7.212480
H	3.341768	3.759567	9.400422
H	2.318052	4.985030	10.162121
H	2.073151	0.709174	7.902873
H	3.098301	2.104561	8.246585
H	3.065155	0.729382	9.375812
H	0.717777	0.171837	10.315597
H	-0.419695	1.541041	10.443200
H	-0.242109	0.669744	8.900288
H	-2.359258	5.097319	9.502566
H	-4.098678	6.119383	9.395181
H	-3.211287	5.800092	11.177113
H	-2.377856	7.064417	9.853779

(CH_3)(BH_4)La@**c**-2
60

B	-0.364442	7.915450	7.530435
La	1.276488	6.000750	8.403991
C	1.633957	6.364944	10.837964
Si	3.509033	4.102377	7.118997
O	3.519332	3.698984	5.509791
Si	3.638903	2.319700	4.599158
O	4.037653	2.723903	3.067394
Si	4.267917	4.187079	2.247957
O	2.195412	1.512605	4.584907
Si	0.778452	0.987923	5.230177
O	1.012638	-0.412123	6.074589

Si	2.215476	-1.242973	6.843964
O	1.790563	-2.825367	6.739312
O	-0.345340	0.779085	4.068118
Si	-0.911079	-0.527793	3.151136
O	0.169702	2.139655	6.278831
Si	0.629420	2.644775	7.770879
O	0.745009	1.407200	8.842439
Si	2.033475	0.514003	9.429417
O	1.620734	-0.045924	10.905752
Si	2.106413	0.260258	12.497835
O	4.806827	1.328806	5.218928
Si	4.980004	0.017983	6.214472
O	6.266098	-0.892444	5.748123
O	5.175317	0.548347	7.771613
Si	4.796484	1.814684	8.761442
O	5.972365	1.966886	9.888253
Si	6.940817	3.248263	10.421583
O	3.673319	-0.985176	6.110182
O	4.681901	3.223566	7.898118
O	3.359612	1.497154	9.531034
O	2.012278	3.535039	7.754999
O	3.396858	5.660442	7.450830
O	-0.430115	3.833569	8.299648
Si	-2.157367	3.819985	8.383591
O	2.319050	-0.760016	8.426609
H	2.455959	-3.450104	7.042702
H	7.091790	-0.411513	5.639668
H	4.557283	3.822242	0.833406
H	3.033131	5.019303	2.325924
H	5.422144	4.924271	2.837638
H	-1.597299	0.061349	1.968585
H	0.229747	-1.384872	2.718509
H	-1.872809	-1.323041	3.966174
H	7.741535	2.710667	11.556529
H	7.843663	3.696070	9.322185
H	6.088641	4.382334	10.879872
H	1.211359	-0.554368	13.364703
H	3.526861	-0.152286	12.682653
H	1.949255	1.710706	12.808198
H	-2.504396	4.833315	9.412891
H	-2.697992	4.177909	7.047370
H	-2.580446	2.453411	8.794876
H	-0.111505	8.088092	8.731455
H	0.717315	7.884026	6.913639
H	-0.868095	6.777457	7.419310
H	0.696698	6.487711	11.401318
H	2.172802	5.516631	11.290636
H	2.238198	7.261516	11.044278
H	-1.090134	8.759921	7.086218

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78

H	1.671717	5.565446	4.862909
O	4.225313	4.171912	6.807911
O	6.982174	4.505156	8.460602
Si	3.524733	5.205645	7.882408
Si	6.173230	5.531016	9.477588
O	4.677818	5.880038	8.864215
O	6.040936	4.841866	10.975138
Si	2.321275	3.593010	10.252086
Si	4.990140	3.892880	11.834233
O	3.451163	4.191526	11.305251
O	2.581262	1.974609	10.038623

O	5.371881	2.293623	11.665981
O	2.405742	4.425139	8.824544
Si	6.049317	1.271692	10.557170
Si	3.384991	0.978376	8.988675
O	4.887953	0.613224	9.583730
O	3.512257	1.682366	7.511392
O	7.163756	2.071633	9.635783
O	6.138129	2.269966	7.135875
O	8.715851	2.669774	7.522768
Si	7.240232	2.893200	8.199217
La	6.642498	1.266839	4.308607
O	7.978877	-0.531350	5.589165
C	7.427686	-1.487812	6.135010
C	8.202434	-2.683953	6.609393
C	8.134919	-2.916658	8.130842
C	6.837122	-3.567133	8.606858
C	5.574105	-2.757616	8.315660
C	5.310501	-2.488131	6.845145
O	6.114279	-1.408150	6.294792
Si	4.562722	2.561387	6.560491
O	4.609275	2.103943	5.031403
O	6.798583	0.040489	11.340817
Si	7.280649	-0.190889	12.945718
O	2.565202	-0.439728	8.858660
Si	0.968923	-0.879890	9.203996
O	2.764339	6.414318	7.080926
Si	2.442015	6.702162	5.444074
O	0.805652	3.745041	10.874364
O	5.130521	4.198623	13.443654
O	7.035863	6.912427	9.636730
Si	6.924045	8.468455	8.987671
Si	10.138256	3.590348	7.450894
C	5.961059	-0.469016	2.634434
B	8.225867	2.974575	3.007572
H	4.962915	5.109152	13.703414
H	8.101554	0.960941	13.416778
H	6.085806	-0.365517	13.819883
H	6.709646	8.405955	7.513183
H	0.375180	4.579373	10.665742
H	1.624764	7.947837	5.405461
H	3.715844	6.899270	4.695738
H	5.799200	9.204728	9.634571
H	8.217197	9.141339	9.293704
H	0.768903	-0.960880	10.679271
H	0.013095	0.095235	8.605952
H	0.777643	-2.226367	8.592088
H	8.098994	-1.437332	12.947440
H	9.926623	4.793326	6.599942
H	10.538307	4.000153	8.829665
H	11.175350	2.700734	6.860895
H	4.293583	-2.125090	6.695997
H	5.456763	-3.378835	6.222972
H	4.702287	-3.306139	8.692134
H	5.582186	-1.801769	8.850696
H	6.904711	-3.741208	9.686399
H	6.745137	-4.559028	8.141329
H	8.301657	-1.967640	8.654817
H	8.977215	-3.564393	8.396002
H	9.231263	-2.513336	6.288183
H	7.835198	-3.573407	6.079013
H	5.360290	-1.265291	3.104627
H	6.807548	-0.959755	2.130474
H	5.332293	-0.043409	1.837275

H	8.866543	2.348931	3.871622
H	8.921917	3.753947	2.417123
H	7.724947	2.132496	2.242465
H	7.295063	3.557461	3.589736

$TS_{G \rightarrow H}$
78

H	1.207323	5.293277	4.786390
O	3.755939	3.941684	6.715900
O	6.906955	4.741851	8.508498
Si	3.169074	5.067001	7.772314
Si	5.878749	5.763656	9.333789
O	4.398095	5.780710	8.615934
O	5.748627	5.260505	10.901142
Si	2.122024	3.663333	10.339054
Si	4.767537	4.318353	11.848991
O	3.212430	4.455141	11.303075
O	2.515493	2.061133	10.266745
O	5.263681	2.743132	11.824227
O	2.116304	4.365663	8.841258
Si	6.013491	1.641230	10.846623
Si	3.366000	0.996973	9.326403
O	4.916586	0.863959	9.892636
O	3.384346	1.485229	7.751386
O	7.124026	2.412539	9.873348
O	5.893682	2.442236	7.443560
O	8.409638	2.726814	7.477730
Si	7.071324	3.107957	8.380985
La	7.021109	1.470668	5.187271
O	8.520305	-0.227178	6.109429
C	7.661989	-1.125762	5.875541
C	8.072088	-2.553053	5.607875
C	8.061217	-3.405010	6.892308
C	6.677780	-3.959189	7.248267
C	5.618178	-2.910913	7.598131
C	5.407050	-1.832165	6.548275
O	6.490052	-0.880502	6.562684
Si	4.337609	2.385135	6.728069
O	4.681021	1.756483	5.302884
O	6.808450	0.547315	11.764457
Si	7.178086	0.420203	13.410470
O	2.660041	-0.479719	9.410193
Si	1.253328	-1.068924	10.140007
O	2.365896	6.222037	6.936853
Si	2.010494	6.441585	5.296160
O	0.608792	3.740661	10.978939
O	4.887524	4.785426	13.420469
O	6.524662	7.264069	9.337650
Si	7.402301	8.202330	8.236535
Si	10.081053	2.634386	7.849881
C	6.957147	-0.739140	3.713451
B	8.131147	3.269963	3.537825
H	4.663642	5.704812	13.592044
H	7.899971	1.640388	13.872367
H	5.928266	0.232626	14.201318
H	6.876136	8.007035	6.855002
H	0.124064	4.542036	10.760419
H	1.213831	7.698413	5.218790
H	3.269616	6.579527	4.510571
H	7.230634	9.618914	8.662963
H	8.841598	7.817733	8.296413
H	1.337119	-0.914102	11.620838

H	0.055881	-0.351778	9.615890
H	1.182463	-2.513889	9.781384
H	8.054307	-0.777431	13.541532
H	10.770494	2.405677	6.555607
H	10.496163	3.927763	8.463728
H	10.310257	1.513757	8.801252
H	4.521033	-1.237289	6.775273
H	5.291856	-2.241216	5.538644
H	4.655129	-3.412375	7.755237
H	5.864559	-2.413400	8.543915
H	6.777471	-4.651337	8.092868
H	6.318767	-4.562765	6.402221
H	8.475394	-2.827730	7.727989
H	8.742794	-4.248428	6.734226
H	9.078677	-2.492166	5.188705
H	7.431796	-3.019238	4.854438
H	6.254260	-1.575876	3.684329
H	7.899500	-1.052899	3.251824
H	6.516831	0.006032	3.018480
H	9.009256	2.629785	4.137194
H	8.606325	4.074775	2.785675
H	7.417929	2.447851	2.934204
H	7.409349	3.813440	4.392054

H

78

H	1.457075	5.929261	4.878029
O	3.713262	4.131965	6.841759
O	6.847825	4.358423	8.677423
Si	3.254064	5.290730	7.926361
Si	5.992898	5.499876	9.550496
O	4.553855	5.804454	8.812546
O	5.762307	4.943124	11.085175
Si	1.960437	3.944591	10.414289
Si	4.631063	4.125794	11.982625
O	3.126074	4.537008	11.435685
O	2.139331	2.312057	10.282942
O	4.882751	2.497259	11.874770
O	2.093542	4.705017	8.949049
Si	5.482555	1.333529	10.869476
Si	2.798702	1.161341	9.295675
O	4.305479	0.764213	9.862502
O	2.890197	1.728282	7.742813
O	6.722685	1.955480	9.942500
O	5.523801	2.238413	7.539712
O	8.058391	2.209936	7.558438
Si	6.775938	2.725492	8.489851
La	6.545120	1.250186	5.259425
O	6.580655	-0.762861	4.243126
C	6.498429	-1.765027	5.159931
C	7.664238	-2.759651	5.038380
C	9.026761	-2.255079	5.520496
C	9.272619	-2.477083	7.018023
C	8.400454	-1.647295	7.962354
C	6.906023	-1.702102	7.674997
O	6.579327	-1.016914	6.464142
Si	4.004657	2.498033	6.781125
O	4.284722	1.896491	5.329491
O	6.105400	0.104475	11.748077
Si	6.033167	-0.343800	13.379603
O	1.880113	-0.190911	9.334546
Si	0.564481	-0.756885	8.435260
O	2.637658	6.572442	7.117976

Si	2.403064	6.914340	5.476116
O	0.459026	4.221191	11.024698
O	4.800265	4.486688	13.576575
O	6.885907	6.863934	9.640063
Si	7.736107	7.841422	8.552515
Si	9.697937	2.740673	7.554589
C	5.145415	-2.468272	5.116554
B	8.181548	2.930107	3.923264
H	4.605825	5.397684	13.815406
H	6.827957	0.612120	14.201944
H	4.617054	-0.371409	13.844532
H	7.116629	7.770334	7.198031
H	0.081428	5.072368	10.784285
H	1.818510	8.283816	5.426593
H	3.706472	6.882137	4.753632
H	7.671879	9.230974	9.083937
H	9.152150	7.378273	8.492816
H	-0.132094	-1.756050	9.292762
H	-0.357075	0.366122	8.097000
H	1.057215	-1.406775	7.187088
H	6.628926	-1.707110	13.454448
H	10.473597	1.637955	6.930410
H	9.806887	4.005375	6.786507
H	10.108575	2.936049	8.974796
H	6.343413	-1.206087	8.472094
H	6.544200	-2.736238	7.617324
H	8.562860	-1.977988	8.996553
H	8.705244	-0.593334	7.928984
H	10.325434	-2.271499	7.247709
H	9.120113	-3.543942	7.235601
H	9.144385	-1.195257	5.255950
H	9.810666	-2.784038	4.966286
H	7.705108	-2.998566	3.970654
H	7.418649	-3.697048	5.554968
H	5.022924	-3.184585	5.935721
H	5.054110	-3.011039	4.171252
H	4.344043	-1.726655	5.165208
H	8.821831	2.123611	4.626546
H	8.922972	3.652113	3.315631
H	7.471935	2.256472	3.158646
H	7.429526	3.572756	4.671065

$TS_{E\rightarrow I}$

78

O	-0.018612	1.902539	6.986684
Si	0.376474	2.560901	8.441592
O	-0.946087	3.310744	9.101211
O	3.559998	2.321332	9.792115
Si	7.538992	3.920332	9.556803
Si	4.703123	3.011118	8.809622
B	-2.111073	6.626471	7.639204
La	0.152209	6.128926	8.995135
O	1.399978	3.847674	8.298133
Si	2.554071	4.717327	7.375033
O	4.042174	4.259168	7.953538
O	1.025031	1.429791	9.448053
Si	2.578509	0.991513	9.860844
O	2.562895	0.379899	11.377073
Si	2.956522	0.966025	12.912170
Si	-2.585661	2.828301	9.235832
O	5.315227	1.873232	7.774784
Si	5.075176	1.271555	6.256980
O	6.567772	0.887341	5.681361

O	5.899904	3.571953	9.775344
Si	0.688387	0.876837	5.882791
O	1.436683	-0.358504	6.691414
Si	2.930833	-0.738429	7.282553
O	3.006032	-2.380232	7.251909
O	0.569267	7.937630	10.318442
C	1.300370	9.130660	10.414457
C	2.807880	8.898081	10.320886
C	3.468429	8.257770	11.545424
C	2.905153	6.915444	12.035628
C	1.569959	7.022689	12.786847
C	0.313108	6.644814	12.040523
O	0.265194	5.564866	11.390936
C	-0.966201	7.287833	12.505360
O	2.083440	6.218198	7.655096
O	2.416288	4.196599	5.805511
Si	2.866040	2.936217	4.836046
O	1.777531	1.696488	4.961703
O	3.114586	-0.180349	8.832450
O	4.116473	-0.078991	6.335693
O	4.367981	2.382177	5.255208
O	2.928351	3.438686	3.281080
Si	2.347502	4.802432	2.463392
O	-0.502123	0.278962	4.938947
Si	-0.957659	-1.261875	4.411807
H	3.781192	-2.760363	7.675670
H	6.610715	0.771129	4.727510
H	2.535215	4.519856	1.012612
H	0.903060	5.012195	2.766959
H	3.136913	6.004153	2.858078
H	-2.029920	-1.052009	3.399955
H	0.205952	-1.961396	3.794716
H	-1.480635	-2.055952	5.560532
H	8.343095	2.684648	9.780253
H	7.784850	4.449161	8.184018
H	7.892281	4.948953	10.575580
H	2.421929	-0.025969	13.886177
H	4.437581	1.073393	13.049211
H	2.326019	2.299222	13.135729
H	-3.157718	3.635424	10.345259
H	-3.283605	3.090587	7.951060
H	-2.617660	1.375336	9.570796
H	0.991084	9.814502	9.608354
H	1.056544	9.648060	11.359879
H	3.297963	9.863981	10.136262
H	2.996023	8.281622	9.431863
H	4.531545	8.113539	11.315185
H	3.441007	8.968619	12.384490
H	2.809262	6.204778	11.206390
H	3.643452	6.472737	12.713600
H	1.567698	6.324273	13.638133
H	1.449122	8.019691	13.222724
H	-0.867887	8.371550	12.583169
H	-1.197636	6.892235	13.503734
H	-1.794120	7.036028	11.840500
H	-1.415244	7.645175	7.782018
H	-1.423317	5.782861	7.043409
H	-2.352614	6.182279	8.777936
H	-3.125538	6.867375	7.045503

I

78

O	-0.034921	2.049372	6.909367

Si	0.196076	2.832062	8.345358
O	-1.226767	3.429367	8.897846
O	3.381931	2.657192	9.883897
Si	7.369618	4.085327	9.641217
Si	4.534084	3.230712	8.842367
B	-2.108347	7.084226	7.595750
La	0.353471	6.782317	8.638573
O	1.175522	4.156218	8.149806
Si	2.410797	4.770543	7.135002
O	3.866091	4.310559	7.797153
O	0.854614	1.795411	9.451414
Si	2.349548	1.377887	10.024756
O	2.210754	1.005140	11.616113
Si	2.255664	-0.438115	12.492362
Si	-2.859057	3.058102	8.601243
O	5.213098	1.977151	7.996261
Si	5.005569	1.232639	6.536447
O	6.499102	0.776757	6.015658
O	5.688680	3.961244	9.747035
Si	0.644712	0.824946	6.025707
O	1.333571	-0.287706	7.042986
Si	2.805222	-0.637332	7.701256
O	2.873891	-2.276456	7.828793
O	0.978601	8.639024	9.574110
C	1.389432	9.896276	10.018202
C	2.808346	9.902870	10.593765
C	3.018753	9.261063	11.972095
C	2.731670	7.753427	12.070174
C	1.250306	7.443385	12.400929
C	0.932236	6.009694	12.091252
O	0.572584	5.672029	10.958155
C	1.085570	4.976886	13.165101
O	2.113125	6.339534	7.167283
O	2.271649	4.019501	5.660001
Si	2.840555	2.700758	4.845144
O	1.790576	1.430884	5.005200
O	2.927577	0.061920	9.202216
O	4.045516	-0.104519	6.744645
O	4.327306	2.241909	5.416260
O	3.005984	3.060912	3.257171
Si	2.522043	4.368590	2.298027
O	-0.546094	0.111623	5.162624
Si	-0.937829	-1.478053	4.745411
H	3.761880	-2.632615	7.926732
H	6.595409	0.772478	5.058614
H	2.835284	3.981657	0.893477
H	1.059138	4.611420	2.451844
H	3.289591	5.589702	2.676027
H	-1.972646	-1.386222	3.678104
H	0.267441	-2.193303	4.234277
H	-1.487004	-2.192137	5.933821
H	8.001251	2.808676	10.083683
H	7.787046	4.403525	8.245135
H	7.763574	5.191742	10.558937
H	1.265668	-1.411840	11.948185
H	3.626017	-1.025864	12.446528
H	1.903228	-0.079036	13.895288
H	-3.644588	3.849563	9.585718
H	-3.223709	3.419041	7.205538
H	-3.074578	1.598032	8.830200
H	1.355949	10.614045	9.183723
H	0.687912	10.281282	10.780775
H	3.134266	10.949827	10.663900

H	3.470900	9.422047	9.861619
H	4.066087	9.423676	12.255234
H	2.421928	9.795153	12.725085
H	3.007696	7.274818	11.123759
H	3.364540	7.303466	12.844459
H	1.060171	7.659000	13.457887
H	0.613010	8.070746	11.773325
H	0.274090	5.105872	13.892698
H	2.022334	5.130620	13.710735
H	1.045019	3.969392	12.750632
H	-1.412451	8.109872	7.498054
H	-1.508324	6.161542	7.023212
H	-2.178300	6.801210	8.805074
H	-3.196715	7.259025	7.120004

4.3 Catalysts of (alkyl or dialkylamido)La@**ac**-1

(NMe$_2$)La@**ac**-1

60

O	2.230794	2.282146	10.535744
O	-0.073141	-1.936830	9.966397
O	1.419361	-0.149102	11.265147
Si	0.626845	-1.588867	11.409008
O	1.653366	-2.834759	11.798573
Si	2.652970	-2.945929	13.127849
O	3.941922	-3.894019	12.933037
La	5.918117	-2.921565	13.602766
Si	0.148626	-3.166742	8.833120
O	-0.575927	-1.495244	12.541648
Si	-1.038071	-0.932125	14.023301
O	-0.179034	-1.591281	15.268906
Si	1.187848	-2.406437	15.705974
O	0.858628	-3.372613	16.992848
Si	-0.566785	-3.974588	17.670505
Si	2.158961	1.228418	11.791539
O	3.709364	0.948627	12.316210
Si	4.205217	-0.103683	13.509440
O	3.120944	-1.375899	13.463243
Si	3.507219	3.063069	9.755478
O	1.293018	1.942340	13.007720
Si	0.411513	1.725037	14.386676
O	-0.135740	3.185503	14.913741
O	-2.609383	-1.346905	14.286402
O	-0.858485	0.713541	14.059187
O	1.298250	1.103319	15.632026
Si	2.669344	0.296561	16.071897
O	3.145420	0.803227	17.560081
Si	2.816931	2.169124	18.497463
O	2.371504	-1.341668	16.213310
O	1.745977	-3.358913	14.477361
O	3.907971	0.575387	15.014980
O	5.717051	-0.641097	13.355913
N	5.207403	-2.896017	16.209905
N	7.935297	-4.017018	13.387771
H	-3.178773	-1.252173	13.517159
H	-0.239448	-4.485865	9.411977
H	-0.741173	-2.836061	7.683796
H	-0.144672	-4.976149	18.691359
H	-0.502716	3.745904	14.223689
H	1.413927	2.122213	19.000304
H	3.768967	2.119032	19.644100
H	3.036493	3.414501	17.706788
H	-1.330380	-2.873505	18.324793

H	-1.407447	-4.632014	16.628677
H	2.891172	3.879839	8.671302
H	4.238294	3.950872	10.706013
H	4.449085	2.066358	9.167339
H	1.569295	-3.211726	8.378478
H	4.312668	-2.401024	16.274705
H	5.050318	-3.813105	16.622858
H	5.844746	-2.407115	16.835104
C	8.039436	-5.437086	13.126505
C	9.233359	-3.377361	13.386228
H	8.631116	-5.967130	13.893871
H	7.044045	-5.907816	13.111399
H	8.510176	-5.659037	12.152206
H	9.903375	-3.777028	14.168070
H	9.764172	-3.491796	12.424300
H	9.137511	-2.296542	13.570405

D

78

Si	-4.805620	10.765943	13.289531
O	-4.280563	9.830231	14.578580
Si	-2.817942	9.150878	14.937785
O	-1.876596	9.286793	13.575792
O	2.192963	8.262291	15.789494
Si	1.816925	6.924732	16.692165
O	3.215993	6.375990	17.363866
O	1.176004	5.685615	15.793364
Si	-0.138591	5.813803	14.762616
O	-1.538766	5.344686	15.567236
Si	-2.596736	6.351962	16.344867
O	0.797953	7.325038	17.930810
O	-3.129409	7.584155	15.369279
O	-1.936400	6.929454	17.748348
Si	-0.696613	7.681632	18.528988
O	-0.909859	9.324374	18.456145
H	-6.193857	11.204816	13.613282
Si	-0.890719	10.381138	17.178941
O	0.566424	10.353148	16.425417
O	-2.159112	10.003872	16.186323
Si	1.591467	9.721085	15.293343
O	0.832330	9.659695	13.815049
O	2.880449	10.732914	15.142687
Si	3.271330	11.945079	14.045426
Si	-0.364845	8.569359	13.387671
O	-0.173975	7.949582	11.917231
O	-3.923981	5.459634	16.737242
Si	-4.566745	4.935067	18.202496
O	-0.795170	7.178014	20.096064
O	-0.337701	7.474728	14.648373
La	-0.133201	5.768865	11.144500
N	-2.000349	3.849518	11.712843
O	0.033597	5.042131	13.369246
O	-1.073521	11.920409	17.741358
Si	4.123151	4.978194	17.123998
N	1.820673	5.145187	10.099916
C	1.990972	3.746932	9.783604
O	-0.975269	7.591674	9.120714
C	-1.723733	6.721949	8.436019
O	-1.786489	5.594596	8.913233
C	3.025159	5.902690	9.853999
C	-0.820882	9.000809	8.806268
C	-2.122685	9.777797	8.868795
C	-3.044044	9.605922	7.659944

C	-3.547434	8.181382	7.427224
C	-2.433781	7.144136	7.183286
H	-1.895996	12.064680	18.218536
H	-0.000599	7.355367	20.608348
H	-5.005556	6.093873	19.033922
H	-5.749180	4.092302	17.857207
H	-3.573543	4.117459	18.958588
H	-4.831802	9.963829	12.026121
H	-3.935344	11.962243	13.086558
H	5.365081	5.142212	17.934127
H	3.375797	3.775169	17.596065
H	4.481143	4.812842	15.684316
H	2.130816	12.890047	13.853240
H	4.438239	12.677437	14.616226
H	3.651501	11.355644	12.726390
H	-0.135592	9.331708	9.586685
H	-0.328613	9.084619	7.830220
H	-1.849188	10.835981	8.959262
H	-2.636147	9.518899	9.802756
H	-3.908936	10.268376	7.776778
H	-2.517415	9.948345	6.757876
H	-4.170403	7.853909	8.269112
H	-4.197758	8.173446	6.546140
H	-2.846069	6.230201	6.751706
H	-1.697825	7.546588	6.474449
H	3.327140	5.886621	8.790054
H	2.885632	6.955816	10.132785
H	3.888811	5.528284	10.432988
H	2.202940	3.567844	8.713186
H	2.806968	3.270392	10.357014
H	1.074180	3.175383	10.013874
H	-1.937673	2.926376	11.293130
H	-1.701842	3.774577	12.686859
H	-2.983910	4.105057	11.709722

$TS_{D\rightarrow E}$

78

Si	-4.850927	11.114971	14.477206
O	-4.297517	9.781668	15.345129
Si	-2.795793	9.143937	15.575352
O	-1.849848	9.624671	14.302196
O	2.213378	8.408522	16.256383
Si	1.984170	6.884949	16.853159
O	3.442637	6.336194	17.375929
O	1.421010	5.810227	15.718172
Si	0.044377	6.004603	14.792553
O	-1.286669	5.360766	15.597433
Si	-2.400471	6.200331	16.487744
O	0.959127	6.895734	18.152162
O	-3.009014	7.492133	15.624661
O	-1.790585	6.681562	17.944601
Si	-0.507854	7.232794	18.823656
O	-0.641903	8.872592	19.017717
H	-6.247879	11.366542	14.934523
Si	-0.876400	10.098799	17.926021
O	0.473508	10.365088	17.033720
O	-2.193956	9.691354	17.008905
Si	1.579313	9.892544	15.899082
O	0.874264	9.961182	14.393558
O	2.829798	10.956804	15.913592
Si	3.243557	12.275507	14.951661
Si	-0.362336	8.969239	13.869542
O	-0.304601	8.602753	12.303092

O	-3.667722	5.184393	16.753328
Si	-4.384308	4.560659	18.147191
O	-0.618473	6.483682	20.287432
O	-0.259149	7.647795	14.890302
La	-0.617986	6.513461	11.415217
N	-2.968748	5.837996	12.625617
O	0.165779	5.442875	13.291489
O	-1.159153	11.506376	18.733834
Si	4.378365	4.995794	16.967180
N	0.676006	5.899145	9.437874
C	0.845317	4.505158	9.087357
O	-1.423361	7.762656	8.985525
C	-1.466681	6.440343	8.623693
O	-2.090157	5.728047	9.435587
C	1.790329	6.687211	8.961474
C	-0.915412	8.781618	8.098355
C	-1.913714	9.133469	7.004764
C	-1.976434	8.134919	5.847285
C	-2.300991	6.694253	6.246965
C	-1.255729	6.059340	7.186223
H	-1.904583	11.468241	19.340312
H	0.189991	6.523932	20.807069
H	-4.893502	5.662405	19.014819
H	-5.524428	3.719086	17.681081
H	-3.413762	3.721160	18.907156
H	-4.854072	10.812192	13.014260
H	-4.007288	12.317999	14.737390
H	5.616888	5.085922	17.792967
H	3.654272	3.729810	17.285099
H	4.735475	5.020809	15.518371
H	2.084483	13.200862	14.783003
H	4.353252	12.979422	15.656011
H	3.713843	11.814215	13.611800
H	-0.744910	9.635044	8.757771
H	0.049910	8.467418	7.688943
H	-1.635826	10.119142	6.611157
H	-2.900187	9.253059	7.470216
H	-2.721353	8.481626	5.121450
H	-1.011760	8.142619	5.320265
H	-3.295150	6.635938	6.707528
H	-2.348639	6.082162	5.339508
H	-1.326284	4.970832	7.157618
H	-0.246121	6.331406	6.860002
H	1.880201	6.682426	7.855930
H	1.698287	7.735951	9.276103
H	2.761828	6.325806	9.343340
H	0.973510	4.350299	7.999097
H	1.727068	4.048829	9.570208
H	-0.034473	3.922137	9.391947
H	-3.773403	5.727808	12.014119
H	-2.830787	4.952731	13.109510
H	-3.228299	6.501362	13.356271

E

78

Si	-5.090289	11.199200	14.882775
O	-4.460374	9.769469	15.515010
Si	-2.927618	9.185416	15.661317
O	-2.043166	9.763052	14.385694
O	2.107908	8.583566	16.129817
Si	1.961213	7.021070	16.645920
O	3.454709	6.502102	17.094549
O	1.404429	5.994876	15.463973

Si	-0.022402	6.168017	14.612360
O	-1.286904	5.456434	15.462159
Si	-2.407112	6.217276	16.411286
O	0.980066	6.911904	17.973673
O	-3.076053	7.524446	15.615377
O	-1.771517	6.662383	17.868620
Si	-0.462307	7.192829	18.720526
O	-0.617895	8.818819	18.996046
H	-6.455162	11.355386	15.462389
Si	-0.954034	10.086953	17.981672
O	0.336251	10.451752	17.038040
O	-2.297337	9.672481	17.104135
Si	1.423798	10.062581	15.855173
O	0.672240	10.172371	14.375661
O	2.644815	11.159459	15.881499
Si	2.954309	12.573026	15.018576
Si	-0.560714	9.181084	13.843012
O	-0.567473	8.917432	12.255515
O	-3.642081	5.161839	16.668291
Si	-4.135436	4.251663	18.000563
O	-0.496898	6.373900	20.150059
O	-0.378237	7.796016	14.764536
La	-0.786672	6.837396	11.299585
N	-3.195770	6.459022	12.466898
O	0.048700	5.651539	13.090413
O	-1.250875	11.439073	18.874032
Si	4.493041	5.319154	16.494329
N	0.372358	5.412963	9.253491
C	-0.046750	4.009977	9.298082
O	-0.019044	7.622659	8.933180
C	-0.638647	6.303461	8.557215
O	-1.796682	6.181072	9.203925
C	1.755116	5.514520	8.785295
C	-0.191757	8.795522	8.134633
C	-1.583515	9.035157	7.553043
C	-1.867402	8.274592	6.255772
C	-1.945174	6.755447	6.400468
C	-0.713757	6.111563	7.039322
H	-1.941414	11.331076	19.534669
H	0.338204	6.387717	20.627210
H	-4.664777	5.143824	19.072315
H	-5.221525	3.355904	17.507734
H	-3.005296	3.434554	18.529695
H	-5.189300	11.096410	13.395945
H	-4.242421	12.370588	15.250071
H	5.751941	5.427858	17.285961
H	3.902276	3.960213	16.673017
H	4.785052	5.553139	15.049089
H	1.744510	13.445659	14.968748
H	4.055327	13.274218	15.738860
H	3.392670	12.244322	13.629914
H	0.076956	9.614663	8.809177
H	0.550693	8.785625	7.322525
H	-1.656046	10.111288	7.348912
H	-2.342340	8.807656	8.310745
H	-2.809041	8.638821	5.826810
H	-1.084038	8.531070	5.527215
H	-2.814094	6.482432	7.008454
H	-2.097141	6.316058	5.407126
H	-0.761396	5.029299	6.870540
H	0.211949	6.461258	6.565257
H	1.893912	5.057244	7.793525
H	2.054068	6.561649	8.738433

H	2.411201	4.991801	9.488815
H	0.113444	3.495216	8.337706
H	0.533228	3.483327	10.062528
H	-1.108010	3.953706	9.545335
H	-3.992015	6.834651	11.956740
H	-3.386918	5.469298	12.610114
H	-3.219041	6.879460	13.398831

$TS_{E \rightarrow F}$

78

C	0.397878	5.550688	11.854353
N	-0.311833	5.497609	10.569585
C	-0.987946	6.760200	10.284573
La	-1.460532	2.921680	10.079297
N	-0.244588	0.736029	11.137000
O	-1.037062	4.579835	8.414792
C	-1.090515	4.779406	7.022347
C	0.061391	4.167412	6.221980
C	1.356087	4.982810	6.199441
C	2.105338	5.115600	7.526409
C	1.333578	5.826081	8.640359
C	0.489881	4.912406	9.502887
O	0.910743	3.747477	9.792146
O	-2.997735	3.097265	11.777841
Si	-4.010869	1.952600	12.280002
O	-4.151827	0.646443	11.241547
Si	-3.641108	0.210750	9.708842
O	-2.631266	1.257686	9.022240
O	-5.071022	-0.014175	8.875892
Si	-6.561496	-0.256252	9.570830
O	-6.992066	0.945564	10.621155
Si	-6.929990	1.521957	12.169697
O	-8.257465	2.466697	12.373594
Si	-8.548110	3.886174	13.232852
O	-2.896237	-1.269722	9.996967
Si	-2.957594	-2.142553	11.401937
O	-1.802319	-3.309604	11.302116
Si	-1.858568	-4.991337	11.178220
O	-7.675715	-0.282360	8.362793
Si	-7.599930	0.067045	6.716619
O	-6.591404	-1.737783	10.304481
Si	-6.068344	-2.803901	11.447492
O	-6.530889	-4.327206	11.022608
O	-4.427695	-2.862724	11.609178
O	-2.550099	-1.193892	12.712880
Si	-3.342107	-0.417100	13.957753
O	-2.397929	-0.627994	15.291406
Si	-2.010627	0.375392	16.587813
O	-6.739525	-2.393348	12.905270
Si	-6.441822	-1.114653	13.919416
O	-7.285580	-1.316834	15.319635
O	-4.814428	-1.104878	14.232296
O	-6.981785	0.290761	13.271067
O	-3.469847	1.213679	13.691551
O	-5.589977	2.461388	12.468946
H	-7.056479	1.438684	6.489395
H	-3.222461	1.065100	17.118151
H	-1.421306	-0.501359	17.640154
H	-7.093986	-2.140266	15.778165
H	-7.420400	-4.376873	10.659816
H	-0.999511	1.391700	16.166110
H	-0.442043	-5.441013	11.050688
H	-2.468372	-5.585761	12.402879

H	-2.631536	-5.405473	9.971654
H	-10.029193	4.023257	13.335760
H	-7.949118	3.818827	14.598249
H	-7.987089	5.058032	12.497241
H	-6.751001	-0.933461	6.005255
H	-8.999628	-0.010727	6.208340
H	-2.035078	4.339524	6.668348
H	-1.151048	5.858831	6.797010
H	-0.285222	4.056004	5.185897
H	0.251802	3.151022	6.592106
H	2.039190	4.533479	5.467450
H	1.126657	5.988204	5.816057
H	2.407621	4.128346	7.893082
H	3.029390	5.674651	7.337749
H	2.047215	6.276883	9.346769
H	0.731519	6.651785	8.249042
H	-0.293645	7.613489	10.253157
H	-1.510812	6.676424	9.332161
H	-1.722216	6.950705	11.073014
H	1.128832	6.373811	11.889099
H	-0.329596	5.705171	12.656298
H	0.925649	4.612113	12.027184
H	0.675017	0.847557	11.556582
H	-0.837623	0.279537	11.832150
H	-0.146325	0.052950	10.387787

F

78

Si	-5.090289	11.199200	14.882775
O	-4.460374	9.769469	15.515010
Si	-2.927618	9.185416	15.661317
O	-2.043166	9.763052	14.385694
O	2.107908	8.583566	16.129817
Si	1.961213	7.021070	16.645920
O	3.454709	6.502102	17.094549
O	1.404429	5.994876	15.463973
Si	-0.022402	6.168017	14.612360
O	-1.286904	5.456434	15.462159
Si	-2.407112	6.217276	16.411286
O	0.980066	6.911904	17.973673
O	-3.076053	7.524446	15.615377
O	-1.771517	6.662383	17.868620
Si	-0.462307	7.192829	18.720526
O	-0.617895	8.818819	18.996046
H	-6.455162	11.355386	15.462389
Si	-0.954034	10.086953	17.981672
O	0.336251	10.451752	17.038040
O	-2.297337	9.672481	17.104135
Si	1.423798	10.062581	15.855173
O	0.672240	10.172371	14.375661
O	2.644815	11.159459	15.881499
Si	2.954309	12.573026	15.018576
Si	-0.560714	9.181084	13.843012
O	-0.567473	8.917432	12.255515
O	-3.642081	5.161839	16.668291
Si	-4.135436	4.251663	18.000563
O	-0.496898	6.373900	20.150059
O	-0.378237	7.796016	14.764536
La	-0.786672	6.837396	11.299585
N	-3.195770	6.459022	12.466898
O	0.048700	5.651539	13.090413
O	-1.250875	11.439073	18.874032
Si	4.493041	5.319154	16.494329

N	0.372358	5.412963	9.253491
C	-0.046750	4.009977	9.298082
O	-0.019044	7.622659	8.933180
C	-0.638647	6.303461	8.557215
O	-1.796682	6.181072	9.203925
C	1.755116	5.514520	8.785295
C	-0.191757	8.795522	8.134633
C	-1.583515	9.035157	7.553043
C	-1.867402	8.274592	6.255772
C	-1.945174	6.755447	6.400468
C	-0.713757	6.111563	7.039322
H	-1.941414	11.331076	19.534669
H	0.338204	6.387717	20.627210
H	-4.664777	5.143824	19.072315
H	-5.221525	3.355904	17.507734
H	-3.005296	3.434554	18.529695
H	-5.189300	11.096410	13.395945
H	-4.242421	12.370588	15.250071
H	5.751941	5.427858	17.285961
H	3.902276	3.960213	16.673017
H	4.785052	5.553139	15.049089
H	1.744510	13.445659	14.968748
H	4.055327	13.274218	15.738860
H	3.392670	12.244322	13.629914
H	0.076956	9.614663	8.809177
H	0.550693	8.785625	7.322525
H	-1.656046	10.111288	7.348912
H	-2.342340	8.807656	8.310745
H	-2.809041	8.638821	5.826810
H	-1.084038	8.531070	5.527215
H	-2.814094	6.482432	7.008454
H	-2.097141	6.316058	5.407126
H	-0.761396	5.029299	6.870540
H	0.211949	6.461258	6.565257
H	1.893912	5.057244	7.793525
H	2.054068	6.561649	8.738433
H	2.411201	4.991801	9.488815
H	0.113444	3.495216	8.337706
H	0.533228	3.483327	10.062528
H	-1.108010	3.953706	9.545335
H	-3.992015	6.834651	11.956740
H	-3.386918	5.469298	12.610114
H	-3.219041	6.879460	13.398831

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O	2.652124	2.634262	10.924171
O	0.543603	-1.654290	9.843839
O	1.919905	0.090300	11.286274
Si	1.095539	-1.341773	11.358224
O	2.045216	-2.625716	11.826131
Si	2.902630	-2.705170	13.252779
O	4.294836	-3.518292	13.173286
La	6.100704	-2.758220	14.319028
Si	0.599306	-3.022558	8.857219
O	-0.205320	-1.238113	12.374692
Si	-0.876172	-0.870987	13.836592
O	-0.139057	-1.624052	15.106772
Si	1.188776	-2.417430	15.677749
O	0.733944	-3.460467	16.863640
Si	-0.751900	-4.101117	17.349395
Si	2.485238	1.450417	12.047673
O	3.960339	1.206488	12.770483

Si	4.279784	0.057866	13.931451
O	3.094844	-1.100457	13.687133
Si	3.063745	2.650424	9.288680
O	1.420000	2.014668	13.179623
Si	0.443218	1.769894	14.485706
O	-0.139404	3.225994	14.986659
O	-2.439957	-1.383737	13.873368
O	-0.804338	0.769483	14.055888
O	1.217451	1.097143	15.780544
Si	2.539912	0.291730	16.346592
O	2.828658	0.733979	17.903242
Si	2.438300	2.095041	18.824313
O	2.269212	-1.358579	16.392232
O	1.931146	-3.295537	14.489560
O	3.890845	0.640796	15.459012
O	5.775137	-0.550251	13.906926
N	5.111243	-2.893265	16.861533
C	8.337993	-3.719978	13.678247
H	-2.977734	-1.083514	13.134758
H	0.004592	-4.199676	9.555358
H	-0.206457	-2.691616	7.647258
H	-0.433156	-5.150480	18.360078
H	-0.195423	3.883679	14.287068
H	0.987522	2.083012	19.167916
H	3.255216	1.997040	20.068211
H	2.780789	3.345502	18.087084
H	-1.592918	-3.037985	17.970714
H	-1.466844	-4.709813	16.190988
H	1.845720	2.415223	8.459682
H	3.615493	4.004921	9.001227
H	4.087736	1.606883	8.989329
H	2.006201	-3.323515	8.463276
H	9.053722	-2.958826	13.328956
H	8.271350	-4.465537	12.869915
H	8.833517	-4.234555	14.520410
H	4.204506	-2.416182	16.815103
H	4.910907	-3.821901	17.228845
H	5.635760	-2.411328	17.589510

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Si	3.188257	2.446349	10.920605
O	1.272374	-0.787833	10.160389
Si	2.023961	-0.440320	11.591204
O	3.247547	-1.531473	11.819761
Si	4.755973	-1.678402	11.147743
O	5.527800	-0.228630	11.224428
O	7.324045	1.763909	11.221048
Si	8.974257	1.432582	11.132479
Si	5.993575	1.162170	10.467592
Si	4.158582	-2.065720	8.030224
O	6.376936	0.876060	8.882482
O	2.562475	-1.638448	7.897452
Si	1.289120	-0.766613	8.506571
O	2.349460	2.751151	9.528964
O	1.236171	0.793640	7.963448
Si	2.465053	1.930124	8.069962
O	2.498892	2.918694	6.803676
La	4.414828	3.261245	5.526793
N	5.112048	4.377021	7.901333
O	4.587377	-2.268935	9.613545
O	5.666887	-2.730540	12.029141
O	4.821217	2.333098	10.614933

Si	5.323104	0.635314	7.598025
O	5.195586	-1.007470	7.288559
O	2.629595	1.088143	11.678216
O	2.970299	3.733748	11.918372
Si	2.363340	3.907874	13.482322
O	0.922247	-0.557688	12.810963
O	4.310805	-3.520554	7.274157
Si	5.421539	-4.094400	6.143491
O	-0.089828	-1.498511	7.978044
Si	-0.392536	-3.016515	7.317459
O	3.833861	0.993492	8.276886
O	5.699684	1.514414	6.308181
C	5.380151	5.533789	4.864052
O	3.455356	2.232942	3.253953
C	2.289885	2.604883	3.136933
O	1.939950	3.666037	3.865600
C	0.560147	4.101241	4.019921
C	-0.327751	3.054716	4.670278
C	-0.835833	1.966470	3.722473
C	0.254088	1.106824	3.082621
C	1.289500	1.907899	2.264220
H	5.435014	-3.654902	11.900903
H	6.820602	-3.931666	6.636279
H	5.117349	-5.543892	5.964161
H	9.587623	2.233364	10.031618
H	0.320007	-1.302456	12.726427
H	3.113613	3.043094	14.438302
H	2.552427	5.343194	13.840861
H	0.911554	3.566172	13.519654
H	9.565829	1.843138	12.437919
H	9.219144	-0.019840	10.894358
H	0.161826	-4.101149	8.180036
H	-1.876400	-3.148424	7.236520
H	0.190243	-3.119111	5.946401
H	5.259323	-3.385426	4.839948
H	0.659063	4.981041	4.655829
H	0.188823	4.421978	3.039247
H	-1.189739	3.588701	5.088195
H	0.215854	2.630867	5.522849
H	-1.520429	1.311505	4.272222
H	-1.431991	2.434478	2.925762
H	0.775454	0.517593	3.846605
H	-0.210411	0.385495	2.402296
H	1.866788	1.241902	1.620472
H	0.778160	2.640725	1.627258
H	4.863839	6.395651	5.319327
H	5.309185	5.692694	3.773088
H	6.448210	5.662014	5.106956
H	5.150709	3.762967	8.714084
H	6.023000	4.820287	7.815436
H	4.451813	5.114444	8.134933

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Si	3.101931	2.114917	10.978849
O	1.858648	-1.539222	11.446327
Si	2.734355	-0.661715	12.536218
O	4.209118	-1.384538	12.746661
Si	5.516226	-1.496517	11.732695
O	5.980832	0.013355	11.273081
O	7.276804	2.204851	10.419081
Si	8.913696	2.080791	10.033074
Si	5.977760	1.230949	10.162726

Si	4.405025	-2.784756	9.008773
O	6.085434	0.627128	8.622126
O	2.756134	-2.662783	9.111069
Si	1.493731	-1.902939	9.875370
O	1.982896	1.949546	9.767878
O	1.002180	-0.530251	9.088363
Si	1.972739	0.734944	8.601403
O	1.611442	1.323586	7.148523
La	3.123728	1.884562	5.518791
N	3.624563	3.689679	7.498804
O	5.112174	-2.482637	10.470989
O	6.801812	-2.133996	12.540940
O	4.641964	2.207258	10.347102
Si	4.863232	-0.142421	7.767711
O	5.064940	-1.799820	7.843484
O	2.979215	0.909377	12.096896
O	2.802190	3.558221	11.707744
Si	2.489551	4.015262	13.301861
O	1.912383	-0.630179	13.963644
O	4.740805	-4.338660	8.587386
Si	5.720573	-5.010352	7.390913
O	0.227200	-2.949530	9.912765
Si	-0.180558	-4.311019	9.008136
O	3.523774	0.117015	8.737818
O	4.721369	0.441577	6.272654
C	3.941030	4.042466	4.073328
O	2.372989	1.707662	3.205561
C	2.073502	2.930638	3.131257
O	1.101667	3.273561	4.043121
C	0.511917	4.585966	4.040391
C	-0.592820	4.701098	3.000427
C	-0.109723	4.835709	1.554875
C	0.831036	3.727177	1.075529
C	2.172750	3.690938	1.833036
H	6.695523	-3.057152	12.788552
H	7.114437	-4.486389	7.489369
H	5.717561	-6.482344	7.630875
H	9.155909	2.699695	8.695815
H	1.319858	-1.378366	14.082571
H	3.579232	3.549706	14.207473
H	2.436144	5.505983	13.297769
H	1.179311	3.464699	13.754369
H	9.663384	2.837995	11.075700
H	9.354004	0.655803	10.015764
H	0.664032	-5.473117	9.411647
H	-1.612023	-4.601887	9.307676
H	-0.012324	-4.050439	7.547816
H	5.167067	-4.721159	6.035484
H	0.099864	4.696669	5.046264
H	1.294729	5.341187	3.905711
H	-1.201236	5.577006	3.258647
H	-1.246145	3.826502	3.108321
H	-0.984648	4.874450	0.895391
H	0.402289	5.801594	1.437932
H	0.340570	2.747893	1.135245
H	1.054265	3.894070	0.015922
H	2.934045	3.169329	1.249503
H	2.529568	4.711728	1.997312
H	3.554341	5.068148	4.075833
H	4.506258	3.893657	3.146894
H	4.704555	4.025975	4.878174
H	4.242504	3.300171	8.212362
H	4.001293	4.600958	7.251461

H	2.741607	3.843866	7.983586

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Si	2.877300	2.011072	10.594815
O	1.848831	-1.600588	10.937246
Si	2.589441	-0.740598	12.133759
O	4.063443	-1.427920	12.450274
Si	5.489394	-1.416656	11.609135
O	5.831961	0.138519	11.176341
O	7.061296	2.400232	10.415637
Si	8.365416	2.349001	11.487234
Si	5.861172	1.337586	10.046009
Si	4.770244	-2.804035	8.831654
O	6.173053	0.749968	8.530227
O	3.116763	-2.791946	8.831408
Si	1.711190	-2.107901	9.369180
O	1.853016	1.666831	9.343155
O	1.199832	-0.837302	8.426031
Si	2.090801	0.540675	8.120721
O	1.848947	1.186624	6.664324
La	3.533200	1.946718	5.319778
N	4.798580	3.567581	7.096697
O	5.372583	-2.455660	10.333338
O	6.727909	-1.903595	12.579581
O	4.443550	2.220285	10.052504
Si	5.112791	-0.137388	7.569013
O	5.432626	-1.768610	7.713197
O	2.805420	0.854268	11.769831
O	2.426158	3.456325	11.234685
Si	1.579991	3.908460	12.622839
O	1.649135	-0.763573	13.485649
O	5.256212	-4.326528	8.452663
Si	6.073340	-4.986423	7.133784
O	0.548650	-3.267362	9.315075
Si	-0.943940	-3.367713	8.537695
O	3.667508	0.051288	8.392571
O	5.084079	0.416681	6.059102
C	3.737803	4.263652	1.937814
O	3.304765	2.197391	3.064433
C	2.771594	3.407635	2.751612
O	2.617175	4.073964	4.097181
C	1.690624	5.145032	4.275960
C	0.325832	4.646353	4.735505
C	-0.486871	3.920388	3.661803
C	0.248861	2.792140	2.930578
C	1.407363	3.274752	2.053800
H	6.832402	-2.858295	12.630901
H	7.470029	-4.464866	7.069518
H	6.096180	-6.460723	7.355640
H	9.172634	3.571724	11.207719
H	1.292970	-1.629607	13.704898
H	2.398465	3.637346	13.839618
H	1.333734	5.374058	12.495474
H	0.280134	3.181784	12.709535
H	7.879761	2.374359	12.896944
H	9.191461	1.129880	11.252103
H	-1.505628	-4.703412	8.889404
H	-1.862308	-2.293708	9.018393
H	-0.776571	-3.263019	7.058601
H	5.359791	-4.677563	5.860015
H	2.126732	5.804842	5.035602
H	1.615130	5.730667	3.350726

H	-0.248070	5.505870	5.106288
H	0.478638	3.985796	5.600110
H	-1.395006	3.518695	4.126734
H	-0.825627	4.652003	2.914123
H	0.604166	2.036269	3.644580
H	-0.476088	2.271100	2.294701
H	1.590214	2.560920	1.243901
H	1.130146	4.221286	1.571126
H	3.365917	5.283134	1.790683
H	3.887726	3.807241	0.955191
H	4.705233	4.306416	2.445794
H	5.792993	3.345937	7.068706
H	4.721095	4.579609	7.031628
H	4.506360	3.313890	8.044167

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C	-6.590531	0.251177	7.126994
C	-5.146897	0.506226	7.470436
O	-4.475075	-0.395231	8.042128
La	-3.215308	-1.638969	6.288350
O	-4.406177	0.170786	5.469321
C	-4.309488	1.235366	4.563065
C	-3.029607	2.052015	4.750690
C	-2.979095	2.948648	5.991521
C	-3.255610	2.292490	7.352412
C	-4.732166	1.953603	7.604760
Si	-0.051759	-2.705671	5.344473
O	-0.831594	-4.169913	5.127633
Si	-2.389570	-4.771836	5.004756
O	-2.435549	-5.399985	3.458259
Si	-1.101064	-5.835487	2.567121
O	-0.027308	-4.595433	2.343681
Si	1.279140	-3.749904	2.917509
O	2.033665	-3.067580	1.627767
Si	1.658559	-2.974144	-0.012919
O	0.857150	-2.531528	3.958764
O	0.938864	-3.028212	6.663855
Si	1.251577	-4.518381	7.313625
O	1.989334	-4.269234	8.762571
Si	3.509147	-4.672566	9.375164
O	-1.042042	-1.467856	5.637780
O	2.373646	-4.740974	3.663566
Si	2.755658	-5.834825	4.836711
O	4.394695	-5.974096	4.927814
O	-0.165156	-5.337547	7.640922
Si	-1.044332	-6.577102	6.955073
O	-2.369996	-6.019930	6.130478
O	2.250596	-5.408402	6.348213
O	2.082176	-7.295453	4.440241
Si	0.511121	-7.825486	4.478767
O	0.468432	-9.445416	4.184575
O	-0.080455	-7.503926	5.992106
O	-0.371959	-7.135766	3.280220
O	-1.590097	-7.494284	8.209232
Si	-3.060861	-8.262531	8.505319
O	-1.617665	-6.273340	1.071078
Si	-3.086602	-6.856909	0.483930
O	-3.539198	-3.690277	5.321153
N	-1.997840	-2.623832	8.531589
H	0.978662	-9.972311	4.806700
H	-4.101715	-7.255488	8.871613
H	-3.641127	-7.910807	1.383118

H	4.839388	-5.888586	4.079228
H	-2.830857	-9.181150	9.657016
H	-3.511470	-9.040012	7.314592
H	3.533826	-4.164025	10.777166
H	3.699755	-6.152090	9.371382
H	4.587322	-4.017503	8.579844
H	-2.802738	-7.434735	-0.860926
H	-4.067171	-5.739263	0.353232
H	2.696979	-2.097395	-0.626545
H	1.707688	-4.327436	-0.639502
H	0.307263	-2.373434	-0.213957
H	-4.335191	0.845026	3.532711
H	-5.190058	1.897299	4.653088
H	-2.884720	2.686596	3.865880
H	-2.181257	1.352862	4.761685
H	-1.985816	3.412878	6.032155
H	-3.689079	3.778566	5.863897
H	-2.639321	1.393982	7.487813
H	-2.923461	2.988407	8.130945
H	-4.995007	2.193167	8.646541
H	-5.382200	2.579592	6.985330
H	-6.905141	0.826443	6.255090
H	-7.203434	0.563907	7.983273
H	-6.768166	-0.811823	6.955144
H	-2.530708	-2.615284	9.397626
H	-1.663084	-3.578648	8.394374
H	-1.157826	-2.072086	8.695726

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C	-6.070637	-0.411283	9.151606
C	-5.157262	-0.179986	7.984876
O	-4.131663	-0.855116	7.856789
La	-2.334112	-1.107034	5.904190
O	-3.152922	0.723695	4.995231
C	-3.581180	1.848421	4.293910
C	-3.637488	3.117451	5.150360
C	-4.764475	3.231961	6.186484
C	-4.743453	2.209909	7.336128
C	-5.498911	0.902183	6.999095
Si	0.575817	-2.902671	5.143824
O	-0.444380	-4.214304	4.933555
Si	-2.098334	-4.450230	4.814532
O	-2.253219	-5.135037	3.296182
Si	-0.991411	-5.774203	2.421746
O	0.254434	-4.707169	2.181514
Si	1.743924	-4.269115	2.771424
O	2.646741	-3.738664	1.504356
Si	2.264025	-3.268292	-0.067549
O	1.661543	-3.047612	3.888870
O	1.307952	-3.291819	6.618902
Si	1.431874	-4.846379	7.198090
O	2.204091	-4.750184	8.648861
Si	3.735253	-5.220897	9.175231
O	-0.154877	-1.478369	5.247586
O	2.538250	-5.564737	3.424299
Si	2.713128	-6.524158	4.756883
O	4.292792	-6.972731	4.898733
O	-0.060519	-5.499861	7.503453
Si	-1.229034	-6.465144	6.828090
O	-2.380025	-5.609221	5.997151
O	2.331430	-5.775945	6.174380
O	1.760518	-7.864275	4.560505

Si	0.117545	-8.034729	4.413012
O	-0.244385	-9.604298	4.064294
O	-0.555283	-7.625271	5.868012
O	-0.442087	-7.152644	3.148366
O	-1.987412	-7.216386	8.084097
Si	-3.612909	-7.444865	8.452473
O	-1.566729	-6.156588	0.930070
Si	-3.109652	-6.503698	0.349453
O	-2.985267	-3.129163	5.052068
N	-0.916275	-1.474894	8.230693
H	-0.020944	-10.221661	4.767117
H	-4.250451	-6.148785	8.837155
H	-3.830501	-7.436495	1.264751
H	4.735433	-7.097588	4.053910
H	-3.653725	-8.377354	9.616097
H	-4.352503	-8.040910	7.301754
H	3.842825	-4.758372	10.589867
H	3.877218	-6.704539	9.118665
H	4.800288	-4.575493	8.353621
H	-2.924774	-7.146047	-0.983732
H	-3.897838	-5.245628	0.192627
H	3.495317	-2.639754	-0.627326
H	1.887074	-4.454485	-0.890353
H	1.147150	-2.277871	-0.070188
H	-2.905626	2.045200	3.445634
H	-4.580109	1.673961	3.852134
H	-3.729323	3.974917	4.469384
H	-2.666977	3.229342	5.653789
H	-4.706417	4.234816	6.627640
H	-5.738850	3.188435	5.679717
H	-3.702661	1.974925	7.587592
H	-5.192450	2.653021	8.233771
H	-6.577313	1.093065	6.994823
H	-5.177691	0.570824	6.007634
H	-7.014929	-0.830256	8.782255
H	-6.320659	0.538756	9.636113
H	-5.625148	-1.101845	9.868258
H	-0.585799	-0.657253	8.736889
H	-1.342713	-2.086799	8.922475
H	-0.081044	-1.952444	7.882724