DFT study of the Ring Opening Polymerization of ε-caprolactone by grafted lanthanide complexes : 1- Effect of the grafting mode on the reactivity of borohydride complexes

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4 - Study of the initiation step of ROP of \varepsilon-Caprolactone

4.1 (BH_4)La@**c**-1 as catalyst form

Study of the hydride transfer and BH_3 trapping steps of the ε-CL ROP reaction with (BH_4)La@**c**-1

(BH_4)La@c-1 :

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O	0.723489	0.573913	3.530641
Si	1.154245	1.701256	4.716543
Si	-0.294809	0.537507	2.253826
O	-0.090582	-0.909368	1.488470
Si	0.071736	-1.879268	0.156005
O	0.385321	-3.411704	0.640046
Si	-0.511308	-4.840910	0.695962
O	-1.872946	0.617240	2.831357
Si	-3.201192	0.474325	1.871466
N	-4.263153	-0.628899	2.608068
O	-0.152225	1.835402	1.250203
Si	0.995915	2.475645	0.240982
O	1.944670	3.440651	1.189473
O	-4.082022	1.888366	1.525414
La	-4.065497	1.862761	-1.170849
O	-2.397436	3.242801	-1.692533
Si	-0.860189	3.507071	-2.156451
O	0.260468	3.378367	-0.915716
O	-2.703335	0.252951	0.299965
Si	-2.114669	-0.496507	-1.126631
O	-1.401197	-1.920538	-0.669850
Si	-5.009058	2.824882	2.642862
O	-3.379964	-0.241668	-2.080344
O	-0.840356	0.488472	-1.568212
Si	-0.172004	0.801206	-3.074214
O	-0.821905	-0.103572	-4.273245
Si	-2.108333	0.096319	-5.356166
B	-6.701098	2.392594	-1.295011
O	-0.383643	2.411989	-3.347946
O	1.417546	0.369240	-2.882821
Si	2.063030	-0.011092	-1.395464
O	1.320285	-1.376065	-0.792436
O	-0.672255	5.012700	-2.802532
Si	0.520320	6.190508	-2.666292
O	1.961199	1.273511	-0.366469
O	3.673338	-0.313852	-1.552064
H	0.797201	1.115058	6.040934
H	2.796360	3.665152	0.802742
H	0.248963	7.199709	-3.729717
H	-0.806267	-5.321061	-0.684374

H	-6.388734	2.273760	2.699083
H	3.885670	-1.129443	-2.015363
H	-1.533330	0.388160	-6.701290
H	1.881122	5.606312	-2.864896
H	0.456252	6.846415	-1.326039
H	2.624694	1.918876	4.635700
H	-4.340663	2.748066	3.970062
H	-4.997233	4.210525	2.105890
H	0.420311	2.982675	4.512593
H	-2.872846	-1.178934	-5.389662
H	-2.987265	1.227805	-4.939615
H	0.330363	-5.833950	1.419513
H	-1.789167	-4.622218	1.437794
H	-5.161390	-0.852904	2.206667
H	-3.886448	-1.372559	3.176811
H	-6.141395	2.393971	-2.410900
H	-7.858862	2.685610	-1.392606
H	-6.540934	1.267725	-0.800390
H	-6.089892	3.215097	-0.585602

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O	0.265511	0.712258	3.676062
Si	0.916995	1.846978	4.660629
O	0.172454	3.311054	4.536098
Si	-1.261478	4.000811	4.982701
O	-1.926081	3.129979	6.229310
Si	-1.922841	2.865303	7.860533
O	-3.353086	2.193241	8.329019
Si	-0.100912	0.603052	2.031086
O	0.893070	1.224821	6.188427
Si	0.798122	1.317252	7.836509
O	-0.711253	1.807285	8.300238
O	2.500832	2.110372	4.190418
Si	3.542462	3.147119	4.943938
O	2.764713	3.785932	6.273277
Si	2.188858	3.860762	7.872087
O	0.593886	4.331321	7.713922
Si	-0.461029	5.267083	8.593352
O	-1.825342	4.316131	8.670003
O	1.027353	-0.177580	8.474524
Si	2.352182	-0.961083	9.163566
O	2.036470	2.294044	8.421303
N	5.031604	2.345896	5.115264
O	3.830694	4.633896	4.198354
Si	4.757667	4.940566	2.787082
O	-2.250773	3.853391	3.666108
O	-1.068632	5.591044	5.343896
Si	-0.212722	6.805011	6.130148
O	-0.894918	8.231842	5.626982
Si	-2.215300	8.566631	4.647106
La	3.547398	6.276566	6.460710
O	1.385471	6.784262	5.922319
O	3.114660	5.025011	8.465832
O	-0.649086	6.676227	7.766936
O	0.029821	5.602474	10.130090
Si	-0.508564	5.024569	11.626719
H	0.714358	-0.506270	1.455700
H	-3.122935	4.243032	3.777293
H	-2.395568	10.048421	4.666488
H	2.645882	-0.394506	10.511633
H	6.202292	4.717172	3.053975
H	-3.342130	1.231733	8.342413

H	-1.905557	5.477511	11.884387
H	-3.458174	7.914342	5.161572
H	-1.971527	8.117137	3.243518
H	-1.550232	0.283771	1.900571
H	4.273268	4.038258	1.704148
H	4.487813	6.364134	2.446175
H	0.214575	1.880114	1.328527
H	-0.428453	3.537331	11.681934
H	0.409467	5.619365	12.641377
H	1.974040	-2.397305	9.284963
H	3.555471	-0.827331	8.288891
H	5.818213	2.835441	5.519551
H	5.050562	1.350254	5.276432
O	3.797843	8.946362	6.552057
C	3.500352	9.189857	7.714622
O	3.247672	8.111339	8.472512
C	2.831175	8.145312	9.869748
C	1.491469	8.826009	10.076361
C	1.522247	10.354564	10.038635
C	1.969770	10.958074	8.707442
C	3.400923	10.569742	8.287164
H	4.079364	10.647654	9.147407
H	3.772000	11.238847	7.508723
H	1.940677	12.050209	8.782968
H	1.269494	10.685917	7.908414
H	0.521234	10.732526	10.274564
H	2.184122	10.722136	10.836122
H	1.132036	8.500761	11.059741
H	0.777662	8.422556	9.349023
H	2.778992	7.083775	10.113202
H	3.637188	8.609897	10.449139
H	5.931471	6.834720	7.227472
B	6.268532	6.202081	6.215853
H	7.460184	6.185596	6.063523
H	5.796837	5.058799	6.340546
H	5.703037	6.728529	5.238242

$TS_{A \rightarrow AB}$

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O	0.951268	0.642039	3.449871
Si	1.160155	1.823867	4.560770
O	0.146312	3.106133	4.358308
Si	-1.478787	3.405895	4.464334
O	-2.182987	2.364196	5.544415
Si	-2.373680	1.963641	7.132780
O	-3.652839	0.926177	7.170839
Si	0.860440	0.556466	1.764603
O	1.049752	1.124794	6.050309
Si	0.591247	1.085329	7.640773
O	-1.048860	1.182329	7.776115
O	2.699888	2.464547	4.374338
Si	3.330215	3.646564	5.334627
O	2.240409	3.994539	6.543711
Si	1.293238	3.871710	7.960380
O	-0.281521	3.986123	7.411187
Si	-1.654958	4.578642	8.162348
O	-2.725617	3.317542	8.036606
O	1.058793	-0.341732	8.299988
Si	2.336139	-0.801357	9.300827
O	1.404569	2.298218	8.483733
N	4.926368	3.215125	5.717671
O	3.347408	5.224426	4.704766
Si	4.164038	5.826008	3.315304

O	-2.101074	3.060937	2.971542
O	-1.724544	4.990724	4.814166
Si	-1.448378	6.311667	5.812232
O	-2.376138	7.540146	5.210918
Si	-3.631485	7.583461	4.095310
La	2.182778	6.581814	6.769024
O	0.109546	6.750837	5.941655
O	1.740082	5.218673	8.707706
O	-2.110968	5.915868	7.314630
O	-1.448287	4.919520	9.752336
Si	-1.027207	6.297302	10.633081
H	1.973272	-0.321102	1.298170
H	-3.054224	2.931946	2.960981
H	-4.237281	8.943814	4.184674
H	2.122281	-0.285457	10.683748
H	5.623436	5.570744	3.433853
H	-3.736831	0.431194	7.991095
H	-2.251290	6.791664	11.329509
H	-4.670315	6.554843	4.404747
H	-3.114905	7.359987	2.711690
H	-0.449645	-0.050203	1.399575
H	3.602616	5.150274	2.113188
H	3.863326	7.282727	3.299913
H	0.996376	1.911661	1.157465
H	-0.003550	5.902512	11.639832
H	-0.498128	7.372977	9.745796
H	2.350361	-2.291158	9.307058
H	3.631863	-0.284785	8.766742
H	5.509546	3.843486	6.251921
H	5.161789	2.242425	5.844751
O	3.306272	8.751511	6.604151
C	3.949572	8.775027	7.709786
O	3.193897	8.103137	8.695531
C	3.728186	7.928418	10.022449
C	3.314856	9.084526	10.917916
C	3.981073	10.425455	10.599860
C	3.858284	10.898274	9.146221
C	4.664708	10.051034	8.150384
H	5.641935	9.811991	8.582948
H	4.849075	10.599426	7.222867
H	4.238769	11.924370	9.085330
H	2.806331	10.944312	8.838945
H	3.551837	11.188752	11.259765
H	5.048423	10.368507	10.857135
H	3.541141	8.803873	11.954519
H	2.223852	9.182021	10.854689
H	3.304386	6.984260	10.371444
H	4.816822	7.811166	9.953209
H	5.044273	7.956943	7.623555
B	5.548157	6.788901	7.218539
H	6.540719	6.654649	7.886781
H	4.662802	6.000420	7.527195
H	5.676023	6.996842	6.036979

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O	0.855818	0.755147	3.328880
Si	1.109212	1.874979	4.493565
O	0.116906	3.184865	4.374524
Si	-1.505073	3.491053	4.515842
O	-2.200455	2.401830	5.554487
Si	-2.374266	1.941510	7.128415
O	-3.669092	0.923273	7.146230

Si	0.739252	0.763781	1.642715
O	1.014034	1.106127	5.949507
Si	0.583500	0.998830	7.544811
O	-1.051555	1.114822	7.717406
O	2.660038	2.491168	4.309269
Si	3.333103	3.601158	5.323786
O	2.252957	3.927789	6.547220
Si	1.336744	3.757256	7.985135
O	-0.242966	3.928033	7.460322
Si	-1.597144	4.500538	8.260704
O	-2.689182	3.263130	8.091149
O	1.040678	-0.464451	8.127414
Si	2.354036	-0.995297	9.042964
O	1.430080	2.158761	8.428384
N	4.917628	3.099676	5.677939
O	3.410569	5.204577	4.769818
Si	4.372545	5.804829	3.472809
O	-2.146949	3.220505	3.015976
O	-1.739742	5.057259	4.946130
Si	-1.432996	6.340804	5.984327
O	-2.380476	7.590055	5.461077
Si	-3.714354	7.664358	4.442590
La	2.211105	6.490752	6.856322
O	0.126848	6.776457	6.079664
O	1.820666	5.062016	8.777333
O	-2.048659	5.885074	7.490287
O	-1.359688	4.758378	9.862143
Si	-0.886812	6.077346	10.804006
H	1.842858	-0.087567	1.110220
H	-3.103103	3.115977	3.007432
H	-4.302256	9.025948	4.604090
H	2.211907	-0.549326	10.458839
H	5.752110	6.063929	3.961852
H	-3.748336	0.397198	7.947390
H	-2.082897	6.558608	11.556091
H	-4.735144	6.635359	4.806405
H	-3.302632	7.466875	3.020424
H	-0.577496	0.179662	1.265417
H	4.370521	4.791395	2.382329
H	3.707952	7.063196	3.041387
H	0.868840	2.151079	1.111815
H	0.153875	5.611378	11.761163
H	-0.359178	7.188819	9.960300
H	2.343853	-2.483354	8.970691
H	3.632611	-0.469808	8.476735
H	5.511966	3.669550	6.263153
H	5.123381	2.113809	5.741017
O	3.659316	8.384843	6.493862
C	4.190738	8.567502	7.663728
O	3.262270	8.077482	8.641213
C	3.557391	8.194965	10.044329
C	2.973434	9.483026	10.602550
C	3.665012	10.765691	10.133086
C	3.813006	10.925232	8.614719
C	4.801249	9.934077	7.983870
H	5.671355	9.816888	8.640139
H	5.172400	10.304076	7.024084
H	4.182148	11.937179	8.412141
H	2.837876	10.851852	8.117727
H	3.106898	11.622599	10.528914
H	4.665280	10.821394	10.585985
H	3.016841	9.427695	11.697946
H	1.909169	9.510173	10.336152

H	3.101500	7.317450	10.509110
H	4.642033	8.125333	10.188634
H	5.185017	7.819879	7.826984
B	5.780823	6.557870	7.787906
H	6.159618	6.445555	8.922267
H	4.813474	5.880464	7.486895
H	6.573812	6.765340	6.910295

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C	3.103754	8.903504	9.824304
C	1.988975	9.897122	9.528935
C	2.368811	11.034355	8.577006
C	3.028966	10.604855	7.260466
C	4.428896	10.007541	7.444828
C	4.474360	8.505365	7.743452
O	3.395505	8.097774	8.679940
La	2.554400	6.252028	7.120643
O	4.288321	7.715753	6.664136
Si	3.416759	3.488759	5.157684
O	3.610629	5.139621	4.838670
Si	4.570286	5.877877	3.615381
O	2.560902	2.604493	4.061107
Si	0.988578	2.073138	4.310985
O	0.954367	1.134271	5.666513
Si	0.629854	0.830364	7.259991
O	1.625119	1.787710	8.225644
Si	1.662207	3.432462	7.988857
O	2.316902	4.572630	8.898346
O	0.557182	1.126278	3.048466
Si	0.328169	1.353929	1.389610
O	0.087519	3.447985	4.437590
Si	-1.497825	3.819054	4.745082
O	-1.615742	5.318063	5.400929
Si	-1.111701	6.462691	6.522775
O	-1.567896	5.869676	8.039497
Si	-1.169626	4.364445	8.576112
O	-0.786995	4.381910	10.170548
Si	-0.047499	5.489751	11.208511
O	-2.182752	2.639483	5.688884
Si	-2.264938	2.027534	7.217538
O	-2.374257	3.248300	8.343706
O	-2.256962	3.785419	3.276462
O	-3.640953	1.122349	7.250518
O	-0.972540	1.041544	7.584051
O	1.011386	-0.729936	7.591312
Si	2.168606	-1.473009	8.566909
O	2.481246	3.709287	6.511800
N	4.962588	2.786363	5.283622
O	0.076132	3.818486	7.599830
O	-2.052347	7.798343	6.259095
Si	-3.427785	8.050954	5.329633
O	0.466920	6.811882	6.470510
B	6.813049	6.309238	8.345704
H	1.325913	0.504915	0.675103
H	-3.217591	3.784791	3.325235
H	-3.952947	9.398075	5.698476
H	1.938994	-1.136797	10.001868
H	5.970840	6.007585	4.098426
H	-3.733332	0.568116	8.030977
H	-1.085518	5.973149	12.166922
H	-4.470615	7.017617	5.608273
H	-3.095449	8.032114	3.873152

H	-1.051177	0.910173	1.046384
H	4.512752	5.015819	2.401454
H	3.955626	7.205035	3.356438
H	0.525521	2.785085	1.021270
H	1.036912	4.791795	11.949362
H	0.495159	6.659193	10.456541
H	2.014187	-2.939713	8.354494
H	3.542605	-1.047236	8.164729
H	5.665441	3.173184	5.895543
H	5.057124	1.789681	5.156101
H	4.960523	10.561269	8.230382
H	5.022886	10.124116	6.532251
H	3.110733	11.488844	6.617652
H	2.384757	9.900935	6.717536
H	1.464385	11.613317	8.355129
H	3.050984	11.723584	9.095421
H	1.644129	10.320104	10.481661
H	1.139860	9.333912	9.119553
H	2.801319	8.210935	10.616299
H	4.022991	9.402426	10.157993
H	5.421300	8.276094	8.284497
H	7.404153	7.055893	9.067178
H	5.842669	5.738547	8.751853
H	7.224899	6.090289	7.246462

B :
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C	2.617043	9.064317	9.761227
C	1.607228	9.896838	8.985547
C	2.212683	10.977242	8.086499
C	3.305710	10.495191	7.125517
C	4.581891	10.029380	7.836022
C	4.590675	8.580668	8.308108
O	3.327502	8.159828	8.896620
La	2.845283	6.115707	7.391783
O	4.747134	7.695850	7.247711
Si	3.506777	3.442936	5.294489
O	3.584637	5.098965	4.943880
Si	4.323264	5.892801	3.610092
O	2.670861	2.492800	4.238124
Si	1.075129	2.016492	4.427789
O	0.952263	1.075157	5.775121
Si	0.589625	0.783008	7.362619
O	1.611963	1.704888	8.336728
Si	1.690217	3.346865	8.098084
O	2.307727	4.478002	9.056195
O	0.651054	1.092129	3.146355
Si	0.453911	1.342940	1.486902
O	0.225555	3.425505	4.530652
Si	-1.341208	3.874668	4.821861
O	-1.375384	5.372998	5.493854
Si	-0.819341	6.457262	6.646757
O	-1.386104	5.889665	8.136650
Si	-1.095548	4.351264	8.650734
O	-0.736356	4.304285	10.248913
Si	0.069871	5.290398	11.355887
O	-2.109160	2.718593	5.730527
Si	-2.253643	2.089278	7.249190
O	-2.357820	3.311760	8.375535
O	-2.088570	3.909096	3.346853
O	-3.658200	1.228529	7.234418
O	-1.011555	1.053051	7.651988
O	0.893846	-0.789516	7.710730

Si	2.148022	-1.599818	8.495871
O	2.610421	3.625154	6.689149
N	5.095311	2.854142	5.392371
O	0.121866	3.747133	7.669651
O	-1.621734	7.878224	6.366094
Si	-3.059266	8.229346	5.569257
O	0.784964	6.688999	6.669568
B	5.852291	6.613417	7.269207
H	1.420860	0.455118	0.777930
H	-3.047719	3.850644	3.390038
H	-3.457272	9.604809	5.990392
H	2.117549	-1.308060	9.958070
H	5.746995	5.483844	3.494111
H	-3.742104	0.597401	7.955230
H	-0.932963	5.718689	12.376347
H	-4.137755	7.263474	5.936984
H	-2.857804	8.205971	4.089412
H	-0.940125	0.966315	1.122385
H	3.568482	5.533067	2.377168
H	4.191098	7.343816	3.907361
H	0.719509	2.766914	1.133624
H	1.148516	4.503439	12.009238
H	0.626147	6.507420	10.695412
H	1.920029	-3.053015	8.259053
H	3.469539	-1.196150	7.929003
H	5.787403	3.364717	5.922570
H	5.268955	1.861334	5.352736
H	4.789875	10.688729	8.688546
H	5.449563	10.110708	7.172789
H	3.566220	11.324515	6.458508
H	2.921379	9.699790	6.473691
H	1.403153	11.438729	7.509384
H	2.633391	11.775781	8.714484
H	0.928681	10.365114	9.710121
H	0.991782	9.211255	8.389348
H	2.111641	8.428378	10.493355
H	3.340766	9.683964	10.304096
H	5.381404	8.414798	9.052182
H	6.588144	6.780909	8.216804
H	5.264010	5.506986	7.424070
H	6.407377	6.601016	6.192430

Study of the ring opening step of the ε-CL ROP reaction with (BH_4)La@**c**-1

$TS_{B\rightarrow C}$
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C	2.367942	9.207990	9.753488
O	2.696523	8.432992	8.632480
La	2.165593	6.547080	7.422336
O	3.328005	5.557772	5.094957
Si	3.803599	6.395074	3.677490
C	2.096350	10.656772	9.375418
C	3.307042	11.405579	8.815500
C	3.938993	10.828054	7.537079
C	5.106673	9.840711	7.728508
C	4.800261	8.417890	8.125527
O	4.549568	7.511994	7.176271
B	6.049445	7.089275	7.227094
O	2.517312	3.967832	6.831392
Si	1.489294	3.625400	8.143525
O	-0.069827	3.793930	7.547272
Si	-1.457896	4.208556	8.395715
O	-1.968316	5.651311	7.782321

Si	-1.386013	6.276342	6.318335
O	-2.411319	7.509054	5.910787
Si	-4.026737	7.816419	6.254933
Si	3.505916	3.919096	5.494390
N	5.163384	3.614893	5.699186
O	1.830525	4.873904	9.095560
O	0.143749	6.788999	6.449061
O	2.920240	2.822280	4.412293
Si	1.412126	2.095587	4.501247
O	1.254708	1.065177	3.240365
Si	1.178744	1.216735	1.558932
O	1.334337	1.202502	5.884010
Si	0.857956	0.898792	7.439116
O	1.370814	-0.593222	7.885539
Si	2.707090	-1.158936	8.745631
O	0.349091	3.352768	4.461267
Si	-1.286531	3.577667	4.591076
O	-1.942877	2.348290	5.491622
Si	-2.126791	1.741282	7.012551
O	-2.501849	2.960022	8.083968
O	-0.785242	0.915418	7.559015
O	1.611048	2.001526	8.468434
O	-3.381203	0.677921	6.920838
O	-1.624317	5.070397	5.179279
O	-1.866150	3.445669	3.048320
O	-1.230038	4.297025	10.016142
Si	-0.714709	5.494819	11.091242
H	2.345409	0.483798	0.985941
H	-2.815702	3.574355	2.965964
H	-4.182217	8.296086	7.660842
H	2.545627	-0.869406	10.199658
H	5.284649	6.365279	3.543127
H	-3.424519	0.055067	7.652333
H	-1.881568	5.843616	11.955772
H	-4.868054	6.598470	6.052037
H	-4.469619	8.888414	5.315753
H	-0.090110	0.592820	1.092260
H	3.150243	5.766364	2.497703
H	3.315088	7.788447	3.873377
H	1.235896	2.651451	1.157166
H	0.383922	4.944281	11.928261
H	-0.270417	6.722349	10.368268
H	2.760611	-2.630708	8.519974
H	3.961664	-0.523466	8.242451
H	5.743071	4.252075	6.227922
H	5.502765	2.665033	5.701332
H	5.803884	10.251153	8.468420
H	5.648619	9.768021	6.779889
H	4.367736	11.658371	6.963085
H	3.170262	10.379479	6.900163
H	2.992194	12.434115	8.600926
H	4.078796	11.492178	9.594226
H	1.726268	11.190593	10.261115
H	1.282890	10.671312	8.637896
H	1.483646	8.790630	10.260938
H	3.188406	9.170185	10.495533
H	4.815194	8.099228	9.164678
H	6.476651	7.912575	8.082651
H	6.154604	5.989390	7.717322
H	6.598607	7.356095	6.190872

C :
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C	2.895033	3.440025	7.313781
O	4.034434	4.244314	7.383415
La	5.507674	5.842990	7.212891
O	4.409826	7.750995	7.752897
Si	3.659299	9.144806	7.431717
O	3.077494	9.205198	5.842532
Si	4.085369	9.238883	4.541333
O	5.610807	8.870443	5.108946
Si	6.632339	7.574034	4.860669
O	7.497703	7.442932	6.316944
Si	8.783139	7.326991	7.347597
N	10.107314	6.331012	6.937806
C	3.142022	1.956838	7.606516
C	3.851561	1.112891	6.536322
C	5.351711	1.384816	6.335077
C	5.665400	2.479348	5.313098
C	7.074310	3.041069	5.407564
O	7.263401	3.696614	6.695340
B	7.861680	3.053363	7.727166
O	5.838079	6.179307	4.851179
O	7.938749	6.606201	8.629693
Si	8.339707	6.520117	10.287494
O	7.697552	8.138807	3.714360
Si	8.199617	9.738225	3.785364
O	8.839702	10.038320	5.283728
Si	8.810605	10.229083	6.919973
O	9.391592	8.831668	7.645339
O	9.385884	9.891775	2.662972
Si	9.722075	11.056713	1.488570
O	6.997919	10.817404	3.428088
Si	5.706126	11.615723	4.114906
O	4.292454	10.760440	3.901538
O	5.527526	13.070001	3.356348
O	5.992551	11.945803	5.704546
Si	5.962464	11.365695	7.258121
O	7.301058	10.434843	7.539660
O	9.831337	11.455472	7.287246
Si	10.200872	12.363186	8.662183
O	6.109798	12.659198	8.278561
O	4.599686	10.527950	7.616654
O	3.554910	8.253804	3.343666
Si	2.669527	6.814956	3.290357
O	2.337986	9.380938	8.402495
Si	1.729726	10.739432	9.176186
H	11.049394	10.693896	0.914982
H	2.591947	11.122447	10.335139
H	8.683428	11.026985	0.417762
H	11.680042	12.302271	8.848788
H	9.517111	11.806432	9.865082
H	5.464381	13.356583	8.129937
H	1.623568	11.902246	8.242689
H	0.369244	10.380326	9.673421
H	9.641198	5.816592	10.460996
H	4.916102	13.041139	2.614404
H	1.314645	7.131106	2.748786
H	9.779092	13.772694	8.430186
H	8.395132	7.889427	10.865789
H	7.235607	5.731225	10.906099
H	3.371689	5.881178	2.367248
H	2.532508	6.210326	4.645707
H	9.784731	12.417424	2.096572
H	9.959495	5.369836	6.669918
H	10.865654	6.757740	6.424560

H	4.952415	3.301856	5.417116
H	5.543739	2.088192	4.294658
H	5.857059	0.460265	6.026815
H	5.778190	1.645532	7.313956
H	3.732620	0.060338	6.821990
H	3.325244	1.219027	5.576811
H	2.157300	1.502315	7.784414
H	3.688938	1.878317	8.556825
H	2.145327	3.802346	8.035628
H	2.428548	3.528564	6.316458
H	7.236853	3.813523	4.653191
H	7.836190	2.258830	5.316094
H	8.402933	1.999322	7.559124
H	7.836374	3.613914	8.785107

$TS_{B \rightarrow BCro}$

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O	9.305477	9.280189	7.695035
O	8.624857	10.450386	5.350371
Si	8.597610	10.624530	6.990036
H	9.275138	8.484205	0.849258
O	6.708278	11.071999	3.527314
Si	7.976577	10.076526	3.875127
O	9.113103	10.307620	2.713090
O	7.576862	8.440646	3.841361
O	7.078890	10.688454	7.623380
Si	5.693002	11.561243	7.387227
O	5.665554	12.171484	5.845158
Si	5.408163	11.821657	4.254665
O	4.043677	10.884051	4.082098
Si	3.954603	9.348859	4.706199
O	3.515274	8.337705	3.492014
O	2.939809	9.219223	5.997056
H	2.278308	11.204683	10.440213
Si	3.505341	9.225330	7.591321
O	4.317710	7.871116	7.948727
O	5.832508	6.406132	5.039583
Si	6.575560	7.829154	5.023941
O	4.381107	10.649116	7.760381
O	5.500451	9.081714	5.286008
O	7.484587	7.732649	6.455202
Si	8.756906	7.733243	7.522080
O	7.902806	7.072157	8.825168
Si	8.431186	6.762139	10.420098
La	5.590627	6.089604	7.422355
O	7.064506	3.916238	6.406144
B	7.831015	3.506533	7.728478
N	10.106233	6.738792	7.239241
O	9.505622	11.937809	7.351605
Si	9.870795	12.815607	8.747008
O	5.790757	12.846949	8.423619
O	5.177913	13.275841	3.514001
Si	10.093478	9.270970	1.817276
Si	2.698324	6.866171	3.382955
O	2.166720	9.406059	8.548297
Si	1.463303	10.745896	9.275058
O	4.186556	4.375988	7.297506
C	2.864270	3.928587	7.191513
C	2.720080	2.408439	7.270648
C	3.592396	1.664553	6.251043
C	5.028849	1.407538	6.749140
C	6.149989	1.783185	5.739736
C	6.321254	3.247796	5.653998

H	11.353743	12.799151	8.912765
H	9.222774	12.205161	9.943455
H	5.164487	13.552390	8.235741
H	1.308781	11.876020	8.309504
H	0.116687	10.317161	9.754661
H	9.496833	5.723306	10.421452
H	5.302472	13.255428	2.560646
H	1.369893	7.122308	2.751646
H	9.400489	14.216186	8.557947
H	8.923351	8.025564	11.034769
H	7.219531	6.265835	11.133343
H	3.494770	5.960049	2.507973
H	2.499392	6.250279	4.724831
H	11.059972	10.134957	1.082463
H	10.836511	8.337666	2.716907
H	9.996877	5.734259	7.213953
H	10.869861	7.077381	6.673867
H	5.902311	1.397736	4.745314
H	7.093958	1.345854	6.078040
H	5.169902	0.346479	6.980582
H	5.211756	1.958063	7.674451
H	3.129621	0.704117	5.997339
H	3.603090	2.239285	5.315158
H	1.662129	2.167928	7.102468
H	2.958327	2.060182	8.284594
H	2.238676	4.380931	7.978612
H	2.435161	4.257146	6.228701
H	5.817469	3.844972	4.887061
H	7.706532	2.334728	7.963605
H	8.965562	3.879891	7.545056
H	7.256693	4.203773	8.564430

BC$_{ro}$

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C	2.915139	3.971335	7.099391
O	4.287307	4.233779	7.070269
La	5.927947	5.722203	6.989208
O	4.722138	7.520205	7.613172
Si	3.814329	8.824922	7.314064
O	3.257918	8.860917	5.714582
Si	4.293117	9.106115	4.457132
O	5.835670	8.907152	5.068548
Si	6.945053	7.689413	4.775612
O	7.814011	7.515442	6.219074
Si	9.059142	7.515089	7.312296
N	10.485648	6.639929	6.987812
C	2.555714	2.600102	7.677773
C	2.907009	1.361880	6.843242
C	4.405663	1.043342	6.712749
C	5.082617	1.776419	5.509862
C	6.484140	1.972388	5.897603
O	6.926597	3.097873	6.181912
B	8.288805	3.399910	6.920548
O	6.217246	6.259994	4.676964
O	8.226463	6.724418	8.554323
Si	8.788961	6.327468	10.114472
O	7.963198	8.390237	3.660740
Si	8.296787	10.028292	3.793249
O	8.874300	10.352383	5.311467
Si	8.803032	10.431604	6.955935
O	9.520206	9.071966	7.616402
O	9.479470	10.331883	2.696254
Si	9.813262	11.644032	1.691056

O	7.003556	11.003034	3.443984
Si	5.646216	11.653249	4.163556
O	4.321901	10.675148	3.907638
O	5.343571	13.125405	3.481796
O	5.881269	11.951799	5.767259
Si	5.865876	11.275419	7.283334
O	7.266993	10.438797	7.548451
O	9.671210	11.744790	7.412453
Si	10.006289	12.513023	8.877136
O	5.869000	12.523493	8.369970
O	4.570762	10.305356	7.557581
O	3.937929	8.139582	3.181819
Si	3.355291	6.570804	2.961693
O	2.457017	8.858433	8.263926
Si	1.630033	10.110893	9.014610
H	11.189282	11.425384	1.160654
H	2.389520	10.616020	10.197950
H	8.839357	11.688919	0.560914
H	11.482954	12.465181	9.089487
H	9.312986	11.831550	10.008124
H	5.251549	13.229072	8.155380
H	1.374671	11.244689	8.074929
H	0.325255	9.548833	9.473530
H	9.775454	5.213842	10.040816
H	4.981034	13.076041	2.592352
H	2.054297	6.685074	2.235555
H	9.560254	13.930813	8.773982
H	9.398490	7.525847	10.754032
H	7.577876	5.886913	10.865272
H	4.322806	5.814090	2.121077
H	3.125467	5.876614	4.260150
H	9.759250	12.925515	2.453448
H	10.419118	5.660104	6.750187
H	11.225773	7.111380	6.487942
H	4.623197	2.751835	5.349390
H	5.013433	1.150623	4.613299
H	4.560540	-0.033669	6.588007
H	4.896093	1.325189	7.652430
H	2.435509	0.493007	7.319412
H	2.454892	1.438755	5.844980
H	1.469262	2.590054	7.840232
H	3.015885	2.509139	8.671551
H	2.392366	4.733346	7.699790
H	2.488042	4.041444	6.081903
H	7.156318	1.115604	6.047741
H	8.881888	2.362198	7.079422
H	8.831607	4.218246	6.213951
H	7.890815	3.886259	7.972780

$TS_{BCro\rightarrow C}$

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C	2.783226	3.545595	7.723403
O	3.983258	4.254833	7.828472
La	5.479423	5.819801	7.538504
O	4.362779	7.743394	7.925880
Si	3.588086	9.105945	7.529619
O	2.981994	9.057064	5.948779
Si	3.979027	9.038269	4.638671
O	5.507815	8.692715	5.208590
Si	6.527800	7.384437	5.035675
O	7.414847	7.350715	6.482040
Si	8.725299	7.260626	7.493366
N	10.046074	6.258814	7.138515

C	2.934206	2.164388	7.069315
C	3.739335	2.207574	5.762459
C	5.243998	2.104323	6.046198
C	6.153063	2.788340	5.003152
C	7.427941	3.249888	5.579733
O	7.467197	3.957803	6.629955
B	8.478593	2.904688	7.485639
O	5.731738	5.991222	5.123509
O	7.891081	6.572681	8.808386
Si	8.428798	6.343798	10.417126
O	7.573343	7.871036	3.836369
Si	8.076427	9.472872	3.811289
O	8.725242	9.861122	5.284135
Si	8.716352	10.140917	6.909128
O	9.307487	8.791092	7.707421
O	9.251746	9.555366	2.669721
Si	9.620961	10.683413	1.469856
O	6.871155	10.529907	3.400368
Si	5.602641	11.385177	4.064520
O	4.181125	10.526936	3.926941
O	5.427177	12.799699	3.234166
O	5.914968	11.811038	5.625027
Si	5.884289	11.315174	7.208239
O	7.214020	10.387977	7.533469
O	9.739269	11.389232	7.188438
Si	10.153313	12.344426	8.517749
O	6.039932	12.660372	8.157298
O	4.514132	10.507142	7.607725
O	3.433119	7.999397	3.492309
Si	2.456885	6.622256	3.513433
O	2.279024	9.384101	8.504223
Si	1.678882	10.774423	9.227627
H	10.946206	10.282608	0.917471
H	2.563827	11.215001	10.348100
H	8.591010	10.643692	0.390691
H	11.627130	12.221274	8.716777
H	9.438153	11.887772	9.744153
H	5.403353	13.355680	7.966638
H	1.545320	11.890687	8.242536
H	0.331903	10.430318	9.769844
H	9.663824	5.514683	10.434508
H	4.931825	12.710258	2.414629
H	1.104277	6.995501	3.004958
H	9.803415	13.758956	8.208382
H	8.662755	7.666626	11.057266
H	7.304412	5.627243	11.086135
H	3.074546	5.621005	2.598413
H	2.336025	6.059872	4.888384
H	9.701206	12.058558	2.042271
H	9.956822	5.252428	7.116394
H	10.824629	6.618754	6.608550
H	5.691236	3.741405	4.676571
H	6.333028	2.179849	4.113237
H	5.544403	1.054167	6.137896
H	5.430305	2.566280	7.017383
H	3.427645	1.402939	5.086143
H	3.521496	3.149280	5.241579
H	1.925716	1.771906	6.886837
H	3.413703	1.466780	7.769664
H	2.326685	3.418121	8.717711
H	2.064116	4.128801	7.122880
H	8.376115	3.074181	5.054071
H	8.308873	1.814147	6.957582

H	9.597110	3.334548	7.364993
H	7.941076	2.925439	8.562827

$TS_{BCro \rightarrow BC'ro}$

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C	2.935683	3.738447	7.488506
C	2.974230	2.206764	7.433542
C	3.867280	1.677487	6.302785
C	5.296989	1.428675	6.791745
C	6.357453	1.321111	5.660971
C	6.616487	2.658269	5.081963
O	7.336048	3.535389	5.587750
B	8.156337	3.501851	6.929392
O	4.200985	4.332733	7.489344
La	5.540537	6.066878	7.285243
O	5.784642	6.460104	4.929346
Si	6.571083	7.860086	4.956497
O	7.579709	8.491844	3.791189
Si	8.005854	10.118390	3.892576
O	9.169070	10.372857	2.762133
Si	10.167744	9.351362	1.868888
O	6.761334	11.146723	3.554604
Si	5.438575	11.868948	4.268367
O	5.216937	13.339283	3.557049
O	8.631988	10.424640	5.393719
Si	8.573844	10.574597	7.035048
O	9.493385	11.868489	7.436614
Si	9.836287	12.720041	8.853670
O	5.658016	12.184458	5.871825
Si	5.670550	11.542697	7.401351
O	5.770176	12.810277	8.460097
O	4.082281	10.929966	4.040453
Si	3.982287	9.390848	4.653452
O	3.570458	8.381967	3.427763
Si	2.857118	6.856221	3.315952
O	4.348951	10.634588	7.749389
Si	3.482228	9.213004	7.525880
O	2.128291	9.362112	8.466356
Si	1.393756	10.682194	9.198345
O	7.043950	10.650688	7.636742
O	9.245470	9.210373	7.738128
Si	8.710530	7.668051	7.493379
O	7.802574	6.973522	8.750491
Si	8.356535	6.627082	10.332372
N	10.079081	6.686413	7.254910
O	7.489512	7.690030	6.373232
O	5.520133	9.125779	5.260754
O	4.293395	7.851214	7.853835
O	2.942860	9.251388	5.923080
H	10.867665	8.380745	2.763352
H	2.177434	11.131258	10.388496
H	9.373906	8.606552	0.848654
H	11.315075	12.685371	9.051374
H	9.156207	12.097558	10.025832
H	5.171310	13.535902	8.260051
H	1.247021	11.825881	8.247695
H	0.041919	10.230879	9.641467
H	9.115134	5.345466	10.331274
H	5.346542	13.337975	2.604142
H	1.532024	7.030414	2.649250
H	9.384970	14.128555	8.677382
H	9.203658	7.747165	10.823856
H	7.120977	6.488217	11.154710

H	3.723937	5.990612	2.469062
H	2.649543	6.239630	4.657387
H	11.169505	10.224964	1.194949
H	9.951647	5.696399	7.085835
H	10.871767	7.072707	6.763630
H	6.007809	0.649840	4.870342
H	7.290522	0.936108	6.083691
H	5.337506	0.495353	7.364673
H	5.592233	2.231865	7.470818
H	3.461801	0.748107	5.883721
H	3.862561	2.409382	5.483409
H	1.943797	1.851121	7.308581
H	3.324228	1.807637	8.395340
H	2.363311	4.043041	8.379612
H	2.359738	4.089702	6.614057
H	6.133620	2.959634	4.145229
H	8.055223	2.439123	7.483053
H	9.279510	3.795282	6.591989
H	7.647910	4.406240	7.584195

BC'$_{ro}$

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Si	10.069939	8.196161	2.103637
O	9.437183	9.485199	2.989222
O	9.755660	11.315084	7.539619
Si	10.182337	12.231107	8.895889
O	6.364712	13.466671	3.168127
O	6.327546	12.469426	5.588756
O	4.615963	11.473296	3.705406
Si	6.044872	12.000691	7.153532
O	6.466364	13.262462	8.135230
Si	6.143247	12.064273	4.001455
H	9.238600	11.976906	10.021477
O	7.276437	10.953399	3.494180
O	8.730877	9.903838	5.541340
Si	8.163534	9.663542	4.004299
O	8.813343	8.843175	8.024833
Si	8.574665	10.257119	7.144965
O	7.293476	8.218403	3.954575
Si	7.946362	7.467343	7.770051
O	6.836623	7.731659	6.574359
Si	6.078494	7.966367	5.056255
O	5.354153	9.467391	5.232456
O	7.063967	10.759644	7.567591
O	4.488499	11.567510	7.431201
O	2.890958	10.430695	5.583966
Si	3.219923	10.480859	7.240851
O	1.905725	11.187122	7.950811
O	3.510405	9.001400	7.829994
Si	2.322829	7.835433	3.253714
O	3.433828	9.111381	3.274569
Si	4.023196	10.106897	4.434545
O	4.970711	6.811754	5.116578
O	6.799829	7.060758	8.965928
Si	7.160949	6.570252	10.574468
N	9.054173	6.177663	7.661024
La	4.483137	6.994485	7.492750
O	3.478360	5.235252	8.289323
C	2.717360	4.162464	8.751261
C	2.854736	2.938195	7.844161
C	2.089912	1.701643	8.324981
C	0.564605	1.821417	8.237363
C	-0.158548	0.553176	8.686846

C	-0.102341	0.301422	10.143879
O	-0.534972	-0.714999	10.697334
B	-1.228131	-1.932168	9.911416
Si	1.565389	12.766126	8.412768
H	1.929693	7.435541	4.637322
H	10.400616	7.055973	3.010356
H	2.304405	13.117146	9.662855
H	9.096082	7.747559	1.067343
H	11.562721	11.823925	9.289126
H	6.092671	14.110636	7.877866
H	1.930830	13.737479	7.337711
H	0.097630	12.833861	8.669060
H	7.397627	5.099878	10.587804
H	6.383496	13.366537	2.211827
H	1.110197	8.307254	2.522611
H	10.167230	13.669152	8.511295
H	8.357127	7.312210	11.053164
H	5.950353	6.911776	11.370125
H	2.940750	6.692750	2.530212
H	11.312625	8.703318	1.457689
H	8.748731	5.238296	7.454394
H	9.977986	6.372053	7.302511
H	0.214642	-0.354536	8.187576
H	-1.230185	0.557913	8.427057
H	0.279386	2.038593	7.201624
H	0.207964	2.672693	8.831396
H	2.402642	0.833342	7.730559
H	2.387004	1.473685	9.360303
H	3.922318	2.695458	7.769677
H	2.528193	3.210286	6.831309
H	3.032950	3.883564	9.771981
H	1.658436	4.459512	8.824037
H	0.331198	1.062458	10.809217
H	-0.377660	-2.323672	9.133585
H	-1.519312	-2.715654	10.775581
H	-2.173187	-1.425852	9.336535

$TS_{BC'RO \rightarrow C'}$

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Si	9.984884	8.182439	2.076240
O	9.386312	9.471172	2.985434
O	9.739456	11.283395	7.540221
Si	10.182707	12.186129	8.899952
O	6.359421	13.487684	3.185943
O	6.313650	12.481364	5.602615
O	4.589269	11.511875	3.716418
Si	6.031982	12.010878	7.167091
O	6.469493	13.265022	8.151583
Si	6.123157	12.084534	4.014137
H	9.235940	11.943185	10.025458
O	7.243733	10.963269	3.501248
O	8.692954	9.890773	5.540303
Si	8.117433	9.661777	4.004695
O	8.769819	8.821254	8.020173
Si	8.544818	10.240734	7.145478
O	7.231153	8.226703	3.953018
Si	7.885042	7.457295	7.762126
O	6.773507	7.742599	6.573029
Si	6.015137	7.985610	5.056315
O	5.306665	9.493429	5.235735
O	7.041417	10.759476	7.573652
O	4.472653	11.592135	7.449245
O	2.857049	10.487061	5.598332

Si	3.189558	10.522719	7.254994
O	1.886305	11.242898	7.970903
O	3.462495	9.036625	7.835100
Si	2.241758	7.910374	3.263153
O	3.375110	9.166568	3.283843
Si	3.981001	10.151471	4.444427
O	4.897713	6.840553	5.116253
O	6.739535	7.057327	8.960725
Si	7.099336	6.556904	10.566358
N	8.977109	6.155100	7.640253
La	4.416163	7.020310	7.493887
O	3.406937	5.257673	8.273516
C	2.657640	4.165683	8.710474
C	3.107584	2.868799	8.035327
C	2.375988	1.611202	8.515200
C	0.893651	1.569455	8.127547
C	0.192106	0.213932	8.391024
C	0.118610	-0.056707	9.858073
O	-0.888850	0.121321	10.559570
B	-1.740020	-1.388274	10.047538
Si	1.574615	12.819406	8.460047
H	1.851763	7.508400	4.646881
H	10.302231	7.023722	2.964027
H	2.324585	13.138239	9.712297
H	8.992889	7.766520	1.043436
H	11.556496	11.754433	9.290391
H	6.091901	14.115217	7.906924
H	1.952230	13.801935	7.399267
H	0.109309	12.908064	8.723424
H	7.320517	5.084010	10.573303
H	6.368237	13.391997	2.229049
H	1.032608	8.406193	2.542347
H	10.191591	13.625817	8.521291
H	8.305156	7.283649	11.044424
H	5.894935	6.908317	11.366881
H	2.836444	6.762023	2.528898
H	11.230979	8.674068	1.424744
H	8.658877	5.220884	7.429606
H	9.900602	6.340646	7.276261
H	0.764924	-0.588754	7.910947
H	-0.820585	0.224233	7.982407
H	0.798326	1.771031	7.053531
H	0.333853	2.361108	8.638197
H	2.875832	0.729758	8.091663
H	2.487448	1.527488	9.605359
H	4.183221	2.751355	8.220316
H	2.989331	2.977815	6.948556
H	2.753458	4.049894	9.804045
H	1.588811	4.342266	8.509836
H	1.068809	-0.319111	10.362162
H	-0.848444	-2.085119	9.593439
H	-2.084202	-1.731088	11.143247
H	-2.538011	-0.992235	9.244628

C' :

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Si	10.315038	8.324846	2.379634
O	9.601290	9.564707	3.272837
O	9.511618	11.231344	7.906928
Si	9.805171	12.077795	9.341019
O	6.412268	13.462306	3.339962
O	6.211495	12.387298	5.718427
O	4.692803	11.400713	3.667836

Si	5.833234	11.852972	7.241823
O	6.162708	13.084643	8.294962
Si	6.169510	12.027329	4.110363
H	8.781982	11.740595	10.371482
O	7.376681	10.968831	3.667183
O	8.704153	9.873871	5.778004
Si	8.252160	9.678984	4.196728
O	8.594502	8.722428	8.221280
Si	8.397414	10.160921	7.373450
O	7.422968	8.220580	4.028828
Si	7.774284	7.339014	7.868962
O	6.773949	7.604530	6.579838
Si	6.131270	7.894086	5.019208
O	5.359808	9.372964	5.201989
O	6.843445	10.612999	7.679126
O	4.270305	11.384377	7.394900
O	2.855875	10.279953	5.386197
Si	3.049154	10.275874	7.065395
O	1.665505	10.932062	7.687395
O	3.327168	8.783994	7.624716
Si	2.548490	7.704403	2.986296
O	3.601028	9.025239	3.096016
Si	4.078370	10.004572	4.320014
O	5.048138	6.719369	4.934817
O	6.532925	6.893929	8.947851
Si	6.730439	6.403733	10.584798
N	8.909989	6.069145	7.838844
La	4.360094	6.803404	7.279034
O	3.389438	4.997225	7.986295
C	2.667055	3.875276	8.402480
C	2.497931	2.861208	7.271010
C	1.787927	1.566246	7.679306
C	0.320582	1.750261	8.079979
C	-0.443673	0.441444	8.299683
C	0.048108	-0.405134	9.465630
O	-0.128729	0.295646	10.696966
B	0.881405	0.520604	11.553609
Si	1.263923	12.482370	8.192949
H	2.079908	7.269236	4.335624
H	10.610402	7.153380	3.258204
H	1.908037	12.791484	9.505119
H	9.420117	7.902548	1.264005
H	11.159988	11.679586	9.823001
H	5.798486	13.936771	8.037091
H	1.681776	13.507489	7.188972
H	-0.219132	12.514664	8.349614
H	7.009398	4.941323	10.619716
H	6.488399	13.395175	2.383634
H	1.366887	8.142642	2.185891
H	9.783816	13.534761	9.035864
H	7.845801	7.177640	11.192150
H	5.431677	6.706631	11.244628
H	3.253236	6.598233	2.286819
H	11.586508	8.879749	1.836621
H	8.634670	5.126922	7.604503
H	9.852951	6.280619	7.545948
H	-0.387742	-0.179634	7.395061
H	-1.505402	0.661944	8.463065
H	-0.191911	2.320629	7.294029
H	0.245603	2.357882	8.989589
H	1.839016	0.859689	6.839364
H	2.346391	1.096749	8.501310
H	3.496902	2.622482	6.883401

H	1.952285	3.341943	6.447203
H	3.184369	3.385623	9.245279
H	1.680100	4.185725	8.779277
H	1.102489	-0.686225	9.347578
H	-0.542769	-1.326159	9.529823
H	1.994170	0.129853	11.307334
H	0.614542	1.120081	12.555447

Study of the alternative mechanism of the ε-CL ROP reaction with (BH_4)La@**c**-1

$TS_{AB\rightarrow Bro}$

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Si	3.511189	3.426981	5.225252
O	2.331154	3.592223	6.378690
Si	1.889730	2.979677	7.904855
O	0.244592	3.206435	7.872259
O	-1.462467	4.880311	5.687030
O	-0.837088	3.393478	10.416193
Si	-1.098072	3.491422	8.800029
O	-1.641621	4.992475	8.381380
Si	-1.113451	5.838772	7.018881
O	0.438515	6.287455	7.129455
O	2.666563	3.975858	8.888588
O	2.779037	2.752307	3.904876
Si	1.260905	2.043092	4.020931
O	1.285551	0.918098	5.230963
Si	1.113653	0.404620	6.793570
O	-0.473750	0.420747	7.243280
Si	-1.878356	1.292948	7.038692
H	-3.222521	3.654429	3.599267
O	-2.137399	2.273104	8.359633
Si	-1.357264	3.498334	4.808844
O	2.077392	1.325292	7.818820
O	0.190110	3.268231	4.272684
La	2.613869	6.015591	7.612825
O	3.929024	5.057138	5.114105
Si	5.026641	5.764328	4.009389
O	1.665614	-1.138999	6.887550
Si	2.735521	-1.935783	7.917175
N	4.934161	2.536050	5.543869
O	0.972687	1.236399	2.625210
Si	0.634418	1.660209	1.027060
Si	-0.690510	4.529199	11.657046
O	-3.139113	0.240836	6.892815
O	-1.874208	2.164213	5.642149
O	-2.274093	3.638305	3.440269
O	-2.115747	7.153422	6.897490
Si	-3.428788	7.475884	5.904060
O	2.999351	7.510489	9.191756
C	2.571747	8.369420	10.207338
C	1.571473	9.421566	9.713726
C	2.125452	10.591230	8.890354
C	2.923937	10.234313	7.626461
C	4.375345	9.832563	7.916179
C	4.858219	8.538853	7.374479
O	4.302013	7.799996	6.575945
H	-4.421912	6.358688	5.926577
H	1.653392	0.997239	0.161751
H	-4.071236	8.716200	6.429782
H	2.325086	-1.769673	9.341816
H	6.332491	5.980253	4.694109
H	-3.186694	-0.419795	7.589985
H	-2.046456	4.973578	12.093537

H	-2.987836	7.708373	4.495498
H	-0.724504	1.157301	0.680878
H	5.198568	4.851679	2.844864
H	4.441767	7.061688	3.576282
H	0.702162	3.139003	0.843661
H	0.003640	3.840215	12.780913
H	0.105518	5.708235	11.210408
H	2.690420	-3.375852	7.536670
H	4.121401	-1.410528	7.730676
H	5.505764	2.754319	6.347194
H	4.918949	1.544425	5.350892
H	4.584774	9.783335	8.993396
H	5.097384	10.578941	7.544749
H	2.930432	11.099037	6.954142
H	2.415897	9.435134	7.076811
H	1.276311	11.216931	8.589807
H	2.749028	11.230003	9.532944
H	1.059544	9.846281	10.587993
H	0.800922	8.897138	9.132948
H	2.092739	7.789928	11.012872
H	3.435740	8.873846	10.679701
H	5.880771	8.250236	7.736724
H	7.834349	8.971510	8.787077
H	7.904499	7.178138	7.751579
H	7.954226	8.971928	6.719094
B	7.885566	8.374045	7.752472

BC_{ro} :

77

Si	3.555690	3.171761	5.526221
O	2.138784	3.368882	6.398713
Si	2.028152	2.829216	8.008312
O	0.782565	3.795826	8.599921
O	0.028697	4.911207	4.890100
O	-1.457783	4.476161	9.884361
Si	-0.855438	4.035488	8.422342
O	-1.143743	5.211444	7.306657
Si	-0.175028	5.978074	6.169640
O	1.233613	6.479707	6.775062
O	3.359784	3.399513	8.692576
O	3.076706	2.696105	4.011531
Si	1.760048	1.677221	3.870220
O	1.781587	0.702658	5.220251
Si	0.976755	0.363716	6.625988
O	-0.634301	0.642397	6.410537
Si	-1.799689	1.816756	6.538566
H	-2.340102	3.573611	2.680856
O	-1.568787	2.608980	7.974525
Si	-0.741955	3.632138	4.219527
O	1.590567	1.230365	7.920805
O	0.354390	2.505757	3.674996
La	3.015962	5.718351	7.975995
O	4.198969	4.730727	5.588509
Si	5.548138	5.272893	4.682258
O	1.201334	-1.225411	6.964262
Si	1.705114	-2.076714	8.331322
N	4.753375	2.098403	6.115279
O	1.996543	0.732188	2.550663
Si	1.177857	0.529592	1.089632
Si	-2.547078	5.665170	10.381603
O	-3.286657	1.110553	6.495271
O	-1.770036	2.857309	5.266770
O	-1.630429	4.170172	2.937662

O	-1.099431	7.252400	5.626990
Si	-0.707622	8.721976	4.918648
O	3.002077	6.877588	9.825144
C	2.809703	7.545418	11.034647
C	2.417881	9.018024	10.871336
C	3.510197	10.006976	10.440986
C	4.108155	9.791558	9.041456
C	5.275665	8.765427	9.049069
C	5.518547	8.269725	7.670735
O	5.006121	7.252467	7.206832
H	-0.281105	8.479301	3.518011
H	1.931192	-0.508481	0.331076
H	-1.915615	9.556863	5.114978
H	0.830278	-1.760815	9.498186
H	6.741138	5.333880	5.573175
H	-3.452492	0.481248	7.203271
H	-3.822228	5.565477	9.613193
H	0.578110	8.871030	5.965107
H	-0.219257	0.065177	1.335073
H	5.790231	4.319180	3.564519
H	5.217863	6.623264	4.152993
H	1.155515	1.808282	0.321351
H	-2.804588	5.413966	11.828239
H	-1.952447	7.021726	10.202185
H	1.592074	-3.521854	7.986382
H	3.122150	-1.740955	8.657270
H	4.974469	2.183642	7.100916
H	4.684702	1.131256	5.829089
H	4.995649	7.914591	9.674320
H	6.180600	9.247669	9.435417
H	4.478890	10.741570	8.640275
H	3.316385	9.453574	8.363932
H	3.072609	11.012722	10.462110
H	4.318145	10.017593	11.186258
H	2.025153	9.365183	11.837026
H	1.580632	9.068889	10.162504
H	2.015377	7.045397	11.610829
H	3.721090	7.483687	11.658257
H	6.166483	8.868788	7.004718
H	0.576197	10.719420	6.612212
H	1.992569	9.956917	5.286504
H	0.171019	10.438269	4.673076
B	0.850353	10.083490	5.633356

$TS_{AB \rightarrow Bintra}$

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C	3.175218	8.710439	9.915277
C	1.999438	9.629186	9.611034
C	2.286995	10.740207	8.599015
C	2.915986	10.281192	7.277964
C	4.341824	9.740669	7.434870
C	4.456608	8.251405	7.769768
O	3.466711	7.841409	8.815873
La	2.415571	6.065212	7.299475
O	4.194806	7.427730	6.734159
Si	2.866765	3.461514	5.010189
O	3.182597	5.113250	4.828301
Si	4.145073	5.885883	3.628546
O	1.845166	2.760928	3.921127
Si	0.284494	2.280167	4.312433
O	0.352898	1.203348	5.561151
Si	0.219084	0.758101	7.149226
O	1.384530	1.560281	8.063805

Si	1.486949	3.217794	8.008609
O	2.366687	4.206543	8.904420
O	-0.347622	1.492364	3.025713
Si	-0.760284	1.886567	1.435561
O	-0.518708	3.669742	4.687651
Si	-2.023920	4.083805	5.240711
O	-1.961354	5.510080	6.048022
Si	-1.279952	6.511806	7.211456
O	-1.597810	5.786987	8.706039
Si	-1.218379	4.224608	9.064952
O	-0.680173	4.084780	10.608062
Si	0.150864	5.086323	11.682596
O	-2.651199	2.851337	6.155342
Si	-2.582985	2.084991	7.612860
O	-2.490898	3.179400	8.863777
O	-2.969036	4.238787	3.892986
O	-3.992240	1.239508	7.726594
O	-1.309258	1.015837	7.709702
O	0.540467	-0.845142	7.276742
Si	1.792665	-1.742038	7.962233
O	2.045031	3.625313	6.443314
N	4.346761	2.621877	4.945045
O	-0.104808	3.731757	7.922665
O	-2.175097	7.904019	7.190041
Si	-3.628230	8.306103	6.451330
O	0.298257	6.804863	7.009331
B	6.239950	6.506725	10.154123
H	0.075945	1.044467	0.530979
H	-3.912405	4.290086	4.073642
H	-4.041678	9.626961	7.009120
H	1.844349	-1.528168	9.437279
H	5.568775	5.877733	4.058149
H	-4.028273	0.623865	8.464522
H	-0.815913	5.572052	12.710808
H	-4.686844	7.291865	6.741160
H	-3.456272	8.426319	4.972137
H	-2.200772	1.566342	1.235840
H	3.979636	5.130462	2.354470
H	3.617320	7.267619	3.496474
H	-0.502473	3.329820	1.162605
H	1.218891	4.277954	12.330557
H	0.743641	6.260998	10.977984
H	1.497141	-3.171042	7.661321
H	3.102639	-1.360456	7.353567
H	5.122991	2.878445	5.536474
H	4.339329	1.639865	4.712009
H	4.878972	10.335609	8.185509
H	4.901906	9.852489	6.500230
H	2.940650	11.138942	6.596074
H	2.276809	9.533838	6.789005
H	1.347995	11.265683	8.388623
H	2.955228	11.482170	9.059594
H	1.663420	10.077007	10.555537
H	1.167916	9.005974	9.255976
H	2.940121	8.056503	10.761171
H	4.079395	9.273771	10.180047
H	5.449328	8.056873	8.226300
H	5.387971	6.144995	10.907814
H	6.502928	5.853835	9.187752
H	6.854492	7.507664	10.378881

B_{intra}
77

C	2.358458	9.244654	9.205872
C	1.814708	9.837487	7.914487
C	2.749467	10.717298	7.074596
C	3.877659	10.039614	6.282005
C	5.096649	9.613216	7.109072
C	5.149226	8.186299	7.545158
O	3.292804	8.195122	8.962538
La	2.766450	5.894592	7.951090
O	4.710391	7.239007	6.880539
Si	2.900348	3.565082	5.206856
O	3.442220	5.160684	5.176830
Si	4.410511	5.891845	3.970134
O	1.857686	3.105635	4.011076
Si	0.298055	2.578002	4.336594
O	0.374528	1.333069	5.418393
Si	0.366262	0.667390	6.933280
O	1.612228	1.334238	7.846682
Si	1.677886	2.976663	8.113204
O	2.702628	3.763165	9.058832
O	-0.335386	1.979154	2.950999
Si	-0.933684	2.624188	1.509706
O	-0.519874	3.893028	4.897840
Si	-1.950781	4.222425	5.659936
O	-1.767248	5.493972	6.681001
Si	-0.987299	6.261351	7.951297
O	-1.361051	5.378596	9.340114
Si	-1.022192	3.771260	9.512398
O	-0.533161	3.427131	11.035500
Si	-0.041301	4.327425	12.380805
O	-2.520101	2.860709	6.413035
Si	-2.404005	1.888027	7.739017
O	-2.306816	2.787212	9.135080
O	-3.017695	4.615693	4.459584
O	-3.798594	1.009642	7.753298
O	-1.113258	0.838701	7.639444
O	0.682257	-0.938067	6.804731
Si	1.981893	-1.915976	7.245375
O	2.022277	3.708880	6.609380
N	4.259062	2.534538	5.127660
O	0.089785	3.409870	8.334455
O	-1.739180	7.727351	8.127489
Si	-3.270417	8.268474	7.699009
O	0.609378	6.455086	7.741136
B	3.626968	7.325974	10.163757
H	-0.206738	1.959101	0.389303
H	-3.939975	4.604445	4.732511
H	-3.515158	9.522357	8.470797
H	2.155593	-1.926127	8.726451
H	5.838628	5.866693	4.390911
H	-3.808070	0.290899	8.392179
H	-1.249354	4.771365	13.137180
H	-4.323418	7.263397	8.035425
H	-3.329272	8.572173	6.237276
H	-2.388552	2.317344	1.419658
H	4.235007	5.133960	2.699082
H	3.930719	7.290007	3.805433
H	-0.708268	4.097388	1.455618
H	0.772770	3.409344	13.225534
H	0.764138	5.507625	11.963778
H	1.660554	-3.286376	6.756791
H	3.240512	-1.436248	6.597502
H	5.007985	2.610040	5.800265
H	4.119494	1.584071	4.816230

H	5.233107	10.245054	7.993545
H	6.020594	9.737046	6.518842
H	4.217713	10.747813	5.518570
H	3.491760	9.171826	5.734042
H	2.122102	11.245750	6.346007
H	3.181955	11.501522	7.712751
H	0.954216	10.454436	8.203780
H	1.393894	9.026950	7.305328
H	1.523797	8.839462	9.794408
H	2.849383	10.014334	9.819300
H	5.748630	7.975801	8.445339
H	2.617753	6.644247	10.421613
H	4.507025	6.548364	9.757784
H	4.001239	7.936101	11.133947

B_{BH3}
73

C	3.816023	2.939502	5.273555
C	2.476204	3.278136	5.915560
C	2.239514	2.655834	7.293296
C	3.361980	2.865457	8.317492
C	4.651210	2.115216	7.969248
C	5.624583	2.857830	7.050157
O	6.329970	3.832743	7.666769
La	6.021837	5.786833	6.504740
O	4.898102	3.578283	5.953440
O	7.296853	8.270083	6.050292
Si	7.113671	7.729181	4.435455
O	7.919723	8.832243	3.500271
Si	8.398100	10.389491	3.862901
O	9.492599	10.801946	2.714963
Si	10.916073	11.708231	2.713957
Si	8.676671	7.934629	6.943087
N	10.064280	7.317654	6.158447
O	9.048687	9.329227	7.750717
Si	8.843118	10.791661	6.961457
O	9.994965	11.828137	7.491888
Si	9.962426	13.220666	8.452204
O	8.075939	6.691620	7.929785
Si	8.992949	5.843166	9.124658
O	5.449001	7.815591	4.232755
Si	4.183694	8.888181	4.115266
O	4.720183	10.321577	3.483225
Si	5.510695	11.633564	4.120512
O	5.191435	11.793448	5.722018
Si	5.712528	11.323327	7.223740
O	5.193096	12.401315	8.357629
O	7.447781	6.165931	4.552600
O	3.098000	8.227425	3.073338
Si	1.441286	8.434318	2.832547
O	3.492404	9.117900	5.591532
Si	3.967694	8.740488	7.159552
O	2.669626	9.145627	8.116132
Si	1.754388	8.186291	9.150364
O	5.197514	9.801742	7.576232
O	4.417437	7.195933	7.315442
O	9.133008	10.474352	5.351546
O	7.365416	11.439416	7.255357
O	7.133880	11.444014	3.825711
O	4.989408	13.020353	3.404381
H	4.312077	12.208914	8.693730
H	0.718455	9.079929	9.746588
H	11.386767	13.613764	8.647189

H	1.080637	7.077799	8.408333
H	10.715975	13.003210	3.427281
H	9.648435	4.669848	8.489721
H	5.123865	13.055171	2.452761
H	1.044231	9.854867	3.056888
H	2.596468	7.609451	10.240971
H	9.221664	14.309081	7.753058
H	10.001681	6.787137	9.678664
H	8.016329	5.427584	10.164111
H	9.326344	12.928636	9.768808
H	1.161367	8.040271	1.422432
H	0.683894	7.545389	3.762166
H	12.010634	10.934640	3.370484
H	11.255249	11.955906	1.284727
H	9.914192	6.558764	5.503806
H	10.739005	7.985329	5.811434
H	4.400130	1.137777	7.535634
H	5.234367	1.907897	8.872798
H	3.003087	2.511913	9.290896
H	3.571982	3.935126	8.448437
H	1.302005	3.058280	7.695664
H	2.078655	1.574549	7.175496
H	1.678614	2.961260	5.230656
H	2.404537	4.372085	5.981836
H	3.845878	3.299567	4.239325
H	3.995473	1.856761	5.246253
H	6.271423	2.129185	6.527090

$TS_{BBH3 \rightarrow Bro\text{-}BH3}$

73

C	3.483466	3.374798	5.187723
C	2.351048	3.463075	6.217487
C	2.439480	2.553591	7.449707
C	3.698791	2.674611	8.323218
C	4.914275	1.930649	7.754856
C	6.157557	2.707057	7.513236
O	6.412979	3.829806	7.948568
La	5.831508	5.747611	6.311506
O	4.648101	4.026681	5.596844
O	7.238025	8.309290	6.014749
Si	7.096262	7.756352	4.408443
O	7.899426	8.860757	3.473234
Si	8.418450	10.400165	3.857912
O	9.535646	10.793873	2.724350
Si	10.985216	11.656178	2.749600
Si	8.581018	7.903851	6.929841
N	9.966579	7.262940	6.152548
O	8.992546	9.286250	7.746860
Si	8.827008	10.754391	6.963264
O	9.987601	11.767624	7.522801
Si	9.959643	13.159264	8.482251
O	7.950737	6.676608	7.907140
Si	8.845091	5.871028	9.130720
O	5.424348	7.810318	4.197543
Si	4.189648	8.921819	4.053634
O	4.793609	10.331076	3.429863
Si	5.551139	11.655907	4.080440
O	5.204729	11.815319	5.676258
Si	5.703290	11.344385	7.185625
O	5.193375	12.439774	8.308159
O	7.437754	6.194940	4.523675
O	3.096807	8.305597	2.993451
Si	1.411920	8.348040	2.917480

O	3.481222	9.179388	5.517584
Si	3.929544	8.781905	7.089090
O	2.615421	9.173016	8.031393
Si	1.692896	8.196193	9.040538
O	5.147268	9.839009	7.545192
O	4.364546	7.232024	7.224369
O	9.141480	10.455581	5.353444
O	7.356842	11.430625	7.235482
O	7.181901	11.487995	3.814349
O	5.021820	13.034850	3.354297
H	4.304167	12.266931	8.632959
H	0.652401	9.077996	9.646787
H	11.386362	13.529612	8.705053
H	1.023861	7.099484	8.276998
H	11.347107	11.911690	1.327101
H	9.487857	4.656244	8.556677
H	5.144916	13.057109	2.400739
H	0.905679	9.728787	3.169718
H	2.525514	7.599126	10.128459
H	9.251026	14.261955	7.771928
H	9.874848	6.802926	9.666578
H	7.868881	5.497418	10.189359
H	9.295245	12.878994	9.787617
H	1.041608	7.911817	1.541179
H	0.829669	7.406771	3.918548
H	10.818603	12.948062	3.477067
H	12.049967	10.841899	3.406207
H	9.789924	6.535802	5.468247
H	10.655034	7.925764	5.822759
H	4.687929	1.433733	6.802319
H	5.232437	1.102116	8.411117
H	3.475792	2.272698	9.317335
H	3.949105	3.729336	8.480314
H	1.568035	2.766250	8.081118
H	2.327011	1.505065	7.137153
H	1.405456	3.233363	5.707307
H	2.277336	4.510909	6.538572
H	3.124229	3.814044	4.243006
H	3.690844	2.312675	4.959483
H	6.934198	2.174911	6.930626

B_{roBH3}

73

C	3.454675	3.450589	4.949874
C	2.296746	3.023770	5.858452
C	2.582448	1.965838	6.933286
C	3.574451	2.371388	8.035768
C	5.051531	2.116175	7.626125
C	5.959319	2.905556	8.497384
O	6.364297	4.033697	8.224070
La	5.746491	5.795424	6.362602
O	4.390268	4.269364	5.580852
O	7.239009	8.335776	6.029341
Si	7.041685	7.763720	4.438095
O	7.835720	8.840467	3.462929
Si	8.399243	10.371495	3.816544
O	9.488034	10.730279	2.643870
Si	10.948991	11.572469	2.612940
Si	8.588010	7.906693	6.923898
N	9.934200	7.213160	6.122151
O	9.060016	9.293335	7.702265
Si	8.907821	10.752397	6.900858
O	10.106631	11.746018	7.414738

Si	10.134263	13.156533	8.345339
O	7.943518	6.724541	7.942067
Si	8.778133	6.011407	9.255773
O	5.364505	7.848771	4.277150
Si	4.149635	8.985094	4.160505
O	4.764807	10.373074	3.500749
Si	5.566970	11.690900	4.109835
O	5.268266	11.881409	5.711880
Si	5.806782	11.419280	7.210398
O	5.358103	12.541460	8.333140
O	7.352414	6.196277	4.559496
O	3.008602	8.386611	3.141428
Si	1.322127	8.410302	3.158425
O	3.495398	9.272518	5.643645
Si	3.981651	8.889165	7.208329
O	2.702386	9.320293	8.182622
Si	1.762468	8.355515	9.186483
O	5.228918	9.933441	7.612322
O	4.388096	7.334486	7.359382
O	9.171773	10.426677	5.287110
O	7.462754	11.469439	7.202883
O	7.186117	11.486373	3.801502
O	5.045371	13.069789	3.377460
H	4.481216	12.384196	8.697078
H	0.745183	9.254950	9.806586
H	11.574261	13.497135	8.527307
H	1.064194	7.279722	8.419080
H	11.266164	11.811741	1.176869
H	9.314304	4.684485	8.840363
H	5.137692	13.072666	2.420182
H	0.815255	9.788246	3.424515
H	2.585019	7.730114	10.266680
H	9.435651	14.262545	7.630074
H	9.891826	6.911324	9.664247
H	7.800919	5.854364	10.367201
H	9.495344	12.919559	9.671962
H	0.882547	7.957757	1.807816
H	0.803009	7.473024	4.197238
H	10.825553	12.872786	3.334130
H	12.024916	10.749239	3.239534
H	9.714468	6.481057	5.455577
H	10.624909	7.853834	5.755054
H	5.191674	2.449168	6.595325
H	5.276962	1.048372	7.723197
H	3.363424	1.814996	8.956340
H	3.431709	3.433113	8.267170
H	1.629732	1.719676	7.418584
H	2.924463	1.034960	6.459451
H	1.498673	2.628738	5.214772
H	1.889973	3.926187	6.334292
H	3.026935	3.976059	4.081663
H	3.943698	2.544723	4.545161
H	6.258798	2.473392	9.470296

$TS_{B \rightarrow Csurf}$

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C	3.153071	8.781976	9.960671
C	2.828037	10.230888	10.284919
C	3.555459	11.268578	9.422542
C	3.087326	11.279915	7.959751
C	3.687746	10.214664	7.029601
C	3.994168	8.841968	7.628032
O	4.045979	7.860405	6.698768

La	2.398170	6.305705	7.243238
O	2.218295	3.803751	6.512197
Si	3.076805	3.625727	5.101271
O	2.142838	2.772896	4.042416
Si	0.647596	2.133193	4.457413
O	0.129026	1.196098	3.219622
Si	-0.343582	1.452666	1.618127
O	2.920829	8.440591	8.592620
O	0.195174	6.691670	6.886390
Si	-1.352989	6.290645	7.117565
O	-1.616994	5.643825	8.660354
Si	-1.090817	4.152851	9.119478
O	-0.575206	4.164250	10.677193
Si	-0.002618	5.343117	11.738227
O	3.244893	5.286147	4.815973
Si	4.116776	6.057896	3.549920
Si	1.719284	3.401371	8.098857
O	1.827950	1.749037	8.230781
Si	0.755306	0.776090	7.381496
O	0.829245	1.152460	5.770778
O	2.482601	4.524532	8.945814
O	-2.363374	7.597468	7.006483
Si	-3.841211	7.825129	6.244723
O	-1.961471	5.155047	6.036930
Si	-1.857962	3.696237	5.295009
O	-2.315562	2.438604	6.276042
Si	-2.185067	1.796191	7.787662
O	-3.493495	0.809496	7.972631
O	0.074364	3.691347	8.021998
O	-2.245186	2.966848	8.970677
O	-0.797573	0.885144	7.942447
O	1.281083	-0.762795	7.591428
Si	0.503390	-2.220302	7.936629
N	4.625736	2.917470	5.096209
O	-0.322284	3.436182	4.735355
O	-2.829698	3.671760	3.957595
B	5.403842	5.511646	8.357516
H	0.614421	0.718730	0.740273
H	-3.772055	3.677919	4.149959
H	-4.369011	9.139760	6.713689
H	-0.032028	-2.202019	9.329443
H	5.533929	6.232694	3.967409
H	-3.696099	0.596973	8.888491
H	-1.120773	5.771153	12.629043
H	-4.811953	6.746169	6.602025
H	-3.675551	7.861042	4.760205
H	-1.714209	0.896252	1.444666
H	4.029036	5.199682	2.335250
H	3.450369	7.366603	3.325351
H	-0.323545	2.905815	1.284818
H	1.084559	4.728114	12.548785
H	0.516921	6.530659	10.998429
H	-0.606981	-2.466967	6.971443
H	1.538982	-3.284273	7.806676
H	5.361456	3.268864	5.690819
H	4.697516	1.923861	4.931516
H	4.635271	10.570801	6.605422
H	3.016636	10.050825	6.178886
H	3.299244	12.263018	7.523227
H	1.994670	11.183307	7.956943
H	3.362814	12.256921	9.856588
H	4.643359	11.122337	9.484375
H	3.071048	10.386861	11.344673

H	1.745506	10.383249	10.186427
H	2.527096	8.109236	10.556051
H	4.204444	8.561868	10.202383
H	4.908102	8.889901	8.251420
H	4.758156	6.266433	9.014768
H	4.963522	5.027206	7.355928
H	6.514096	5.230162	8.688550

C_{surf}

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C	4.031730	8.807412	9.349027
C	3.939681	10.223051	9.893500
C	4.224864	11.333672	8.875090
C	3.140415	11.468655	7.795054
C	3.214659	10.490849	6.610987
C	3.738276	9.087211	6.904321
O	3.359722	8.172037	5.977617
La	2.222567	6.515193	7.084789
O	2.398179	3.928206	6.791509
Si	3.252614	3.690039	5.370684
O	2.346273	2.837098	4.291844
Si	0.791916	2.235541	4.431038
O	0.349936	1.607179	2.989212
Si	-0.013747	2.210564	1.452541
O	3.194509	8.595721	8.205521
O	-0.012058	6.712236	6.898630
Si	-1.491240	6.168248	7.244548
O	-1.563524	5.453025	8.770458
Si	-0.953270	4.008469	9.269296
O	-0.644622	4.022628	10.875808
Si	-0.558187	5.208463	12.077069
O	3.359581	5.332968	4.997370
Si	4.285506	6.113477	3.764008
Si	1.946143	3.128104	8.230614
O	1.925199	1.505724	7.935379
Si	0.808523	0.574322	7.121088
O	0.776449	1.002497	5.524031
O	2.957998	3.597788	9.388967
O	-2.627411	7.368544	7.262789
Si	-4.177417	7.498244	6.631829
O	-2.046261	5.022720	6.145363
Si	-1.763676	3.629439	5.333705
O	-2.211747	2.317956	6.244404
Si	-2.061728	1.648209	7.743519
O	-3.387655	0.695863	7.963426
O	0.399020	3.706065	8.351443
O	-2.017233	2.769746	8.963159
O	-0.686075	0.716617	7.806727
O	1.314347	-0.977988	7.230793
Si	0.601120	-2.425949	7.727076
N	4.793961	2.977219	5.460000
O	-0.160341	3.501909	4.913021
O	-2.604007	3.590658	3.912577
B	3.300922	5.046950	9.484288
H	1.036423	1.718426	0.513681
H	-3.559700	3.538847	4.008453
H	-4.739484	8.785880	7.132574
H	0.261017	-2.361852	9.178291
H	5.551847	6.615921	4.356715
H	-3.621416	0.559777	8.886455
H	-1.936292	5.533257	12.549009
H	-5.044445	6.368023	7.085029
H	-4.143516	7.518256	5.138198

H	-1.343818	1.677642	1.049177
H	4.574690	5.077778	2.730498
H	3.443566	7.194533	3.198444
H	-0.023538	3.701471	1.463016
H	0.236368	4.623326	13.192206
H	0.101993	6.440698	11.560060
H	-0.629276	-2.698972	6.929409
H	1.615308	-3.490543	7.486987
H	5.436634	3.255644	6.187810
H	4.879440	1.999296	5.223087
H	3.864707	10.893470	5.823862
H	2.222405	10.377930	6.159915
H	3.162091	12.487471	7.390968
H	2.164371	11.364796	8.284695
H	4.286180	12.280775	9.424273
H	5.214489	11.189522	8.418927
H	4.645408	10.293202	10.732011
H	2.938219	10.378207	10.315442
H	3.714156	8.078295	10.100217
H	5.068643	8.567594	9.070040
H	4.834181	9.108423	7.054513
H	2.255865	5.761522	9.447101
H	4.007182	5.408743	8.504317
H	3.890682	5.318552	10.501613

$TS_{Csurf \rightarrow Csurf\_ro}$

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H	-3.834222	0.873571	8.520355
O	-3.498924	1.000266	7.627750
O	1.070156	-0.997789	7.054082
O	-0.798064	0.832755	7.653370
Si	-2.097818	1.865803	7.564482
Si	0.703775	0.597696	7.008350
O	0.759987	1.098895	5.431876
O	-2.089127	2.639516	6.107440
Si	-1.486060	3.955037	5.299117
Si	0.981000	2.381790	4.421917
O	2.590883	2.839079	4.436291
O	0.107377	3.703498	4.900492
O	-1.652038	5.316908	6.191431
H	4.808368	1.575692	5.679843
Si	3.481729	3.511131	5.651095
N	4.869047	2.558872	5.904528
Si	-1.071316	6.324975	7.405007
O	2.507105	3.861643	6.963167
O	-1.341448	5.530848	8.865577
Si	1.971304	2.983154	8.327592
Si	-0.916416	4.004286	9.313921
O	-2.076563	2.902673	8.858319
O	1.871893	1.390672	7.891251
O	2.997473	3.287267	9.528911
O	-0.728744	3.902630	10.935623
O	-2.286397	4.089259	3.859648
O	0.608613	1.877075	2.912556
Si	-3.668556	7.869406	6.947926
O	-2.072424	7.643350	7.414806
H	5.436759	2.725310	6.724148
B	3.413435	4.714108	9.688217
La	2.695836	6.474043	7.341122
O	3.901844	5.116513	5.319552
Si	4.842054	5.689078	3.995028
O	0.444878	3.592454	8.464740
Si	0.215802	-2.389572	7.482928

O	0.472972	6.742604	7.201491
Si	0.297777	2.596398	1.416114
Si	-0.515478	5.020241	12.187180
O	3.491700	8.320380	8.326613
C	3.615625	9.197790	6.163276
O	3.444839	8.128923	5.545513
C	4.287172	9.104456	9.167400
C	3.602519	10.398155	9.594350
C	3.245556	11.362888	8.457085
C	2.139723	10.869875	7.502651
C	2.595077	10.293165	6.150668
H	1.308194	2.073608	0.450510
H	-3.245596	4.076454	3.930145
H	-4.127226	9.145628	7.570123
H	-0.164767	-2.339257	8.924599
H	5.983426	6.460739	4.556697
H	-1.849723	5.533987	12.616433
H	-4.539363	6.747078	7.412017
H	-3.769250	7.982715	5.461047
H	-1.069847	2.202396	0.979149
H	5.334640	4.502801	3.241195
H	3.975528	6.534418	3.135256
H	0.412101	4.080037	1.512279
H	0.125637	4.279294	13.308765
H	0.347634	6.152445	11.748729
H	-1.007030	-2.530096	6.640537
H	1.139402	-3.533175	7.239117
H	3.063131	11.100682	5.563699
H	1.729730	9.934405	5.584503
H	1.469913	11.702496	7.259236
H	1.525776	10.118904	8.008170
H	2.911157	12.302304	8.912595
H	4.152901	11.624112	7.892570
H	4.266286	10.912534	10.302721
H	2.689802	10.144597	10.149451
H	4.558640	8.529226	10.065430
H	5.241830	9.357959	8.665593
H	4.618711	9.450134	6.539419
H	2.412509	5.475548	9.577127
H	4.212467	5.055970	8.767135
H	3.937559	4.928973	10.752340

C_{Sruf_ro}

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H	-3.883161	0.957771	8.447880
O	-3.523951	1.083103	7.564420
O	1.016562	-0.997589	6.992790
O	-0.829679	0.847725	7.610840
Si	-2.101674	1.915833	7.543482
Si	0.677546	0.604813	6.981544
O	0.764016	1.142553	5.418508
O	-2.054903	2.736889	6.113666
Si	-1.418008	4.050988	5.329780
Si	1.018811	2.438892	4.433592
O	2.639146	2.857955	4.466178
O	0.170219	3.770198	4.929977
O	-1.555614	5.403680	6.240164
H	4.762939	1.472999	5.759211
Si	3.527836	3.465900	5.717305
N	4.867795	2.451995	5.986380
Si	-0.980663	6.358767	7.498950
O	2.528385	3.825526	7.006716
O	-1.306253	5.526400	8.926658

Si	1.975445	2.940257	8.358438
Si	-0.900828	3.988174	9.352671
O	-2.071594	2.908377	8.871459
O	1.845320	1.355391	7.900138
O	3.005395	3.203410	9.566238
O	-0.726910	3.855799	10.973868
O	-2.210502	4.225715	3.889799
O	0.645927	1.970211	2.912616
Si	-3.569983	7.946308	7.151734
O	-1.953218	7.699300	7.526807
H	5.424713	2.588198	6.819071
B	3.464155	4.614483	9.745741
La	2.798133	6.438380	7.437274
O	4.023444	5.057547	5.422905
Si	4.977422	5.619976	4.106804
O	0.460514	3.575114	8.505254
Si	0.129159	-2.384561	7.366145
O	0.574414	6.750601	7.343763
Si	0.327065	2.721131	1.433779
Si	-0.487121	4.950442	12.240800
O	3.621916	8.258821	8.365882
C	3.541323	9.185011	5.954443
O	3.349731	8.062136	5.473530
C	4.285830	9.204108	9.148626
C	3.431448	10.426814	9.472772
C	3.040555	11.309972	8.280569
C	1.993894	10.714461	7.313882
C	2.513219	10.266097	5.928781
H	1.316350	2.198106	0.446572
H	-3.169992	4.224913	3.957377
H	-3.995197	9.196589	7.846667
H	-0.274313	-2.369957	8.802366
H	6.024086	6.510910	4.677741
H	-1.807193	5.501551	12.667657
H	-4.420673	6.806446	7.609959
H	-3.742157	8.122225	5.677340
H	-1.052232	2.357947	1.006700
H	5.598809	4.437871	3.448463
H	4.100433	6.350357	3.155701
H	0.467965	4.200732	1.553289
H	0.121718	4.175443	13.357399
H	0.415059	6.059602	11.822592
H	-1.081833	-2.477341	6.500310
H	1.035175	-3.538071	7.103263
H	2.979543	11.131673	5.434376
H	1.677923	9.921749	5.311755
H	1.221707	11.462720	7.104392
H	1.480661	9.870566	7.783787
H	2.638188	12.247284	8.682046
H	3.947479	11.601755	7.730576
H	3.992056	11.041357	10.190583
H	2.523427	10.093100	9.992051
H	4.613651	8.743339	10.093352
H	5.207795	9.544746	8.638318
H	4.538989	9.443448	6.344671
H	2.486619	5.408379	9.648421
H	4.271121	4.946017	8.828144
H	3.995914	4.797081	10.812004

4.2 $(X_1)(X_2)$La@c-2 as catalyst forms

$(BH_4)(CH_3)$La@c-2

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

A :
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C	3.396760	5.680184	10.105434
La	1.939835	5.427375	8.076128
O	0.933549	7.495264	7.388365
Si	2.055539	8.327643	6.615744
O	2.466108	9.806343	7.257800
Si	3.820575	10.677631	7.629676
O	4.199989	11.723641	6.406781
Si	4.104384	11.823374	4.757128
O	5.490010	11.269897	4.052047
Si	6.689630	10.159870	4.312022
O	6.933651	9.984249	5.942716
Si	6.444928	9.033017	7.206628
O	7.638421	8.957023	8.320979
Si	9.277021	9.365017	8.350096
B	1.726170	3.136551	6.624601
O	4.740669	5.131775	6.717924
Si	5.574028	3.691803	6.318411
O	0.396997	4.146184	9.955514
C	-0.695682	4.657523	9.768803
O	-0.706000	5.651930	8.864133
C	-1.873974	6.409965	8.453003
C	-2.472556	7.236745	9.576150
C	-3.310138	6.452887	10.588107
C	-2.551087	5.372447	11.358710
C	-1.954800	4.258435	10.477779
O	3.407093	7.296562	6.782723
Si	4.795800	6.672128	6.135670
O	4.739557	6.672823	4.487501
Si	5.008396	7.761483	3.265731
O	5.321871	6.896910	1.915674
Si	5.116698	7.131599	0.255563
O	6.119790	7.495635	6.666939
O	5.087627	9.652367	7.909719
O	3.539972	11.585573	8.965246
Si	2.637508	11.368069	10.373983
O	1.800334	8.538584	4.983731
Si	2.371426	9.447049	3.727087
O	1.193863	9.593291	2.595928
Si	-0.322619	8.879697	2.394787
O	3.684320	8.721016	3.028418
O	2.788920	10.960997	4.241218
O	6.313213	8.696736	3.653528
O	8.068501	10.673845	3.578378
O	3.983039	13.395795	4.287980
H	8.179703	11.629146	3.568311
H	3.195225	13.851316	4.598793
H	-0.824580	9.337687	1.068766
H	-0.211209	7.392453	2.416315
H	-1.252401	9.332224	3.471462
H	3.696763	6.867070	-0.115978
H	5.488608	8.525935	-0.123481
H	6.014794	6.156046	-0.422389
H	3.238027	12.256868	11.408038
H	1.220895	11.768972	10.126441
H	2.687614	9.946773	10.823256
H	9.999293	8.694425	7.230253
H	9.437025	10.844368	8.241457
H	9.801719	8.888403	9.659848
H	5.573601	2.853975	7.545301
H	4.883638	3.016871	5.189557
H	6.969245	4.057765	5.934310
H	4.292751	6.293976	9.925924
H	2.849072	6.164503	10.931647

H	3.749479	4.714359	10.498650
H	-1.459390	7.047854	7.671657
H	-2.598909	5.714634	8.013887
H	-3.105564	7.997016	9.102412
H	-1.661494	7.783526	10.073192
H	-3.746252	7.155674	11.307223
H	-4.157738	5.987590	10.065239
H	-1.753924	5.822891	11.963274
H	-3.236808	4.894839	12.066432
H	-1.690203	3.387199	11.079692
H	-2.692500	3.934614	9.731263
H	0.646348	3.455644	7.151404
H	1.615307	2.134824	5.969323
H	2.080165	4.098177	5.922139
H	2.559421	2.991466	7.530665

$TS_{A \rightarrow AB}$

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C	3.240733	6.757007	11.020133
La	2.096602	6.225024	8.857241
O	1.203692	8.305326	8.164281
Si	2.240334	8.935921	7.127257
O	2.952785	10.382251	7.529371
Si	4.467246	11.045878	7.583046
O	4.826736	11.822165	6.167941
Si	4.511451	11.755298	4.545458
O	5.682201	10.898802	3.754993
Si	6.746396	9.667998	4.044125
O	7.163292	9.661063	5.649428
Si	6.757001	8.973765	7.096996
O	8.080508	8.859083	8.046866
Si	9.702992	9.312778	7.914967
B	0.761053	4.357072	6.501833
O	4.398714	5.423822	7.435951
Si	5.059692	3.838073	7.321767
O	0.930115	4.172558	9.545528
C	-0.173560	4.337805	8.917976
O	-0.496484	5.722500	8.928483
C	-1.675405	6.196398	8.259835
C	-2.852093	6.232982	9.220290
C	-3.387042	4.863183	9.643397
C	-2.346131	3.890957	10.209964
C	-1.341609	3.381619	9.163996
O	3.494318	7.765002	7.150722
Si	4.684632	6.809799	6.544255
O	4.486244	6.491109	4.944814
Si	4.640940	7.430616	3.577347
O	4.596561	6.411208	2.304008
Si	4.107362	6.509359	0.687834
O	6.175163	7.429122	6.853026
O	5.593832	9.860578	7.857088
O	4.535833	12.153335	8.784333
Si	3.675063	12.402184	10.218520
O	1.720967	9.040579	5.551064
Si	2.313968	9.589789	4.109718
O	1.078935	9.733808	3.043372
Si	-0.591586	9.495951	3.137638
O	3.422208	8.534891	3.479774
O	3.024626	11.068764	4.307420
O	6.099485	8.203422	3.644296
O	8.081849	9.876047	3.108675
O	4.566033	13.261969	3.889946
H	8.269053	10.792308	2.884307

H	3.929217	13.887066	4.248525
H	-1.138786	9.893193	1.810031
H	-0.897155	8.063766	3.412030
H	-1.176322	10.356078	4.207045
H	2.629169	6.335869	0.604091
H	4.499913	7.827182	0.110524
H	4.798921	5.402467	-0.028922
H	4.480607	13.362702	11.025256
H	2.341171	12.992693	9.908251
H	3.507188	11.118916	10.957703
H	10.348753	8.579789	6.787045
H	9.808926	10.784256	7.691336
H	10.343898	8.940106	9.206270
H	4.418843	3.080716	8.428761
H	4.731219	3.260988	5.992324
H	6.533702	3.934338	7.514713
H	4.111989	7.422723	10.909306
H	2.558140	7.262774	11.721460
H	3.599854	5.855771	11.541065
H	-1.415720	7.199784	7.911701
H	-1.866739	5.569307	7.378961
H	-3.659237	6.807448	8.747876
H	-2.541165	6.805596	10.104553
H	-4.174912	5.015082	10.390510
H	-3.874779	4.384928	8.782173
H	-1.811306	4.341779	11.055606
H	-2.874465	3.017797	10.611936
H	-0.873086	2.448122	9.489640
H	-1.866942	3.169189	8.226393
H	0.006492	4.122405	7.608293
H	0.304810	3.581294	5.703141
H	0.567858	5.535124	6.295953
H	1.851842	4.063202	6.957712

AB :

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C	2.598385	6.886092	11.151983
La	1.891216	6.502760	8.777144
O	1.098346	8.592660	7.949735
Si	2.227676	9.132752	6.964526
O	2.980910	10.564202	7.352707
Si	4.521656	11.152009	7.479129
O	4.998385	11.874912	6.070624
Si	4.772145	11.764628	4.435301
O	5.950676	10.833655	3.746799
Si	6.934529	9.560355	4.127347
O	7.270014	9.578593	5.751971
Si	6.733692	8.956502	7.186486
O	7.985117	8.803328	8.225006
Si	9.626890	9.205901	8.200220
B	-0.199681	4.795067	5.786566
O	4.179885	5.527612	7.471277
Si	4.687140	3.887186	7.296098
O	1.110828	4.261475	8.599145
C	-0.172078	4.362927	8.351141
O	-0.565883	5.697281	8.759145
C	-1.944929	6.088291	8.714604
C	-2.613108	5.842706	10.058995
C	-2.818778	4.370058	10.422409
C	-1.572261	3.480525	10.329966
C	-1.084107	3.255981	8.892557
O	3.434672	7.916655	7.143666
Si	4.586193	6.884092	6.581401

O	4.432399	6.554223	4.979836
Si	4.744578	7.420294	3.589255
O	4.741131	6.346451	2.361212
Si	4.333499	6.383651	0.720085
O	6.091053	7.433864	6.948187
O	5.569277	9.920507	7.844325
O	4.579660	12.283657	8.660166
Si	3.619048	12.641296	10.004620
O	1.840431	9.174512	5.348290
Si	2.507356	9.685420	3.925487
O	1.324032	9.865378	2.810173
Si	-0.357597	9.684419	2.842325
O	3.598442	8.579328	3.352531
O	3.271887	11.135662	4.136910
O	6.233543	8.117273	3.739771
O	8.325421	9.674846	3.259146
O	4.930636	13.242461	3.731320
H	8.561960	10.572810	3.008390
H	4.272055	13.891927	3.994592
H	-0.836742	10.088115	1.490390
H	-0.718828	8.264484	3.114686
H	-0.951445	10.574585	3.881566
H	2.854031	6.277939	0.571379
H	4.821554	7.647727	0.096298
H	5.000762	5.207592	0.096514
H	4.416196	13.577223	10.846175
H	2.357551	13.302472	9.561462
H	3.304912	11.399741	10.767897
H	10.330954	8.414502	7.150450
H	9.794872	10.664522	7.936764
H	10.157361	8.861478	9.548286
H	4.531218	3.278967	8.642581
H	3.828683	3.223459	6.282823
H	6.114722	3.898639	6.870909
H	3.587544	7.367543	11.223721
H	1.901178	7.548723	11.689652
H	2.661797	5.957690	11.740801
H	-1.943160	7.153416	8.467119
H	-2.442446	5.557757	7.893739
H	-3.584222	6.354728	10.055757
H	-2.005677	6.337899	10.827613
H	-3.220077	4.320028	11.441942
H	-3.595399	3.944347	9.770850
H	-0.757889	3.886197	10.943005
H	-1.819005	2.502707	10.759676
H	-0.485767	2.343206	8.818972
H	-1.947901	3.122670	8.229991
H	-0.399048	4.349404	7.175095
H	0.178312	3.734378	5.371722
H	-1.324543	5.152398	5.559559
H	0.627240	5.643370	6.018984

$TS_{AB \rightarrow B}$

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C	2.618036	6.998178	11.037486
La	1.880660	6.454269	8.703477
O	1.152991	8.498044	7.722673
Si	2.305410	8.943292	6.716870
O	1.933478	8.905211	5.097374
Si	2.654067	9.295855	3.661957
O	3.737276	8.127731	3.214945
Si	4.838543	6.944544	3.502325
O	4.482338	6.164680	4.933723

Si	4.601998	6.599129	6.513637
O	6.114975	7.127364	6.880350
Si	6.800937	8.643011	7.035608
O	5.657726	9.682732	7.604205
Si	4.654674	10.921200	7.145785
O	4.731398	12.122407	8.254367
Si	3.789454	12.568719	9.585506
O	-0.598032	5.699626	8.792472
C	-0.226163	4.326699	8.493321
O	1.057685	4.217694	8.754552
O	3.472203	7.701211	6.977007
O	4.135013	5.317193	7.481345
Si	4.589197	3.653244	7.424038
C	-1.966790	6.115673	8.760071
C	-2.599049	5.987595	10.137450
C	-2.830726	4.552328	10.616340
C	-1.610938	3.625794	10.557950
C	-1.167208	3.288364	9.126729
O	3.099603	10.370957	7.031321
O	8.025225	8.534417	8.111729
Si	9.712947	8.535749	8.015658
O	7.388221	9.140772	5.572176
Si	7.078310	9.043868	3.945836
O	6.130039	10.312966	3.478212
Si	4.971402	11.328660	4.075655
O	5.174809	11.540468	5.703909
O	6.355709	7.595077	3.614120
O	8.485709	9.072302	3.096521
O	4.793719	5.815761	2.325031
Si	5.748890	5.432121	0.982886
O	3.453986	10.737192	3.789438
O	5.196996	12.748219	3.276550
O	1.507585	9.435139	2.504465
Si	-0.140410	9.058946	2.429706
B	0.278061	2.876201	6.465536
H	8.774843	9.952600	2.838165
H	4.529495	13.419977	3.444238
H	10.174652	7.487842	7.059549
H	10.197203	9.875510	7.574660
H	10.206402	8.235134	9.388005
H	2.530924	13.217735	9.117083
H	3.469646	11.377431	10.423082
H	4.606102	13.542181	10.363369
H	6.055741	6.662659	0.198179
H	7.013942	4.785826	1.435971
H	4.949069	4.481097	0.162546
H	-0.563596	9.356572	1.032444
H	-0.356934	7.617112	2.739039
H	-0.902468	9.911102	3.387361
H	6.010990	3.587498	6.986842
H	3.698249	2.946118	6.467541
H	4.427370	3.147626	8.811184
H	1.930099	7.699827	11.536184
H	2.675928	6.107866	11.680450
H	3.611861	7.473432	11.072278
H	0.459740	1.784196	7.103323
H	-0.689280	3.036317	5.637325
H	1.258674	3.630262	6.298765
H	-2.499881	5.536482	8.000585
H	-1.951916	7.159921	8.433266
H	-1.959155	6.522558	10.848147
H	-3.556508	6.525047	10.120975
H	-3.637849	4.103707	10.019019

H	-3.203729	4.589922	11.646299
H	-1.873822	2.687808	11.062177
H	-0.769417	4.051614	11.118273
H	-2.051001	3.142312	8.492495
H	-0.602972	2.354294	9.105254
H	-0.456685	4.218690	7.312040

B:

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C	2.748935	6.041079	10.640764
La	1.888571	5.658473	8.322757
O	1.098332	7.797463	7.612150
Si	2.229777	8.433138	6.687203
O	1.848575	8.564621	5.071112
Si	2.524256	9.197161	3.700791
O	3.670567	8.174848	3.086809
Si	4.857102	7.049603	3.258569
O	4.550417	6.084743	4.582870
Si	4.673789	6.308444	6.208794
O	6.150309	6.907845	6.616060
Si	6.730917	8.430202	6.969951
O	5.524265	9.305739	7.673577
Si	4.429508	10.511436	7.368082
O	4.415004	11.566358	8.619428
Si	3.451095	11.752022	9.996096
O	-0.662851	5.382630	8.226234
C	-0.802789	3.980866	8.559632
O	0.485273	3.634335	8.942145
O	3.460644	7.247026	6.802920
O	4.324134	4.889891	7.006121
Si	5.058184	3.334295	6.887795
C	-1.826548	6.203094	8.057185
C	-2.195528	6.899646	9.358149
C	-2.723381	5.984633	10.464953
C	-1.849339	4.767141	10.793936
C	-1.813138	3.722745	9.672212
O	2.919960	9.866413	7.169610
O	7.975980	8.255637	8.012842
Si	9.596590	8.734676	8.044648
O	7.262291	9.168901	5.587886
Si	6.948619	9.236989	3.961063
O	5.911182	10.484611	3.645827
Si	4.691657	11.327561	4.375421
O	4.896307	11.343158	6.017239
O	6.321781	7.790201	3.466641
O	8.341582	9.461099	3.117236
O	4.899435	6.077773	1.947347
Si	5.987460	5.829368	0.676098
O	3.219951	10.662129	4.017803
O	4.802412	12.851418	3.767246
O	1.350220	9.409861	2.579367
Si	-0.270305	8.944468	2.479280
B	1.361871	2.923469	7.911101
H	8.568924	10.383214	2.964708
H	4.121764	13.460876	4.067526
H	10.353748	8.046661	6.959384
H	9.699717	10.213473	7.877051
H	10.122660	8.329262	9.377262
H	2.152041	12.380696	9.618359
H	3.210493	10.433310	10.648045
H	4.204502	12.653193	10.912498
H	6.324901	7.128006	0.025774
H	7.225973	5.176767	1.189777

H	5.294973	4.931654	-0.289415
H	-0.727043	9.322117	1.112671
H	-0.402985	7.471393	2.676087
H	-1.077155	9.666794	3.505523
H	6.360943	3.517556	6.184675
H	4.159050	2.443971	6.112105
H	5.272859	2.849451	8.274792
H	2.031999	6.612166	11.252349
H	2.944637	5.103294	11.181986
H	3.688556	6.616785	10.652072
H	2.503094	3.005341	8.377687
H	1.040839	1.780785	7.697759
H	1.328637	3.587548	6.851133
H	-2.647550	5.588767	7.664864
H	-1.552257	6.939377	7.298327
H	-1.304318	7.439322	9.701598
H	-2.947280	7.666696	9.130084
H	-3.725407	5.624945	10.189107
H	-2.858672	6.585090	11.372711
H	-2.254305	4.289530	11.693325
H	-0.829491	5.078978	11.052025
H	-2.814448	3.625954	9.232328
H	-1.555294	2.734475	10.066995
H	-1.089196	3.444015	7.642206

$TS_{B\rightarrow C}$

78

C	2.189707	7.483029	11.221339
La	1.366491	6.857285	8.933364
O	1.002478	9.255338	7.630377
Si	2.459183	9.688535	7.008788
O	3.426048	8.498582	7.661991
Si	5.138812	8.358667	7.742654
O	-0.806947	7.714897	8.592618
Si	-0.694857	9.049555	7.727590
O	-1.318159	10.443452	8.382000
Si	-0.880988	12.018422	8.624451
O	-1.354207	12.969585	7.358325
Si	-1.613659	12.910946	5.725498
O	-2.779341	13.986937	5.291039
O	0.944110	4.617033	9.180850
O	-1.238562	8.932069	6.157326
Si	-1.362195	9.939515	4.852082
O	-2.303538	9.224080	3.719833
Si	-3.189014	7.786454	3.669315
O	0.122585	10.244759	4.197218
Si	1.747561	10.483503	4.167871
O	2.368054	9.990984	2.740906
Si	3.078938	10.753259	1.409213
O	-2.053137	11.375208	5.295669
O	2.480956	9.588147	5.365641
O	2.087025	12.084656	4.414710
Si	1.382121	13.422104	5.081823
O	1.988755	14.723694	4.280982
O	2.928670	11.183524	7.510888
Si	2.131477	12.562856	8.001251
O	1.772892	13.506473	6.691251
O	0.763096	12.118469	8.803937
O	3.119508	13.381901	9.012711
Si	3.942472	14.856908	8.954557
O	-1.614792	12.589216	9.971138
Si	-2.209319	11.882904	11.387582
O	-0.261177	13.390382	4.906436

H	1.382901	15.468393	4.220915
H	-3.651129	13.812498	5.657717
H	4.872868	14.880306	7.788836
H	2.969613	15.982669	8.851083
H	4.709038	14.953777	10.227517
H	-3.528802	11.243669	11.114191
H	-1.248636	10.869875	11.911522
H	-2.373895	12.992664	12.367933
H	2.188818	11.835453	0.898694
H	4.402891	11.320201	1.795785
H	3.253251	9.697195	0.373874
H	-3.834379	7.745585	2.327277
H	-2.281844	6.613887	3.836691
H	-4.229069	7.779975	4.738635
H	5.698235	9.681177	8.137588
H	5.654335	7.942484	6.412166
H	5.401580	7.332447	8.783585
H	2.293214	8.570929	11.361067
H	1.503769	7.137346	12.011227
H	3.172919	7.043786	11.455078
O	2.723981	5.264365	7.413323
C	2.300816	4.013454	7.604783
B	3.963646	4.698256	6.647878
H	3.716890	3.463821	6.761110
H	3.878872	4.954601	5.475636
H	4.975501	4.916787	7.263496
H	2.706884	3.442722	8.437278
C	1.245156	3.440117	6.695899
C	0.429137	2.254523	7.236088
C	0.666351	3.512663	9.991567
C	-0.806512	2.641168	8.068771
C	-0.613536	2.783444	9.584331
H	1.743305	3.152656	5.764042
H	0.578245	4.268091	6.430162
H	0.087997	1.688265	6.362523
H	1.079826	1.564645	7.790570
H	-1.203270	3.583000	7.672324
H	-1.591630	1.894232	7.900467
H	-1.484732	3.312025	9.990123
H	-0.603647	1.792770	10.059729
H	1.510754	2.797913	9.947458
H	0.595742	3.813771	11.048252

C :
78

C	2.683871	7.770907	11.024197
La	1.616188	6.670826	9.018616
O	1.203351	9.078233	7.609616
Si	2.666480	9.563294	7.055797
O	3.680989	8.432307	7.733513
Si	5.294130	8.574922	8.287325
O	-0.566473	7.487769	8.598063
Si	-0.479185	8.811586	7.715027
O	-1.157473	10.194956	8.340032
Si	-0.787229	11.785534	8.579675
O	-1.272876	12.709601	7.296612
Si	-1.499910	12.622977	5.660614
O	-2.697877	13.650125	5.195104
O	1.259035	4.665914	9.813074
O	-1.017757	8.653792	6.142767
Si	-1.126997	9.649830	4.828696
O	-2.008974	8.900061	3.669413
Si	-2.933205	7.488158	3.628070

O	0.366696	9.992551	4.213785
Si	1.979679	10.302261	4.198321
O	2.634047	9.816272	2.782134
Si	3.342066	10.601700	1.462845
O	-1.873280	11.067823	5.239009
O	2.741856	9.457463	5.412199
O	2.247922	11.920596	4.418672
Si	1.483265	13.235831	5.064213
O	2.056675	14.553706	4.264928
O	3.071537	11.078305	7.561041
Si	2.215412	12.434512	8.008412
O	1.836797	13.343725	6.679751
O	0.845840	11.962169	8.794740
O	3.177922	13.295883	9.009658
Si	3.487241	14.937244	9.263972
O	-1.570813	12.334948	9.908091
Si	-2.248732	11.591800	11.267237
O	-0.154071	13.144352	4.855777
H	1.419617	15.269009	4.177110
H	-3.562149	13.463718	5.573477
H	4.378936	15.453962	8.185986
H	2.210969	15.710044	9.280291
H	4.167060	15.036717	10.585174
H	-3.516269	10.903075	10.887884
H	-1.292844	10.614775	11.862704
H	-2.535905	12.687302	12.235685
H	2.407067	11.620425	0.904300
H	4.617593	11.252047	1.879826
H	3.612742	9.542584	0.450938
H	-3.558113	7.440845	2.276383
H	-2.060579	6.294062	3.826661
H	-3.989970	7.523089	4.680318
H	5.364072	9.523260	9.428412
H	6.150195	9.037302	7.158055
H	5.681787	7.198757	8.704123
H	2.775431	8.865634	10.950922
H	2.084042	7.570030	11.926335
H	3.691827	7.383488	11.247719
O	2.640682	5.137501	6.814321
C	2.065634	3.807791	6.974507
B	3.491668	5.404327	5.789502
H	2.687220	3.098553	6.419230
H	3.790370	4.528805	5.027484
H	3.906304	6.518604	5.709813
H	2.131237	3.598045	8.040117
C	0.618085	3.788413	6.496395
C	-0.284734	2.779104	7.236386
C	0.937098	3.359658	10.164234
C	-1.033540	3.350999	8.464967
C	-0.516737	2.987139	9.861900
H	0.608302	3.592156	5.417390
H	0.192412	4.792336	6.619483
H	-1.028121	2.419505	6.517058
H	0.296723	1.889713	7.517565
H	-1.078601	4.443378	8.381974
H	-2.077050	3.016683	8.417006
H	-1.166642	3.486999	10.591735
H	-0.630733	1.906922	10.034182
H	1.599720	2.646371	9.634765
H	1.126827	3.191007	11.236367

$(BH_4)(NMe_2)$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

A :
83

N	3.020682	5.516591	10.139539
La	1.842989	5.435180	8.171527
O	3.546355	7.240197	6.922493
Si	4.990334	6.780870	6.234627
O	6.224835	7.736250	6.765814
Si	6.561837	9.263013	7.303792
O	5.223266	9.897357	8.034481
Si	3.883213	10.790736	7.672433
O	3.488596	11.694504	8.983975
Si	2.144117	11.795978	9.991912
O	1.044685	7.543246	7.424824
Si	2.232948	8.304593	6.672851
O	2.039086	8.479840	5.030417
Si	2.503611	9.434547	3.766052
O	2.826521	10.972943	4.277630
Si	4.112472	11.893947	4.772125
O	3.920751	13.449350	4.271330
O	5.206019	5.236923	6.732220
Si	5.921567	3.847568	6.067003
O	-0.003276	3.966418	9.578934
C	-0.967571	4.715493	9.587711
C	-2.286765	4.397210	10.225600
C	-2.669959	5.349982	11.374480
C	-3.209700	6.707006	10.921220
C	-2.232696	7.553745	10.103917
C	-1.777471	6.928879	8.798008
O	-0.769018	5.900804	8.985438
O	2.619116	9.797720	7.295562
O	4.209134	11.823625	6.423841
O	5.516701	11.374435	4.082936
Si	6.786321	10.363408	4.410750
O	8.183639	10.984761	3.807625
O	7.032546	10.217821	6.035342
O	6.466908	8.884895	3.736940
Si	5.196535	7.908154	3.343845
O	3.842730	8.804424	3.024920
O	7.771799	9.184737	8.400194
Si	9.366862	9.738768	8.458181
O	4.893607	6.855496	4.586902
O	5.618868	7.060839	2.009623
Si	4.784610	6.266193	0.774981
O	1.286945	9.502238	2.668094
Si	-0.226665	8.764850	2.556126
B	1.925098	3.426142	6.342288
H	8.143108	11.252592	2.884825
H	3.078131	13.848806	4.505792
H	-0.802339	9.195316	1.250705
H	-0.094079	7.280027	2.594421
H	-1.109232	9.222013	3.670537
H	3.485937	5.731872	1.277467
H	4.542817	7.218938	-0.347254
H	5.658758	5.151014	0.314855
H	2.463285	12.825799	11.020127
H	0.939104	12.214275	9.215068
H	1.877924	10.484343	10.652558
H	10.154525	9.168254	7.327359
H	9.397531	11.228614	8.400869

H	9.920346	9.264718	9.757753
H	5.898754	2.815656	7.137677
H	5.163939	3.398262	4.868895
H	7.332242	4.165098	5.692171
C	3.498006	4.343398	10.837815
H	-1.248210	7.644220	8.166795
H	-2.610194	6.495559	8.231794
H	-2.713144	8.506043	9.847961
H	-1.344250	7.809531	10.695008
H	-3.517665	7.275524	11.806094
H	-4.122329	6.546101	10.329832
H	-1.807013	5.483575	12.038779
H	-3.437916	4.846016	11.970699
H	-2.199982	3.370158	10.584833
H	-3.066601	4.411355	9.452058
H	0.792558	3.565898	6.836853
H	1.945043	2.518477	5.554083
H	2.229043	4.502408	5.808761
H	2.716425	3.215250	7.275480
H	3.123417	4.289335	11.876365
H	3.167547	3.424698	10.332858
H	4.600467	4.303099	10.893336
C	3.456196	6.734111	10.785956
H	3.084119	6.817927	11.824083
H	4.556340	6.820127	10.835772
H	3.092507	7.618170	10.243661

$TS_{A \rightarrow AB}$

83

N	3.067177	6.654004	10.924900
La	2.128607	6.286761	8.871164
O	3.582272	7.828349	7.184324
Si	4.744417	6.850799	6.560336
O	6.249371	7.435990	6.872723
Si	6.868702	8.965060	7.112696
O	5.730528	9.884355	7.873734
Si	4.621104	11.080704	7.595907
O	4.725900	12.182927	8.802730
Si	3.631522	12.851345	9.900795
O	1.302262	8.414622	8.206068
Si	2.347338	9.017718	7.163545
O	1.822843	9.134276	5.589098
Si	2.404438	9.669325	4.138542
O	3.143082	11.136460	4.325583
Si	4.649577	11.784864	4.549873
O	4.726415	13.289987	3.891681
O	4.441677	5.452668	7.424099
Si	5.084845	3.866125	7.270438
O	1.044576	4.118130	9.206958
C	-0.099657	4.330601	8.660902
C	-1.207213	3.284032	8.809606
C	-2.168975	3.560141	9.974285
C	-3.286995	4.551701	9.627770
C	-2.842242	5.998465	9.397402
C	-1.717663	6.175306	8.388788
O	-0.483379	5.673293	8.923230
O	3.091449	10.452922	7.560179
O	4.979451	11.839219	6.170283
O	5.790833	10.896681	3.754429
Si	6.865157	9.678999	4.068782
O	8.266222	9.922114	3.245405
O	7.286111	9.642720	5.664189
O	6.173043	8.239539	3.625106

Si	4.702900	7.493270	3.579781
O	3.479786	8.593479	3.487944
O	8.194504	8.814391	8.053609
Si	9.786463	9.382125	7.987157
O	4.540190	6.563340	4.955108
O	4.665913	6.498934	2.284585
Si	3.479326	5.994614	1.189924
O	1.156467	9.826479	3.089573
Si	-0.524685	9.815912	3.257335
B	0.734422	4.769584	6.265350
H	8.157119	10.180794	2.325511
H	4.073321	13.913337	4.222703
H	-1.073677	10.220838	1.932506
H	-1.000124	8.448513	3.613087
H	-0.948782	10.791489	4.303952
H	2.193226	5.737277	1.898417
H	3.289131	7.042088	0.145430
H	3.990426	4.740858	0.569152
H	4.403162	13.840843	10.703915
H	2.525593	13.540006	9.172129
H	3.070769	11.793506	10.788896
H	10.514103	8.720837	6.866340
H	9.800078	10.862131	7.804718
H	10.408065	9.017343	9.290619
H	4.414063	3.076300	8.335979
H	4.775222	3.336583	5.916535
H	6.555984	3.931848	7.492509
C	3.456225	5.554414	11.783269
H	-1.533496	7.232928	8.184743
H	-1.926642	5.679601	7.431976
H	-3.701043	6.591645	9.057334
H	-2.511528	6.445454	10.343390
H	-4.033343	4.543362	10.431338
H	-3.805379	4.186822	8.729402
H	-1.606948	3.898425	10.853298
H	-2.632122	2.606915	10.255026
H	-0.678002	2.337779	8.950910
H	-1.777842	3.196337	7.878394
H	0.015623	4.335298	7.346990
H	0.121228	4.296724	5.345318
H	0.658296	5.973961	6.388526
H	1.799632	4.262220	6.541047
H	2.916591	5.561624	12.747184
H	3.237274	4.586125	11.309457
H	4.535190	5.564586	12.021136
C	3.321877	7.932203	11.554463
H	2.783054	8.040736	12.513005
H	4.393500	8.088633	11.771655
H	2.996695	8.755858	10.906636

AB :

83			
N	2.740916	6.800779	10.971965
La	1.993285	6.503399	8.829954
O	3.538537	7.937635	7.166017
Si	4.666506	6.899916	6.570866
O	6.184713	7.427135	6.920313
Si	6.852961	8.935032	7.165702
O	5.718730	9.912262	7.857897
Si	4.671307	11.148678	7.519145
O	4.774184	12.263062	8.715154
Si	3.664588	12.982880	9.764410
O	1.229213	8.627511	8.045012

Si	2.341528	9.164347	7.039172
O	1.908326	9.240174	5.435270
Si	2.544092	9.750337	3.998943
O	3.329566	11.190876	4.199614
Si	4.848322	11.791725	4.468444
O	5.002840	13.277539	3.780801
O	4.270054	5.527282	7.434725
Si	4.769971	3.893659	7.217758
O	1.227859	4.236257	8.637514
C	-0.036664	4.339333	8.330049
C	-0.957220	3.171527	8.704379
C	-1.560216	3.266851	10.112650
C	-2.830436	4.124330	10.179607
C	-2.629851	5.624652	9.952035
C	-1.868471	5.987765	8.686100
O	-0.486926	5.623811	8.806832
O	3.118887	10.584560	7.429872
O	5.116912	11.870649	6.099239
O	5.990326	10.847886	3.740501
Si	7.000167	9.593692	4.118611
O	8.436972	9.762522	3.339558
O	7.364919	9.571078	5.728272
O	6.263818	8.174123	3.682328
Si	4.768097	7.487998	3.574247
O	3.599916	8.634249	3.381976
O	8.126596	8.747776	8.170089
Si	9.735366	9.270434	8.180789
O	4.489522	6.606577	4.963118
O	4.754879	6.455134	2.309005
Si	3.648505	6.060447	1.092195
O	1.331992	9.945585	2.915750
Si	-0.354187	9.965779	3.039437
B	0.127068	4.970436	5.838953
H	8.370218	10.030789	2.418375
H	4.340379	13.920951	4.048883
H	-0.858527	10.365282	1.695261
H	-0.861716	8.611493	3.398448
H	-0.785998	10.962901	4.062104
H	2.288340	5.864734	1.670279
H	3.619514	7.145561	0.069380
H	4.139459	4.794062	0.481091
H	4.441853	13.950161	10.588890
H	2.613838	13.704976	8.988321
H	3.031142	11.955204	10.639266
H	10.503509	8.568466	7.113022
H	9.800865	10.745857	7.974108
H	10.275077	8.913082	9.522256
H	4.670616	3.261807	8.559052
H	3.872554	3.239536	6.231839
H	6.179216	3.907540	6.734216
C	2.990167	5.708721	11.888856
H	-1.876959	7.068951	8.522455
H	-2.290535	5.514601	7.790921
H	-3.608734	6.120417	9.916337
H	-2.090540	6.064648	10.800751
H	-3.306516	3.984096	11.157762
H	-3.545455	3.740455	9.437698
H	-0.805770	3.633936	10.819253
H	-1.816065	2.251938	10.438725
H	-0.330042	2.281056	8.604541
H	-1.764355	3.075460	7.968101
H	-0.199722	4.415609	7.125822
H	-0.965838	5.350198	5.513126

H	0.917380	5.811567	6.204705
H	0.573684	3.964245	5.360361
H	2.359676	5.765538	12.794701
H	2.777882	4.740645	11.413106
H	4.039314	5.678301	12.233995
C	3.000202	8.083638	11.590665
H	2.372870	8.253962	12.484297
H	4.050974	8.191383	11.913557
H	2.790623	8.903247	10.890501

$TS_{AB \rightarrow B}$

83

N	2.175973	6.699032	10.862434
La	1.706618	6.208987	8.663411
O	1.060234	8.804365	7.649930
Si	2.165311	9.963283	7.023258
O	-0.126693	4.660523	8.474250
Si	-1.406449	5.517830	8.077738
O	-2.687544	5.549681	9.143475
Si	-3.652012	6.673545	9.877035
O	-5.052661	6.884787	9.019809
Si	-5.613636	6.832843	7.464441
O	-7.193521	6.375123	7.432251
O	3.452169	4.473895	7.873380
C	4.024330	3.182745	8.073057
C	4.922096	3.161130	9.303481
C	6.233524	3.938316	9.162556
C	6.095137	5.380750	8.659699
C	5.637677	5.478628	7.200417
C	4.120420	5.449024	6.977274
O	3.497239	6.618515	7.233057
O	-0.779207	7.116119	8.080629
Si	-0.587237	8.634318	7.481738
O	-1.418681	9.726864	8.389493
Si	-2.782525	9.630681	9.341644
O	-4.132041	9.936968	8.434929
Si	-4.739106	9.755931	6.904247
O	-5.734519	11.012156	6.536351
O	-2.023728	5.255746	6.552155
Si	-3.324760	5.737384	5.655451
O	-3.557251	4.672624	4.433814
Si	-2.731307	3.297578	3.902401
O	-3.073622	7.238671	5.007242
Si	-2.442149	8.754935	5.062944
O	-2.131007	9.286186	3.550102
Si	-2.760993	10.493744	2.548603
O	-4.690865	5.778080	6.586909
O	-0.997075	8.750193	5.891703
O	-3.490968	9.785635	5.820842
O	-2.867679	8.125536	10.011497
O	-2.640095	10.761034	10.513055
Si	-3.669430	11.914145	11.196223
O	-4.045302	6.156589	11.381100
Si	-3.781576	4.731347	12.247102
O	-5.593754	8.344717	6.796822
B	2.630446	5.949215	4.124277
H	-6.669726	10.814451	6.643946
H	-7.355482	5.457329	7.669363
H	-3.930605	13.005976	10.214706
H	-4.956717	11.281285	11.606754
H	-2.957975	12.452656	12.388552
H	-4.336503	3.563044	11.502330
H	-2.324141	4.531722	12.489670

H	-4.499172	4.895388	13.542502
H	-4.231274	10.309498	2.379414
H	-2.478129	11.837293	3.130614
H	-2.069162	10.344732	1.238113
H	-3.480997	2.801511	2.714073
H	-1.333944	3.647539	3.516067
H	-2.719501	2.257045	4.970895
H	1.489680	11.292617	7.041806
H	2.542562	9.584497	5.638263
H	3.331792	9.950067	7.942396
C	1.317051	6.277576	11.948786
C	3.317729	7.437782	11.353199
H	2.774745	7.127333	4.005034
H	3.388327	5.196646	3.585662
H	1.695059	5.514391	4.729545
H	4.564349	2.878527	7.166329
H	3.185561	2.490179	8.200415
H	4.338578	3.562613	10.142662
H	5.143288	2.114710	9.552514
H	6.900576	3.395920	8.476803
H	6.739272	3.941171	10.136010
H	7.072628	5.868487	8.752839
H	5.412431	5.947804	9.304956
H	6.117909	4.683225	6.614480
H	5.963310	6.424813	6.755369
H	3.920941	5.069989	5.948656
H	3.024650	8.347594	11.908480
H	3.949303	6.841452	12.037449
H	3.960192	7.762084	10.522951
H	0.915714	7.129577	12.526794
H	0.453198	5.711942	11.570884
H	1.836988	5.621281	12.670819

B:

83

N	2.448317	7.196969	10.225980
La	2.047167	6.665438	8.036640
O	0.944790	9.267905	7.159102
Si	1.759168	10.621744	6.482610
O	0.352705	4.989045	8.046268
Si	-1.053159	5.704966	7.815000
O	-2.194095	5.570114	9.020198
Si	-3.196854	6.566136	9.879136
O	-4.700320	6.610119	9.188203
Si	-5.425033	6.501241	7.704723
O	-6.933261	5.859130	7.842364
O	3.374444	4.507731	7.530343
C	3.250072	3.100851	7.767532
C	3.592539	2.757632	9.210788
C	5.067696	2.904114	9.586378
C	5.700857	4.260205	9.249777
C	5.849446	4.502270	7.743362
C	4.617373	5.059967	7.039093
O	4.463008	6.419645	7.274748
O	-0.595711	7.350974	7.771715
Si	-0.670947	8.883349	7.182193
O	-1.534070	9.858998	8.188691
Si	-2.752103	9.603407	9.295923
O	-4.225369	9.755414	8.557570
Si	-4.965810	9.509608	7.094821
O	-6.127764	10.645466	6.842649
O	-1.801995	5.374219	6.364326
Si	-3.248433	5.690995	5.629526

O	-3.488385	4.599055	4.433305
Si	-2.519037	3.413049	3.720130
O	-3.257284	7.210384	4.976756
Si	-2.794092	8.788757	4.990296
O	-2.718439	9.363117	3.463292
Si	-3.671378	10.401863	2.529077
O	-4.492400	5.563560	6.711142
O	-1.272929	8.937891	5.649279
O	-3.859660	9.688279	5.881247
O	-2.578292	8.098913	9.947811
O	-2.611584	10.731057	10.470332
Si	-3.580470	11.991596	11.042413
O	-3.348967	5.999522	11.408523
Si	-2.905316	4.574683	12.196720
O	-5.656609	8.007918	7.067029
B	4.006772	7.293090	6.105175
H	-6.997639	10.402355	7.173451
H	-6.958117	4.918519	8.040780
H	-3.826123	12.984397	9.956663
H	-4.879442	11.455685	11.543265
H	-2.821843	12.624465	12.156682
H	-3.491284	3.392918	11.497568
H	-1.420665	4.447047	12.245037
H	-3.457347	4.673316	13.576875
H	-5.101418	9.982804	2.587789
H	-3.528294	11.801119	3.023975
H	-3.157838	10.293206	1.135399
H	-3.316026	2.850136	2.594312
H	-1.254557	4.013450	3.204630
H	-2.206423	2.341868	4.710309
H	0.789415	11.754586	6.440872
H	2.223687	10.277301	5.114659
H	2.892164	10.934952	7.391116
C	1.723062	6.709591	11.379065
C	3.511298	8.101703	10.608526
H	3.588868	8.323869	6.655255
H	4.879746	7.553068	5.314615
H	3.045718	6.732683	5.546392
H	3.876152	2.553255	7.050846
H	2.203651	2.866147	7.557230
H	2.976277	3.398729	9.854166
H	3.266826	1.726520	9.401358
H	5.648974	2.116043	9.085650
H	5.169833	2.716310	10.662186
H	6.697852	4.294783	9.703760
H	5.128625	5.076997	9.707037
H	6.151586	3.568395	7.251452
H	6.645726	5.226120	7.540261
H	4.667690	4.862595	5.957132
H	3.134395	9.000081	11.129529
H	4.248077	7.628190	11.282502
H	4.068635	8.450111	9.726850
H	1.238932	7.523219	11.948055
H	0.932016	6.011364	11.075710
H	2.376362	6.170766	12.089764

$TS_{B\rightarrow C}$

83

N	2.072862	12.500651	7.847084
La	0.063015	12.532489	6.737796
Si	-2.494139	11.606508	8.519943
O	-2.596512	11.048485	10.083911
Si	-2.633999	11.665368	11.617478

O	-1.810962	13.101201	11.679645
Si	-2.067501	14.730422	11.740293
O	-1.776079	15.378596	10.234661
Si	-1.973229	14.834092	8.692169
O	-3.376899	15.401548	8.046063
Si	-4.969503	15.405838	8.527718
O	-5.614971	13.900915	8.381278
Si	-5.522289	12.251554	8.427368
O	-6.675873	11.629594	7.445873
Si	-6.638165	10.713205	6.027619
O	-3.618137	15.053132	12.216298
Si	-5.148381	15.299051	11.630680
O	-5.994492	13.877985	11.656521
Si	-5.699631	12.255830	11.537950
O	-6.859229	11.544214	12.462322
O	-1.016340	15.425531	12.781339
Si	-1.135921	16.107169	14.323150
O	-4.191521	11.903518	12.119400
O	-5.814580	11.737955	9.971831
O	-1.925926	10.603439	12.644280
Si	-1.094393	9.146944	12.442862
O	-5.938246	16.407659	12.553281
O	-5.051403	15.914970	10.100663
O	-5.779138	16.445858	7.563725
Si	-6.670357	17.861173	7.808892
O	-4.040948	11.728707	7.913960
O	-1.439062	10.900550	7.554426
O	-0.689724	15.269192	7.728111
Si	0.081991	16.781740	7.486613
O	-0.557633	13.973087	4.685346
C	-0.240653	13.321379	3.559172
C	-1.289163	12.503776	2.848629
C	-0.777891	11.395323	1.913085
C	-0.493577	10.045189	2.596156
C	0.928533	9.811356	3.123252
C	1.528614	11.010611	3.858681
O	0.594313	11.669238	4.660138
O	-1.878773	13.197245	8.612842
B	-0.722895	15.268070	3.841642
C	3.192017	13.307391	7.418257
H	-2.010800	8.104159	11.896340
H	0.068302	9.331688	11.527760
H	-0.425526	14.785934	2.706683
H	-1.879911	15.589025	3.775144
H	0.133229	16.071247	4.113962
H	0.787188	13.356016	3.204329
H	-6.525007	16.022753	13.211175
H	-6.901590	10.585793	12.395698
H	-1.855594	17.411072	14.247019
H	-1.857231	15.181163	15.243913
H	0.261096	16.317380	14.794507
H	-0.621940	8.750129	13.798966
H	-7.827769	17.590275	8.709473
H	-5.800114	18.917816	8.401043
H	-7.151673	18.283935	6.464521
H	-8.054044	10.577569	5.584544
H	-5.838339	11.411061	4.979067
H	-6.055239	9.367071	6.297973
H	0.405685	17.367419	8.817588
H	-0.822069	17.681099	6.721881
H	1.321885	16.477208	6.726375
C	2.412025	11.678328	8.987355
H	-1.924101	13.198125	2.288570

H	-1.930753	12.074671	3.626079
H	-1.557630	11.239130	1.159429
H	0.099010	11.746235	1.351755
H	-1.200650	9.928489	3.425300
H	-0.725162	9.238427	1.890155
H	0.903008	8.942725	3.792714
H	1.601147	9.544762	2.296043
H	1.941049	11.713717	3.107856
H	2.394201	10.680793	4.454760
H	2.704796	12.276061	9.869292
H	1.556592	11.058899	9.289674
H	3.250196	10.989270	8.776935
H	3.540399	14.006320	8.200567
H	4.067129	12.701769	7.119845
H	2.923337	13.922488	6.544290

C :

83

N	1.790017	11.949422	7.464340
La	-0.163423	11.504472	6.309002
Si	-2.686334	11.507958	8.512794
O	-2.574296	11.212649	10.146322
Si	-2.408408	11.859769	11.650023
O	-1.667333	13.339043	11.561522
Si	-2.075927	14.925820	11.368084
O	-2.098996	15.298205	9.752113
Si	-2.394128	14.624845	8.272893
O	-3.974144	14.825338	7.851957
Si	-5.459938	15.004357	8.562023
O	-6.186733	13.533306	8.729344
Si	-5.768021	11.935303	8.868701
O	-6.914008	11.024959	8.132376
Si	-6.896720	9.975587	6.808361
O	-3.553043	15.229132	12.047250
Si	-5.157712	15.294253	11.634693
O	-5.868387	13.831455	11.933019
Si	-5.474867	12.225870	11.949692
O	-6.463186	11.556591	13.082193
O	-0.941639	15.878166	12.063399
Si	-0.734215	16.572746	13.589069
O	-3.887104	12.030313	12.373886
O	-5.731142	11.527232	10.472344
O	-1.485795	10.879299	12.583145
Si	-0.721148	9.395234	12.322736
O	-5.927545	16.454742	12.510168
O	-5.289094	15.722312	10.044711
O	-6.357927	15.964951	7.589083
Si	-7.573468	17.111390	7.838939
O	-4.305034	11.674285	8.153491
O	-1.879312	10.500479	7.582632
O	-1.439856	15.426673	7.175073
Si	-0.758311	16.979595	7.350390
O	-0.336672	13.746063	4.828478
C	0.807817	14.418710	4.238092
C	0.979508	14.113271	2.757748
C	1.249060	12.641702	2.409489
C	-0.017650	11.793817	2.250467
C	0.219307	10.283040	2.203343
C	0.948404	9.739264	3.441845
O	0.432751	10.248480	4.628339
O	-1.961127	13.034176	8.198491
B	-1.566636	14.342413	4.850395
C	3.124014	11.611559	7.018422

H	-1.731556	8.344670	12.003434
H	0.268285	9.505347	11.213463
H	0.683208	15.493920	4.399606
H	-2.459600	13.664315	5.269590
H	-1.731778	15.413418	4.348507
H	1.676285	14.079530	4.811768
H	-6.323042	16.133747	13.326141
H	-6.459235	10.595226	13.106592
H	-1.591101	17.787573	13.708823
H	-1.085878	15.595893	14.660729
H	0.703720	16.949034	13.687899
H	-0.027562	9.060980	13.598575
H	-8.515605	16.652428	8.900257
H	-6.960964	18.413893	8.229622
H	-8.289944	17.253591	6.540410
H	-8.305951	9.530490	6.617175
H	-6.416990	10.685871	5.586937
H	-6.022302	8.801169	7.090826
H	0.381564	16.928555	8.306304
H	-1.792610	17.948173	7.809730
H	-0.271987	17.355543	5.992546
C	1.811032	12.465828	8.815936
H	1.826509	14.732417	2.433394
H	0.104911	14.485839	2.207531
H	1.828248	12.594744	1.478746
H	1.894954	12.209417	3.184398
H	-0.699186	12.000852	3.081617
H	-0.547706	12.110482	1.342113
H	-0.755109	9.786546	2.111707
H	0.796642	10.009377	1.308828
H	2.023505	9.980425	3.360955
H	0.885169	8.639124	3.429790
H	2.412112	13.389778	8.905748
H	0.797506	12.713521	9.160084
H	2.231913	11.746770	9.542788
H	3.800113	12.487260	7.002598
H	3.609247	10.855906	7.663713
H	3.102643	11.197027	6.001880

4.3 (BH_4)La@**ac**-1 as catalyst form

(BH_4)La@**ac**-1

56

O	4.655671	-0.425772	5.578244
Si	4.649397	-1.526623	4.345437
O	4.148574	-3.013568	4.866635
O	9.389315	0.418702	7.316336
O	2.766093	-5.058230	5.849432
Si	2.477532	-6.708301	5.642222
O	5.430620	-5.193302	5.984021
Si	7.017794	-4.704035	6.088974
O	7.514277	-4.594390	7.684071
Si	7.685497	-3.205544	8.573235
O	6.222599	-2.617841	9.055535
Si	4.616854	-2.437258	8.717049
O	4.067856	-3.476492	7.559568
Si	4.123211	-4.161150	6.056248
Si	8.204084	-0.638358	6.902063
H	10.843833	2.470983	7.689464
Si	9.407833	2.070952	7.674836
O	6.738983	-0.031162	7.350390
Si	5.111805	0.059228	7.088026
O	4.342208	-0.884190	8.210707

O	3.585961	-1.008491	3.209726
Si	3.709561	-0.677856	1.559226
O	6.162149	-1.565603	3.645669
Si	7.543967	-2.103674	4.400593
O	8.283668	-0.873169	5.262659
O	6.974152	-3.102698	5.612360
O	8.048548	-5.593402	5.211699
La	9.669151	-4.764290	3.890997
N	10.878125	-3.612987	5.978167
O	8.545534	-2.062072	7.708092
O	8.598082	-3.561810	9.889562
Si	8.260729	-3.831727	11.523568
O	3.832093	-2.726584	10.134162
O	4.710366	1.641882	7.293125
O	8.598102	-2.843931	3.419241
B	11.457803	-6.091668	2.378624
H	4.610603	0.488820	1.329222
H	3.852905	1.885368	6.931933
H	2.878369	-2.819511	10.052334
H	0.998724	-6.859097	5.534716
H	3.131661	-7.199154	4.394370
H	2.982940	-7.478741	6.815885
H	4.226050	-1.869382	0.824539
H	2.330292	-0.353037	1.097598
H	7.875781	-2.551745	12.184233
H	7.168638	-4.835959	11.673602
H	9.522510	-4.354303	12.121313
H	8.671773	2.840514	6.631016
H	8.798136	2.309524	9.014252
H	10.177550	-3.123262	6.543846
H	11.347534	-4.256272	6.613391
H	11.570082	-2.909187	5.725704
H	12.253469	-6.680185	1.704458
H	10.586313	-6.856741	2.828581
H	11.995737	-5.536713	3.362156
H	10.884162	-5.197622	1.730946

A :
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C	4.672751	-0.532267	5.594531
O	4.881902	-1.466872	4.498168
La	4.452442	-4.202265	4.155357
O	3.150360	-6.012350	3.649941
Si	1.549463	-6.140241	3.715206
O	0.860475	-5.835273	2.206959
Si	-0.519240	-4.941974	1.969049
O	-0.348118	-3.402915	2.577495
Si	-0.806482	-2.516426	3.910104
O	-1.090561	-0.982865	3.384393
Si	-2.469782	-0.012718	3.349306
C	4.191655	0.827198	5.125610
C	5.278128	1.723629	4.531045
C	5.970609	1.163438	3.287964
C	6.728624	-0.158955	3.512294
C	5.851147	-1.372350	3.577168
O	5.939463	-2.328685	2.815958
N	3.097799	-3.492909	1.879341
O	2.870602	-3.422428	5.599528
Si	1.287537	-3.722351	5.637872
O	0.793126	-4.987932	4.665170
O	0.410280	-2.426575	5.028560
O	0.704238	-4.155629	7.141791
Si	-0.487465	-5.290952	7.391084

O	-0.119892	-6.769877	6.747067
Si	-0.259209	-7.762670	5.429712
O	-0.230061	-9.314767	5.965099
Si	0.903856	-10.558030	5.847194
O	-2.195706	-3.112219	4.574271
Si	-2.914378	-4.186340	5.598909
O	-4.190927	-3.378581	6.256181
O	-1.925629	-4.724724	6.803790
O	-3.454611	-5.488492	4.729300
Si	-2.662861	-6.556199	3.740931
O	-3.751508	-7.488299	2.928475
O	-0.654047	-5.484275	9.014526
Si	0.197365	-4.889635	10.341793
O	0.981710	-7.578753	4.338760
O	-1.710773	-7.535477	4.667231
O	-1.840727	-5.705193	2.592724
O	-0.710635	-4.774215	0.343815
Si	-1.771225	-5.462106	-0.774496
H	-4.018907	-8.278936	3.406427
H	-4.600013	-3.829175	7.000908
H	-0.401954	-5.536151	11.544346
H	1.644598	-5.239625	10.245771
H	0.043866	-3.407761	10.441973
H	2.242479	-10.101407	6.321475
H	0.403613	-11.658981	6.719607
H	1.002452	-11.039123	4.437908
H	-3.563312	-0.673857	2.579761
H	-2.932178	0.292212	4.734092
H	-2.064476	1.249761	2.664665
H	-1.739761	-6.950595	-0.685077
H	-3.158848	-4.965831	-0.546096
H	-1.292098	-5.024391	-2.117586
H	3.915023	-1.046445	6.186691
H	5.599228	-0.473415	6.176221
H	3.754605	1.324903	5.999693
H	3.366822	0.681059	4.416952
H	4.838131	2.694958	4.278825
H	6.036891	1.923892	5.300519
H	5.246331	1.035552	2.473413
H	6.701790	1.896154	2.930777
H	7.433778	-0.347444	2.700593
H	7.310991	-0.105998	4.442570
H	2.261544	-2.940577	2.064461
H	3.604856	-3.021502	1.135175
H	2.749324	-4.376339	1.506813
B	6.736751	-4.886438	5.423545
H	7.753466	-5.199045	5.979500
H	6.449744	-3.694705	5.638451
H	6.836553	-5.031682	4.192597
H	5.774843	-5.569309	5.807669

$TS_{A \rightarrow AB}$

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C	6.392373	-1.293490	6.095967
O	5.562661	-1.618555	4.968164
La	3.678587	-3.233926	4.003300
O	2.883094	-5.337306	3.621109
Si	1.351091	-5.812597	3.771037
O	0.574496	-5.906099	2.286719
Si	-0.896546	-5.250645	1.900676
O	-0.971593	-3.648852	2.366942
Si	-1.700478	-2.766751	3.583357
O	-2.281731	-1.401290	2.879774

Si	-3.749483	-0.571605	2.960886
C	6.253585	0.175972	6.464573
C	6.914207	1.154551	5.490952
C	6.524233	0.984337	4.018443
C	7.028146	-0.327532	3.399372
C	6.096408	-1.517652	3.635565
O	5.132800	-1.714068	2.792758
N	2.092232	-2.534547	1.977775
O	2.016727	-2.670778	5.438390
Si	0.532665	-3.308039	5.472266
O	0.385560	-4.728051	4.604596
O	-0.588465	-2.311066	4.723782
O	0.017632	-3.733198	7.001561
Si	-0.964246	-5.031879	7.347800
O	-0.346449	-6.472897	6.826241
Si	-0.132517	-7.583722	5.620145
O	0.170007	-9.031729	6.333826
Si	1.456892	-10.117401	6.238083
O	-2.951893	-3.604588	4.258119
Si	-3.480967	-4.645370	5.422946
O	-4.937407	-4.055880	5.916358
O	-2.470057	-4.753136	6.723267
O	-3.665719	-6.153335	4.764004
Si	-2.691817	-7.068989	3.785806
O	-3.565246	-8.270120	3.073696
O	-1.106518	-5.124199	8.982021
Si	-0.527429	-4.177925	10.250201
O	1.153587	-7.232501	4.626102
O	-1.499646	-7.748510	4.702742
O	-2.134136	-6.123609	2.554994
O	-1.037519	-5.250987	0.263992
Si	-1.732118	-6.310302	-0.852066
H	-3.715779	-9.034111	3.638137
H	-5.284945	-4.472242	6.710564
H	-1.045883	-4.798020	11.503017
H	0.965276	-4.178103	10.268533
H	-1.027957	-2.776442	10.136209
H	2.727453	-9.466936	6.673412
H	1.121620	-11.239246	7.161192
H	1.605649	-10.635955	4.846740
H	-4.839048	-1.385175	2.348710
H	-4.090242	-0.243752	4.375608
H	-3.555134	0.684734	2.181374
H	-1.342172	-7.719226	-0.554964
H	-3.216969	-6.175925	-0.829598
H	-1.206432	-5.907747	-2.188220
H	6.038572	-1.927215	6.914465
H	7.428644	-1.580636	5.880439
H	6.682799	0.315816	7.465047
H	5.181973	0.394480	6.553768
H	6.673405	2.175471	5.810438
H	8.006497	1.061561	5.573141
H	5.437615	1.064198	3.891962
H	6.959862	1.813489	3.449379
H	7.100520	-0.248122	2.311240
H	8.035425	-0.548011	3.770634
H	1.122098	-2.835711	2.097470
H	2.070821	-1.527662	1.830220
H	2.408214	-2.944352	1.100823
B	7.146123	-3.841071	3.717104
H	8.046286	-3.861200	4.511681
H	6.926938	-2.470267	3.602512
H	7.342097	-4.086931	2.560112

H	6.072375	-4.212686	4.170664

AB :

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C	6.405758	-1.328828	6.086900
O	5.584747	-1.666200	4.956490
La	3.682052	-3.238130	3.987629
O	2.884874	-5.343757	3.615759
Si	1.352029	-5.814450	3.770989
O	0.571430	-5.911342	2.288928
Si	-0.898377	-5.253133	1.903181
O	-0.968856	-3.649720	2.364875
Si	-1.694466	-2.762618	3.579681
O	-2.273544	-1.397955	2.872710
Si	-3.739100	-0.564364	2.953730
C	6.230743	0.133765	6.467614
C	6.871351	1.136354	5.505174
C	6.489641	0.970941	4.029990
C	7.021438	-0.325655	3.402178
C	6.109956	-1.534441	3.620450
O	5.139698	-1.723270	2.781088
N	2.089687	-2.534427	1.968589
O	2.026222	-2.666592	5.427489
Si	0.541601	-3.302104	5.466296
O	0.391274	-4.724211	4.602684
O	-0.580100	-2.305996	4.717357
O	0.028966	-3.722305	6.997787
Si	-0.956287	-5.016927	7.349470
O	-0.344317	-6.461212	6.830286
Si	-0.133084	-7.576440	5.627859
O	0.167471	-9.022388	6.346494
Si	1.448561	-10.114611	6.247894
O	-2.946841	-3.595918	4.258212
Si	-3.475409	-4.631253	5.428164
O	-4.930216	-4.037761	5.921580
O	-2.462490	-4.734827	6.727264
O	-3.663170	-6.141589	4.775568
Si	-2.694163	-7.061673	3.796636
O	-3.572424	-8.262167	3.089421
O	-1.095464	-5.104532	8.984216
Si	-0.512492	-4.155345	10.248448
O	1.152798	-7.230777	4.631639
O	-1.501079	-7.741972	4.711808
O	-2.137394	-6.120592	2.562121
O	-1.041960	-5.257623	0.266752
Si	-1.739656	-6.318594	-0.845790
H	-3.726000	-9.023359	3.656817
H	-5.276867	-4.450132	6.718252
H	-1.031603	-4.769388	11.503968
H	0.980223	-4.159860	10.265407
H	-1.008990	-2.752820	10.129791
H	2.723878	-9.469644	6.677458
H	1.111152	-11.233151	7.174229
H	1.589732	-10.636360	4.856948
H	-4.831367	-1.376416	2.344366
H	-4.077481	-0.232794	4.368151
H	-3.542388	0.689882	2.171443
H	-1.351148	-7.727359	-0.546035
H	-3.224284	-6.182160	-0.821322
H	-1.215477	-5.919840	-2.183671
H	6.067902	-1.977912	6.900109
H	7.448695	-1.588681	5.869844
H	6.653576	0.274752	7.470662

H	5.154014	0.326174	6.555584
H	6.606597	2.148521	5.833445
H	7.965217	1.067258	5.589737
H	5.402030	1.029579	3.900379
H	6.909972	1.813650	3.469432
H	7.099313	-0.234387	2.315293
H	8.030234	-0.531910	3.777673
H	1.120553	-2.838538	2.089426
H	2.065069	-1.526837	1.826346
H	2.404330	-2.938620	1.088549
B	7.189589	-3.842232	3.687313
H	8.005065	-3.844632	4.568728
H	6.944804	-2.470758	3.560050
H	7.509893	-4.063264	2.553543
H	6.082735	-4.243965	4.015404

$TS_{AB \rightarrow B}$

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Si	-2.390767	9.002572	6.825266
Si	-2.186046	10.861986	9.237616
O	-1.833117	9.538760	8.324348
Si	-2.857535	15.198683	12.451803
O	-2.947423	16.610346	13.286250
Si	-3.713646	17.071131	14.714073
O	-1.261988	14.769892	12.364732
Si	-0.077131	13.803060	11.748387
O	1.338606	14.111576	12.531707
O	-3.497714	15.460741	10.953065
Si	-3.647876	15.051779	9.358835
O	-4.138257	16.400262	8.564373
Si	-5.192952	16.670380	7.276602
O	-3.682763	14.044354	13.319038
Si	-3.971713	12.475043	12.834098
O	-5.369126	11.869368	13.360749
La	-6.762929	10.673180	11.990345
N	-4.744502	8.842034	12.013007
O	-3.725920	11.339844	8.858681
Si	-4.737187	12.333116	9.761771
O	-4.781483	13.862009	9.097814
O	-1.087964	12.049683	8.920153
Si	-0.817637	13.682225	8.811091
O	0.012714	14.030529	7.432726
O	-2.059582	10.363145	10.826246
Si	-1.448348	10.986288	12.251430
O	-0.686568	9.742358	13.010268
Si	0.887216	9.507692	13.574649
O	-0.359902	12.190898	11.960830
O	0.086577	14.119273	10.131042
O	-2.204312	14.553103	8.726363
O	-2.674304	11.487226	13.243112
O	-3.852806	12.536360	11.168589
O	-6.180148	11.659410	10.005810
O	-8.715606	9.575745	12.560326
C	-9.601283	10.484430	13.024665
O	-8.866599	11.775644	12.942303
C	-9.324617	12.919118	13.671217
C	-8.673383	13.002785	15.045499
C	-9.152713	11.956745	16.054520
C	-9.114416	10.502029	15.569470
C	-10.108333	10.204546	14.441866
B	-11.168202	9.702326	10.236337
H	0.874534	13.608074	7.371831
H	1.514882	15.046908	12.670767

H	-2.478308	10.129448	5.851970
H	-1.407697	7.988438	6.348058
H	-3.731817	8.364071	6.981226
H	1.228295	10.522831	14.612202
H	0.907527	8.141797	14.173062
H	1.861926	9.581086	12.447868
H	-4.928250	18.057848	6.800230
H	-4.945878	15.696626	6.173404
H	-6.607167	16.558134	7.740283
H	-3.427543	18.523393	14.891407
H	-5.187611	16.855947	14.614853
H	-3.172127	16.304947	15.874880
H	-10.938156	8.531529	10.217082
H	-12.206054	10.101055	10.677590
H	-10.384940	10.477748	9.771805
H	-10.420313	12.893164	13.732265
H	-9.052297	13.790633	13.066915
H	-7.588001	12.924037	14.902882
H	-8.859081	14.006475	15.449963
H	-10.184595	12.190447	16.353977
H	-8.545784	12.049953	16.963186
H	-9.345540	9.851585	16.420906
H	-8.097411	10.227357	15.256196
H	-11.041597	10.754317	14.621783
H	-10.376605	9.142703	14.431519
H	-10.475771	10.611865	12.348950
H	-4.892797	7.909368	11.633739
H	-3.945735	9.233644	11.506506
H	-4.410457	8.715334	12.967180

B:

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Si	-2.979029	9.669599	6.395567
Si	-2.501512	11.012246	9.103507
O	-2.335055	9.857783	7.942240
Si	-2.532425	14.774275	13.041739
O	-2.430246	16.021180	14.106925
Si	-2.879849	16.188038	15.722895
O	-0.994612	14.373187	12.583131
Si	0.062066	13.526141	11.641618
O	1.589024	13.731502	12.224707
O	-3.432849	15.295877	11.757166
Si	-3.843399	15.127478	10.165268
O	-4.440641	16.579977	9.687661
Si	-5.508527	17.061068	8.476871
O	-3.215922	13.486237	13.844024
Si	-3.588486	12.020115	13.138775
O	-4.912541	11.323055	13.742524
La	-6.610922	10.358704	12.582685
N	-4.886868	8.604064	11.480679
O	-4.079586	11.522437	9.087747
Si	-4.860414	12.369102	10.310151
O	-5.021154	13.979588	9.901454
O	-1.468530	12.257023	8.788596
Si	-1.178336	13.884896	8.907784
O	-0.609154	14.468154	7.476742
O	-2.109075	10.259792	10.539266
Si	-1.246260	10.649934	11.915656
O	-0.389623	9.304273	12.307265
Si	1.167355	9.033242	12.899541
O	-0.200815	11.897411	11.638003
O	-0.033462	14.095070	10.087424
O	-2.531983	14.750957	9.232940

O	-2.265115	10.990841	13.176028
O	-3.697396	12.397008	11.512540
O	-6.239531	11.657703	10.744842
O	-8.654540	9.626489	13.854921
C	-9.701548	10.358969	13.305035
O	-9.011370	11.303462	12.449726
C	-9.731321	12.415490	11.894372
C	-9.588494	13.649153	12.773503
C	-10.291055	13.568790	14.130710
C	-9.977839	12.323316	14.970036
C	-10.550111	11.029817	14.379430
B	-8.338709	8.263996	13.224888
H	0.235598	14.096095	7.206639
H	1.781129	14.629423	12.511183
H	-3.140218	10.988277	5.716562
H	-2.024927	8.814267	5.633715
H	-4.303036	8.984150	6.484257
H	1.430284	9.879938	14.099265
H	1.222241	7.590742	13.273188
H	2.177845	9.321402	11.841168
H	-5.253360	18.509092	8.231791
H	-5.283959	16.283552	7.223041
H	-6.916529	16.872177	8.937206
H	-2.519670	17.581219	16.113093
H	-4.349753	15.983749	15.884417
H	-2.140135	15.215912	16.579939
H	-7.195316	8.004811	13.628458
H	-9.118372	7.395878	13.519487
H	-8.284350	8.417209	11.985564
H	-10.780367	12.128612	11.748103
H	-9.287491	12.589767	10.910772
H	-8.515436	13.834981	12.913344
H	-9.973025	14.511010	12.213189
H	-11.378742	13.614571	13.977024
H	-10.030444	14.464991	14.706022
H	-10.412341	12.465181	15.965828
H	-8.896193	12.224179	15.129026
H	-11.549553	11.229308	13.972070
H	-10.682789	10.269543	15.156169
H	-10.319736	9.713933	12.662949
H	-5.254426	8.160756	10.641515
H	-4.017319	9.063951	11.202245
H	-4.624570	7.848698	12.110437

$TS_{B\rightarrow C}$

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Si	2.100270	12.391712	7.068913
O	-1.580583	12.445457	6.564565
O	0.758039	11.962022	7.927882
O	-1.305771	13.221304	9.128071
O	0.990654	14.548964	9.610475
Si	2.333037	14.988890	8.756380
O	3.589143	15.212095	9.788120
Si	3.721870	15.502033	11.446766
O	3.227303	11.205581	7.188014
Si	3.195790	9.584638	7.661698
O	2.781764	13.771981	7.709144
O	1.751963	12.621177	5.471758
Si	1.116252	13.924842	4.638556
O	1.946478	14.336732	3.322373
La	2.973437	16.382506	3.659095
N	4.629240	15.156702	5.412663
Si	-1.768307	13.683980	5.482067

O	-0.511929	13.669656	4.399700
Si	-0.886613	12.068262	8.016058
O	-1.406627	10.581271	8.493221
Si	-0.656103	14.639001	9.684146
O	-1.025427	14.867608	11.271919
O	-1.869431	15.125934	6.273789
Si	-1.523170	16.407719	7.249366
O	-2.801248	17.434549	7.256956
Si	-2.999545	19.037072	6.760924
O	-3.163371	13.427367	4.660484
Si	-3.549079	13.324234	3.019879
O	-0.190962	17.237503	6.714723
Si	1.365827	16.711434	6.446161
O	2.239430	17.638266	5.462257
O	-1.269081	15.896525	8.803919
O	2.088509	16.391983	7.920854
O	1.253638	15.214172	5.700558
O	4.862940	16.836022	2.397316
C	6.169552	17.317132	2.280616
C	7.071363	16.391022	1.462992
C	6.396659	15.775631	0.230183
C	5.548910	16.713433	-0.647897
C	4.059908	16.786801	-0.275960
C	3.679699	17.751622	0.810611
O	2.536274	17.590533	1.465377
B	1.849368	18.687019	0.551460
H	2.146604	8.838192	6.908994
H	4.543494	9.035733	7.337428
H	2.825990	18.991556	-0.179899
H	1.040245	18.146475	-0.154679
H	1.563685	19.644489	1.220822
H	4.317784	18.595125	1.067147
H	-1.917526	15.190064	11.430293
H	-2.353448	10.440743	8.400008
H	2.807043	16.604210	11.862123
H	3.407576	14.260323	12.210370
H	5.139527	15.898396	11.683409
H	2.944256	9.482294	9.127961
H	-4.437249	19.361353	6.983119
H	-2.141265	19.943379	7.577583
H	-2.661479	19.181524	5.315179
H	-5.032676	13.198501	2.952098
H	-3.108558	14.554800	2.300373
H	-2.908611	12.122527	2.410900
H	3.471368	17.060496	-1.158578
H	3.688939	15.801481	0.027667
H	5.593444	16.347077	-1.679135
H	5.982538	17.722295	-0.681548
H	5.761257	14.941926	0.551095
H	7.182658	15.328657	-0.389996
H	7.434266	15.570952	2.095779
H	7.960535	16.961865	1.162010
H	6.163212	18.315147	1.802385
H	6.620351	17.479556	3.273904
H	5.267404	15.786312	5.893924
H	4.078827	14.699080	6.143121
H	5.201587	14.430335	4.988374

C :
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Si	2.081612	12.203936	7.469839
O	-1.572987	12.667337	6.612058
O	0.608761	12.106313	8.211769

O	-1.332831	13.757045	9.062918
O	1.043717	15.005964	9.381564
Si	2.497205	15.074762	8.599295
O	3.679199	15.388622	9.696148
Si	3.699113	16.132899	11.210888
O	3.019993	10.954824	7.975694
Si	2.739324	9.566279	8.892371
O	2.872206	13.605711	7.909107
O	1.944701	12.107018	5.827329
Si	1.468440	13.284259	4.731155
O	2.438576	13.388592	3.453650
La	3.803105	15.255371	3.311995
N	5.036809	14.250857	5.497394
Si	-1.474584	13.539425	5.207899
O	-0.142688	13.057846	4.347375
Si	-1.008881	12.417928	8.143594
O	-1.761294	11.095826	8.774747
Si	-0.585502	15.222951	9.251748
O	-1.052095	15.920815	10.668429
O	-1.489789	15.162456	5.511528
Si	-1.035222	16.500157	6.364650
O	-2.163708	17.662192	6.082062
Si	-2.071877	19.279513	5.624620
O	-2.806486	13.193382	4.309588
Si	-3.030332	12.324501	2.881976
O	0.438843	17.095869	5.886864
Si	1.899227	16.278401	5.903725
O	2.956086	16.811409	4.812838
O	-1.008581	16.200848	7.990559
O	2.512893	16.274733	7.463440
O	1.477660	14.682266	5.651678
O	5.707404	15.393011	2.207302
C	6.783890	16.116923	1.696225
C	6.541298	16.592829	0.256643
C	5.169531	17.235353	0.041018
C	4.873977	18.454660	0.922105
C	3.421408	18.951792	0.834782
C	2.441668	18.307475	1.802631
O	2.369136	16.860642	1.637851
B	1.422657	16.285689	0.848260
H	1.651781	8.746787	8.284113
H	4.019118	8.801062	8.883361
H	1.433433	18.708683	1.662455
H	0.612436	16.966276	0.290359
H	1.464411	15.093705	0.764459
H	2.734782	18.460871	2.845422
H	-1.978633	16.176273	10.701005
H	-2.678349	10.998577	8.502062
H	2.922374	17.406379	11.184233
H	3.135987	15.214201	12.241772
H	5.131059	16.417830	11.514726
H	2.378791	9.932267	10.292853
H	-3.468795	19.800026	5.639262
H	-1.230847	20.058460	6.580261
H	-1.506916	19.403961	4.247397
H	-4.504607	12.236901	2.676315
H	-2.404246	13.038814	1.730570
H	-2.453497	10.953331	2.998797
H	3.380482	20.025770	1.058384
H	3.046055	18.842192	-0.191505
H	5.549299	19.269773	0.633729
H	5.115232	18.237037	1.971800
H	4.408402	16.466281	0.207188

H	5.069845	17.531730	-1.011761
H	6.627010	15.735520	-0.422646
H	7.342492	17.293562	-0.018048
H	6.997502	16.997394	2.330812
H	7.702291	15.507840	1.710229
H	5.714598	14.892092	5.903265
H	4.374651	14.028542	6.243196
H	5.539106	13.388991	5.295837