Supporting Information

Ring-Opening Polymerization of Racemic β-Butyrolactone Promoted by Rare Earth Trisborohydride Complexes towards PHB-diol: An Experimental and DFT Study

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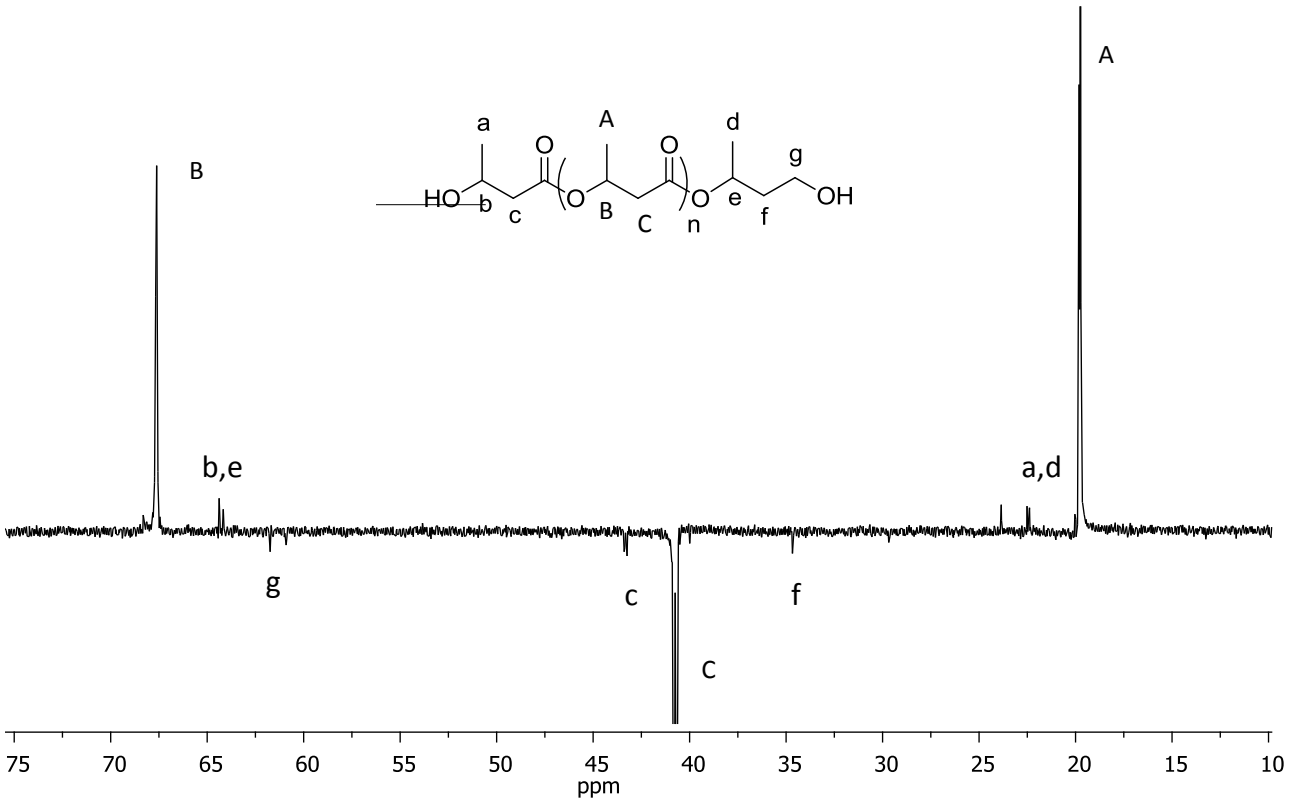

Figure S1. ^{13}C DEPT (125 MHz,$CDCl_3$, 298 °K) NMR spectrum of a PHB produced from $[La(BH_4)_3(THF)_3]$ (Table 1, entry 4).

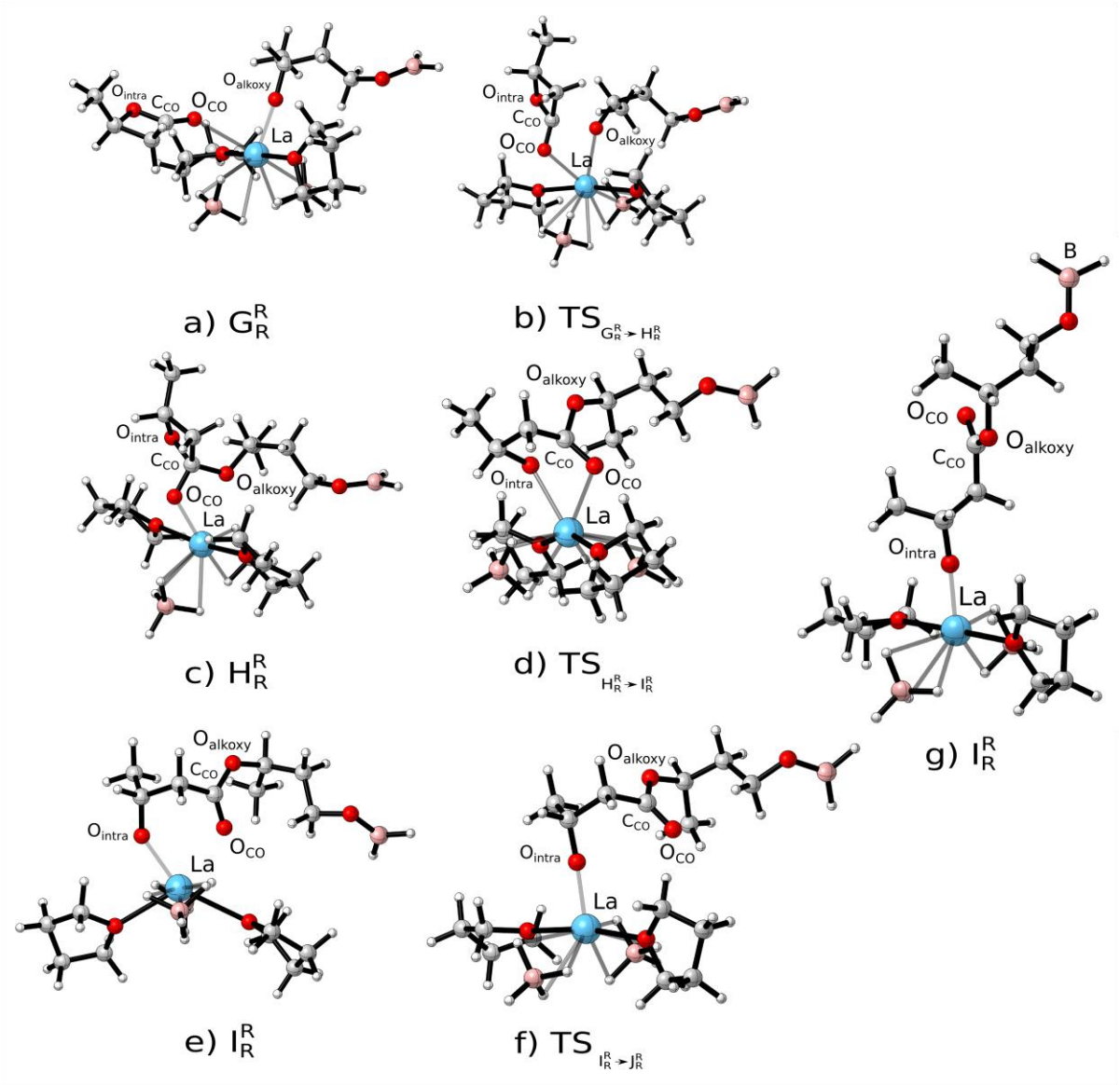

Figure S2. Optimized structures of complexes involved in the propagation ROP step of BBL-R mediated by F_R with alkoxyborane arm as propagator.

	$Ln\text{-}O_{CO}$	$Ln\text{-}O_{intra}$	$C_{CO}\text{-}O_{CO}$	$C_{CO}\text{-}O_{intra}$	$C_{CO}\text{-}H_t$	$B\text{-}H_t$	$O_{CO}\text{-}B$	$B\text{-}H_{t2}$	$C_{CO}\text{-}H_{t2}$	$Ln\text{-}O_{alkoxy}$	$C_{CO}\text{-}O_{alkoxy}$
BBL-R	-	-	1,190	1,369	-	-	-	-	-	-	-
BH_4^- as propagator											
Nucleophilic Attack											
$\mathbf{F_RA_R}$	2.714	-	1.209	1.347	-	~1.23	-	-	-	-	-
TS($\mathbf{F_RA_R}$ →$\mathbf{F_RB_R}^R$)	2/325	-	1.303	1.434	1.197	1.456	-	-	-	-	-
$\mathbf{F_RB_R}^R$	2.395	2.634	1.304	1.506	1.153	1.587	3.463	-	-	-	-
BH_3 Trapping											
TS($\mathbf{F_RB_R}^R$ →$\mathbf{F_RC_R}^R$)	2.363	2.611	1.324	1.539	1.108	-	2.540	-	-	-	-
$\mathbf{F_RC_R}^R$	2.560	2.726	1.367	1.479	1.095	-	1.553	-	-	-	-
Ring-opening + Hydrogen transfer											
TS($\mathbf{F_RC_R}^R$ →$\mathbf{F_RD_R}^R$)	3.863	2.296	1.238	2.444	1.098	-	1.585	1.217	-	-	-
$\mathbf{F_RD_R}^R$	3.271	2.303	1.246	2.809	1.098	-	1.583	1.215	-	-	-
TS($\mathbf{F_RD_R}^R$ →$\mathbf{F_RE_R}^R$)	2.888	2.293	1.268	2.865	1.099	-	1.702	1.229	2.140	-	-
$\mathbf{F_RE_R}^R$	2.899	2.239	1.446	2.896	1.099	-	1.354	-	1.099	-	-
TS($\mathbf{F_RC_R}^R$ →$\mathbf{F_RE_R}^R$)	2.615	2.369	1.333	2.009	1.088	-	1.565	1.262	1.771	-	-
Arm Decoordination											
TS($\mathbf{F_RE_R}^R$ →$\mathbf{F_RE_R}$)	3.660	2.215	1.437	2.847	1.097	-	1.346	-	1.097	-	-
$\mathbf{F_RE_R}$	-	2.239	1.429	2.980	1.097	-	1.342	-	1.098	-	-
Alkoxyborane arm as propagator											
Nucleophilic Attack											
$\mathbf{G_R}$	2.700	-	1.210	1.347	-	-	-	-	-	2.194	-
TS($\mathbf{G_R}$ →$\mathbf{H_R}^R$)	2.471	-	1.241	1.377	-	-	-	-	-	2.402	1.986
$\mathbf{H_R}^R$	2.317	-	1.324	1.448	-	-	-	-	-	2.729	1.452
Ring-opening											
TS($\mathbf{H_R}^R$ →$\mathbf{I_R}^R$)	2.390	2.530	1.303	1.663	-	-	-	-	-	-	1.362
$\mathbf{I_R}^R$	2.619	2.223	1.235	2.899	-	-	-	-	-	-	1.324
Arm Decoordination											
TS($\mathbf{I_R}^R$ →$\mathbf{J_R}^R$)	4.241	2.180	1.218	2.926	-	-	-	-	-	-	1.341
$\mathbf{J_R}^R$	-	1.393	1.213	-	-	-	-	-	-	-	1.348

Table S1. Selected bond lengths (Å) of the stationary points calculated for the propagation step of the ROP of **BL-R** mediated by $\mathbf{F_R}$. The labels refer to the intermediates and transition states shown in Figures 7 and 8.

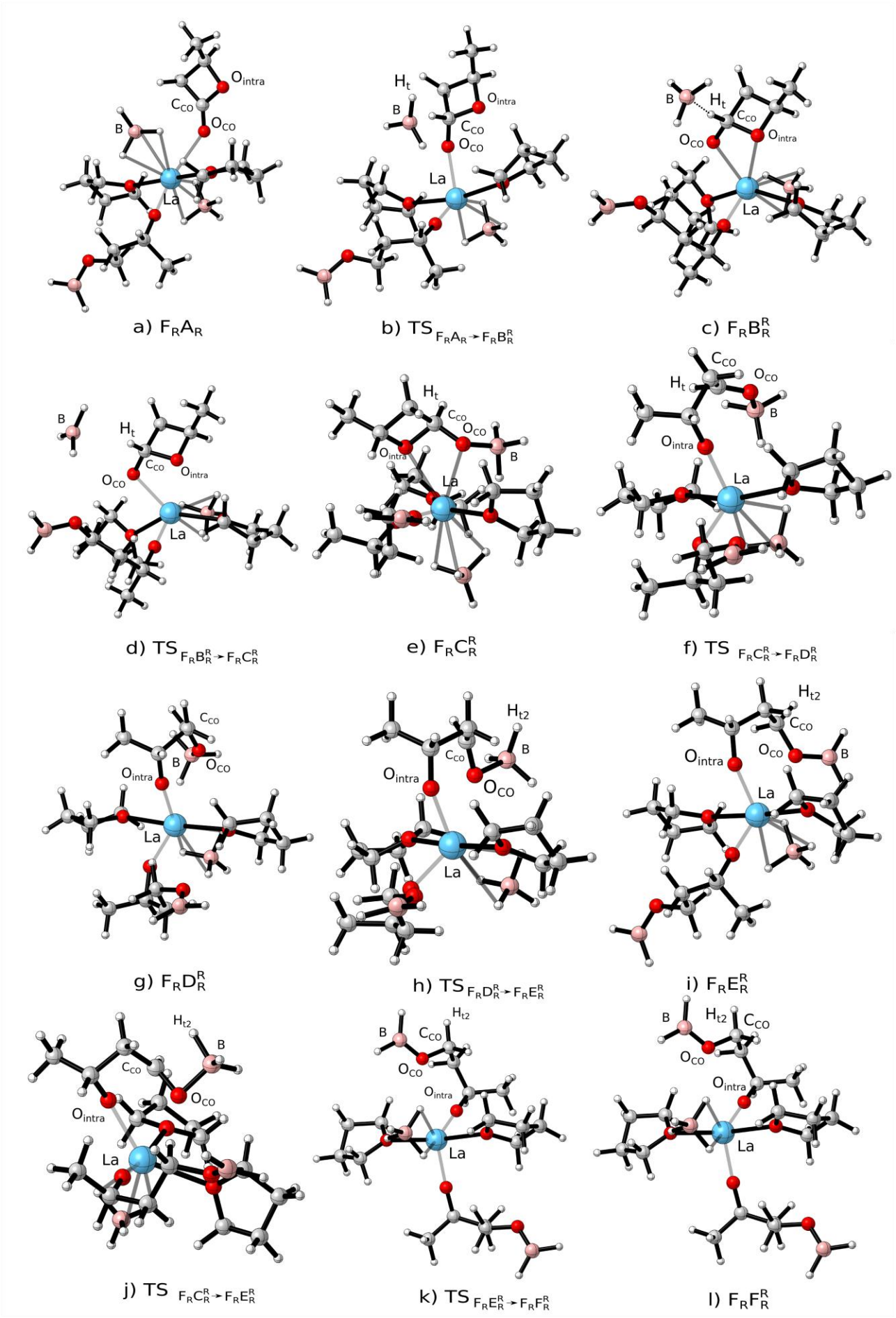

Figure S3. Optimized structures of complexes involved in the propagation ROP step mediated by $\mathbf{F_R}$ with borohydride as propagator.

Cartesian Coordinates

Initiation Step of *rac*-BL ROP polymerization mediated by $[La(BH_4)_3(THF)_3]$.

BBL-R

G = -306,297886 kcal.mol^{-1}

H	-0.069978	-1.397155	-2.593485
C	-0.083116	-0.426973	-2.087066
C	-1.198415	-0.282939	-1.040901
C	-0.045058	-0.321469	-0.047810
O	0.920235	-0.443341	-1.010894
O	0.104578	-0.278760	1.136315
H	-1.899458	-1.115300	-0.948555
H	-1.746805	0.662361	-1.053402
C	0.149063	0.710333	-3.050526
H	-0.634236	0.722684	-3.815438
H	0.140312	1.671314	-2.527073
H	1.114866	0.600385	-3.551776

BBL-S

G = -306,297846 kcal.mol^{-1}

C	-0.023749	0.075958	0.122513
O	0.145700	0.181906	1.299986
O	0.923571	-0.117408	-0.846639
C	-1.190541	0.096631	-0.855289
C	-0.093798	-0.114243	-1.909801
C	-0.088922	-1.403892	-2.692233
H	-1.896262	-0.728089	-0.727814
H	-1.732212	1.044413	-0.888792
H	0.076286	0.753033	-2.555376
H	-0.882538	-1.390313	-3.446421
H	0.867547	-1.541038	-3.204539
H	-0.251191	-2.260559	-2.030904

$Ln(BH_4)_3(THF)_3$

G = -810,211634 kcal.mol^{-1}

C	-5.079014	-1.316743	1.083200
C	-3.895321	-0.391516	1.326306
O	-3.020558	-0.570195	0.182928
C	-3.721088	-1.295638	-0.858889
C	-5.185007	-1.298040	-0.441829
La	-0.443719	0.217321	0.008305
B	-1.063860	0.123602	-2.628772
B	-0.972712	0.956116	2.559724
B	2.231927	-0.012731	0.001754
O	-0.271797	-2.375170	0.397952
C	0.085283	-2.909283	1.701602
C	0.585324	-4.324353	1.441424
C	1.184427	-4.198448	0.039247
C	0.190619	-3.273212	-0.643889
O	-0.335484	2.794659	-0.387854
C	0.091657	3.352016	-1.663485
C	0.431196	4.817971	-1.391760
C	-0.340503	5.119699	-0.104651
C	-0.213446	3.804244	0.642213
H	-1.113191	-0.994816	-2.091156
H	-1.837246	0.863137	-2.000780
H	0.084466	0.543807	-2.469427
H	-1.363500	0.061984	-3.792380
H	1.883404	1.162792	-0.181743
H	1.742283	-0.370842	1.082641
H	1.711626	-0.688659	-0.897446
H	3.428083	-0.131991	0.002138
H	-1.788167	1.435365	1.757071
H	-1.010040	-0.277066	2.415144
H	0.155114	1.325184	2.224171
H	-1.237748	1.275822	3.688816
H	-3.524739	-0.796828	-1.808999
H	-3.312917	-2.312744	-0.903401
H	-5.681002	-0.381514	-0.780274
H	-5.730489	-2.151376	-0.853523
H	-5.983872	-0.969358	1.588930
H	-4.857640	-2.329267	1.439646
H	-4.204188	0.659488	1.363147
H	-3.326098	-0.615591	2.229471
H	0.869755	-2.273570	2.125934
H	-0.799209	-2.859137	2.341355
H	-0.676738	-3.818787	-1.035425
H	0.625688	-2.671723	-1.444648
H	2.170327	-3.724312	0.083135
H	1.282838	-5.155747	-0.479333
H	-0.246785	-5.037497	1.441997
H	1.309386	-4.645775	2.194422
H	0.765751	3.703769	1.126664
H	-0.993496	3.615277	1.380308
H	-0.739665	3.227326	-2.362231
H	0.946230	2.775467	-2.026770
H	-1.393023	5.333946	-0.320788
H	0.073291	5.960179	0.458824
H	1.506515	4.937593	-1.223239
H	0.148462	5.463313	-2.227459

THF

G = -232,28445 kcal.mol^{-1}

O	-0.029262	0.112527	0.099196
C	0.053065	0.115359	1.521769
C	1.479866	0.536964	1.873516
C	2.260769	-0.011519	0.677059
C	1.273619	0.235306	-0.463155
H	-0.707307	0.797139	1.920935
H	1.559052	1.629535	1.909626
H	3.225131	0.479697	0.519218
H	1.403194	1.245720	-0.882166
H	-0.164499	-0.893674	1.905348
H	1.815425	0.141122	2.836266
H	2.441940	-1.085400	0.801066
H	1.373880	-0.484087	-1.284334

A_R

G = -884,228819 kcal.mol^{-1}

C	-2.938570	1.824364	0.506751
O	-3.126157	1.129897	1.772346
C	-4.388574	1.528142	2.353215
C	-4.629260	2.923422	1.805628
C	-4.125457	2.779922	0.367039
La	-1.809580	-1.054707	2.370366
O	0.077584	-0.733111	4.222711
C	0.204368	-0.441098	5.389714
C	-0.471184	0.445492	6.406358
C	0.618318	-0.096594	7.345985
C	0.203830	-0.958841	8.508510
O	-0.687878	-3.342619	2.876213
C	0.735456	-3.622947	2.892981
C	0.846475	-5.135801	2.762835
C	-0.424983	-5.612040	3.469063
C	-1.441843	-4.573837	3.018073
B	0.103481	0.047317	0.832327
B	-3.300513	-2.515679	0.693821
O	1.148220	-0.913433	6.222585
B	-3.288836	-0.890537	4.666340
H	1.143859	-3.258270	3.840976
H	-3.573400	-1.309585	0.603062
H	-2.089156	-2.636789	0.457647
H	-0.722443	-6.626385	3.190727
H	-2.627772	0.137689	4.443637
H	-2.491853	-1.836343	4.726098

H	-4.027799	-1.081984	3.699433
H	-3.916886	-0.773806	5.689574
H	-1.499418	0.146775	6.623961
H	-0.437104	1.510545	6.167847
H	1.383276	0.634687	7.619965
H	-0.220895	-0.331985	9.299042
H	1.063957	-1.493203	8.921284
H	-0.551216	-1.689234	8.203564
H	-0.226409	0.794075	1.768839
H	0.954410	0.550053	0.148007
H	-0.912699	-0.217044	0.178571
H	0.487325	-1.016526	1.340240
H	-3.490978	-2.838904	1.876057
H	-3.965051	-3.183448	-0.052549
H	-4.283047	1.469315	3.436795
H	-5.169410	0.826173	2.033470
H	-5.679569	3.220620	1.866951
H	-4.030585	3.655964	2.358359
H	-4.903673	2.334707	-0.261575
H	-3.832321	3.730770	-0.085517
H	-1.976178	2.339163	0.564569
H	-2.891629	1.082822	-0.294790
H	1.198809	-3.069245	2.073243
H	1.764895	-5.521280	3.213337
H	0.831211	-5.432506	1.708563
H	-2.246073	-4.393836	3.736011
H	-1.882110	-4.818381	2.045874
H	-0.295456	-5.579334	4.556693

TS($A_R \rightarrow B^R_R$)

G = -884,201902 kcal.mol^{-1}

C	-3.302789	1.681960	0.259960
O	-2.968482	1.054592	1.528833
C	-3.572808	1.790763	2.623661
C	-3.873308	3.161484	2.042132
C	-4.268548	2.811208	0.604657
La	-1.592399	-1.102160	1.775469
O	-1.427011	-0.424135	3.941248
C	-1.343761	-0.581681	5.245087
C	-0.826852	0.525962	6.180125
C	0.099192	-0.567600	6.735265
C	-0.173470	-1.070505	8.136013
O	-0.432639	-3.243930	2.533205
C	0.910988	-3.229180	3.095779
C	1.284640	-4.695539	3.255719
C	-0.070719	-5.339056	3.559608
C	-1.004997	-4.575694	2.632451
B	0.374882	-0.179599	0.215800
B	-3.466431	-2.621983	0.601166
O	-0.353217	-1.503412	5.713134
B	-3.829755	-1.262864	5.861291
H	0.861330	-2.704519	4.054922
H	-3.533080	-1.438759	0.228478
H	-2.322451	-3.016300	0.324866
H	-0.091995	-6.414880	3.367289
H	-2.365363	-0.980055	5.667166
H	-3.891523	-2.103898	5.004892
H	-4.239128	-0.158850	5.621603
H	-3.724425	-1.604540	7.008336
H	-1.553019	0.954846	6.873337
H	-0.315337	1.315254	5.625474
H	1.168660	-0.366646	6.596727
H	0.150146	-0.329914	8.875754
H	0.373870	-1.999552	8.323514
H	-1.240262	-1.264982	8.281711
H	0.398986	0.384031	1.319478
H	1.251383	0.212254	-0.503966
H	-0.746716	0.013443	-0.285862
H	0.463235	-1.404767	0.413715
H	-3.580809	-2.624268	1.839486
H	-4.311504	-3.299411	0.084342
H	-2.862894	1.782325	3.451651
H	-4.487296	1.270968	2.932785
H	-4.662816	3.680297	2.591866
H	-2.974865	3.788235	2.055084
H	-5.303940	2.455963	0.570711
H	-4.176172	3.652340	-0.086966
H	-2.370970	2.048447	-0.182270
H	-3.734407	0.919313	-0.394119
H	1.553217	-2.681477	2.400058
H	2.020140	-4.845379	4.050207
H	1.700231	-5.093738	2.323604
H	-2.025842	-4.480718	3.008723
H	-1.036678	-5.006364	1.625992
H	-0.347743	-5.169537	4.605242

B^R_R

G = -884,204468 kcal.mol^{-1}

O	0.365503	-0.571732	0.724125
C	0.185418	-0.504300	-0.714351
C	1.561663	-0.170959	-1.284089
C	2.232877	0.569156	-0.123832
C	1.724451	-0.210083	1.077316
H	1.678101	0.360968	2.006905
H	2.297039	-1.131267	1.241116
H	1.889354	1.608040	-0.075819
H	3.324203	0.569496	-0.186550
H	1.491114	0.427126	-2.196187
H	2.114007	-1.086902	-1.520418
H	-0.206476	-1.465411	-1.059184
H	-0.555914	0.274302	-0.917340
La	-1.407770	-1.088141	2.505465
O	-0.155365	0.538831	3.671745
H	-1.032597	1.484692	5.259306
C	-0.590759	0.486684	4.905581
H	-2.546870	2.860379	4.958170
B	-1.652543	2.884911	5.755603
H	-1.852862	2.506045	6.877652
H	-0.657736	3.508458	5.515780
H	0.431590	0.440993	6.898244
H	1.102808	-0.677262	5.667977
C	0.198332	-0.193379	6.040977
C	-1.007052	-1.130572	6.206974
H	-0.794085	-2.181099	5.983769
H	-2.060600	0.051906	7.674456
H	-1.269712	-1.404076	8.318621
C	-1.827408	-0.996573	7.468268
H	-2.766425	-1.552104	7.382541
H	0.468911	-4.494889	2.891487
H	-0.899684	-3.268426	3.735007
H	0.701868	-2.488687	2.834641
B	-0.092429	-3.435005	2.811329
H	-0.736278	-3.360548	1.745123
O	-1.689632	-0.523743	5.052434
O	-3.510115	-2.487237	3.179744
B	-3.110451	0.112454	0.777753
C	-3.757577	-3.837738	2.716913
C	-5.001538	-4.287579	3.466759
C	-5.792797	-2.981863	3.574981
C	-4.695112	-1.954268	3.825357
H	-3.595067	0.044152	1.916989
H	-2.065635	0.763498	0.869261
H	-2.810110	-1.048766	0.434005
H	-3.881897	0.600612	-0.003409
H	-4.473010	-1.836186	4.891150
H	-4.908149	-0.973233	3.392874
H	-3.928262	-3.810492	1.633177
H	-2.862493	-4.427401	2.925660
H	-4.733504	-4.661896	4.461041
H	-5.540525	-5.077849	2.937775
H	-6.307672	-2.768840	2.632053
H	-6.537718	-2.990139	4.374868

TS($B^R_R \rightarrow C^R_R$)

G = -884,205222 kcal.mol^{-1}

O	0.297479	-0.568226	0.768132
C	0.087825	-0.403567	-0.657150
C	1.434176	0.044069	-1.220973
C	2.090068	0.725937	-0.016925
C	1.643019	-0.167614	1.128060
H	1.586559	0.327735	2.099762
H	2.263127	-1.068581	1.211822
H	1.696578	1.739308	0.116509
H	3.178707	0.786334	-0.096064
H	1.315511	0.706503	-2.082265
H	2.027626	-0.820657	-1.537080
H	-0.258901	-1.356291	-1.067956
H	-0.696719	0.347440	-0.790302
La	-1.439005	-1.159368	2.571247

O	-0.216740	0.404311	3.790801
H	-1.147011	1.351250	5.344631
C	-0.721351	0.382095	5.020124
H	-0.461058	4.100019	4.026572
B	-0.695219	3.817601	5.162126
H	-1.826871	3.770491	5.546485
H	0.201395	3.615075	5.927000
H	0.252041	0.200815	7.037075
H	0.899831	-0.887706	5.771264
C	0.007540	-0.382277	6.145683
C	-1.230698	-1.281415	6.250624
H	-1.046224	-2.338066	6.027766
H	-2.283677	-0.085415	7.712104
H	-1.571510	-1.581523	8.351923
C	-2.084320	-1.138537	7.491045
H	-3.042838	-1.652037	7.366357
H	0.487128	-4.559630	2.868567
H	-0.865525	-3.348889	3.758141
H	0.701383	-2.550960	2.815896
B	-0.084599	-3.503200	2.808124
H	-0.760296	-3.430478	1.762906
O	-1.858776	-0.637901	5.092904
O	-3.531933	-2.661723	3.101052
B	-3.162194	0.214432	0.982318
C	-3.681884	-4.051211	2.723117
C	-4.889206	-4.542129	3.505798
C	-5.777294	-3.295684	3.526528
C	-4.761153	-2.171133	3.695718
H	-3.608610	0.079181	2.131989
H	-2.095321	0.826673	1.082428
H	-2.915068	-0.925848	0.544088
H	-3.945455	0.783240	0.269104
H	-4.558409	-1.951046	4.749210
H	-5.040678	-1.246115	3.185750
H	-3.855141	-4.104750	1.640718
H	-2.746803	-4.561063	2.961415
H	-4.595059	-4.825333	4.522539
H	-5.365804	-5.405865	3.034834
H	-6.309092	-3.191164	2.574698
H	-6.518790	-3.303496	4.329650

C^R_R

G = -884,242782 kcal.mol^{-1}

O	0.117287	-0.186130	0.720291
C	-0.371717	0.307156	-0.553281
C	0.744367	0.010994	-1.541131
C	1.988837	0.225248	-0.677626
C	1.559076	-0.361354	0.661702
H	2.000274	0.145897	1.523759
H	1.767310	-1.433043	0.736218
H	2.204343	1.294659	-0.578982
H	2.882223	-0.266543	-1.071121
H	0.704816	0.665336	-2.416010
H	0.687954	-1.027571	-1.885922
H	-1.314967	-0.197512	-0.767864
H	-0.562680	1.381979	-0.460724
La	-1.238795	-0.470258	2.927449
O	0.042858	0.556961	4.914110
H	-1.157250	1.400372	6.339504
C	-0.851853	0.426168	5.938764
H	0.453488	1.516382	2.988674
B	-0.122213	1.807252	4.043121
H	-1.333631	1.934046	3.791911
H	0.319864	2.809990	4.543242
H	-0.499463	-0.362166	7.997918
H	0.326871	-1.253819	6.681317
C	-0.559073	-0.678422	6.954319
C	-1.886080	-1.315778	6.514705
H	-1.787009	-2.305194	6.056780
H	-3.139243	-0.291886	7.948626
H	-2.852501	-2.008917	8.302328
C	-3.031125	-1.284226	7.500315
H	-3.974966	-1.544274	7.011694
H	1.046865	-3.629748	3.261922
H	-0.410558	-2.536664	4.139190
H	1.034114	-1.609848	3.147344
B	0.362299	-2.643826	3.175997
H	-0.331858	-2.674051	2.145318
O	-2.053361	-0.303434	5.462529
O	-3.091249	-2.363628	3.218093
B	-3.219561	0.623245	1.451167
C	-2.903514	-3.780248	2.983102
C	-4.163353	-4.434361	3.524017
C	-5.230815	-3.405837	3.146400
C	-4.509350	-2.077901	3.362582
H	-3.509577	0.556691	2.655923
H	-2.185568	1.294231	1.379955
H	-2.958238	-0.529709	1.067059
H	-4.113247	1.107510	0.808395
H	-4.663907	-1.680833	4.371542
H	-4.781068	-1.309550	2.636548
H	-2.794895	-3.950630	1.904333
H	-1.979859	-4.079200	3.479541
H	-4.098670	-4.547421	4.612155
H	-4.338604	-5.421578	3.088244
H	-5.511941	-3.520865	2.094069
H	-6.140876	-3.481063	3.747325

$TS(C^R_R \rightarrow D^R_R)$

G = -884,226409 kcal.mol^{-1}

C	-1.404931	-2.480066	2.201060
O	-1.288909	-2.463539	3.649459
C	-2.601056	-2.327737	4.250369
C	-3.545743	-1.999477	3.101331
C	-2.881086	-2.719758	1.926309
La	0.786193	-3.051989	5.115828
O	2.512476	-0.093153	6.516031
C	1.499277	0.487016	6.928523
C	0.837733	0.065932	8.170177
C	-0.404922	-0.782275	7.663840
C	-1.602319	0.127255	7.382249
O	2.917497	-3.609133	6.499164
C	2.959207	-4.542316	7.613315
C	4.428004	-4.643546	8.010685
C	5.147412	-4.337092	6.695143
C	4.267955	-3.247124	6.107091
O	-0.029663	-1.514555	6.556740
B	1.871887	-3.710073	2.711578
B	-0.267293	-5.277843	6.167267
B	2.970273	-0.002706	5.004428
H	0.017196	-4.469888	7.061168
H	-1.051452	-4.701470	5.394001
H	0.759803	-5.520769	5.516947
H	-0.750326	-6.283374	6.614603
H	2.355033	0.908948	4.495087
H	4.170099	0.097412	5.014333
H	2.621605	-1.099978	4.573520
H	1.044968	1.249754	6.282221
H	4.498340	-2.260958	6.524363
H	1.514249	-0.568783	8.746300
H	0.506038	0.918612	8.770848
H	4.293580	-3.188002	5.017163
H	6.179849	-4.005566	6.833137
H	5.152415	-5.216474	6.042113
H	2.553419	-5.496440	7.264936
H	2.314148	-4.158086	8.407674
H	-0.672996	-1.441764	8.507316
H	-1.396498	0.818847	6.558091
H	-1.886286	0.709162	8.266268
H	-2.460484	-0.487216	7.095854
H	4.678850	-3.889801	8.765308
H	4.672417	-5.627129	8.420014
H	2.680517	-3.889540	3.634866
H	0.889109	-4.422132	2.959150
H	2.353406	-3.954977	1.637087
H	-2.854574	-3.280134	4.730567
H	-2.539924	-1.549705	5.013804
H	-1.070816	-1.507679	1.820512
H	-0.739582	-3.256204	1.821990
H	-3.106390	-3.791366	1.955676
H	-3.187194	-2.332489	0.950979
H	-3.574086	-0.918975	2.921288
H	-4.566057	-2.338496	3.298719
H	1.509387	-2.522071	2.774127

D^R_R

G = -884,231463 kcal.mol^{-1}

C	-4.678258	-1.325805	4.283353
O	-3.799237	-0.589213	3.388428

C	-4.585576	0.309225	2.570861
C	-5.972750	-0.308622	2.549921
C	-6.093807	-0.836647	3.981055
La	-1.166454	-0.595007	3.642660
B	-1.312557	0.964017	1.403261
O	-1.268560	1.927645	5.084068
C	0.231953	-2.135615	0.618351
B	-1.583886	-2.983087	4.857256
H	-3.483315	2.098186	5.313461
H	-2.392422	2.009697	7.047607
H	-2.590231	0.372901	5.872496
H	-0.364531	2.958196	6.544026
H	0.790771	2.631673	3.722363
H	1.660347	3.307546	5.151665
C	2.096068	0.845658	6.429944
H	1.900040	-2.051150	3.357430
H	1.176362	-3.640147	2.997436
H	3.087569	-3.676963	1.476033
H	2.948721	-1.936067	1.162455
H	1.006218	-4.130440	0.264919
H	1.748006	-2.890062	-0.760012
H	0.364747	-1.138551	0.187684
H	-0.762693	-2.503950	0.353480
H	-2.079017	-2.043536	5.498173
H	-0.374272	-2.750960	4.762349
H	-1.796249	-4.039828	5.391486
H	-2.068796	-2.954570	3.713989
H	-1.901688	1.498876	2.349027
H	-0.131632	0.812890	1.731989
H	-1.810301	-0.166236	1.250740
H	-1.419408	1.610049	0.392552
H	-4.542033	-2.389518	4.069483
H	-4.367258	-1.132207	5.312544
H	-4.592976	1.301263	3.039015
H	-4.099096	0.379713	1.597285
H	-6.013627	-1.130487	1.826275
H	-6.747709	0.417407	2.289604
H	-6.372356	-0.024246	4.660506
H	-6.832995	-1.634865	4.088624
H	2.626042	-0.109276	6.484959
H	2.774023	1.635669	6.772017
H	1.244700	0.782684	7.115301

$TS(D^{R}_{R} \rightarrow E^{R}_{R})$

G = -884,212843 kcal.mol^{-1}

C	-4.436935	-1.038402	4.551823
O	-3.631886	-0.519017	3.456199
C	-4.481317	0.180194	2.511207
C	-5.884542	-0.326400	2.799811
C	-5.844290	-0.501449	4.319100
La	-1.015106	-0.662306	3.404803
C	-0.277173	2.540609	5.533302
C	0.973942	2.536480	4.795710
C	1.630407	1.069122	4.989899
O	0.767173	0.113112	4.564503
B	-2.571343	1.597292	5.924549
H	2.520046	1.136058	4.337738
B	-1.279827	0.854873	1.154792
O	-1.599132	1.195274	5.345453
C	-0.742657	1.904064	5.960749
C	0.464336	2.391786	5.299024
C	1.453350	1.149503	5.075570
O	0.838191	0.186479	4.333025
B	-2.908174	2.189686	5.772623
H	2.287466	1.613382	4.519186
O	0.413500	-2.135733	1.845947
C	1.624767	-2.758480	2.343743
C	2.505472	-2.934851	1.116377
C	1.470399	-3.212915	0.023587
C	0.335552	-2.269447	0.403566
B	-1.410607	-2.928883	4.854605
H	-3.452030	2.295410	4.705934
H	-2.384779	3.264813	6.052691
H	-3.449917	1.643769	6.695647
H	-0.852612	1.999009	7.048094
H	0.220175	2.766587	4.301499
H	0.958159	3.163618	5.894095
C	1.997150	0.610021	6.400082
H	2.046125	-2.100529	3.108031
H	1.356094	-3.716227	2.803247
H	3.231115	-3.742844	1.241082
H	3.053231	-2.010708	0.901863
H	1.138535	-4.255850	0.070274
H	1.842866	-3.019188	-0.985632
H	0.452784	-1.272906	-0.032935
H	-0.656614	-2.651589	0.149573
H	-1.769995	-1.912239	5.470713
H	-0.211778	-2.781041	4.594189
H	-1.607955	-3.925708	5.498467
H	-2.036149	-2.957378	3.781777
H	-1.787126	1.406109	2.143111
H	-0.084008	0.678608	1.403777
H	-1.813416	-0.265020	1.043667
H	-1.445451	1.503027	0.154418
H	-4.388344	-2.130678	4.508556
H	-3.997584	-0.701288	5.493039
H	-4.392447	1.257122	2.691980
H	-4.115073	-0.039360	1.507276
H	-6.056657	-1.287949	2.303033
H	-6.653324	0.374984	2.464692
H	-5.969385	0.466099	4.816140
H	-6.609864	-1.183023	4.699186
H	2.745141	-0.158859	6.187981
O	0.301614	-2.008314	2.060668
C	1.481288	-2.679287	2.567671
C	2.379913	-2.852787	1.353449
C	1.356924	-3.092954	0.240403
H	2.471649	1.393996	7.000937
H	1.204834	0.137503	6.989816

E^{R}_{R}

G = -884,283214 kcal.mol^{-1}

C	-2.669488	-3.008410	4.599015
O	-1.309244	-3.238365	4.154354
C	-1.299909	-3.719200	2.786746
C	-2.763199	-3.960533	2.431601
C	-3.489002	-2.946250	3.319591
La	0.647082	-2.366007	5.579411
B	1.736826	-1.689406	3.150991
O	2.944186	-3.751673	5.767449
C	4.163671	-3.451105	5.046840
C	5.033902	-4.690784	5.189215
C	4.640271	-5.191893	6.579900
C	3.141639	-4.924201	6.600894
B	-0.176757	-4.144242	7.483374
O	-0.458171	-0.551347	6.091582
C	-0.584400	0.755837	6.548658
C	0.610840	1.124230	7.449731
C	1.967572	0.750862	6.870601
O	2.260494	-0.661426	7.064974
B	3.159184	-1.057270	7.999285
C	-0.743501	1.725113	5.375014
H	0.739825	-3.405076	7.885915
H	-1.113490	-3.408870	7.158684
H	0.230307	-4.725768	6.465640
H	-0.499081	-4.935790	8.331183
H	2.770177	1.317801	7.352159
H	3.334846	-2.231803	8.112181
H	3.737360	-0.237109	8.655597
H	2.015132	0.920140	5.791261
H	4.636177	-2.575759	5.511163
H	0.509157	0.628839	8.423075
H	0.609746	2.204497	7.645241
H	3.894500	-3.200150	4.019786
H	6.098677	-4.462729	5.091779
H	4.772341	-5.431404	4.425174
H	2.573482	-5.753354	6.165102
H	2.734916	-4.711444	7.591125
H	-1.490354	0.843393	7.174040
H	0.139001	1.712793	4.725776
H	-0.911128	2.752467	5.718867
H	-1.599530	1.422461	4.765278
H	5.147467	-4.606090	7.354717

H	4.872108	-6.247266	6.745906
H	2.388857	-1.240943	4.110384
H	1.663589	-2.920883	3.299377
H	2.267084	-1.416442	2.104272
H	-2.968661	-3.842961	5.243365
H	-2.673362	-2.084464	5.182809
H	-0.836712	-2.947711	2.164077
H	-0.685587	-4.622926	2.745596
H	-3.062685	-4.980571	2.696196
H	-2.954015	-3.816733	1.364957
H	-3.436725	-1.943841	2.881088
H	-4.540295	-3.193605	3.488464
H	0.599927	-1.221542	3.231595

$TS(C^{R}_{R} \rightarrow E^{R}_{R})$

G = -884,206140 $kcal.mol^{-1}$

C	-2.596728	-2.283966	4.175339
O	-1.264516	-2.482458	3.633311
C	-1.281726	-2.324398	2.187959
C	-2.755004	-2.228832	1.812262
C	-3.372752	-1.597200	3.062642
La	0.702418	-3.155635	5.155447
B	1.947246	-3.836550	2.857307
B	-0.388186	-5.304654	6.330542
O	1.777557	-0.800959	5.313939
C	0.897454	-0.037479	5.968244
C	0.906923	0.090218	7.480544
C	-0.178617	-0.962164	7.768232
C	-1.468577	-0.403270	8.344753
O	-0.374215	-1.466140	6.448927
O	2.764509	-3.566253	6.671880
C	4.050096	-2.950144	6.373384
C	5.091798	-3.852204	7.022586
C	4.323542	-4.440752	8.208065
C	2.945000	-4.662738	7.607303
B	2.683084	0.456200	5.095330
H	-0.126483	-4.424464	7.165677
H	-1.158087	-4.795025	5.499015
H	0.662004	-5.575137	5.725138
H	-0.862447	-6.280765	6.844578
H	1.986721	1.315843	5.711688
H	3.709259	0.342143	5.717642
H	2.707291	0.762974	3.932993
H	0.170282	0.520434	5.380726
H	4.046134	-1.941620	6.796651
H	1.896086	-0.165768	7.867154
H	0.660028	1.107269	7.800481
H	4.150554	-2.877237	5.287251
H	5.986354	-3.297303	7.316501
H	5.395270	-4.646799	6.332645
H	2.886351	-5.605872	7.053458
H	2.123811	-4.626868	8.325396
H	0.190868	-1.753812	8.438136
H	-1.859044	0.399867	7.710156
H	-1.308756	-0.002301	9.352138
H	-2.224847	-1.191589	8.404823
H	4.273749	-3.720609	9.032478
H	4.759847	-5.367422	8.589785
H	2.663747	-4.075892	3.842400
H	0.899928	-4.483299	3.021533
H	2.491400	-4.116487	1.823303
H	-3.018299	-3.266873	4.418186
H	-2.487580	-1.701776	5.092484
H	-0.734782	-1.407373	1.943464
H	-0.757875	-3.174882	1.748350
H	-3.173709	-3.226822	1.643116
H	-2.909083	-1.637833	0.905766
H	-3.193159	-0.516285	3.077811
H	-4.449626	-1.765491	3.145641
H	1.656247	-2.630385	2.897694

$TS(E^{R}_{R} \rightarrow F^{R}_{R})$

G = -884,280272$kcal.mol^{-1}$

C	0.580416	-0.978225	0.611032
O	0.612299	-0.794527	2.049343
C	1.954380	-0.989370	2.552553
C	2.849179	-0.933947	1.322740
C	1.946968	-1.545025	0.247503
La	-1.529399	-0.750175	3.495924
O	-0.863665	0.160024	5.351411
C	-0.437489	0.744681	6.541700
C	0.705455	1.744018	6.280032
C	0.419562	2.784350	5.202437
O	0.738428	2.272724	3.899906
B	1.475897	2.978944	3.025696
B	-1.177946	-3.440408	3.652924
O	-3.980187	-1.136824	4.307941
C	-5.187901	-0.935166	3.525678
C	-6.285988	-1.671554	4.281781
C	-5.810123	-1.564284	5.732196
C	-4.308111	-1.749491	5.578198
B	-2.718848	0.775183	1.576333
C	-1.612605	1.396744	7.274736
H	1.609799	1.196966	5.988656
H	0.942652	2.263671	7.217528
H	-1.300458	1.823961	8.234412
H	-2.065220	2.191514	6.671756
H	-0.640338	3.058201	5.188856
H	1.003881	3.696606	5.373392
H	1.687824	2.470161	1.962109
H	1.909436	4.061720	3.322273
H	-0.028526	-0.035030	7.207785
H	-0.102503	-2.844529	3.799322
H	-1.657328	-3.104112	2.555396
H	-1.036922	-4.633244	3.712277
H	-1.937196	-3.029603	4.540711
H	-7.269575	-1.225352	4.113506
H	-5.372978	0.141916	3.464232
H	-1.494954	0.952272	1.590562
H	-3.136276	1.037634	2.715568
H	-3.257863	1.461764	0.748530
H	-2.925794	-0.431344	1.363298
H	-6.330339	-2.721400	3.972183
H	-3.715217	-1.255118	6.351960
H	-6.036527	-0.572654	6.139333
H	-6.253314	-2.315132	6.391472
H	-2.387015	0.649678	7.472707
H	1.998383	-1.966541	3.048758
H	2.152013	-0.200684	3.282042
H	3.093658	0.104513	1.075410
H	3.783149	-1.483466	1.466117
H	1.942781	-2.637235	0.327587
H	2.244313	-1.277666	-0.769777
H	0.393909	-0.001765	0.152502
H	-0.248404	-1.648879	0.367277
H	-4.026202	-2.807791	5.535857
H	-5.011021	-1.315362	2.517568

F_{R}

G = -884,286670 $kcal.mol^{-1}$

C	-2.517277	1.986482	0.213388
O	-2.370586	1.405856	1.535460
C	-3.314983	2.008195	2.449911
C	-3.670935	3.339394	1.809028
C	-3.676813	2.974214	0.321682
La	-1.257535	-0.888809	2.007195
B	0.867331	-0.285832	0.431522
O	-0.181120	-3.241380	2.332388
C	1.144848	-3.642431	1.902969
C	1.044478	-5.142294	1.683602
C	0.083685	-5.557663	2.799839
C	-0.909342	-4.400359	2.833927
B	-3.558909	-2.173251	1.370793
O	-1.167359	-0.371834	4.117709
C	-0.920492	-0.201607	5.483224
C	-0.853272	-1.566433	6.183072
C	-2.169079	-2.322573	6.106013
O	-1.965031	-3.707602	6.402443
B	-2.491742	-4.301110	7.487219
C	0.363406	0.596221	5.703489
H	-2.570560	-2.268447	5.089490
H	-1.756562	0.369673	5.927912
H	-0.072772	-2.162822	5.694144
H	-0.558199	-1.441896	7.232801
H	1.223971	0.047927	5.304354
H	0.304099	1.556886	5.183223
H	0.539313	0.790179	6.767440
H	0.108057	0.685503	0.562781
H	-1.569060	2.471162	-0.038374

H	-2.704828	1.181174	-0.503669
H	-4.621287	2.488813	0.054603
H	-3.541303	3.836532	-0.335870
H	-2.898000	4.085274	2.023682
H	-2.823944	2.083534	3.422190
H	1.219934	-0.622561	1.573597
H	0.203574	-1.215135	-0.056400
H	-3.697801	-0.941641	1.317636
H	-4.580805	-2.744479	1.098750
H	-3.185767	-2.446603	2.522475
H	-2.647500	-2.483023	0.587421
H	1.859892	-3.396842	2.698148
H	1.394670	-3.066478	1.010811
H	0.612033	-5.354861	0.699771
H	-1.764106	-4.561963	2.170679
H	-1.271032	-4.177002	3.840585
H	0.616827	-5.635980	3.753425
H	-0.412402	-6.513174	2.611759
H	-2.912236	-1.901333	6.795472
H	-3.171655	-3.675158	8.258438
H	-2.246728	-5.464226	7.636304
H	1.815914	-0.016825	-0.255476
H	-4.191530	1.352909	2.536460
H	-4.630632	3.727043	2.160307
H	2.018128	-5.635683	1.744255

$TS(A_R \rightarrow B^S_R)$

G = -884,202721 kcal.mol^{-1}

C	-1.143028	-4.966381	1.964362
O	-0.613186	-3.664298	2.327832
C	0.689825	-3.804791	2.944924
C	1.082523	-5.261444	2.731330
C	-0.277817	-5.963601	2.719399
La	-1.637512	-1.363228	1.776237
B	-3.407771	-1.755680	4.306833
O	-2.706656	0.960072	1.504529
C	-3.002218	1.561955	0.213520
C	-3.595759	2.929785	0.529237
C	-2.932679	3.274621	1.865345
C	-2.922238	1.926423	2.566109
B	0.388638	-0.596628	0.210293
B	-3.414959	-2.648296	0.232009
O	-0.782731	-0.644026	3.906057
C	-1.291280	-0.556482	5.067982
C	-0.740170	-1.075308	6.403122
C	-1.318059	0.235516	6.959473
C	-0.403061	1.186824	7.690207
O	-1.602709	0.695249	5.598447
H	-2.261836	0.093192	7.499263
H	0.591436	-3.556002	4.007428
H	-3.520770	-1.413577	0.143394
H	-2.248707	-2.921182	-0.091715
H	-0.255669	-6.941549	2.231793
H	-2.515640	-1.160604	5.081100
H	-2.774832	-2.707674	3.889079
H	-3.639106	-0.886077	3.481936
H	-4.325142	-2.010225	5.039379
H	0.379916	0.065729	1.256487
H	1.285991	-0.274860	-0.519863
H	-0.717419	-0.454210	-0.339795
H	0.464695	-1.796523	0.524707
H	-3.551670	-2.936019	1.431364
H	-4.222472	-3.216743	-0.451345
H	-2.127872	1.802962	3.303948
H	-3.885673	1.705506	3.040291
H	-3.476493	4.032008	2.435904
H	-1.908964	3.631226	1.707695
H	-4.682448	2.860831	0.648686
H	-3.385907	3.656926	-0.259269
H	-2.061562	1.636402	-0.341685
H	-3.681870	0.894658	-0.322392
H	1.368772	-3.090427	2.470527
H	1.752465	-5.625930	3.514369
H	1.586508	-5.384382	1.766751
H	-2.199381	-4.984049	2.238915
H	-1.055369	-5.081038	0.878837
H	-0.649816	-6.098446	3.741023
H	-0.164693	0.791561	8.683248
H	0.529422	1.329800	7.136385
H	-0.882423	2.161946	7.817968
H	-1.139754	-2.016889	6.779864
H	0.353253	-1.097182	6.387361

B^S_R

G = -884,205221 kcal.mol^{-1}

C	-3.836264	1.337055	2.533022
O	-2.899628	0.753215	1.591766
C	-2.846984	1.556586	0.379802
C	-3.879122	2.664260	0.574141
C	-3.959895	2.787101	2.097880
La	-1.384739	-1.303007	1.954261
O	-1.687355	-0.258633	4.445425
C	-0.989612	-0.271483	5.739043
C	0.486676	0.010960	5.624639
O	0.046060	-3.427808	2.313292
C	-0.598762	-4.686991	2.630764
C	0.550612	-5.660529	2.822829
C	1.532424	-5.194372	1.743995
C	1.371969	-3.675495	1.768986
B	0.946439	-0.039327	1.490725
B	-2.453688	-2.319137	-0.284539
O	-2.489154	-2.337201	3.796009
C	-2.399238	-1.513968	4.805069
C	-1.470568	-1.701739	6.017319
B	-4.664104	-0.644034	6.001755
H	-1.477728	0.462699	6.390002
H	2.091220	-3.184837	2.431424
H	-1.988468	-1.180307	-0.456474
H	-1.517901	-3.020667	0.128631
H	0.238788	-6.700937	2.700166
H	-3.452206	-1.187551	5.170438
H	-4.831295	-1.653107	6.626687
H	-5.322687	-0.446872	5.018296
H	-4.089616	0.276552	6.516055
H	0.983952	-0.738367	2.516062
H	1.991677	0.525080	1.311888
H	0.007409	0.760676	1.635730
H	0.652273	-0.782819	0.543602
H	-3.298998	-2.248851	0.619803
H	-2.922846	-2.754297	-1.300404
H	-3.426999	1.194752	3.534335
H	-4.792200	0.805879	2.451097
H	-4.889297	3.245422	2.445478
H	-3.119892	3.373786	2.485481
H	-4.849026	2.361681	0.165242
H	-3.578741	3.591978	0.080599
H	-1.828049	1.948410	0.290256
H	-3.056902	0.904438	-0.471216
H	1.436023	-3.214873	0.780261
H	2.564364	-5.499290	1.935956
H	1.238056	-5.594567	0.768164
H	-1.223554	-4.514953	3.508559
H	-1.237321	-4.978129	1.786420
H	0.985716	-5.547154	3.822023
H	0.946005	-0.030402	6.618336
H	0.985088	-0.718981	4.980648
H	0.663013	1.007700	5.209620
H	-1.952342	-1.895535	6.976334
H	-0.707522	-2.457588	5.811261

$TS(B^R_R \rightarrow C^S_R)$

G = -884,203029 kcal.mol^{-1}

C	-3.513211	1.665578	2.700551
O	-2.867447	0.854408	1.691128
C	-3.046423	1.457429	0.379521
C	-3.923816	2.685483	0.606866
C	-3.633780	3.041643	2.067331
La	-1.370179	-1.238623	2.025165
O	-1.455798	-0.107127	4.464405
C	-0.688946	-0.163431	5.707993
C	0.794319	0.037303	5.520277
O	0.037251	-3.390563	2.338980
C	-0.620223	-4.622648	2.727659
C	0.516019	-5.605992	2.951061
C	1.498428	-5.196867	1.850120
C	1.367025	-3.676092	1.827914
B	0.981585	-0.076048	1.371002
B	-2.629847	-2.232416	-0.138272
O	-2.425677	-2.167204	3.905607

C	-2.269402	-1.316538	4.910601
C	-1.236019	-1.557873	6.029797
B	-5.623809	-1.584662	5.537905
H	-1.088620	0.600529	6.388738
H	2.085580	-3.182925	2.489925
H	-1.971316	-1.214544	-0.405411
H	-1.832981	-3.056192	0.335350
H	0.187334	-6.645455	2.871319
H	-3.224679	-0.916153	5.309975
H	-5.278709	-2.145778	6.535257
H	-5.972912	-2.211345	4.584970
H	-5.653741	-0.388131	5.513113
H	1.031224	-0.688224	2.450046
H	2.038949	0.437682	1.119040
H	0.072306	0.763929	1.470625
H	0.637969	-0.885561	0.498591
H	-3.439408	-1.940468	0.753750
H	-3.182169	-2.658847	-1.116611
H	-2.892931	1.621026	3.597320
H	-4.499284	1.235452	2.918737
H	-4.420006	3.644709	2.529180
H	-2.686184	3.584419	2.153646
H	-4.981481	2.430226	0.481126
H	-3.685681	3.492152	-0.091021
H	-2.053050	1.722140	0.001236
H	-3.492216	0.710242	-0.280672
H	1.458167	-3.241932	0.829824
H	2.525766	-5.515909	2.044387
H	1.188036	-5.622646	0.890036
H	-1.229341	-4.398029	3.605030
H	-1.276467	-4.942830	1.907980
H	0.960020	-5.461056	3.942388
H	1.299903	-0.022219	6.490556
H	1.218967	-0.723241	4.859367
H	1.004645	1.019315	5.085956
H	-1.623264	-1.732548	7.035938
H	-0.543178	-2.356089	5.747913

C^S_R

G = -884,244233 kcal.mol^{-1}

C	-3.841902	1.512649	2.655060
O	-2.713104	0.987467	1.917004
C	-2.433537	1.825194	0.764517
C	-3.572307	2.837303	0.711681
C	-3.981361	2.951233	2.182330
La	-1.671115	-1.354872	2.307460
O	-1.695302	0.038343	4.732797
C	-0.721618	0.431978	5.761960
C	0.565712	0.994784	5.220940
O	-0.529832	-3.692929	2.380703
C	-0.934195	-4.838620	3.165675
C	0.228749	-5.808626	3.046602
C	0.658447	-5.595547	1.592810
C	0.466143	-4.092368	1.400871
B	0.838711	-0.504308	1.827019
B	-2.809294	-1.935554	-0.046605
O	-2.127395	-2.252278	4.697057
C	-2.031572	-1.161416	5.517706
C	-0.769312	-0.983539	6.356681
B	-3.523108	-2.452038	4.081252
H	-1.211023	1.161667	6.421078
H	1.374303	-3.518934	1.607971
H	-1.956712	-1.044441	-0.174518
H	-2.233204	-2.920395	0.436697
H	-0.065438	-6.839050	3.263223
H	-2.972060	-0.990256	6.059803
H	-4.337598	-2.854948	4.872822
H	-3.343742	-3.222057	3.140295
H	-3.881331	-1.357726	3.601736
H	0.783473	-1.198375	2.854640
H	1.958401	-0.122251	1.613037
H	0.053834	0.443095	1.979914
H	0.403593	-1.192124	0.894949
H	-3.639843	-1.549717	0.790370
H	-3.332817	-2.198670	-1.095756
H	-3.615482	1.402331	3.717141
H	-4.729510	0.917265	2.408418
H	-4.995191	3.335825	2.321092
H	-3.288933	3.602756	2.726991
H	-4.403620	2.446722	0.115185
H	-3.256695	3.787721	0.273667
H	-1.460152	2.300320	0.928515
H	-2.375207	1.182369	-0.116794
H	0.097815	-3.826678	0.405893
H	1.688314	-5.903893	1.395144
H	0.002351	-6.156588	0.918861
H	-1.140942	-4.484707	4.176455
H	-1.853612	-5.256222	2.737095
H	1.033406	-5.527691	3.735229
H	1.231857	1.239344	6.055801
H	1.069206	0.284674	4.561634
H	0.381023	1.913941	4.656788
H	-0.866671	-1.086165	7.438974
H	0.042503	-1.614843	5.985101

TS($C^S_R \rightarrow D^S_R$)

G = -884,229031 kcal.mol^{-1}

C	-0.311239	-4.381480	3.442674
O	-0.347523	-3.466691	2.319008
C	0.217219	-4.096902	1.138931
C	0.319290	-5.574108	1.489658
C	0.586064	-5.527304	2.995935
La	-1.308584	-1.071250	2.178372
B	1.050966	-0.392345	1.097635
O	-2.316763	1.326419	1.878844
C	-2.082328	2.144135	0.704047
C	-3.414708	2.819251	0.414617
C	-4.000678	2.986229	1.818614
C	-3.574334	1.688826	2.494055
B	-3.119766	-1.635226	0.235232
O	-1.124116	-0.440944	4.331549
C	-0.863281	0.105082	5.582368
C	-1.358477	-0.931269	6.649898
C	-2.555366	-1.475643	5.980801
O	-2.589128	-2.621319	5.513171
B	-3.654451	-2.997778	4.400733
C	0.603409	0.461963	5.778733
H	-1.467543	1.018808	5.729639
H	1.196012	-3.643736	0.948228
H	-2.290072	-0.796674	-0.149223
H	-2.489937	-2.654933	0.549044
H	0.343487	-6.462020	3.508142
H	-3.424260	-0.823635	5.815246
H	-3.945667	-4.152574	4.574714
H	-3.000183	-2.854125	3.369422
H	-4.560082	-2.195867	4.488735
H	1.220799	-0.985672	2.171004
H	2.093086	-0.074492	0.590375
H	0.343923	0.599074	1.340727
H	0.397467	-1.132462	0.345926
H	-3.645598	-1.200350	1.275183
H	-3.950823	-1.857992	-0.604836
H	-3.407636	1.785843	3.570484
H	-4.294611	0.882180	2.309362
H	-5.086122	3.114613	1.822755
H	-3.551764	3.849163	2.322926
H	-4.048696	2.162408	-0.189932
H	-3.291010	3.765512	-0.118424
H	-1.293600	2.865781	0.945773
H	-1.736039	1.492677	-0.101178
H	-0.446998	-3.885871	0.296794
H	1.109216	-6.076629	0.925615
H	-0.627865	-6.083797	1.283071
H	0.068600	-3.837037	4.310970
H	-1.334765	-4.710497	3.648434
H	1.638178	-5.292197	3.190800
H	0.785016	0.900506	6.766425
H	1.229659	-0.428884	5.667440
H	0.906257	1.184417	5.015318
H	-1.599187	-0.447126	7.602619
H	-0.620459	-1.723035	6.802201

D^S_R

G = -884,236165 kcal.mol^{-1}

C	0.418514	-3.925410	3.175006
O	-0.640537	-3.424805	2.307799
C	-1.110067	-4.489760	1.437781
C	-0.634681	-5.770147	2.101712
C	0.710967	-5.340171	2.689910

La	-1.411497	-0.968313	2.232613
O	-1.618063	-0.543604	4.378932
C	-1.735627	-0.043116	5.666395
C	-1.167136	-1.070649	6.676848
C	-1.882737	-2.361421	6.579504
O	-1.294109	-3.432330	6.405340
B	-2.047465	-4.846245	6.353390
O	-2.114003	1.424644	1.447405
C	-1.359401	2.306831	0.571939
C	-2.347738	3.377628	0.132784
C	-3.268215	3.484131	1.350356
C	-3.391262	2.028208	1.775452
B	1.029516	-0.242721	1.305465
B	-3.758740	-1.840468	1.208188
C	-1.023002	1.299014	5.823848
H	-2.803044	0.100597	5.915911
H	-0.657508	-4.353061	0.447476
H	-2.881816	-1.752589	0.329655
H	-3.344041	-2.603617	2.090355
H	1.046813	-5.984209	3.506231
H	-2.978712	-2.383248	6.672416
H	-1.563098	-5.453194	7.280720
H	-1.723641	-5.301244	5.277209
H	-3.230528	-4.595999	6.463172
H	1.107379	-1.254230	2.014893
H	2.102109	0.083187	0.873013
H	0.528456	0.648245	2.005023
H	0.235100	-0.497254	0.380915
H	-3.873207	-0.726629	1.738634
H	-4.800282	-2.216571	0.742782
H	-3.566010	1.890377	2.846075
H	-4.174427	1.501336	1.220007
H	-4.240213	3.929112	1.122726
H	-2.795256	4.079866	2.138952
H	-2.912343	3.045759	-0.745304
H	-1.849267	4.317492	-0.117872
H	-0.525512	2.722793	1.146471
H	-0.953632	1.709215	-0.246467
H	-2.194126	-4.394293	1.356275
H	-0.551045	-6.596431	1.390838
H	-1.323856	-6.062053	2.900431
H	1.272376	-3.247340	3.089251
H	0.037815	-3.921375	4.199914
H	1.485825	-5.331580	1.915491
H	-1.138613	1.704613	6.834980
H	0.044979	1.190129	5.608725
H	-1.438349	2.022268	5.116272
H	-1.320807	-0.690046	7.697999
H	-0.096505	-1.224969	6.515209

$TS(D^S_R \rightarrow E^S_R)$

G = -884,213644 kcal.mol^{-1}

C	0.503425	-3.851113	3.130847
O	-0.524793	-3.366450	2.218742
C	-0.946666	-4.437365	1.334827
C	-0.488950	-5.711285	2.024462
C	0.827714	-5.265983	2.664996
La	-1.352177	-0.922970	2.161410
O	-1.625171	-0.545890	4.304565
C	-1.752634	-0.186619	5.638082
C	-1.367007	-1.385267	6.545659
C	-2.215195	-2.559241	6.223033
O	-1.765885	-3.608606	5.697523
B	-2.346739	-4.554329	6.961203
O	-2.099830	1.462640	1.436679
C	-1.459401	2.284954	0.423861
C	-2.481376	3.357031	0.071913
C	-3.239227	3.527846	1.390615
C	-3.323922	2.092339	1.888000
B	1.091798	-0.145654	1.283116
B	-3.637369	-1.851069	1.040518
C	-0.893279	1.028939	5.980718
H	-2.807098	0.061243	5.857925
H	-0.453033	-4.302648	0.364139
H	-2.722488	-1.756308	0.202238
H	-3.248232	-2.595153	1.950822
H	1.141089	-5.904195	3.494923
H	-3.304771	-2.439734	6.331960
H	-1.375846	-5.232090	7.174982
H	-3.379431	-5.044096	6.592197
H	-2.471737	-3.770805	7.906719
H	1.177717	-1.125966	2.035771
H	2.169064	0.198993	0.877488
H	0.536224	0.753659	1.928387
H	0.341526	-0.462793	0.341482
H	-3.801017	-0.732388	1.547088
H	-4.647069	-2.257602	0.531890
H	-3.367791	1.998735	2.976480
H	-4.171888	1.553847	1.449818
H	-4.226493	3.980401	1.268075
H	-2.662596	4.144780	2.088521
H	-3.157702	3.002785	-0.713465
H	-2.006217	4.277353	-0.277068
H	-0.545900	2.703422	0.857989
H	-1.183885	1.642554	-0.415514
H	-2.026938	-4.351832	1.205212
H	-0.369208	-6.540726	1.322573
H	-1.210615	-6.008306	2.792495
H	1.354561	-3.166647	3.072408
H	0.080299	-3.838203	4.139149
H	1.630851	-5.253669	1.920108
H	-1.024113	1.337763	7.023496
H	0.165019	0.806843	5.809938
H	-1.170565	1.867718	5.335628
H	-1.545398	-1.113119	7.593786
H	-0.313007	-1.644340	6.413232

E^S_R

G = -884,285293 kcal.mol^{-1}

C	-3.359745	1.384624	0.836957
O	-2.532137	1.064116	1.982268
C	-1.833883	2.251665	2.437299
C	-2.186015	3.347817	1.435810
C	-3.548322	2.890821	0.907973
La	-1.561674	-1.290970	2.545988
O	-1.077020	-0.314760	4.463700
C	-1.317060	0.091787	5.769648
C	-0.010319	0.359917	6.514011
O	-0.413001	-3.566769	3.066642
C	-0.405310	-4.649115	2.095708
C	0.779797	-5.529664	2.475725
C	1.738924	-4.524733	3.119148
C	0.779966	-3.627696	3.884699
B	0.586115	-0.881699	0.935424
B	-3.687653	-2.205497	1.099803
C	-2.177869	-0.942368	6.512048
C	-3.430693	-1.351458	5.752668
O	-3.133508	-2.310643	4.710781
B	-3.650684	-3.563109	4.754817
H	-1.895560	1.037982	5.759671
H	-0.281466	-4.208418	1.100675
H	-2.926341	-1.559501	0.370739
H	-3.023852	-3.129813	1.597479
H	2.482165	-4.990719	3.771490
H	-3.893041	-0.487592	5.261840
H	-4.369273	-3.875891	5.664098
H	-3.344312	-4.308378	3.876394
H	-4.169695	-1.805162	6.421286
H	0.939267	-1.017454	2.115427
H	1.531482	-0.683885	0.218061
H	-0.216232	0.064563	0.895891
H	-0.032078	-1.898028	0.589534
H	-4.041905	-1.468930	2.036349
H	-4.642435	-2.624186	0.498810
H	-0.764044	2.031900	2.481268
H	-2.190741	2.480476	3.446736
H	-2.208060	4.337196	1.900306
H	-1.453374	3.370815	0.622156
H	-4.344998	3.145295	1.616134
H	-3.802354	3.323210	-0.063318
H	-2.831084	1.084879	-0.075689
H	-4.277184	0.800075	0.921078
H	-1.372787	-5.154250	2.146629
H	1.205881	-6.037229	1.606729
H	0.478701	-6.292446	3.202351
H	1.144177	-2.607495	4.028633
H	0.510001	-4.054751	4.858914
H	2.263333	-3.945981	2.351903
H	-0.189306	0.729125	7.530651

H	0.583447	-0.558713	6.578596
H	0.580343	1.104794	5.973462
H	-2.488417	-0.532860	7.482657
H	-1.585492	-1.842775	6.722848

$TS(C^S_R \rightarrow E^S_R)$

G = -884,208937 kcal.mol^{-1}

C	-1.655317	1.563183	0.417193
O	-2.344902	0.865828	1.487434
C	-3.559114	1.572540	1.841307
C	-3.370022	2.973081	1.281171
C	-2.591051	2.690871	-0.005714
La	-1.569978	-1.247354	2.786269
B	0.876510	-0.340214	2.045571
O	-0.634399	-3.544191	2.004939
C	0.685974	-3.822584	1.473821
C	0.591286	-5.234223	0.920943
C	-0.342413	-5.901015	1.932659
C	-1.347334	-4.794962	2.235734
B	-3.984484	-2.227264	2.062066
O	-1.210124	-2.550277	4.961899
C	-1.745046	-1.773185	5.892556
C	-0.936496	-0.759422	6.668977
C	-1.520943	0.475637	5.971992
C	-0.553639	1.606859	5.687409
O	-2.028605	-0.143527	4.792879
B	-1.003990	-3.728325	6.002353
H	-2.801231	-1.909375	6.129320
H	-2.369845	0.864523	6.555992
H	0.124476	-0.902964	6.445142
H	-1.091600	-0.820963	7.749327
H	0.299551	1.248687	5.102926
H	-1.051500	2.398324	5.118154
H	-0.181185	2.042945	6.621132
H	0.223714	0.564761	2.575668
H	-0.705454	1.930807	0.816731
H	-1.445504	0.847414	-0.381874
H	-3.271525	2.353575	-0.795030
H	-2.041945	3.558874	-0.379612
H	-2.773030	3.583881	1.967269
H	-3.661638	1.531832	2.928439
H	0.981121	-1.254876	2.871537
H	0.195799	-0.773988	1.093657
H	-4.099049	-1.108933	2.577359
H	-5.047348	-2.668678	1.715188
H	-3.437723	-2.954203	2.901325
H	-3.209214	-2.119945	1.094734
H	1.415137	-3.752982	2.289120
H	0.915752	-3.056206	0.732018
H	0.139153	-5.225793	-0.077117
H	-2.207549	-4.810979	1.559768
H	-1.702276	-4.802490	3.268630
H	0.209663	-6.175478	2.837756
H	-0.830078	-6.800042	1.547015
H	-1.430521	-3.189935	7.051147
H	0.176077	-3.923683	6.137100
H	-1.737848	-4.640547	5.715055
H	1.949033	0.040771	1.657763
H	-4.409826	1.055216	1.383666
H	-4.321878	3.481816	1.108044
H	1.569901	-5.716415	0.850600

$TS(E^S_R \rightarrow F^S_R)$

G = -884,281347 kcal.mol^{-1}

C	-2.875978	1.525673	0.211649
O	-2.281745	1.370270	1.524884
C	-1.955715	2.666853	2.083180
C	-2.181751	3.665840	0.954232
C	-3.284313	2.988509	0.136692
La	-1.406538	-0.909600	2.431189
O	-1.642681	-0.453034	4.539885
C	-1.805150	-0.086270	5.876765
C	-0.709368	0.884218	6.312762
O	-0.468573	-3.313141	2.522163
C	-0.696227	-4.355726	1.543217
C	-0.194248	-5.627799	2.207211
C	0.993190	-5.110499	3.023109
C	0.486583	-3.761215	3.521328
B	1.039917	-0.105333	1.559246
B	-3.636360	-1.957041	1.264649
C	-1.836833	-1.325356	6.782757
C	-2.901741	-2.351635	6.388826
O	-2.295864	-3.516388	5.809109
B	-2.577822	-4.756881	6.239807
H	-2.779428	0.425809	5.987222
H	-0.122418	-4.117597	0.638601
H	-2.740053	-1.752527	0.425804
H	-3.181384	-2.715653	2.130801
H	1.271222	-5.772074	3.847507
H	-3.571756	-1.934891	5.630073
H	-3.347084	-4.935711	7.147571
H	-2.017571	-5.659545	5.683256
H	-3.504005	-2.663102	7.250298
H	1.140190	-0.991078	2.419940
H	2.117721	0.253039	1.165074
H	0.413681	0.828461	2.079900
H	0.351011	-0.556195	0.626683
H	-3.886099	-0.882125	1.827122
H	-4.615411	-2.418964	0.740511
H	-0.922034	2.635939	2.438214
H	-2.626092	2.847048	2.931405
H	-2.462411	4.653642	1.328760
H	-1.272366	3.773684	0.353601
H	-4.262479	3.137661	0.606967
H	-3.341593	3.348915	-0.893619
H	-2.119102	1.278995	-0.543282
H	-3.702640	0.816444	0.137901
H	-1.761947	-4.357035	1.305466
H	0.083667	-6.393130	1.477820
H	-0.964111	-6.041730	2.866826
H	1.272198	-3.004182	3.601105
H	-0.047394	-3.841700	4.472605
H	1.870428	-4.979022	2.380471
H	-0.849457	1.210137	7.349685
H	0.273664	0.408215	6.228534
H	-0.710218	1.771102	5.672226
H	-1.997394	-1.002115	7.818728
H	-0.856350	-1.815479	6.752122

A_s

G = -884,229398 kcal.mol^{-1}

La	-1.835700	-0.928686	2.340995
B	-3.225666	-0.507554	4.660557
H	-4.005855	-0.748916	3.737559
H	-2.461692	-1.476761	4.767863
H	-3.812440	-0.292077	5.692233
H	-2.541692	0.475532	4.333376
O	0.140736	-0.568727	4.083551
C	0.333480	-0.175478	5.211491
O	1.347476	-0.547290	6.012219
H	0.552363	-0.317403	7.940814
C	0.849989	0.325137	7.108234
C	1.879210	1.347698	7.510601
H	2.769999	0.862361	7.918671
H	1.464455	2.005158	8.281358
H	2.178172	1.960569	6.654918
C	-0.313543	0.759819	6.202613
H	-1.322152	0.457194	6.491534
H	-0.317809	1.807696	5.893220
B	0.083294	-0.118308	0.633454
H	-1.804015	1.854123	0.002871
H	-1.001283	-0.276644	0.058539
H	0.940275	0.254870	-0.122795
H	-0.086786	0.693569	1.557916
H	0.369400	-1.204364	1.158123
H	-3.686351	-1.201876	0.673492
H	-2.292025	-2.621428	0.567201
H	-4.218207	-3.092682	0.181979
B	-3.482300	-2.413091	0.845991
H	-3.635220	-2.635467	2.056452
C	-2.446120	2.344674	0.734951
H	-1.843044	3.048134	1.322481
C	-3.677938	3.015036	0.147555
H	-4.055920	2.437937	-0.703331
H	-3.471723	4.033237	-0.193076
C	-4.659802	2.951440	1.319114
H	-4.441365	3.743313	2.044405
H	-5.705654	3.048171	1.016277
C	-4.363010	1.581364	1.915261

H	-4.503131	1.524028	2.996521
H	-4.950489	0.788917	1.437763
O	-0.820375	-3.232515	2.991209
C	0.586576	-3.581150	3.029676
C	-1.634093	-4.416869	3.200158
C	-0.662117	-5.495847	3.657093
C	0.621794	-5.098493	2.925407
O	-2.960869	1.326945	1.630203
H	-2.116669	-4.667060	2.250118
H	1.004594	-3.224075	3.976956
H	1.084234	-3.063453	2.206775
H	1.525674	-5.521730	3.371511
H	0.577523	-5.411467	1.876646
H	-1.014560	-6.498793	3.402736
H	-0.514570	-5.450485	4.741930
H	-2.404908	-4.171239	3.935141

$TS(A_R \rightarrow B^R_R)$

G = -884,203096 kcal.mol^{-1}

La	-1.862250	-1.028006	2.109546
B	-3.277611	-0.816559	4.860057
H	-4.094810	-0.888580	5.737852
H	-2.810452	-1.881357	4.499898
H	-2.234190	-0.235460	5.416681
H	-3.548751	-0.035878	3.960112
O	-0.670350	-0.003927	3.936334
C	-0.907419	0.059962	5.182715
O	-0.258016	-0.801456	6.062357
H	-1.016934	-0.077557	7.885386
C	-0.275705	0.203296	7.128386
C	1.093748	0.382328	7.735729
H	1.432964	-0.550266	8.195452
H	1.063223	1.154785	8.510509
H	1.818998	0.677931	6.972588
C	-0.782146	1.258687	6.133562
H	-1.695636	1.800968	6.378088
H	-0.003085	1.946978	5.793958
B	-0.170897	-0.343305	0.151592
H	-4.515998	0.742470	0.179023
H	-1.343208	-0.448807	-0.247141
H	0.572488	-0.056277	-0.747087
H	-0.156387	0.505387	1.053989
H	0.128459	-1.435266	0.662315
H	-4.013570	-1.484835	0.924480
H	-2.598561	-2.832969	0.554353
H	-4.537110	-3.420148	0.630270
B	-3.709765	-2.680090	1.087754
H	-3.569381	-2.849609	2.308232
C	-3.725385	1.485572	0.303663
H	-3.000879	1.382622	-0.512160
C	-4.221664	2.915312	0.450316
H	-5.175252	2.938000	0.989002
H	-4.362681	3.403477	-0.517340
C	-3.110780	3.549793	1.290765
H	-2.248529	3.793470	0.661166
H	-3.424416	4.460018	1.808402
C	-2.759695	2.429522	2.262708
H	-1.706940	2.418306	2.557726
H	-3.385704	2.449266	3.162092
O	-0.535389	-3.104849	2.827309
C	0.827247	-3.008389	3.330338
C	-0.881757	-4.491596	2.586056
C	0.111694	-5.283338	3.419297
C	1.377054	-4.430913	3.289822
O	-3.046500	1.197949	1.553525
H	-0.774163	-4.698816	1.514856
H	0.776464	-2.600567	4.343315
H	1.378083	-2.312635	2.690794
H	2.102577	-4.610708	4.087284
H	1.869241	-4.627092	2.331318
H	0.239503	-6.304502	3.050730
H	-0.218119	-5.331735	4.462738
H	-1.926847	-4.624679	2.870125

B^R_S

G = -884,206660 kcal.mol^{-1}

C	0.311785	-4.013192	3.102847
O	-0.991386	-3.506270	2.711583
C	-2.000482	-4.543113	2.875420
C	-1.279815	-5.709587	3.541216
C	0.163502	-5.525054	3.065570
La	-1.480488	-1.101353	1.962054
O	0.139143	-0.860185	4.091646
C	0.925787	0.138676	4.824878
C	1.738119	1.034894	3.924363
O	-2.271863	1.319622	1.562610
C	-3.475154	1.795226	2.217956
C	-3.603545	3.240186	1.768415
C	-3.123415	3.155619	0.316469
C	-1.990400	2.134568	0.390927
O	-2.146820	-0.473078	4.173136
C	-1.063113	-0.528213	4.896232
C	-0.340581	0.691412	5.493828
B	0.546199	-0.638291	0.256409
B	-3.643712	-2.074342	0.708968
B	-0.894061	-2.348528	6.868076
H	-2.380354	-4.793503	1.880410
H	-4.324385	1.189756	1.875674
H	-3.337354	1.645613	3.290073
H	0.688713	-1.704815	0.882372
H	0.426197	0.259040	1.106940
H	1.475441	-0.423508	-0.473427
H	-0.525377	-0.720526	-0.359034
H	-2.945354	3.885860	2.360388
H	-4.626166	3.614456	1.861987
H	-1.012345	2.599985	0.546226
H	-2.783861	4.114136	-0.084272
H	-1.933786	1.481107	-0.483026
H	-3.929276	2.786564	-0.326364
H	-2.615839	-2.720966	0.448612
H	-3.413847	-0.899284	0.382491
H	-4.600075	-2.517329	0.133853
H	-3.799998	-2.093933	1.939703
H	-2.817406	-4.134261	3.474724
H	-1.334060	-5.621588	4.631110
H	-1.710318	-6.672098	3.253377
H	0.894776	-6.026181	3.705004
H	0.286633	-5.898117	2.042939
H	0.537924	-3.644644	4.108401
H	1.045717	-3.615585	2.397476
H	-1.145691	-1.362500	5.705424
H	0.281597	-2.146554	7.004965
H	-0.340189	0.772090	6.581494
H	-0.697636	1.620262	5.040879
H	2.285415	1.765385	4.530118
H	2.465174	0.455497	3.347939
H	1.572364	-0.394048	5.531192
H	-1.249563	-3.304252	6.233353
H	-1.670720	-1.822136	7.614652
H	1.099143	1.576319	3.220829

$TS(B^R_S \rightarrow C^R_S)$

G = -884,202962 kcal.mol^{-1}

O	-0.159522	-0.186490	0.953702
C	0.376934	1.162885	0.835976
C	1.297387	1.140044	-0.384385
C	1.653812	-0.342864	-0.520213
C	0.350955	-1.011145	-0.116901
H	0.458288	-2.024556	0.272044
H	-0.374065	-1.013097	-0.941652
H	1.970992	-0.619858	-1.529185
H	2.449984	-0.618193	0.179853
H	2.170968	1.782440	-0.246705
H	0.764216	1.484068	-1.277205
H	0.903525	1.379718	1.768615
H	-0.462847	1.855391	0.731504
La	-1.575983	-0.823753	3.028482
B	-0.645665	-3.324003	2.493109
H	0.286652	-2.517936	2.616336
H	-0.244763	-4.423077	2.213267
H	-1.284785	-3.320002	3.549601
H	-1.405092	-2.894175	1.604124
O	-0.029496	0.645065	3.968430
C	-0.178300	0.544585	5.284034
H	-0.515976	1.480451	5.770859
O	-1.236536	-0.510553	5.609690
C	-0.356007	-1.081928	6.629641
H	-0.721222	-0.754294	7.611592
H	1.384914	0.323286	6.893680

H	1.521935	-0.807096	5.510154
C	0.830498	-0.243226	6.142557
H	0.436259	-2.939953	7.342199
C	-0.267637	-2.587643	6.580086
H	0.079517	-2.934066	5.602268
H	-1.240807	-3.046189	6.782777
H	-0.739831	3.916056	6.490989
H	0.019778	4.390784	4.625154
B	0.179881	3.963137	5.727874
H	1.265679	3.610165	6.082564
O	-3.618556	-2.061140	4.104168
B	-3.543651	0.758991	2.048328
C	-4.340458	-3.061235	3.345917
C	-5.538326	-3.425114	4.210723
C	-5.848548	-2.090381	4.892855
C	-4.456499	-1.531402	5.159950
H	-3.615697	0.662084	3.282918
H	-2.439990	1.245245	1.787983
H	-4.442480	1.421885	1.603678
H	-4.049508	-1.873327	6.117853
H	-4.410083	-0.440253	5.121221
H	-4.653512	-2.617154	2.392429
H	-3.652868	-3.887504	3.151016
H	-5.260686	-4.183550	4.951058
H	-6.371878	-3.813031	3.619598
H	-6.397298	-1.432404	4.210822
H	-6.433655	-2.196790	5.810139
H	-3.573016	-0.393976	1.577178

C^R_S

G = -884,244095 kcal.mol^{-1}

La	-1.536361	-0.604860	2.832322
O	-0.025321	1.167557	3.980211
H	3.631581	0.268290	0.352423
B	-0.951121	2.112633	3.195695
H	-2.126204	1.814550	3.483300
H	-0.771976	1.812417	2.015835
H	-0.739163	3.278157	3.419033
H	2.446324	0.089222	2.473418
H	1.370306	1.205645	1.600651
C	1.825958	0.214819	1.578050
C	2.601658	-0.095767	0.308102
H	2.112162	0.360982	-0.558910
H	2.670556	-2.025668	-0.757827
C	2.498437	-1.621168	0.242896
H	3.221635	-2.082534	0.924538
H	0.350040	-1.849234	-0.100561
C	1.073328	-1.871811	0.721929
H	0.947372	-2.801602	1.281239
O	0.761574	-0.766457	1.613158
C	-0.305593	1.050836	5.313414
H	-0.800257	1.952709	5.698351
H	1.558415	-0.018851	5.649255
C	0.764811	0.460569	6.228289
H	1.194476	1.121978	6.982802
C	-0.320671	-0.530527	6.672604
H	-0.811972	-0.207934	7.600097
H	0.473133	-2.343961	5.807980
C	-0.021802	-2.005891	6.721024
H	0.630058	-2.213857	7.576854
H	-0.938983	-2.589204	6.843786
O	-1.171845	-0.119585	5.547160
H	-0.992433	-4.382037	3.600729
H	-2.094582	-2.740011	4.016430
B	-1.158803	-3.217076	3.355234
H	-0.149233	-2.547171	3.621184
H	-1.424181	-3.030570	2.161769
O	-3.899997	-0.469231	3.891691
B	-2.879009	-0.532308	0.518558
C	-5.007659	0.274896	3.316945
C	-6.232012	-0.148384	4.116131
C	-5.634221	-0.442830	5.493345
C	-4.310995	-1.101068	5.129170
H	-2.942267	0.545935	1.128516
H	-1.674972	-0.776677	0.347356
H	-3.473518	-0.475226	-0.524269
H	-4.424385	-2.175636	4.944380
H	-3.516672	-0.941863	5.860333
H	-4.789891	1.343082	3.430058
H	-5.058659	0.030852	2.254557
H	-6.673594	-1.055235	3.688877
H	-7.000103	0.629136	4.133448
H	-5.461205	0.488551	6.043983
H	-6.261872	-1.092297	6.109343
H	-3.324857	-1.420502	1.256859

TS($C^R_S \rightarrow D^R_S$)

G = -884,229340 kcal.mol^{-1}

C	1.473338	-2.098044	1.768231
O	0.608135	-0.946131	1.591444
C	1.151381	-0.066280	0.569833
C	2.207484	-0.896393	-0.143500
C	2.741833	-1.774011	0.990447
La	-1.722313	-0.733932	2.716405
B	-1.837155	-3.410699	2.616344
O	-3.998831	-0.450622	3.956359
C	-4.183875	-1.071852	5.252777
C	-5.654788	-0.871439	5.601868
C	-6.311513	-0.813217	4.220565
C	-5.281053	-0.038090	3.415732
B	-3.093515	0.224688	0.584302
O	0.645504	1.911219	4.066195
B	-0.213932	2.616843	2.939956
O	-0.922411	-0.420593	4.810587
C	-0.396543	-0.393915	6.096046
C	0.127557	-1.747864	6.554466
C	0.157764	1.698030	5.184327
C	0.724466	0.698227	6.110771
H	2.975796	-0.273004	-0.608120
H	-0.607687	1.655640	2.280237
H	0.542405	3.294537	2.294813
H	-1.122916	3.199120	3.491990
H	1.578238	0.811763	1.065663
H	0.325074	0.253644	-0.068775
H	1.748345	-1.513591	-0.923275
H	3.248663	-2.676537	0.639209
H	3.443694	-1.207901	1.612910
H	0.954183	-2.976255	1.371361
H	1.635246	-2.240729	2.839662
H	-0.765575	2.226833	5.457373
H	1.661845	0.307645	5.706311
H	0.884811	1.106836	7.114708
H	-1.167840	-0.057773	6.814504
H	0.922387	-2.093149	5.885729
H	0.520982	-1.704701	7.576366
H	-0.680412	-2.484404	6.522862
H	-1.906423	-4.609700	2.565320
H	-2.874261	-2.915482	3.089302
H	-0.897042	-3.039665	3.331018
H	-1.687319	-2.917832	1.488379
H	-3.112414	0.997043	1.558484
H	-1.900495	0.032643	0.301032
H	-3.709947	0.682240	-0.340830
H	-3.925843	-2.132763	5.156753
H	-3.492749	-0.601584	5.955912
H	-5.381936	1.044658	3.557579
H	-5.277486	-0.256981	2.347579
H	-6.435744	-1.821235	3.810450
H	-7.288001	-0.321905	4.225718
H	-5.800392	0.075461	6.133698
H	-6.039927	-1.676941	6.232489
H	-3.548438	-0.867776	0.953990

D^R_S

G = -884,230763 kcal.mol^{-1}

C	1.461863	-2.056616	1.746424
O	0.572805	-0.927380	1.550694
C	1.091146	-0.058306	0.505837
C	2.181277	-0.869187	-0.178310
C	2.729228	-1.709036	0.977693
La	-1.730554	-0.741240	2.725728
B	-1.853940	-3.414021	2.536154
O	-4.020830	-0.526982	3.969248
C	-4.204961	-1.203401	5.237773
C	-5.683994	-1.052414	5.578048
C	-6.327255	-0.950730	4.193084
C	-5.306610	-0.117795	3.435120
B	-3.122007	0.303078	0.647164
O	0.750058	1.721669	3.967680

B	-0.004317	2.608488	2.898389
O	-0.942133	-0.454667	4.816951
C	-0.463811	-0.279980	6.087933
C	-0.114081	-1.595479	6.781449
C	0.459450	1.746825	5.171417
C	0.831694	0.645186	6.058616
H	2.935520	-0.230666	-0.645368
H	-0.696194	1.775548	2.317888
H	0.843568	3.056561	2.168367
H	-0.671366	3.416828	3.507163
H	1.480819	0.848314	0.979159
H	0.258033	0.212663	-0.146442
H	1.752515	-1.515306	-0.952088
H	3.266978	-2.602051	0.648610
H	3.405923	-1.110602	1.597744
H	0.968048	-2.951012	1.352664
H	1.616314	-2.185371	2.820927
H	-0.207151	2.547304	5.524684
H	1.664240	0.078020	5.635521
H	1.061922	0.988286	7.071538
H	-1.197895	0.258946	6.717377
H	0.638324	-2.140483	6.203108
H	0.265598	-1.433891	7.796704
H	-1.008695	-2.221731	6.841087
H	-1.934208	-4.610426	2.450109
H	-2.888833	-2.925434	3.020675
H	-0.913818	-3.073159	3.265761
H	-1.696140	-2.889927	1.424230
H	-3.144542	1.024989	1.659831
H	-1.928787	0.140317	0.350232
H	-3.747371	0.802082	-0.250152
H	-3.920163	-2.253155	5.102591
H	-3.533598	-0.745067	5.967741
H	-5.433244	0.954991	3.625427
H	-5.288327	-0.286925	2.358158
H	-6.422412	-1.942778	3.738586
H	-7.315321	-0.483167	4.207609
H	-5.857733	-0.132224	6.147225
H	-6.056562	-1.892628	6.169779
H	-3.564147	-0.811337	0.960833

$TS(D^R_S \rightarrow E^R_S)$

G = -884,210959 $kcal.mol^{-1}$

La	-1.682783	-0.970930	2.938651
O	-0.689662	1.328589	3.635648
H	3.046803	0.227797	0.029084
B	-0.205309	2.829436	3.643019
H	-1.081182	3.543258	3.231177
H	0.902012	2.892764	3.171235
H	-0.090706	3.015674	4.883253
H	1.882358	0.628498	2.124562
H	0.516484	0.735261	0.990045
C	1.320302	0.091039	1.354380
C	2.218638	-0.449566	0.252404
H	1.643888	-0.603224	-0.667141
H	3.027673	-2.493100	0.075382
C	2.668646	-1.792000	0.833198
H	3.467809	-1.645083	1.568400
H	0.738166	-2.808700	0.810509
C	1.398621	-2.285754	1.509770
H	1.567256	-2.926094	2.377874
O	0.719791	-1.083927	1.967757
C	-0.671095	1.304910	4.963966
H	-1.539278	1.696785	5.494988
H	1.349691	0.620495	5.095562
C	0.504558	0.792191	5.768595
H	0.813222	1.475666	6.564421
C	-0.164328	-0.514379	6.214043
H	-0.636469	-0.369997	7.199802
H	1.236389	-1.897802	5.320527
C	0.722178	-1.742840	6.274825
H	1.477046	-1.641415	7.062780
H	0.122368	-2.633259	6.485328
O	-1.179619	-0.595640	5.222337
H	-1.663946	-4.849923	2.883032
H	-2.716753	-3.199624	3.406505
B	-1.670430	-3.649297	2.908940
H	-0.730308	-3.198489	3.581707
H	-1.583843	-3.168791	1.767874
O	-4.042284	-0.596414	3.921220
B	-2.768034	-0.051770	0.643586
C	-5.181946	0.075573	3.316982
C	-6.379741	-0.318851	4.171159
C	-5.746422	-0.528164	5.548870
C	-4.426644	-1.192109	5.187756
H	-2.808397	0.790917	1.554218
H	-1.578296	-0.367006	0.483438
H	-3.261062	0.375738	-0.365354
H	-4.542097	-2.272629	5.038425
H	-3.610244	-1.013095	5.890367
H	-4.991152	1.153718	3.347662
H	-5.247661	-0.240648	2.274703
H	-6.819189	-1.254187	3.808051
H	-7.158663	0.447922	4.163337
H	-5.571192	0.434173	6.042898
H	-6.352171	-1.148435	6.214616
H	-3.346707	-1.072637	1.047615

E^R_S

G = -884,284526 $kcal.mol^{-1}$

H	-1.066327	3.275593	2.185503
B	-1.746184	2.332187	2.529172
H	-0.283533	3.194554	4.296288
H	-2.887514	2.617675	2.800114
O	-1.047949	1.460775	3.510296
C	-0.531348	2.180629	4.634968
H	-1.322181	2.274446	5.395004
C	0.708466	1.539634	5.243731
H	1.460582	1.398342	4.454644
H	1.126374	2.268030	5.952245
C	0.484953	0.207464	5.972440
H	-0.265396	0.387204	6.766137
H	2.563077	-0.414957	5.911892
C	1.765863	-0.275387	6.650932
H	2.117894	0.437920	7.404905
H	1.586419	-1.237265	7.139261
O	0.000717	-0.768393	5.096930
La	-1.191488	-1.047377	3.292648
O	1.001863	-1.373285	1.925075
C	2.262616	-1.714155	2.552322
H	2.534525	-0.893255	3.218230
H	2.124640	-2.624585	3.147860
C	3.226720	-1.938132	1.398388
H	4.062664	-2.584537	1.677982
H	3.633281	-0.983480	1.046733
C	2.309734	-2.558169	0.341267
H	2.145519	-3.619664	0.554381
H	2.699090	-2.470936	-0.676215
C	1.016817	-1.772954	0.528184
H	0.989019	-0.862063	-0.078880
H	0.118971	-2.365362	0.330259
H	-1.864784	-3.352580	4.056797
B	-1.916146	-3.644290	2.850728
H	-0.795966	-3.397084	2.377083
H	-2.218904	-4.798238	2.698977
H	-2.727823	-2.881744	2.305999
B	-2.284861	0.677378	1.101299
O	-3.445545	-0.848708	4.587540
C	-4.113181	0.402856	4.862919
C	-5.589786	0.049775	4.864732
C	-5.576077	-1.323859	5.541620
C	-4.289143	-1.957048	5.010306
H	-3.003020	0.258827	1.989312
H	-1.658274	1.780154	1.320679
H	-1.325914	-0.053971	0.876735
H	-2.910059	0.939386	0.111977
H	-4.456234	-2.589769	4.135256
H	-3.747792	-2.536887	5.762486
H	-3.787558	0.772440	5.844615
H	-3.818284	1.118737	4.092667
H	-5.959550	-0.024432	3.836542
H	-6.195911	0.787670	5.396763
H	-5.530114	-1.208949	6.629967
H	-6.454512	-1.929549	5.305086

$TS(C^R_S \rightarrow E^R_S)$

G = -884,206953 $kcal.mol^{-1}$

La	-1.682783	-0.970930	2.938651
O	-0.689662	1.328589	3.635648

H	3.046803	0.227797	0.029084
B	-0.205309	2.829436	3.643019
H	-1.081182	3.543258	3.231177
H	0.902012	2.892764	3.171235
H	-0.090706	3.015674	4.883253
H	1.882358	0.628498	2.124562
H	0.516484	0.735261	0.990045
C	1.320302	0.091039	1.354380
C	2.218638	-0.449566	0.252404
H	1.643888	-0.603224	-0.667141
H	3.027673	-2.493100	0.075382
C	2.668646	-1.792000	0.833198
H	3.467809	-1.645083	1.568400
H	0.738166	-2.808700	0.810509
C	1.398621	-2.285754	1.509770
H	1.567256	-2.926094	2.377874
O	0.719791	-1.083927	1.967757
C	-0.671095	1.304910	4.963966
H	-1.539278	1.696785	5.494988
H	1.349691	0.620495	5.095562
C	0.504558	0.792191	5.768595
H	0.813222	1.475666	6.564421
C	-0.164328	-0.514379	6.214043
H	-0.636469	-0.369997	7.199802
H	1.236389	-1.897802	5.320527
C	0.722178	-1.742840	6.274825
H	1.477046	-1.641415	7.062780
H	0.122368	-2.633259	6.485328
O	-1.179619	-0.595640	5.222337
H	-1.663946	-4.849923	2.883032
H	-2.716753	-3.199624	3.406505
B	-1.670430	-3.649297	2.908940
H	-0.730308	-3.198489	3.581707
H	-1.583843	-3.168791	1.767874
O	-4.042284	-0.596414	3.921220
B	-2.768034	-0.051770	0.643586
C	-5.181946	0.075573	3.316982
C	-6.379741	-0.318851	4.171159
C	-5.746422	-0.528164	5.548870
C	-4.426644	-1.192109	5.187756
H	-2.808397	0.790917	1.554218
H	-1.578296	-0.367006	0.483438
H	-3.261062	0.375738	-0.365354
H	-4.542097	-2.272629	5.038425
H	-3.610244	-1.013095	5.890367
H	-4.991152	1.153718	3.347662
H	-5.247661	-0.240648	2.274703
H	-6.819189	-1.254187	3.808051
H	-7.158663	0.447922	4.163337
H	-5.571192	0.434173	6.042898
H	-6.352171	-1.148435	6.214616
H	-3.346707	-1.072637	1.047615

$TS(E^R_S \rightarrow F^R_S)$

G = -884,280924 kcal.mol^{-1}

C	2.034594	-0.764842	2.312599
O	0.761706	-0.950441	1.651869
C	0.963562	-1.369391	0.274905
C	2.457698	-1.643155	0.152923
C	3.052800	-0.681840	1.185396
La	-1.566746	-0.806906	2.752909
B	-2.113869	-3.250850	1.750458
O	-3.843709	-0.451714	3.993506
C	-4.204151	-1.406612	5.021212
C	-5.408928	-0.793412	5.715130
C	-6.128607	-0.121153	4.542697
C	-4.972465	0.414438	3.702819
B	-2.568955	1.120323	1.035905
O	-0.287046	1.506137	3.750099
B	-0.497704	2.517261	2.840018
O	-0.859634	-1.115863	4.817761
C	-0.517563	-0.663083	6.086544
C	0.390000	-1.660394	6.803411
C	-0.636506	1.709053	5.139574
C	0.126188	0.732290	6.019698
H	2.824908	-1.470269	-0.861815
H	-0.999221	3.544639	3.201407
H	0.002486	2.376110	1.767726
H	-0.397219	2.745682	5.396445
H	0.636344	-0.549591	-0.373815
H	0.334796	-2.244487	0.094268
H	2.680452	-2.680657	0.424280
H	4.056640	-0.965385	1.512436
H	3.096814	0.336391	0.783821
H	2.218737	-1.627637	2.964149
H	1.962500	0.137620	2.922871
H	-1.720913	1.575869	5.251309
H	1.153601	0.657684	5.640194
H	0.192404	1.152441	7.031854
H	-1.439146	-0.554958	6.695967
H	1.328908	-1.780510	6.251733
H	0.626016	-1.333760	7.822993
H	-0.096872	-2.638205	6.855312
H	-2.361143	-4.352686	1.338513
H	-2.986669	-2.857227	2.544704
H	-1.035651	-3.230640	2.363266
H	-2.057696	-2.423346	0.830983
H	-2.345053	1.631197	2.161353
H	-1.513535	0.630442	0.621067
H	-2.996839	1.962542	0.292609
H	-4.455200	-2.360456	4.540438
H	-3.325609	-1.549224	5.653478
H	-4.691542	1.433972	3.987907
H	-5.156813	0.392245	2.627264
H	-6.702849	-0.862302	3.976418
H	-6.813882	0.672783	4.850934
H	-5.090512	-0.048798	6.453495
H	-6.020109	-1.542156	6.225728
H	-3.370757	0.197486	1.211154

F^R_S

G = -884,287651 kcal.mol^{-1}

C	-4.981116	0.423049	3.112357
O	-3.960069	-0.414692	3.714256
C	-4.476968	-1.049863	4.911929
C	-5.817685	-0.378103	5.180864
C	-6.282197	-0.010792	3.769411
La	-1.550547	-0.809060	2.841859
O	-0.562837	-0.374978	4.722206
C	0.083915	-0.192906	5.950300
C	0.656428	1.226520	6.050500
C	-0.389188	2.324082	5.963585
O	-1.207023	2.313955	7.138412
B	-2.547118	2.289726	7.091664
O	0.600172	-1.327528	1.470733
C	1.815854	-0.542540	1.546602
C	2.644101	-0.949641	0.332207
C	2.178522	-2.386800	0.084359
C	0.692989	-2.290901	0.391743
B	-2.126256	-3.447176	2.532275
B	-1.898083	1.433488	1.341752
C	1.174854	-1.243703	6.146548
H	2.368914	-2.732441	-0.934931
H	-3.123022	2.286211	8.143180
H	-3.128799	2.271317	6.036754
H	0.095120	3.306043	5.918094
H	0.126983	-1.909224	-0.467161
H	0.236721	-3.219236	0.740286
H	2.667983	-3.078250	0.778854
H	3.717553	-0.866988	0.520697
H	2.399622	-0.315832	-0.526883
H	2.316572	-0.790648	2.489121
H	1.540431	0.516068	1.552388
H	-1.012313	2.199414	5.070294
H	1.374583	1.371420	5.232284
H	1.207777	1.337960	6.992501
H	-0.652930	-0.313754	6.762430
H	1.956799	-1.130737	5.386412
H	1.641885	-1.154588	7.133650
H	0.752814	-2.248687	6.053731
H	-2.389249	-4.611822	2.392440
H	-2.780260	-2.941214	3.455264
H	-0.930690	-3.277420	2.809489
H	-2.378169	-2.805280	1.496981
H	-2.349504	1.576818	2.486481
H	-0.698117	1.145525	1.464087
H	-2.046816	2.427270	0.681860
H	-4.582136	-2.120969	4.707556
H	-3.746610	-0.909210	5.713500

H	-4.737891	1.468940	3.327238	H	-7.034313	0.782179	3.755005	H	-2.467365	0.459611	0.819242
H	-4.949558	0.270072	2.031528	H	-5.680822	0.524134	5.786162				
H	-6.697392	-0.887459	3.260420	H	-6.509866	-1.041023	5.706209				

Insertion of a second BBL-R monomer : propagation step.

G_R^R

G = -1190,575877 kcal.mol^{-1}

C	-3.749133	1.618389	0.306257
O	-2.846979	1.439277	1.429205
C	-2.783482	2.651752	2.213985
C	-3.967252	3.489489	1.752262
C	-4.062900	3.108438	0.273137
La	-1.789179	-0.884778	2.047604
B	-4.114938	-1.868612	1.063580
O	-0.883080	-3.267005	2.608139
C	-1.522296	-4.129613	3.585805
C	-1.002758	-5.532390	3.292154
C	0.376575	-5.253505	2.690380
C	0.102693	-4.011426	1.856411
O	-0.003056	1.006803	2.768771
C	0.492938	1.461224	3.774554
O	0.896856	2.733784	3.949363
C	1.315055	2.447177	5.346405
C	2.778139	2.735308	5.555822
B	-2.117385	-0.752891	4.816021
C	0.863524	0.990514	5.159411
H	-1.827554	3.148563	2.011663
H	-3.419181	-2.767538	1.559701
H	-4.328575	-1.037389	1.956501
H	-5.043974	3.311398	-0.164021
O	-0.423233	-0.964645	0.332898
H	1.653452	0.235864	5.181003
H	0.005799	0.643656	5.740377
H	0.676277	3.029864	6.015121
H	3.064422	2.469172	6.578397
H	2.990170	3.797780	5.407785
H	3.395025	2.157417	4.860999
H	-0.996080	-1.154712	4.461316
H	-2.163697	-0.660812	6.020665
H	-2.962366	-1.530182	4.376752
H	-2.300623	0.350475	4.279627
H	-3.435208	-1.327427	0.179838
H	-5.143040	-2.301702	0.612331
H	0.970677	-3.363838	1.715324
H	-0.311019	-4.267931	0.875064
H	0.761210	-6.079288	2.086247
H	1.104711	-5.035543	3.479957
H	-1.642806	-6.032721	2.557575
H	-0.967235	-6.153690	4.190872
H	-1.237666	-3.772669	4.580742
H	-2.604725	-4.030321	3.471537
H	-2.824421	2.371449	3.269636
H	-3.807817	4.558454	1.916926
H	-4.877023	3.191150	2.284351
H	-3.247609	1.251758	-0.592436
H	-4.638679	1.006912	0.486741

H	-3.310579	3.650647	-0.310560
C	0.362810	-0.819105	-0.807835
H	1.349691	-0.410655	-0.524415
C	-0.275737	0.173373	-1.784222
H	-0.387144	1.148450	-1.299953
H	-1.270710	-0.168101	-2.089970
H	0.336273	0.305680	-2.684115
C	0.633295	-2.188835	-1.458123
H	1.307227	-2.072788	-2.316987
H	1.156647	-2.814351	-0.726785
C	-0.630948	-2.923852	-1.876626
H	-1.400860	-2.798620	-1.109596
H	-1.025823	-2.556921	-2.831501
O	-0.362505	-4.328151	-1.980448
B	-0.469499	-5.002843	-3.135900
H	-0.214149	-6.173703	-3.101373
H	-0.802759	-4.442153	-4.148208

$TS(G_R^R \rightarrow H^R_R)$

$G = -1190{,}552126\ kcal.mol^{-1}$

C	-4.536656	2.015414	1.463740
O	-3.324984	1.622565	2.154694
C	-3.005381	2.595754	3.188298
C	-4.160566	3.591952	3.185387
C	-4.677663	3.501203	1.747835
La	-2.274242	-0.756238	2.145021
B	-3.696452	-1.112244	-0.130730
O	-1.550652	-3.260778	2.191614
C	-2.475663	-4.357728	1.963294
C	-1.737248	-5.602568	2.432523
C	-0.893350	-5.053429	3.585137
C	-0.459570	-3.700127	3.039918
O	-0.645984	0.493404	3.520665
C	0.417081	0.701309	2.903344
O	0.747727	1.928956	2.375239
C	2.130967	1.804145	2.864353
C	3.181171	2.135614	1.835824
B	-3.642148	-1.494559	4.369691
C	1.851327	0.344997	3.265076
H	-2.050200	3.056666	2.920828
H	-2.894610	-2.042689	0.042582
H	-4.427137	-1.066653	0.870346
H	-5.708148	3.848293	1.635174
O	-0.057986	-0.374122	1.302692
H	2.313501	-0.394173	2.611171
H	1.993125	0.074790	4.313040
H	2.230394	2.458498	3.737941
H	4.174380	2.054385	2.290142
H	3.056080	3.162096	1.478708
H	3.140239	1.462599	0.975750
H	-2.433626	-1.760852	4.456326

H	-4.234117	-1.837470	5.359175
H	-4.083525	-2.059098	3.356754
H	-3.737731	-0.274700	4.175008
H	-3.031213	-0.067511	-0.158653
H	-4.336856	-1.252386	-1.138564
H	-0.307279	-2.946642	3.818639
H	0.440116	-3.776982	2.419789
H	-0.039813	-5.687474	3.838708
H	-1.508114	-4.922463	4.481731
H	-1.092933	-5.992779	1.637338
H	-2.424577	-6.394979	2.739653
H	-3.378580	-4.170470	2.554887
H	-2.733902	-4.356368	0.901796
H	-2.889043	2.064691	4.135864
H	-3.834712	4.596735	3.467063
H	-4.939331	3.278283	3.888796
H	-4.413551	1.758285	0.410687
H	-5.377710	1.442987	1.873491
H	-4.042823	4.081920	1.069387
C	0.742685	-0.316291	0.149859
H	1.506752	0.461595	0.310499
C	-0.059987	0.111653	-1.079243
H	-0.500701	1.098422	-0.910308
H	-0.878185	-0.584012	-1.288271
H	0.580832	0.170076	-1.966843
C	1.504825	-1.636726	-0.065821
H	2.295560	-1.489823	-0.813823
H	2.001731	-1.906208	0.873786
C	0.630176	-2.810150	-0.480742
H	-0.275156	-2.847436	0.131350
H	0.339153	-2.747599	-1.535607
O	1.332228	-4.038640	-0.249265
B	1.745059	-4.833437	-1.251208
H	2.333051	-5.829796	-0.938517
H	1.523908	-4.542022	-2.397818

H^{R}_{R}

G = -1190,565123 kcal.mol^{-1}

C	-4.398796	2.062841	1.415891
O	-3.290448	1.531377	2.176029
C	-2.769112	2.552746	3.077312
C	-3.608088	3.802620	2.809678
C	-4.155124	3.561918	1.399212
La	-2.573260	-0.926622	2.330946
B	-3.661385	-1.393123	-0.117265
O	-1.499622	-3.254608	2.670679
C	-2.128509	-4.516976	2.334206
C	-1.060530	-5.560674	2.613891
C	-0.379281	-4.978229	3.855294
C	-0.372508	-3.481939	3.557867
O	-0.721480	-0.007360	3.378046

C	0.279417	0.228388	2.544306
O	0.546580	1.627812	2.286889
C	1.784446	1.568423	3.044992
C	2.938229	2.243817	2.340201
B	-4.271694	-1.545869	4.315295
C	1.715875	0.035818	3.084286
H	-1.709876	2.676422	2.840417
H	-2.936575	-2.325367	0.278618
H	-4.567752	-1.259208	0.711551
H	-5.064750	4.130004	1.187297
O	-0.095258	-0.425672	1.303123
H	2.411862	-0.445389	2.391686
H	1.760372	-0.446705	4.061261
H	1.630987	2.015069	4.036250
H	3.848772	2.167679	2.944404
H	2.724424	3.305604	2.182375
H	3.134632	1.787606	1.364524
H	-3.119761	-1.413480	4.753889
H	-5.050634	-1.827328	5.185154
H	-4.242189	-2.421805	3.434548
H	-4.581900	-0.483741	3.749667
H	-2.964906	-0.367154	-0.094489
H	-4.077438	-1.608026	-1.224676
H	-0.499382	-2.854986	4.443896
H	0.532269	-3.170266	3.026491
H	0.628999	-5.367552	4.018125
H	-0.974434	-5.188422	4.750257
H	-0.357911	-5.617500	1.775911
H	-1.484996	-6.553891	2.781076
H	-3.011092	-4.648129	2.971698
H	-2.444735	-4.459408	1.290174
H	-2.862098	2.185699	4.103173
H	-3.013099	4.716079	2.889251
H	-4.433426	3.874728	3.525930
H	-4.382903	1.582591	0.435609
H	-5.337172	1.809280	1.925983
H	-3.405714	3.814950	0.641474
C	0.752417	-0.281731	0.147984
H	1.589004	0.361833	0.437316
C	-0.015260	0.420691	-0.962262
H	-0.297321	1.424147	-0.634063
H	-0.927821	-0.120019	-1.227555
H	0.608188	0.512224	-1.858342
C	1.319505	-1.650843	-0.236878
H	2.107218	-1.510793	-0.988463
H	1.798131	-2.091173	0.645313
C	0.292982	-2.644518	-0.763006
H	-0.585556	-2.673246	-0.113098
H	-0.038624	-2.387410	-1.775454
O	0.860207	-3.957472	-0.759037
B	1.116400	-4.631850	-1.894424

H	1.600379	-5.720795	-1.772897
H	0.866480	-4.145423	-2.966151

$TS(H^{R}_{R} \rightarrow I^{R}_{R})$

G = -1190,559379 $kcal.mol^{-1}$

C	4.164342	-1.192091	5.600288
O	3.335343	-2.368807	5.805971
C	3.795180	-3.099288	6.970083
C	5.213545	-2.606271	7.204366
C	5.098568	-1.133571	6.803759
La	1.152081	-2.986199	4.504550
O	0.953083	-4.957888	3.167998
C	1.316198	-5.945738	3.936940
O	2.191144	-6.874187	3.458992
C	3.273448	-6.579627	2.545534
C	2.880832	-6.947271	1.111531
C	1.889071	-6.030615	0.409855
O	1.555020	-6.605555	-0.857151
B	1.849345	-6.005968	-2.021940
O	-1.173178	-2.615938	3.405191
C	-2.199517	-1.691697	3.843630
C	-3.378186	-1.941435	2.915135
C	-2.676836	-2.305245	1.604351
C	-1.495394	-3.135467	2.088664
O	1.942672	-5.249736	5.311652
C	1.109987	-6.146026	6.101959
C	1.947502	-7.177805	6.829382
B	2.138887	-1.207734	2.707262
B	-0.264951	-2.534899	6.770079
C	0.327019	-6.653196	4.887586
C	3.917503	-5.207626	2.704523
H	-0.799896	-3.408397	6.071474
H	0.874950	-2.925476	7.042348
H	-0.143910	-1.515679	6.065822
H	-0.911690	-2.301597	7.756353
H	-1.746121	-4.195330	2.197294
H	-0.674997	-6.227652	4.796271
H	0.287141	-7.736422	4.755237
H	-0.606681	-3.044728	1.459753
H	-3.312658	-2.861670	0.910774
H	-2.326488	-1.400999	1.095045
H	-1.813606	-0.670100	3.741602
H	-2.399589	-1.894007	4.897373
H	0.509529	-5.567341	6.812825
H	2.548090	-7.751406	6.117836
H	1.302218	-7.869256	7.382643
H	2.619091	-6.695295	7.546502
H	-3.979932	-2.782355	3.277447
H	-4.029163	-1.067395	2.830684
H	1.220063	-1.851591	2.192474
H	1.684513	-0.655504	3.726931

H	2.604150	-0.396738	1.951649
H	3.136775	-2.859083	7.813818
H	3.708921	-4.162824	6.739900
H	4.703913	-1.326051	4.658019
H	3.512275	-0.321108	5.505486
H	4.646768	-0.553928	7.616090
H	6.058571	-0.674594	6.553634
H	5.916935	-3.131874	6.548926
H	5.536353	-2.749898	8.238856
H	2.997053	-2.022151	3.075632
H	4.022903	-7.320317	2.848980
H	4.147306	-5.017577	3.756337
H	3.295625	-4.396601	2.324317
H	4.860334	-5.196111	2.147284
H	3.801780	-6.992736	0.514941
H	2.464141	-7.960576	1.122524
H	0.969504	-5.942752	0.991665
H	2.299104	-5.024597	0.262222
H	1.525565	-6.583634	-3.020883
H	2.410851	-4.940528	-2.041963

I^{R}_{R}

G = -1190,593442 $kcal.mol^{-1}$

C	2.653941	-2.150671	8.089514
O	2.550241	-1.654561	6.730459
C	3.293678	-0.418890	6.588083
C	3.701341	-0.026281	8.003451
C	3.820074	-1.385983	8.696598
La	1.653289	-3.253301	4.903724
B	3.592593	-2.081931	3.353812
O	0.061011	-2.452980	2.869805
C	0.490158	-1.795044	1.657897
C	-0.705315	-0.960464	1.232390
C	-1.867359	-1.893671	1.580798
C	-1.387305	-2.570110	2.866114
B	-0.729160	-3.202958	6.239027
O	1.428816	-5.472712	3.531380
C	1.696726	-6.605577	3.942372
O	2.029934	-7.610790	3.147898
C	2.202882	-7.481881	1.698694
C	0.865577	-7.575149	0.962455
C	-0.042502	-6.351688	0.964554
O	-1.196018	-6.654117	0.178756
B	-1.520983	-5.957647	-0.923893
O	2.682131	-4.863786	6.040042
C	2.830719	-6.228487	6.169740
C	4.224822	-6.684109	5.735006
C	1.703069	-6.980938	5.391784
C	3.119668	-6.336948	1.293494
H	-0.708156	-4.051895	5.329326
H	0.177828	-3.488105	7.023053

H	-0.465292	-2.102918	5.726795
H	-1.803991	-3.178232	6.781135
H	0.737280	-2.552680	0.901813
H	0.745610	-6.666990	5.821287
H	1.808884	-8.063187	5.495374
H	1.391221	-1.226786	1.890216
H	-0.671301	-0.687480	0.174257
H	-0.753640	-0.039892	1.824561
H	-1.756706	-2.077410	3.768709
H	-1.654945	-3.629025	2.920607
H	2.687770	-6.533667	7.222150
H	4.410777	-6.422180	4.687767
H	4.360286	-7.764788	5.856701
H	4.976944	-6.169324	6.338966
H	-2.010456	-2.630435	0.782864
H	-2.815901	-1.370086	1.725701
H	2.985666	-2.978943	2.747718
H	2.741801	-1.262505	3.744700
H	4.400154	-1.544068	2.639715
H	1.709323	-1.941386	8.604551
H	2.803093	-3.231507	8.029651
H	4.155649	-0.615525	5.942839
H	2.647387	0.314556	6.098419
H	2.918454	0.575562	8.478014
H	4.629646	0.550839	8.017519
H	4.769348	-1.867809	8.438166
H	3.752132	-1.323718	9.785931
H	4.116876	-2.592333	4.345824
H	2.727350	-8.418947	1.487692
H	4.059843	-6.389867	1.849236
H	2.682837	-5.353255	1.458859
H	3.357298	-6.444986	0.230059
H	1.102163	-7.815931	-0.082011
H	0.308349	-8.432084	1.356690
H	-0.386007	-6.111625	1.972747
H	0.467259	-5.471137	0.557436
H	-2.508049	-6.301481	-1.507004
H	-0.836720	-5.035180	-1.288040

$TS(I^{R}_{R} \rightarrow J^{R}_{R})$

G = -1190,583944 kcal.mol^{-1}

C	-4.412867	-2.539621	4.452641
O	-4.041171	-1.270133	3.858748
C	-5.221021	-0.465715	3.604214
C	-6.301136	-1.086766	4.475535
C	-5.937332	-2.573325	4.424164
La	-1.606343	-0.814472	3.147499
B	-0.704300	-1.186046	5.681893
O	0.925625	-0.739421	2.496526
C	2.061653	-0.750218	3.398743
C	3.229441	-1.240864	2.557392

C	2.894852	-0.658333	1.182731
C	1.382779	-0.832809	1.121546
O	-1.930985	1.218633	2.430176
C	-1.975630	2.532384	1.983442
C	-3.204808	3.268697	2.581226
C	-3.256442	3.233292	4.087857
O	-2.542675	4.233789	4.624806
C	-2.375765	4.381401	6.065917
C	-3.603243	5.010933	6.732242
C	-4.802351	4.120385	7.037322
O	-5.786057	4.914910	7.704842
B	-6.207877	4.644592	8.951497
B	-1.806418	-2.681784	1.192274
C	-0.658998	3.257695	2.260856
O	-3.869352	2.402037	4.733360
C	-1.821427	3.133292	6.739769
H	-4.109025	2.774311	2.218294
H	-3.204493	4.308345	2.238986
H	-0.680489	4.286750	1.886141
H	-0.448597	3.288437	3.333333
H	-2.140594	2.545094	0.891802
H	-2.906626	-2.495203	1.728741
H	-1.009834	-3.038189	2.075327
H	-1.873621	-3.500068	0.313830
H	-1.427070	-1.585233	0.752078
H	4.192236	-0.903293	2.949895
H	2.223612	0.271457	3.762853
H	-1.938764	-1.100126	5.665173
H	-0.259987	-0.145113	5.168528
H	-0.280611	-1.327891	6.798362
H	-0.381872	-2.139109	4.954011
H	3.239431	-2.335588	2.518694
H	0.872894	-0.060413	0.539416
H	3.164900	0.402780	1.141444
H	3.399448	-1.169724	0.358939
H	0.159477	2.728317	1.764076
H	-5.469428	-0.544850	2.537932
H	-4.973675	0.567259	3.857033
H	-6.228428	-0.705014	5.499534
H	-7.306645	-0.876815	4.101467
H	-6.293733	-3.021661	3.490620
H	-6.349115	-3.149540	5.256644
H	-4.013139	-2.558377	5.472369
H	-3.950348	-3.340399	3.866784
H	1.091928	-1.814666	0.735051
H	1.811847	-1.390620	4.245847
H	-1.596755	5.150249	6.094733
H	-0.914615	2.797246	6.229713
H	-2.532041	2.308083	6.746568
H	-1.551491	3.378737	7.772333
H	-3.256844	5.435424	7.683802

H	-3.934324	5.858642	6.121938
H	-5.255639	3.731904	6.124305
H	-4.520587	3.268503	7.666829
H	-7.035321	5.379460	9.410044
H	-5.762581	3.706296	9.561177

J^{R}_{R}

G = -1190,585365 kcal.mol^{-1}

C	-5.169997	-0.565910	2.775885
O	-4.111059	-1.275513	3.458082
C	-4.653380	-2.408096	4.185683
C	-6.141737	-2.439613	3.847804
C	-6.438330	-0.976596	3.505952
La	-1.575515	-0.862179	3.139615
O	-2.120329	1.056079	2.261930
C	-2.336834	2.313123	1.701718
C	-2.392483	3.369077	2.828629
C	-2.757047	4.756139	2.358844
O	-4.005905	4.767755	1.851877
C	-4.581214	5.965896	1.262120
C	-5.093594	6.951111	2.317596
C	-4.084004	7.844889	3.029056
O	-4.804464	8.707095	3.913498
B	-4.774246	10.045376	3.800157
O	0.972398	-0.494190	2.774172
C	1.629981	-0.779382	1.509409
C	3.097806	-0.426115	1.722123
C	3.277614	-0.661622	3.223635
C	1.958859	-0.151117	3.780687
B	-1.352750	-2.964315	1.440896
B	-1.078770	-0.901231	5.800402
C	-1.258895	2.641349	0.670242
O	-2.028817	5.724553	2.425116
C	-3.716826	6.567475	0.160587
H	-1.421935	3.429107	3.327811
H	-3.139293	3.038216	3.558473
H	-1.430430	3.613022	0.194503
H	-0.273686	2.666999	1.148673
H	-3.315721	2.324689	1.195091
H	-2.470947	-2.939872	1.977361
H	-0.508783	-3.036059	2.346537
H	-1.251805	-3.883155	0.672629
H	-1.200944	-1.877536	0.857878
H	4.136758	-0.133053	3.644664
H	1.965314	0.938780	3.904563
H	-2.292829	-0.995047	5.560379
H	-0.689377	0.151501	5.267688
H	-0.860119	-0.896629	6.981801
H	-0.511973	-1.850800	5.237132
H	3.393525	-1.729908	3.436101
H	1.145463	-0.185623	0.729596

H	3.282893	0.625211	1.475909
H	3.758575	-1.040065	1.104886
H	-1.245911	1.875435	-0.110914
H	-5.188099	-0.880424	1.724653
H	-4.937263	0.499265	2.825272
H	-6.562441	-0.382635	4.417892
H	-7.332170	-0.851125	2.889454
H	-6.324613	-3.078491	2.977400
H	-6.741708	-2.819306	4.678526
H	-4.466950	-2.234554	5.250589
H	-4.118375	-3.308390	3.867971
H	1.481861	-1.840947	1.288728
H	1.651883	-0.614169	4.719814
H	-5.476218	5.547519	0.789312
H	-3.457393	5.798267	-0.572935
H	-2.795508	7.003208	0.545481
H	-4.290012	7.342950	-0.358555
H	-5.815748	7.604950	1.810705
H	-5.662745	6.390407	3.067539
H	-3.385356	7.261865	3.630388
H	-3.502236	8.442496	2.318051
H	-5.415604	10.667299	4.598222
H	-4.131714	10.574327	2.929448

F_RA_R

G = -1190,580029 $kcal.mol^{-1}$

C	0.091827	-4.351913	1.519130
O	-0.894108	-3.711079	2.373606
C	-1.210439	-4.573758	3.496498
C	-0.586928	-5.920151	3.156724
C	0.640744	-5.507275	2.342230
La	-1.879267	-1.329529	1.886480
B	-3.731437	-2.040385	3.755394
O	-2.867631	1.007869	1.300894
C	-2.849683	1.487350	-0.064468
C	-3.333370	2.930457	0.008960
C	-4.280692	2.890388	1.211102
C	-3.546441	1.954521	2.160249
O	-2.805189	-1.940032	0.012741
C	-3.413482	-2.397796	-1.153678
C	-2.930289	-3.822362	-1.485030
C	-3.321458	-4.854781	-0.439845
O	-2.493233	-6.020171	-0.563378
B	-2.971284	-7.201695	-0.986590
O	-1.081365	0.434069	3.789012
C	-0.100731	1.107615	4.003133
C	1.384989	0.903064	4.167786
C	1.397968	2.426278	4.374137
C	2.097165	3.282506	3.351728
O	-0.076165	2.442092	4.183371
C	-4.938031	-2.301536	-1.044942

B	0.699574	-0.702423	1.050699
H	-2.794629	2.481172	2.757830
H	-3.818767	3.250705	-0.916700
H	1.833326	-0.417855	0.744275
H	-0.007811	0.312837	1.122136
H	0.680654	-1.251617	2.163087
H	0.188141	-1.464196	0.231081
H	1.865138	0.530440	3.259290
H	1.663166	0.283846	5.023202
H	1.607967	2.742822	5.399374
H	3.180535	3.213102	3.492856
H	1.805607	4.331154	3.458387
H	1.859213	2.949696	2.337395
H	-2.595488	-1.998383	4.248878
H	-4.553080	-2.344443	4.581072
H	-3.718246	-2.841185	2.811736
H	-3.964506	-0.920487	3.272320
H	0.832955	-3.598686	1.244652
H	-0.417152	-4.713463	0.619212
H	1.032429	-6.309829	1.711988
H	1.445470	-5.164791	3.002812
H	-1.268673	-6.512557	2.537365
H	-0.343986	-6.499094	4.051806
H	-0.768222	-4.137272	4.400053
H	-2.295283	-4.592184	3.614092
H	-4.199345	1.389229	2.829317
H	-4.459583	3.873276	1.654992
H	-5.247813	2.463702	0.923342
H	-1.831044	1.379759	-0.447599
H	-3.519671	0.854620	-0.655965
H	-2.494823	3.607501	0.206035
H	-3.098380	-1.763903	-2.002058
H	-5.238781	-1.259667	-0.896937
H	-5.304246	-2.871106	-0.184800
H	-5.432078	-2.674361	-1.949865
H	-3.305335	-4.128242	-2.470687
H	-1.836586	-3.795738	-1.549741
H	-3.152460	-4.450249	0.562118
H	-4.374139	-5.147981	-0.527195
H	-2.185376	-8.103587	-1.064911
H	-4.135574	-7.330451	-1.264610

$TS(F_RA_R \rightarrow F_RB^R{}_R)$

$G = -1190{,}549997\ kcal.mol^{-1}$

C	-0.318372	-4.169186	2.038868
O	-1.532963	-3.780370	2.739602
C	-1.701493	-4.586164	3.934039
C	-0.705890	-5.727329	3.785392
C	0.436573	-5.057703	3.017382
La	-2.682867	-1.519886	2.213120
B	-4.489061	-1.974787	4.191022

O	-3.369041	0.911107	1.743569
C	-3.173619	1.553171	0.456548
C	-2.879267	3.010012	0.781227
C	-3.707151	3.228225	2.049991
C	-3.499042	1.913514	2.788517
O	-3.141900	-2.060254	0.154224
C	-3.378502	-2.426037	-1.173075
C	-2.606972	-3.712786	-1.517572
C	-3.059467	-4.927663	-0.722801
O	-2.036704	-5.932341	-0.731292
B	-2.181774	-7.102470	-1.375826
O	-0.595254	-0.639427	2.736041
C	0.315073	0.266952	2.520691
C	1.545255	0.468630	3.424962
C	1.142870	1.951428	3.405917
C	2.038669	2.909067	2.650639
O	-0.078457	1.637447	2.674360
C	-4.880895	-2.541407	-1.440204
B	0.946820	-0.223540	0.020612
H	-2.566866	1.922516	3.362777
H	-3.154986	3.678916	-0.038309
H	0.725419	0.190576	1.399268
H	-0.206633	-0.194128	-0.326071
H	1.444758	-1.294772	0.248778
H	1.662570	0.690543	-0.293203
H	2.515050	0.214487	2.992909
H	1.415922	-0.025669	4.389969
H	0.881010	2.360053	4.389714
H	2.960888	3.091186	3.213531
H	1.536281	3.870324	2.503148
H	2.303846	2.505204	1.669128
H	-3.385342	-1.730197	4.697390
H	-5.325684	-2.179195	5.029258
H	-4.363869	-2.954765	3.436211
H	-4.801219	-1.010024	3.469271
H	0.217933	-3.256385	1.765121
H	-0.607473	-4.714305	1.134218
H	1.088712	-5.769051	2.504532
H	1.051250	-4.452590	3.692781
H	-1.139020	-6.539951	3.192405
H	-0.399025	-6.134550	4.752275
H	-1.479491	-3.962241	4.807533
H	-2.746162	-4.900273	3.983948
H	-4.334727	1.618114	3.428071
H	-3.372975	4.085436	2.640121
H	-4.765387	3.371943	1.804731
H	-2.356801	1.044461	-0.061521
H	-4.096255	1.435061	-0.123514
H	-1.814430	3.134861	0.998733
H	-2.979137	-1.641713	-1.838723
H	-5.370103	-1.582423	-1.244598

H	-5.340445	-3.285991	-0.781643
H	-5.084018	-2.824138	-2.479492
H	-2.683919	-3.920235	-2.592690
H	-1.547949	-3.534666	-1.299482
H	-3.218283	-4.648287	0.322906
H	-3.989742	-5.353165	-1.117123
H	-1.256635	-7.862379	-1.326230
H	-3.200837	-7.356583	-1.963786

$F_RB^R{}_R$

G = -1190,553753 kcal.mol^{-1}

C	0.056387	-0.992817	0.826950
O	-0.101356	-0.537794	-0.538692
C	1.128436	0.064418	-1.011687
C	1.994258	0.235788	0.229195
C	1.554395	-0.947997	1.094789
La	-2.191890	-1.320948	-1.925678
O	-1.707341	-3.255298	-1.009962
O	-3.235197	-2.602271	-3.943875
C	-2.431107	-3.198330	-4.991379
C	-3.327294	-3.249400	-6.227538
C	-4.732372	-3.271591	-5.619530
C	-4.569141	-2.330743	-4.438314
O	-4.536417	-0.945376	-1.612359
C	-4.606342	-0.064629	-0.653177
O	-3.240076	0.306399	-0.139382
C	-3.549750	1.735184	-0.282425
C	-3.526282	2.444774	1.051252
B	-1.091265	0.285234	-3.874925
C	-4.922158	1.423731	-0.898003
B	-6.217329	-0.805910	1.412655
H	-5.263654	-2.490718	-3.613091
H	-4.623782	-1.280302	-4.750365
H	-4.992188	-4.278508	-5.274530
H	-5.506978	-2.935997	-6.314032
H	-3.110905	-4.116793	-6.856435
H	-3.191415	-2.347391	-6.833107
H	-1.536723	-2.584252	-5.136345
H	-2.134750	-4.196620	-4.651953
H	-5.171837	-0.464012	0.269280
H	-7.190240	-0.728882	0.716323
H	-5.722908	-1.876737	1.624712
H	-5.921878	0.128029	2.107666
H	-5.786405	1.814745	-0.357830
H	-5.008003	1.646702	-1.963238
H	-2.837062	2.191107	-0.979237
H	-4.223875	1.978125	1.752392
H	-3.811805	3.494364	0.920537
H	-2.522921	2.417934	1.487566
H	-0.546081	0.936901	-4.727591
H	-1.166053	0.901554	-2.802814

H	-2.238572	-0.035031	-4.200787
H	-0.443845	-0.760333	-3.658172
H	-0.495803	-0.310512	1.483935
H	-0.384160	-1.990504	0.894118
H	1.589272	-0.614568	-1.738476
H	0.875611	0.996528	-1.520197
H	1.765991	1.182532	0.731393
H	3.061224	0.227061	-0.008412
H	2.033317	-1.872060	0.752581
H	1.782121	-0.819165	2.156107
C	-1.381471	-4.531060	-0.549004
H	-0.353003	-4.520774	-0.141991
C	-1.393364	-5.544112	-1.697573
H	-0.662838	-5.250234	-2.458235
H	-2.378375	-5.584332	-2.173927
H	-1.136021	-6.551036	-1.349858
C	-2.294819	-4.943732	0.618928
H	-1.980792	-5.924444	1.000147
H	-2.161537	-4.225702	1.436773
C	-3.774941	-4.988488	0.275185
H	-4.097681	-4.023648	-0.126649
H	-3.999000	-5.767773	-0.464144
O	-4.529614	-5.229488	1.464580
B	-5.345652	-6.285809	1.601142
H	-5.925151	-6.389882	2.644652
H	-5.472362	-7.084952	0.707515

TS($F_RB^R{}_R \rightarrow F_RC^R{}_R$)

G = -1190,549351 kcal.mol^{-1}

C	0.302673	-0.982617	0.722402
O	0.055867	-0.512114	-0.623432
C	1.257155	0.076031	-1.177534
C	2.208692	0.229504	0.001485
C	1.816195	-0.956281	0.886841
La	-2.150075	-1.264497	-1.865810
O	-1.657257	-3.194404	-0.920687
O	-3.240912	-2.574899	-3.847849
C	-2.467349	-3.174848	-4.914725
C	-3.386046	-3.197320	-6.135205
C	-4.780165	-3.200242	-5.502190
C	-4.577879	-2.274047	-4.315102
O	-4.450425	-0.897490	-1.467449
C	-4.497384	-0.038393	-0.460810
O	-3.071781	0.311336	0.000950
C	-3.360959	1.738879	-0.127337
C	-3.317289	2.433516	1.216204
B	-1.137577	0.330849	-3.884916
C	-4.745886	1.464100	-0.726580
B	-7.258386	-1.599458	0.713019
H	-5.259293	-2.428526	-3.477956
H	-4.618440	-1.219735	-4.615975

H	-5.051970	-4.205841	-5.162331
H	-5.560828	-2.843928	-6.179477
H	-3.196574	-4.061801	-6.776778
H	-3.244722	-2.291391	-6.733599
H	-1.564356	-2.576201	-5.070571
H	-2.183250	-4.182045	-4.590830
H	-5.025282	-0.420631	0.435303
H	-7.793581	-1.742897	-0.345129
H	-6.595053	-2.477016	1.177121
H	-7.419439	-0.583832	1.325247
H	-5.592219	1.909105	-0.196880
H	-4.824812	1.670718	-1.795982
H	-2.647164	2.202200	-0.819201
H	-4.019764	1.972438	1.917440
H	-3.583909	3.490245	1.103639
H	-2.313428	2.379982	1.649156
H	-0.635840	0.978264	-4.768010
H	-1.139011	0.946432	-2.809718
H	-2.306479	0.027621	-4.142606
H	-0.492157	-0.723104	-3.708680
H	-0.194506	-0.301112	1.423060
H	-0.145152	-1.975450	0.809539
H	1.658268	-0.604652	-1.937532
H	0.982425	1.013777	-1.663883
H	2.024673	1.174534	0.524738
H	3.256798	0.212237	-0.308779
H	2.260198	-1.882564	0.505506
H	2.118440	-0.838748	1.930829
C	-1.380039	-4.468985	-0.433417
H	-0.361355	-4.484656	-0.000821
C	-1.394814	-5.501751	-1.564973
H	-0.640881	-5.239259	-2.314114
H	-2.369911	-5.522203	-2.062737
H	-1.172709	-6.509868	-1.196431
C	-2.332218	-4.835999	0.719961
H	-2.053744	-5.815522	1.131054
H	-2.200995	-4.101586	1.523496
C	-3.802723	-4.849952	0.336103
H	-4.083617	-3.893670	-0.114334
H	-4.030360	-5.653071	-0.375918
O	-4.601803	-5.016490	1.511245
B	-5.403453	-6.076727	1.694381
H	-6.019476	-6.117540	2.721715
H	-5.485864	-6.939028	0.856300

$F_RC^R_R$

G = -1190,593545 kcal.mol^{-1}

C	4.838810	-2.684478	5.899409
O	3.758556	-2.180191	5.085254
C	4.289906	-1.407101	3.973024
C	5.801961	-1.376967	4.178401

C	6.057081	-2.649498	4.990476
La	1.176870	-2.365743	5.459330
B	1.216988	0.342877	5.243579
O	-1.171154	-2.263863	4.397063
C	-1.505247	-1.313834	3.351673
C	-2.936539	-1.648660	2.964076
C	-2.960287	-3.169480	3.133852
C	-2.114612	-3.371083	4.385135
O	0.414116	-2.616071	7.514022
C	-0.209891	-2.097720	8.655663
C	-1.740925	-2.184623	8.516435
C	-2.261710	-3.607626	8.398614
O	-3.581137	-3.607950	7.840921
B	-4.660480	-3.994707	8.541167
O	0.903022	-4.615662	4.268345
B	1.289345	-4.077655	2.863850
O	2.369093	-4.738954	6.072568
C	1.775462	-5.663071	7.048686
C	2.831056	-6.386863	7.850281
C	0.312188	-2.789885	9.916846
C	1.739276	-5.459641	4.945246
C	1.074031	-6.437895	5.922747
H	2.317657	-4.611294	2.493964
H	0.350885	-4.232252	2.112604
H	1.497636	-2.849074	2.994616
H	2.510402	-5.864028	4.280513
H	-0.813444	-1.465542	2.515016
H	-0.014869	-6.367044	5.916645
H	1.376773	-7.481608	5.809965
H	-1.364978	-0.311838	3.761675
H	-3.173626	-1.323777	1.947567
H	-3.642848	-1.170789	3.651953
H	-2.712345	-3.311515	5.301032
H	-1.537521	-4.298525	4.372235
H	1.103485	-5.095180	7.699790
H	3.518854	-6.934174	7.197674
H	2.357171	-7.103019	8.530487
H	3.410277	-5.682093	8.454850
H	-2.486813	-3.655683	2.274888
H	-3.968030	-3.576533	3.251531
H	0.140364	-0.042909	5.715899
H	2.111964	-0.048554	6.007024
H	1.244490	1.536346	5.095147
H	4.968637	-2.024161	6.767556
H	4.550806	-3.681152	6.237044
H	4.003467	-1.923442	3.051302
H	3.823984	-0.418964	3.993834
H	6.094228	-0.492800	4.755058
H	6.342841	-1.355057	3.228895
H	6.068619	-3.529161	4.337773
H	6.995295	-2.623775	5.551193

H	1.374620	-0.236795	4.152439
H	0.028806	-1.024450	8.747423
H	1.394075	-2.647633	9.998286
H	0.118883	-3.867985	9.888036
H	-0.155143	-2.381918	10.820481
H	-2.226106	-1.677866	9.360715
H	-2.024937	-1.641158	7.608077
H	-1.624856	-4.173033	7.711171
H	-2.276980	-4.121208	9.367408
H	-5.716016	-3.943357	7.976722
H	-4.549323	-4.375010	9.678206

$TS(F_RC^R{}_R \rightarrow F_RD^R{}_R)$

G = -1190,576947 kcal.mol^{-1}

C	-2.184699	-3.585513	4.730888
O	-1.288759	-2.490868	4.414098
C	-1.875730	-1.642537	3.390843
C	-3.327209	-2.089400	3.289385
C	-3.230612	-3.579794	3.624673
La	1.091383	-2.249044	5.442721
O	1.114894	-4.541063	5.414142
C	1.035019	-5.920787	5.495033
C	2.138877	-6.508746	6.375838
O	3.675958	-2.123952	5.665739
C	4.403672	-2.494679	6.858504
C	5.872094	-2.301919	6.505532
C	5.811765	-1.118383	5.536290
C	4.546340	-1.413311	4.742102
B	0.953221	0.349641	4.554178
O	0.646169	-1.980944	7.566908
C	0.102226	-1.426516	8.725511
C	0.848162	-1.929644	9.964040
C	-1.410966	-1.711458	8.785053
C	-1.741762	-3.194796	8.828177
O	-3.091408	-3.416261	8.395127
B	-4.053876	-3.849185	9.225716
C	1.106715	-6.480723	4.029015
C	2.022065	-5.527109	3.369641
O	1.632186	-4.716557	2.519668
B	2.538436	-3.489253	2.089017
H	3.678013	-3.768477	2.411449
H	2.357357	-3.326757	0.910476
H	2.068756	-2.569763	2.749791
H	3.078327	-5.491611	3.666234
H	-1.329542	-1.809199	2.455538
H	0.130227	-6.438278	3.541129
H	1.497433	-7.504260	3.992681
H	-1.738962	-0.604809	3.699345
H	-3.749158	-1.894227	2.300093
H	-3.942486	-1.569907	4.032095
H	-2.631562	-3.398220	5.714093

H	-1.585372	-4.497748	4.777188
H	0.066909	-6.246711	5.916677
H	3.133512	-6.272649	5.980678
H	2.051184	-7.597528	6.466687
H	2.067278	-6.072072	7.376165
H	-2.875983	-4.144359	2.755080
H	-4.178965	-4.013501	3.952389
H	-0.029391	0.051301	5.249388
H	1.953038	0.182163	5.268755
H	0.880676	1.477966	4.139764
H	4.091456	-1.836148	7.677685
H	4.136977	-3.524248	7.111748
H	4.731319	-2.069264	3.885604
H	4.015190	-0.519964	4.404716
H	5.708675	-0.177363	6.087364
H	6.691903	-1.041686	4.892830
H	6.265593	-3.191270	6.000965
H	6.487601	-2.109490	7.388216
H	1.018811	-0.462088	3.616959
H	0.208936	-0.328366	8.696049
H	1.902258	-1.641915	9.904712
H	0.805636	-3.022034	10.031697
H	0.430631	-1.506879	10.885223
H	-1.862897	-1.198386	9.643883
H	-1.864428	-1.287514	7.881465
H	-1.091117	-3.733305	8.132624
H	-1.610093	-3.615919	9.831953
H	-5.148449	-3.987295	8.757090
H	-3.808168	-4.086571	10.380213

$F_R D^R{}_R$

G = -1190,578915 kcal.mol^{-1}

C	-4.304454	-0.348944	5.031172
O	-3.302174	-1.148988	4.348487
C	-3.446505	-2.542078	4.714025
C	-4.848575	-2.653153	5.293002
C	-4.996047	-1.302764	5.998832
La	-1.414297	-0.291045	2.738958
O	0.229540	-0.844600	4.084858
O	0.387545	0.457586	1.004436
C	0.453097	1.709614	0.275878
C	1.934919	1.932932	0.016043
C	2.442344	0.500754	-0.170676
C	1.636515	-0.264641	0.872756
B	-2.085294	2.169587	3.733011
O	-3.671552	-0.673243	0.402947
B	-3.324781	0.751210	-0.194035
O	-1.745757	-2.324063	1.708279
C	-2.182863	-3.324448	0.913073
C	-1.237790	-3.616215	-0.257245
C	-3.643742	-1.719503	-0.272721

C	-3.683953	-3.017066	0.381283
H	-2.334416	-4.268326	1.472099
H	-4.293922	1.438287	0.005784
H	-3.019775	0.582411	-1.357461
H	-2.377474	1.101142	0.496690
H	-3.456077	-1.620601	-1.349927
H	-4.316900	-2.979131	1.270208
H	-4.005758	-3.809605	-0.298328
H	-3.273776	-3.134688	3.812995
H	-2.685398	-2.798851	5.459953
H	-4.951475	-3.508025	5.966391
H	-5.592088	-2.752415	4.493653
H	-4.474077	-1.320684	6.961679
H	-6.035731	-1.019259	6.182296
H	-4.994235	0.043202	4.275938
H	-3.800161	0.491930	5.510672
H	-1.150156	2.253538	2.919206
H	-3.028243	1.614290	3.144387
H	-1.703085	1.422071	4.642783
H	-2.418131	3.250727	4.144766
H	-0.117838	1.599695	-0.652761
H	-0.017761	2.478768	0.892218
H	2.125425	-0.275294	1.852143
H	1.406701	-1.294203	0.584239
H	2.207728	0.142408	-1.179108
H	3.519501	0.397292	-0.015698
H	2.410047	2.399529	0.885892
H	2.110885	2.571485	-0.853539
H	-0.269082	-3.927238	0.144640
H	-1.611402	-4.416429	-0.906352
H	-1.071720	-2.717893	-0.861321
C	0.973955	-0.737141	5.260430
H	0.929757	0.299769	5.637161
C	2.446388	-1.069110	5.002210
H	2.870382	-0.357256	4.286968
H	2.554086	-2.073238	4.578208
H	3.038357	-1.014681	5.923229
C	0.356348	-1.620582	6.361353
H	0.897859	-1.485942	7.306823
H	-0.670894	-1.276277	6.528222
C	0.305300	-3.093918	5.992092
H	-0.022168	-3.196451	4.953241
H	1.280610	-3.581942	6.105758
O	-0.661163	-3.772856	6.807119
B	-0.319234	-4.705671	7.710169
H	-1.211855	-5.196981	8.341875
H	0.832471	-5.022467	7.861266

$TS(F_RD^R{}_R \rightarrow F_RE^R{}_R)$

G = -1190,558039 $kcal.mol^{-1}$

C	4.630630	-2.421367	4.746965

O	3.250252	-2.502878	4.332879
C	3.123480	-2.007122	2.982640
C	4.547746	-1.718605	2.493593
C	5.415980	-2.540853	3.451978
La	1.366322	-2.347893	6.309708
B	2.261443	0.222082	6.536126
O	-0.416946	-1.768712	4.492622
C	-0.812345	-0.394685	4.231028
C	-2.212823	-0.480178	3.637174
C	-2.189093	-1.841977	2.939072
C	-1.397542	-2.683270	3.927035
O	-0.119017	-2.553055	7.899308
C	-1.108647	-2.425484	8.873808
C	-2.500508	-2.591022	8.235961
C	-2.720870	-3.959127	7.609295
O	-3.752123	-3.883164	6.615965
B	-4.916112	-4.544171	6.728393
O	0.980675	-4.704209	5.244184
B	0.635960	-5.824860	4.207823
O	2.822062	-4.104818	6.945421
C	2.612952	-5.226778	7.800344
C	3.876704	-5.593671	8.557625
C	-0.865016	-3.402675	10.026345
C	2.091607	-5.367493	5.563347
C	2.143001	-6.274898	6.774456
H	1.574919	-6.636993	4.437031
H	-0.384841	-6.377770	4.525727
H	0.774522	-5.409361	3.082364
H	2.962112	-5.237579	4.923612
H	-0.092181	0.036415	3.526683
H	1.158173	-6.703399	6.973392
H	2.857298	-7.089028	6.614779
H	-0.759534	0.166098	5.167706
H	-2.423113	0.352878	2.961443
H	-2.967867	-0.474937	4.430454
H	-2.038888	-3.055552	4.733534
H	-0.855357	-3.518210	3.478962
H	1.813390	-5.012219	8.525594
H	4.690309	-5.818626	7.859447
H	3.713510	-6.469003	9.196807
H	4.191645	-4.759160	9.191569
H	-1.666076	-1.776785	1.978290
H	-3.186063	-2.251983	2.759938
H	1.142239	0.111336	7.050235
H	3.011783	-0.602871	7.091209
H	2.695558	1.338301	6.649735
H	4.805935	-1.453681	5.235949
H	4.792276	-3.222689	5.470716
H	2.625886	-2.785105	2.394451
H	2.496725	-1.108728	2.989314
H	4.778028	-0.653575	2.599166

H	4.686425	-1.990441	1.443982
H	5.467925	-3.587513	3.132040
H	6.435749	-2.157321	3.541354
H	2.174101	-0.108102	5.342652
H	-1.077631	-1.404962	9.293105
H	0.110370	-3.204696	10.480673
H	-0.863636	-4.438174	9.669053
H	-1.631357	-3.305970	10.804047
H	-3.285825	-2.380300	8.973328
H	-2.593882	-1.839664	7.443062
H	-1.808404	-4.279246	7.097418
H	-2.989909	-4.716445	8.355068
H	-5.705492	-4.398770	5.838291
H	-5.137025	-5.241925	7.684037

$F_R E^R_R$

G = -1190,628006 kcal.mol^{-1}

C	-0.565102	-0.333789	-0.031675
O	-0.138654	-0.326737	1.353047
C	1.309209	-0.392692	1.427170
C	1.775990	-0.642283	-0.001949
C	0.677775	0.033845	-0.826865
La	-1.894745	-0.465247	3.294425
O	-2.839483	-2.289460	2.493888
C	-3.343345	-3.491775	2.013642
C	-3.308333	-4.573725	3.098468
O	-3.735189	-0.497716	5.180295
C	-3.691300	-1.140200	6.477697
C	-5.113734	-1.619088	6.744100
C	-5.951607	-0.591243	5.978772
C	-5.105673	-0.364744	4.734485
B	0.255793	-1.308598	4.827180
O	-3.010780	1.181500	2.267758
C	-3.421955	2.482863	2.035037
C	-2.850413	3.014469	0.715367
O	-1.448511	2.113887	4.541742
B	-1.150616	2.238396	5.856938
C	-3.061812	3.404079	3.221189
C	-1.624066	3.278839	3.703985
C	-2.594283	-3.916965	0.735367
C	-1.112559	-4.173899	0.959023
O	-0.400941	-4.075243	-0.284005
B	0.166332	-5.138814	-0.875976
H	-3.719637	3.189984	4.073011
H	-3.240785	4.452090	2.945634
H	-3.217737	4.021942	0.486890
H	-1.754549	3.045054	0.741317
H	-0.927390	3.170988	2.866885
H	-1.328082	4.157354	4.287438
H	-1.061514	1.229881	6.487362
H	-1.003336	3.331513	6.332700

H	-4.524100	2.522943	1.937014
H	2.773647	-0.235058	-0.186469
H	1.671684	0.566659	1.814477
H	-0.806295	-1.268082	5.472851
H	0.441425	-0.175917	4.354746
H	1.178609	-1.632127	5.531448
H	0.086688	-2.099165	3.891912
H	1.796513	-1.715864	-0.215240
H	-1.394268	0.371430	-0.122539
H	0.818934	1.120617	-0.846348
H	0.629150	-0.325651	-1.857922
H	-3.145739	2.349858	-0.101965
H	-5.295505	-1.124184	3.966398
H	-5.213875	0.624429	4.284399
H	-6.044068	0.335897	6.555534
H	-6.957461	-0.945038	5.737968
H	-5.265934	-2.620407	6.326918
H	-5.342691	-1.658086	7.812246
H	-3.363798	-0.396698	7.213399
H	-2.951568	-1.943336	6.440055
H	-0.910104	-1.341910	-0.286809
H	1.579128	-1.178939	2.134715
H	-4.399829	-3.359050	1.714641
H	-3.917003	-4.262613	3.953428
H	-2.286766	-4.728825	3.461086
H	-3.699254	-5.530528	2.732398
H	-3.067258	-4.803819	0.293066
H	-2.693845	-3.103409	0.007528
H	-0.701037	-3.408226	1.622961
H	-0.928569	-5.158707	1.404085
H	0.721870	-4.940816	-1.920006
H	0.111979	-6.228751	-0.367919

$TS(F_RC^R{}_R \rightarrow F_RE^R{}_R)$

G = -1190,554549 $kcal.mol^{-1}$

C	4.630630	-2.421367	4.746965
O	3.250252	-2.502878	4.332879
C	3.123480	-2.007122	2.982640
C	4.547746	-1.718605	2.493593
C	5.415980	-2.540853	3.451978
La	1.366322	-2.347893	6.309708
B	2.261443	0.222082	6.536126
O	-0.416946	-1.768712	4.492622
C	-0.812345	-0.394685	4.231028
C	-2.212823	-0.480178	3.637174
C	-2.189093	-1.841977	2.939072
C	-1.397542	-2.683270	3.927035
O	-0.119017	-2.553055	7.899308
C	-1.108647	-2.425484	8.873808
C	-2.500508	-2.591022	8.235961
C	-2.720870	-3.959127	7.609295

O	-3.752123	-3.883164	6.615965
B	-4.916112	-4.544171	6.728393
O	0.980675	-4.704209	5.244184
B	0.635960	-5.824860	4.207823
O	2.822062	-4.104818	6.945421
C	2.612952	-5.226778	7.800344
C	3.876704	-5.593671	8.557625
C	-0.865016	-3.402675	10.026345
C	2.091607	-5.367493	5.563347
C	2.143001	-6.274898	6.774456
H	1.574919	-6.636993	4.437031
H	-0.384841	-6.377770	4.525727
H	0.774522	-5.409361	3.082364
H	2.962112	-5.237579	4.923612
H	-0.092181	0.036415	3.526683
H	1.158173	-6.703399	6.973392
H	2.857298	-7.089028	6.614779
H	-0.759534	0.166098	5.167706
H	-2.423113	0.352878	2.961443
H	-2.967867	-0.474937	4.430454
H	-2.038888	-3.055552	4.733534
H	-0.855357	-3.518210	3.478962
H	1.813390	-5.012219	8.525594
H	4.690309	-5.818626	7.859447
H	3.713510	-6.469003	9.196807
H	4.191645	-4.759160	9.191569
H	-1.666076	-1.776785	1.978290
H	-3.186063	-2.251983	2.759938
H	1.142239	0.111336	7.050235
H	3.011783	-0.602871	7.091209
H	2.695558	1.338301	6.649735
H	4.805935	-1.453681	5.235949
H	4.792276	-3.222689	5.470716
H	2.625886	-2.785105	2.394451
H	2.496725	-1.108728	2.989314
H	4.778028	-0.653575	2.599166
H	4.686425	-1.990441	1.443982
H	5.467925	-3.587513	3.132040
H	6.435749	-2.157321	3.541354
H	2.174101	-0.108102	5.342652
H	-1.077631	-1.404962	9.293105
H	0.110370	-3.204696	10.480673
H	-0.863636	-4.438174	9.669053
H	-1.631357	-3.305970	10.804047
H	-3.285825	-2.380300	8.973328
H	-2.593882	-1.839664	7.443062
H	-1.808404	-4.279246	7.097418
H	-2.989909	-4.716445	8.355068
H	-5.705492	-4.398770	5.838291
H	-5.137025	-5.241925	7.684037

$TS(F_RE^R{}_R \rightarrow F_RF^R{}_R)$

G = -1190,624409 kcal.mol^{-1}

C	-3.824020	-1.831413	6.204863
O	-3.708691	-0.782305	5.213028
C	-4.715915	0.230807	5.433069
C	-5.257700	-0.043793	6.828943
C	-5.144242	-1.567976	6.918333
La	-1.923148	-0.745968	3.305580
B	0.138404	-1.331161	5.050111
O	-0.002986	-0.510781	1.525150
C	1.409986	-0.321332	1.796120
C	2.101738	-0.472513	0.447869
C	1.034435	0.039641	-0.522265
C	-0.237213	-0.523853	0.095419
O	-2.931246	1.036196	2.467525
C	-3.562222	2.152114	1.942613
C	-3.409254	3.356757	2.898964
C	-2.001123	3.539353	3.453760
O	-1.771593	2.680390	4.582225
B	-1.395191	3.168781	5.778829
O	-2.787348	-2.536007	2.364985
C	-3.386922	-3.600130	1.699357
C	-2.630118	-3.910892	0.393714
C	-1.189483	-4.341572	0.618320
O	-0.426121	-4.151254	-0.581440
B	0.084894	-5.176123	-1.283061
C	-3.031861	2.475519	0.541824
C	-3.499375	-4.822551	2.615556
H	-4.091378	3.246820	3.750641
H	-3.706201	4.279487	2.382931
H	-3.558605	3.326070	0.093581
H	-1.961375	2.710810	0.571072
H	-1.248378	3.284127	2.700734
H	-1.835433	4.577258	3.767531
H	-1.242295	2.376301	6.662414
H	-1.239893	4.352901	5.931937
H	-4.647211	1.965133	1.836974
H	3.038422	0.089116	0.400525
H	1.546154	0.683505	2.213056
H	-0.971309	-1.434893	5.595464
H	0.225816	-0.175298	4.604983
H	1.030451	-1.555738	5.827900
H	0.154040	-2.121609	4.096862
H	2.323722	-1.525820	0.245625
H	-1.131092	0.073404	-0.101611
H	1.010809	1.135285	-0.526237
H	1.180740	-0.304669	-1.549236
H	-3.168657	1.608355	-0.111706
H	-5.492189	0.122150	4.665804
H	-4.239176	1.206205	5.319606
H	-4.624695	0.432493	7.585508

H	-6.279496	0.323021	6.957392
H	-5.973575	-2.044990	6.384400
H	-5.139579	-1.942849	7.944984
H	-2.964425	-1.757472	6.879786
H	-3.785101	-2.793841	5.687496
H	-0.408862	-1.557814	-0.223482
H	1.711419	-1.054254	2.546535
H	-4.412524	-3.318654	1.398215
H	-4.115010	-4.579280	3.487233
H	-2.513400	-5.128114	2.981148
H	-3.960139	-5.673884	2.100858
H	-3.165701	-4.675271	-0.184445
H	-2.621881	-2.996916	-0.211626
H	-0.734470	-3.712763	1.389254
H	-1.117150	-5.389523	0.932047
H	0.695658	-4.897046	-2.276072
H	-0.072084	-6.311561	-0.915639

$F_RF^R_R$

G = -1190,630329 kcal.mol^{-1}

C	-0.243329	-0.475460	0.231427
O	-0.036116	-0.538077	1.665907
C	1.346301	-0.231347	1.983132
C	2.082925	-0.298515	0.653632
C	1.011777	0.180144	-0.329201
La	-1.958702	-0.921871	3.410970
O	-2.838304	-2.595543	2.289180
C	-3.412287	-3.633652	1.559668
C	-3.534741	-4.897424	2.415886
O	-3.808898	-1.054385	5.257781
C	-3.920612	-2.081042	6.275444
C	-5.258366	-1.831753	6.966465
C	-5.455244	-0.326384	6.768488
C	-4.913391	-0.128333	5.361949
B	0.044214	-1.467774	5.215176
O	-2.880853	1.028796	2.910632
C	-3.546400	2.173006	2.479680
C	-3.333593	2.397557	0.978947
C	-3.146697	3.398032	3.324630
C	-1.663314	3.723194	3.283516
O	-1.360041	4.723481	4.258526
B	-0.844640	5.918619	3.930578
C	-2.621973	-3.875456	0.259757
C	-1.185795	-4.314133	0.498340
O	-0.391545	-4.054633	-0.666840
B	0.153066	-5.037115	-1.403943
H	-3.416276	3.203260	4.369663
H	-3.723234	4.275264	3.002693
H	-3.867850	3.285345	0.621493
H	-2.270213	2.520744	0.746738
H	-1.084650	2.830657	3.540339

H	-1.348969	4.071848	2.291807
H	-0.636872	6.682088	4.830231
H	-0.609608	6.192347	2.780672
H	-4.635119	2.045304	2.630334
H	2.983744	0.320672	0.649447
H	1.386492	0.774496	2.418348
H	-1.083055	-1.709312	5.676521
H	0.058828	-0.273654	4.872195
H	0.904226	-1.690539	6.026925
H	0.178429	-2.170100	4.202886
H	2.374572	-1.329907	0.428073
H	-1.158131	0.094346	0.045773
H	0.925253	1.272077	-0.300456
H	1.204857	-0.121209	-1.361840
H	-3.701534	1.530763	0.420808
H	-5.663146	-0.383303	4.601774
H	-4.526099	0.870535	5.154601
H	-4.857964	0.239942	7.491330
H	-6.497558	-0.010463	6.862045
H	-6.060058	-2.388459	6.468933
H	-5.239445	-2.132277	8.017085
H	-3.070725	-1.970011	6.956512
H	-3.856171	-3.058530	5.788639
H	-0.365180	-1.496047	-0.146445
H	1.686054	-0.951204	2.729909
H	-4.432799	-3.345637	1.249067
H	-4.169576	-4.698220	3.284920
H	-2.554353	-5.214542	2.786935
H	-3.978948	-5.726764	1.853252
H	-3.140363	-4.610667	-0.369418
H	-2.602050	-2.932323	-0.298609
H	-0.753982	-3.728147	1.315379
H	-1.117581	-5.377619	0.755694
H	0.789662	-4.700784	-2.361966
H	-0.001482	-6.191053	-1.098935

References and Notes