Supplementary Information for:

Kinetics of Thermoneutral Intermolecular Hydrogen Migration in Alkyl Radicals

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Contents:

SI Table 1: Energies, zero point energies, moments of inertia values for reactants, products and transition states of the reactions R1-R8. All data calculated with GAUSSIAN 03 program at the BH&HLYP/cc-pVDZ level of theory.

Specie	Energy (Hartree)		Moments of inertia (AMU)	ZPE (Hartree)
	BH&HLYP/cc-pVDZ	CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ	BH&HLYP/cc-pVDZ	BH&HLYP/cc-pVDZ
R1 reagent/product CCC.	-118.3937093	-118.113618	54.5946 199.9492 230.6975	0.0904997
R1 TS	-118.3201963	-118.0437131	71.1745 161.5352 197.1772	0.0860685
R2 reagent/product CCCC.	-157.682257	-157.311738	128.3375 363.79629 422.11434	0.120059
R2 TS	-157.6361994	-157.268945	154.44813 269.41561 362.9143	0.116791
R3 reagent/product CCCCC.	-196.9685288	-196.507665	249.454 518.9572 681.9103	0.1493748
R3 TS	-196.9368017	-196.4784784	269.3915 412.1531 597.776	0.1462626
R4,R5,R6 reagent/R4product CCCCCC.	-236.2527839	-235.7019505	414.2243 707.4946 968.7717	0.1787817
R4 TS	-236.2267003	-235.6777814	421.4809 593.6902 898.5078	0.1757586

SI Table 1 cont.: Energies, zero point energies, moments of inertia values for reactants, products and transition states of the reactions R1-R8. All data calculated with GAUSSIAN 03 program at the BH&HLYP/cc-pVDZ level of theory.

Specie	Energy (Hartree)		Moments of inertia (AMU)	ZPE (Hartree)
	BH&HLYP/cc-pVDZ	CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ	BH&HLYP/cc-pVDZ	BH&HLYP/cc-pVDZ
R5 TS	-236.2282224		344.4233 762.90971 985.91463	0.175389
R5 product CCCCC.C	-236.2626926		322.4424 946.4408 1155.1047	0.1789117
R6 TS	-236.2164991		224.3257 1038.8106 1163.725	0.175457
R6 Product CCC.CCC	-236.2641655		191.448 1266.218 1353.341	0.1792441
R7,R8 Reagent CCCCCCCC.	-314.8291965		536.4022 1874.4065 2219.5525	0.2375954
R7 TS	-314.7680751		233.8059 3287.6278 3322.0125	0.2326704
R7 Product CCC.CCCCC	-314.8346587		578.7623 1823.9144 2225.1469	0.2379863
R8 TS	-314.8052339		395.6007 2219.6556 2440.1164	0.2341677
R8 Product CCCC.CCCC	-314.8310248		516.8205 1988.3968 2282.2884	0.2377748

SI Tables 2-18: Optimized geometries and frequencies for reactants, products and transition states of the reactions R1-R8. All data calculated with GAUSSIAN 03 program at the BH&HLYP/cc-pVDZ level of theory.

SI Table 2. Reaction R1 reagent/product: CCC.				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	1.2194	-0.2417	-0.0351
2	H	1.2917	-0.7785	-0.986
3	H	1.2773	-0.9829	0.769
4	H	2.0923	0.4118	0.0509
5	C	-0.0775	0.5514	0.0483
6	H	-0.0868	1.1232	0.9924
7	H	-0.1022	1.3132	-0.7416
8	C	-1.2972	-0.2941	-0.0344
9	H	-1.2783	-1.3249	0.3069
10	H	-2.2623	0.1445	-0.2645
Frequencies (cm^{-1})				
126	263	378	473	779
913	949	1082	1128	1207
1307	1403	3034	3115	3117
3191	3197	3223	3333	1451
1493	1498	1522	1531	

SI Table 3. Reaction R1 TS				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-1.1002	-0.3305	0
2	C	1.1002	-0.3305	0
3	C	0	0.722	0
4	H	-1.6675	-0.4744	0.9182
5	H	1.6673	-0.4744	0.9183
6	H	0	1.3623	-0.8844
7	H	1.6676	-0.4744	-0.9181
8	H	-1.6675	-0.4745	-0.9181
9	H	0	1.3623	0.8844
10	H	-0.0002	-1.1928	-0.0003
Frequencies (cm^{-1})				
164	512	670	775	903
948	978	1024	1082	1215
1302	1360	1440	1460	1523
1833	3155	3179	3185	3204
3290	3291	2285i		

SI Table 4. Reaction R2 reagent/product: CCCC.

Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	0.6404	0.5948	-0.3263
2	C	1.5261	-0.5426	0.1584
3	C	-1.5831	-0.5932	-0.1253
4	C	-0.7607	0.577	0.2811
5	H	0.5544	0.5552	-1.4197
6	H	1.6597	-0.5004	1.245
7	H	-1.4771	-1.0194	-1.1189
8	H	-0.6891	0.6195	1.3761
9	H	-2.4278	-0.9166	0.4733
10	H	2.5182	-0.4982	-0.3006
11	H	1.1168	1.5538	-0.094
12	H	-1.2798	1.5069	-0.0086
13	H	1.0891	-1.5169	-0.0806
Frequencies (cm^{-1})				
158	238	324	437	488
800	854	871	983	1031
1104	1144	1213	1270	1334
1403	1429	1454	1489	1496
1519	1522	1534	3031	3106
3115	3116	3147	3188	3196
3221	3331			

SI Table 5. Reaction R2 TS				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-0.7359	0.7108	0.2197
2	C	-1.2418	-0.6732	-0.1319
3	C	1.2416	-0.6735	0.1319
4	C	0.7361	0.7106	-0.2198
5	H	-0.7927	0.8561	1.3044
6	H	-1.4861	-0.8321	-1.1838
7	H	1.4855	-0.8323	1.1839
8	H	0.7934	0.8562	-1.3045
9	H	1.9552	-1.149	-0.5393
10	H	-1.9552	-1.1487	0.5396
11	H	-1.3136	1.5183	-0.242
12	H	1.3138	1.5179	0.2425
13	H	-0.0002	-1.2345	-0.0002
Frequencies (cm^{-1})				
231	342	569	579	652
863	873	916	959	988
1012	1084	1117	1218	1266
1287	1365	1387	1413	1478
1487	1513	1534	1684	3118
3123	3155	3166	3174	3175
3261	3262	2073i		

SI Table 6. Reaction R3 reagent/product: CCCCC.

Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	1.6016	0.9306	0.0165
2	C	1.2586	-0.5328	-0.2215
3	C	-0.0629	-1.0083	0.3781
4	C	-1.3282	-0.4376	-0.2663
5	C	-1.6454	0.9728	0.0811
6	H	-0.1012	-2.0999	0.2911
7	H	1.2504	-0.735	-1.3006
8	H	2.0622	-1.1539	0.1917
9	H	1.6247	1.1608	1.0874
10	H	2.5868	1.1708	-0.3951
11	H	-1.2676	-0.5505	-1.3567
12	H	-2.1767	-1.0754	0.0376
13	H	-2.2615	1.5807	-0.5728
14	H	-1.4517	1.3466	1.082
15	H	-0.0777	-0.7911	1.4547
16	H	0.8732	1.6013	-0.4471
Frequencies (cm^{-1})				
153	166	252	330	342
464	496	785	817	883
895	958	1027	1087	1128
1160	1205	1262	1301	1352
1409	1423	1441	1458	1488
1497	1513	1517	1525	1534
3023	3099	3101	3115	3116
3139	3148	3184	3201	3222
3332				

SI Table 7. Reaction R3 TS				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	1.3084	0.9982	0.0594
2	C	1.2614	-0.4826	-0.2363
3	C	-0.0004	-1.128	0.339
4	C	-1.2618	-0.4818	-0.2366
5	C	-1.3086	0.9986	0.0597
6	H	-0.0007	-2.2029	0.1314
7	H	1.2739	-0.6423	-1.3214
8	H	2.151	-0.9905	0.1588
9	H	1.5639	1.2508	1.0906
10	H	1.8468	1.6189	-0.6569
11	H	-1.2741	-0.6413	-1.3217
12	H	-2.1518	-0.9894	0.1582
13	H	-1.8455	1.6205	-0.6567
14	H	-1.5624	1.2515	1.0912
15	H	-0.0006	-1.0201	1.4321
16	H	0.0055	1.3188	-0.0164
Frequencies (cm^{-1})				
154	305	358	438	474
588	671	837	848	884
913	948	1031	1034	1087
1131	1134	1225	1248	1294
1326	1395	1403	1422	1437
1481	1483	1510	1512	1528
1546	3092	3093	3103	3132
3138	3161	3161	3164	3245
3248	1923i			

SI Table 8. Reactions R4,R5,R6 reagent/R4 product CCCCCC.

Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	1.737	1.0862	-0.3638
2	C	1.5198	-0.1589	0.4853
3	C	-1.552	1.2962	0.3892
4	C	0.6247	-1.2289	-0.1492
5	C	-1.6354	0.0605	-0.4331
6	C	-0.8789	-1.1499	0.1195
7	H	2.1895	0.8252	-1.3268
8	H	1.1151	0.1239	1.4648
9	H	0.7961	-1.2424	-1.2342
10	H	-1.7899	2.2636	-0.0404
11	H	-1.3123	0.2672	-1.462
12	H	2.4096	1.7899	0.1366
13	H	2.4997	-0.6063	0.6875
14	H	-1.4695	1.232	1.47
15	H	0.9538	-2.2102	0.2112
16	H	-2.6985	-0.2225	-0.5255
17	H	-1.3298	-2.0534	-0.306
18	H	-1.0557	-1.2117	1.2017
19	H	0.801	1.6133	-0.5645
Frequencies (cm^{-1})				
100	149	182	230	298
330	398	466	495	762
814	824	898	937	945
1031	1059	1118	1134	1173
1204	1241	1291	1333	1348
1408	1416	1442	1446	1454
1487	1496	1510	1517	1519
1527	1535	3023	3096	3099
3108	3115	3117	3140	3145
3148	3184	3207	3222	3331

SI Table 9. Reaction R4 TS				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	1.3037	1.2644	-0.2506
2	C	1.6197	-0.1015	0.3033
3	C	-1.3037	1.2644	0.2506
4	C	0.7279	-1.2206	-0.2361
5	C	-1.6197	-0.1015	-0.3033
6	C	-0.7279	-1.2206	0.2361
7	H	1.3717	1.339	-1.3387
8	H	1.5454	-0.0802	1.3984
9	H	0.7503	-1.201	-1.3345
10	H	-1.8107	2.0956	-0.2418
11	H	-1.5454	-0.0802	-1.3984
12	H	1.8107	2.0956	0.2418
13	H	2.6662	-0.3531	0.0817
14	H	-1.3717	1.339	1.3387
15	H	1.1726	-2.1789	0.0548
16	H	-2.6662	-0.3531	-0.0818
17	H	-1.1726	-2.1789	-0.0548
18	H	-0.7503	-1.201	1.3345
19	H	0	1.4495	0
Frequencies (cm^{-1})				
125	177	315	345	384
424	533	545	625	797
841	847	901	965	966
986	1050	1091	1096	1158
1178	1221	1272	1287	1329
1333	1409	1424	1432	1442
1449	1479	1481	1484	1506
1512	1514	1524	3084	3084
3096	3096	3124	3125	3145
3145	3154	3154	3235	3236
1881i				

SI Table 10. Reaction R5 TS				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	1.0891	1.4503	0.1455
2	C	1.769	0.2081	-0.3796
3	C	1.147	-1.0615	0.2064
4	C	-0.3435	-1.1454	-0.1199
5	C	-1.1067	0.036	0.4366
6	C	1.667	-1.9451	-0.1773
7	H	1.6764	0.1709	-1.4719
8	H	2.8456	0.2263	-0.1641
9	H	1.3526	1.7202	1.1701
10	H	1.0797	2.3167	-0.5159
11	H	-0.4655	-1.1736	-1.211
12	H	-0.7593	-2.0895	0.2584
13	H	-1.1911	-0.0015	1.5272
14	H	1.2836	-1.0669	1.296
15	H	-0.1958	1.0013	0.2752
16	H	-2.3985	0.4044	-0.2416
17	H	-2.8487	1.2967	0.2028
18	H	-2.2462	0.6001	-1.3086
19	H	-3.1364	-0.4065	-0.1651
Frequencies (cm^{-1})				
112	170	209	302	342
422	459	506	602	831
849	861	904	952	957
1007	1050	1088	1117	1145
1175	1220	1250	1280	1325
1364	1400	1419	1431	1445
1456	1481	1508	1512	1512
1518	1528	1566	3082	3087
3091	3102	3121	3136	3150
3157	3160	3163	3192	3247
-1926i				

SI Table 11. Reaction R5 product CCCCC.C				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	1.3225	0.1568	0.3925
2	C	0.5504	-0.987	-0.1674
3	C	-0.9026	-1.1017	0.2945
4	C	-1.881	-0.1142	-0.3382
5	H	-1.2523	-2.115	0.0682
6	H	0.5853	-0.9539	-1.2661
7	H	1.0682	-1.9261	0.0999
8	H	1.0883	0.4814	1.4041
9	H	-1.8156	-0.2021	-1.4306
10	H	-2.8983	-0.4272	-0.0746
11	H	-0.9416	-1.0075	1.3881
12	C	2.6345	0.5463	-0.1881
13	H	2.9801	1.5115	0.192
14	H	3.4206	-0.1909	0.0467
15	H	2.5881	0.6076	-1.282
16	C	-1.6994	1.3425	0.0635
17	H	-0.7271	1.7331	-0.2477
18	H	-2.4734	1.9702	-0.3891
19	H	-1.7688	1.463	1.1503
Frequencies (cm^{-1})				
61	77	111	165	248
266	335	372	459	502
800	808	870	929	946
1018	1029	1075	1133	1140
1172	1210	1261	1298	1347
1366	1421	1435	1440	1458
1470	1491	1502	1508	1513
1518	1525	1534	3010	3044
3090	3101	3103	3115	3131
3139	3147	3183	3189	3202
3240				

SI Table 12. Reaction R6 TS				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-1.9981	0.6145	0.0559
2	C	-2.113	-0.8848	-0.1203
3	C	0.2367	-0.2265	0.4611
4	C	-0.5129	0.9267	-0.1809
5	C	-2.2691	0.885	1.0826
6	C	-2.1331	-1.238	-1.1529
7	H	0.2798	-0.1542	1.5529
8	H	-0.308	0.9321	-1.2591
9	H	-2.8018	-1.4299	0.5231
10	H	-2.6556	1.1853	-0.6082
11	H	-0.2241	1.9104	0.2041
12	H	-0.802	-1.0836	0.2717
13	H	1.5205	-0.7137	-0.1557
14	H	1.8094	-1.664	0.3079
15	H	1.3534	-0.9268	-1.219
16	H	2.6731	0.2794	-0.0192
17	H	2.8866	0.4923	1.0334
18	H	3.5884	-0.1127	-0.4737
19	H	2.439	1.2302	-0.5082
Frequencies (cm^{-1})				
84	124	198	251	312
384	486	579	604	796
834	883	919	937	973
985	1045	1047	1082	1125
1182	1217	1261	1273	1321
1353	1381	1386	1423	1444
1449	1483	1510	1514	1522
1531	1532	1690	3104	3107
3113	3119	3138	3148	3157
3167	3174	3188	3193	3262
-2067i				

SI Table 13. Reaction R6 product CCC.CCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-0.4265	-0.2848	0.3963
2	H	-0.2582	-0.4471	1.4603
3	C	0.4732	0.6723	-0.3074
4	H	0.0836	1.6998	-0.1993
5	H	0.4501	0.47	-1.3878
6	C	1.9176	0.6505	0.1874
7	H	2.4676	1.4742	-0.2812
8	H	1.9274	0.8538	1.2657
9	C	2.6345	-0.6616	-0.0914
10	H	3.6629	-0.6408	0.2813
11	C	-1.7352	-0.7095	-0.1781
12	H	-2.0343	-1.6702	0.2571
13	H	-1.6244	-0.8773	-1.2571
14	C	-2.8647	0.3029	0.0476
15	H	-2.6291	1.2684	-0.4108
16	H	-3.8039	-0.0539	-0.3869
17	H	-3.0314	0.474	1.1158
18	H	2.1217	-1.5033	0.3838
19	H	2.6741	-0.8663	-1.167
Frequencies (cm^{-1})				
26	61	140	197	237
292	313	380	466	539
781	811	869	919	926
1002	1064	1080	1106	1121
1187	1216	1270	1307	1339
1364	1390	1419	1437	1453
1474	1494	1508	1518	1521
1521	1532	1533	3023	3095
3101	3111	3114	3115	3140
3146	3187	3190	3195	3196
3223				

SI Table 14. Reactions R7,R8 reagent CCCCCCCC.				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-1.0155	0.1331	0.6188
2	C	-0.3763	-0.8548	-0.3519
3	C	1.8196	1.7085	-0.3906
4	C	0.9248	-1.4923	0.1498
5	C	2.4858	0.5989	0.3414
6	C	2.2384	-0.8025	-0.2222
7	H	-1.2699	-0.3976	1.5468
8	H	-0.1977	-0.359	-1.3148
9	H	0.8732	-1.6021	1.2413
10	H	1.659	2.6693	0.0869
11	H	2.214	0.6289	1.4045
12	H	-1.0945	-1.6553	-0.5583
13	H	1.6918	1.6548	-1.4676
14	H	0.9865	-2.5129	-0.2437
15	H	3.575	0.7782	0.3248
16	H	3.0526	-1.4522	0.1181
17	H	2.3276	-0.7626	-1.3161
18	H	-0.2829	0.8978	0.894
19	C	-2.2618	0.8306	0.082
20	H	-2.5777	1.588	0.8088
21	H	-1.9992	1.3808	-0.8308
22	C	-3.4354	-0.0958	-0.2045
23	H	-4.3148	0.4708	-0.5251
24	H	-3.2061	-0.8162	-0.9952
25	H	-3.7159	-0.6647	0.6891
Frequencies (cm^{-1})				
34	72	82	130	148
176	209	282	289	318
374	453	496	500	744
804	811	823	899	907
941	983	999	1029	1087
1114	1130	1151	1170	1206
1235	1261	1304	1317	1344
1368	1383	1410	1422	1437
1445	1453	1460	1487	1496
1508	1513	1516	1519	1526
1528	1534	3023	3093	3098
3100	3103	3107	3114	3117

3137	3141	3147	3149	3169
3185	3195	3221	3330	

SI Table 15. Reaction R7 TS

Optimized geometry (Angstrom)

Atom number	Atom Symbol	X	Y	Z
1	C	3.7415	0.8657	-0.4534
2	C	2.0516	-0.1414	0.5542
3	C	3.3795	-0.5614	-0.0681
4	H	4.5195	1.3661	0.1208
5	H	2.036	-0.1214	1.6458
6	H	3.2597	-1.2302	-0.9245
7	H	3.7085	1.1339	-1.5081
8	H	4.0763	-1.0267	0.632
9	H	2.4927	1.1189	0.1435
10	C	0.7661	-0.5572	-0.1036
11	H	0.6359	-1.6445	0.0165
12	H	0.8429	-0.3892	-1.1862
13	C	-0.4628	0.1588	0.4383
14	H	-0.5323	-0.0129	1.5204
15	H	-0.3311	1.2408	0.3124
16	C	-1.761	-0.2761	-0.2248
17	H	-1.8892	-1.3597	-0.0991
18	H	-1.6909	-0.1054	-1.3075
19	C	-2.9901	0.44	0.3164
20	H	-3.0607	0.268	1.3979
21	H	-2.8607	1.5224	0.1915
22	C	-4.2829	0.0021	-0.3532
23	H	-5.1471	0.5327	0.0566
24	H	-4.2554	0.1947	-1.431
25	H	-4.456	-1.0707	-0.2161

Frequencies (cm^{-1})

46	59	91	99	139
154	241	261	297	381
424	495	647	749	760
786	846	903	926	950
970	1006	1039	1055	1095
1102	1119	1131	1176	1212
1253	1265	1289	1303	1326
1346	1363	1363	1370	1403
1443	1454	1460	1471	1506
1515	1518	1519	1524	1530
1540	1822	3059	3091	3097
3105	3109	3113	3116	3136

3145	3153	3181	3184	3185
3191	3201	3289	2279i	

SI Table 16. Reaction R7 product CCC.CCCCC

Optimized geometry (Angstrom)

Atom number	Atom Symbol	X	Y	Z
1	C	-1.0284	-0.0454	0.4419
2	C	-0.3644	-1.0637	-0.4197
3	C	0.975	-1.5924	0.0985
4	C	2.2903	0.6388	0.4943
5	C	2.2198	-0.7434	-0.164
6	H	-0.885	-0.1221	1.5185
7	H	-0.2433	-0.6687	-1.4383
8	H	0.8864	-1.7775	1.1773
9	H	1.7932	0.6056	1.4713
10	H	-1.0436	-1.9273	-0.5338
11	H	1.1525	-2.5734	-0.356
12	H	3.3415	0.8688	0.703
13	H	3.0773	-1.3333	0.1794
14	H	2.3567	-0.631	-1.2481
15	C	-2.1693	0.7786	-0.0521
16	H	-2.2252	1.7115	0.5215
17	H	-1.9905	1.0659	-1.0961
18	C	-3.5249	0.0679	0.0379
19	H	-4.3304	0.7112	-0.3302
20	H	-3.5317	-0.8508	-0.5568
21	H	-3.7575	-0.2042	1.0722
22	C	1.7158	1.7763	-0.3392
23	H	0.6536	1.6317	-0.5505
24	H	1.8213	2.735	0.1781
25	H	2.2407	1.8589	-1.2973

Frequencies (cm^{-1})

30	51	74	97	136
214	227	274	297	324
363	416	489	534	762
788	819	851	905	916
960	1010	1017	1073	1089
1099	1134	1164	1187	1209
1238	1286	1310	1337	1348
1365	1392	1413	1438	1441
1443	1452	1474	1492	1508
1509	1516	1518	1521	1526
1533	1535	3014	3093	3096
3100	3104	3108	3114	3117

3139	3140	3144	3147	3183
3190	3195	3210	3228	

SI Table 17. Reaction R8 TS

Optimized geometry (Angstrom)

Atom number	Atom Symbol	X	Y	Z
1	C	2.2467	1.4175	0.1201
2	C	2.8022	0.1614	-0.5076
3	C	2.1711	-1.0927	0.1006
4	C	0.6532	-1.0947	-0.0822
5	C	0.0084	0.1121	0.5658
6	H	2.6046	-1.9891	-0.3542
7	H	2.6016	0.1674	-1.586
8	H	3.8941	0.1155	-0.3996
9	H	2.6228	1.6361	1.1215
10	H	2.2195	2.3065	-0.5099
11	H	0.4272	-1.0925	-1.1572
12	H	0.2346	-2.0282	0.3165
13	H	0.0019	0.0436	1.6589
14	H	2.4103	-1.1392	1.1714
15	H	0.9591	1.0276	0.3594
16	C	-1.3022	0.604	0.0038
17	H	-1.556	1.5684	0.4612
18	H	-1.1884	0.7959	-1.0718
19	C	-2.4705	-0.3594	0.2125
20	H	-2.2383	-1.3221	-0.2581
21	H	-2.579	-0.5637	1.285
22	C	-3.7826	0.1731	-0.3419
23	H	-4.6031	-0.5318	-0.1788
24	H	-4.0578	1.12	0.1347
25	H	-3.7111	0.3567	-1.4193

Frequencies (cm^{-1})

63	88	97	141	254
264	304	315	356	455
491	525	647	768	833
848	856	898	920	926
984	1011	1046	1076	1088
1099	1127	1151	1176	1222
1243	1271	1303	1327	1342
1364	1382	1401	1420	1424
1447	1448	1454	1482	1508
1511	1513	1520	1523	1527
1536	1561	3085	3091	3092
3101	3108	3112	3121	3124

3135	3145	3154	3159	3163
3186	3190	3247	-1924i	

SI Table 18. Reaction R8 product CCCC.CCCC

Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	1.1945	0.0444	0.6316
2	C	0.4841	-0.6031	-0.5501
3	C	3.5457	0.0005	-0.306
4	C	2.4395	0.8347	0.2336
5	H	1.4793	-0.7327	1.3539
6	H	0.1672	0.1757	-1.254
7	H	3.7084	-1.0051	0.0712
8	H	2.1682	1.6095	-0.4956
9	H	4.3209	0.4366	-0.9266
10	H	0.5081	0.7133	1.1607
11	H	2.7987	1.3885	1.1178
12	C	-0.7003	-1.4897	-0.1734
13	H	-1.0793	-1.9669	-1.0857
14	H	-0.3289	-2.3077	0.4573
15	C	-1.881	-0.8371	0.5485
16	H	-2.5681	-1.6459	0.8214
17	H	-1.5522	-0.4011	1.5002
18	C	-2.6676	0.211	-0.2452
19	H	-3.7032	0.2103	0.1134
20	H	-2.7196	-0.0963	-1.2979
21	C	-2.143	1.6382	-0.1507
22	H	-2.1179	1.9753	0.8914
23	H	-1.1324	1.741	-0.5532
24	H	-2.7876	2.3288	-0.7033
25	H	1.2069	-1.2166	-1.1005

Frequencies (cm^{-1})				
42	67	70	137	150
195	227	251	270	362
377	451	487	517	762
768	819	845	874	909
944	968	1005	1053	1092
1096	1137	1150	1166	1196
1237	1260	1284	1340	1347
1364	1383	1413	1418	1440
1449	1454	1462	1490	1495
1508	1514	1518	1521	1528
1533	1537	3031	3094	3099
3103	3107	3113	3116	3119

3132	3141	3145	3150	3165
3184	3208	3221	3331	

SI Table 19: Potential energy data along the MEP for reaction C.CC = CCC. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction CCC. = C.CC

$E_{CCC.}$ = -118.11361 hartree $ZPE_{CCC.}$ = 0.0904996 hartree

Reaction coordinate ($amu^{1/2}$ bohr)	V_C (Hartree)	ZPE (Hartree)	V_{ag} (Hartree)	$V_c - E_{CCC.}$ (kcal/mol)	$V_{ag}-E_{CCC.}$ (kcal/mol)
-1.50	-118.09203	0.08856	-118.00347	13.54	69.12
-1.48	-118.09166	0.08856	-118.00310	13.78	69.35
-1.46	-118.09128	0.08855	-118.00273	14.02	69.58
-1.44	-118.09089	0.08855	-118.00235	14.26	69.82
-1.42	-118.09050	0.08854	-118.00196	14.51	70.07
-1.40	-118.09010	0.08854	-118.00156	14.76	70.31
-1.38	-118.08969	0.08853	-118.00116	15.01	70.57
-1.36	-118.08928	0.08852	-118.00076	15.28	70.82
-1.34	-118.08885	0.08851	-118.00034	15.54	71.08
-1.32	-118.08842	0.08850	-117.99992	15.81	71.35
-1.30	-118.08798	0.08849	-117.99949	16.09	71.62
-1.28	-118.08753	0.08848	-117.99905	16.37	71.89
-1.26	-118.08708	0.08847	-117.99861	16.66	72.17
-1.24	-118.08661	0.08846	-117.99815	16.95	72.45
-1.22	-118.08614	0.08844	-117.99769	17.25	72.74
-1.20	-118.08565	0.08843	-117.99723	17.55	73.04
-1.18	-118.08516	0.08841	-117.99675	17.86	73.34
-1.16	-118.08465	0.08839	-117.99626	18.17	73.64
-1.14	-118.08414	0.08837	-117.99577	18.50	73.95
-1.12	-118.08362	0.08835	-117.99527	18.83	74.27
-1.10	-118.08308	0.08833	-117.99476	19.16	74.59
-1.08	-118.08254	0.08830	-117.99424	19.50	74.91
-1.06	-118.08198	0.08827	-117.99371	19.85	75.24
-1.04	-118.08141	0.08824	-117.99318	20.21	75.58
-1.02	-118.08084	0.08820	-117.99263	20.57	75.92
-1.00	-118.08025	0.08817	-117.99208	20.94	76.27
-0.98	-118.07965	0.08812	-117.99152	21.32	76.62
-0.96	-118.07903	0.08808	-117.99095	21.70	76.97
-0.94	-118.07841	0.08803	-117.99038	22.10	77.33
-0.92	-118.07777	0.08797	-117.98980	22.50	77.70
-0.90	-118.07712	0.08790	-117.98922	22.90	78.06
-0.88	-118.07646	0.08783	-117.98863	23.32	78.43
-0.86	-118.07578	0.08775	-117.98803	23.74	78.81
-0.84	-118.07509	0.08766	-117.98743	24.18	79.19

-0.82	-118.07438	0.08756	-117.98682	24.62	79.57
-0.80	-118.07366	0.08746	-117.98620	25.07	79.95
-0.78	-118.07293	0.08735	-117.98558	25.53	80.34
-0.76	-118.07218	0.08723	-117.98495	26.01	80.74
-0.74	-118.07141	0.08710	-117.98430	26.49	81.15
-0.72	-118.07062	0.08697	-117.98365	26.98	81.56
-0.70	-118.06981	0.08684	-117.98297	27.49	81.98
-0.68	-118.06898	0.08670	-117.98228	28.01	82.41
-0.66	-118.06814	0.08657	-117.98157	28.54	82.86
-0.64	-118.06727	0.08643	-117.98084	29.08	83.32
-0.62	-118.06638	0.08630	-117.98008	29.64	83.80
-0.60	-118.06548	0.08618	-117.97930	30.21	84.29
-0.58	-118.06455	0.08606	-117.97850	30.79	84.79
-0.56	-118.06361	0.08611	-117.97751	31.38	85.41
-0.54	-118.06266	0.08609	-117.97657	31.98	86.00
-0.52	-118.06169	0.08606	-117.97563	32.58	86.59
-0.50	-118.06071	0.08602	-117.97469	33.20	87.18
-0.48	-118.05973	0.08599	-117.97374	33.82	87.77
-0.46	-118.05874	0.08598	-117.97276	34.44	88.39
-0.44	-118.05775	0.08604	-117.97171	35.06	89.05
-0.42	-118.05676	0.08605	-117.97071	35.68	89.68
-0.40	-118.05578	0.08606	-117.96972	36.29	90.30
-0.38	-118.05481	0.08606	-117.96875	36.90	90.90
-0.36	-118.05386	0.08606	-117.96780	37.50	91.50
-0.34	-118.05292	0.08606	-117.96686	38.09	92.09
-0.32	-118.05200	0.08606	-117.96594	38.66	92.67
-0.30	-118.05111	0.08606	-117.96506	39.22	93.22
-0.28	-118.05026	0.08606	-117.96420	39.76	93.76
-0.26	-118.04944	0.08606	-117.96338	40.27	94.28
-0.24	-118.04866	0.08606	-117.96260	40.76	94.77
-0.22	-118.04792	0.08606	-117.96186	41.23	95.23
-0.20	-118.04723	0.08606	-117.96117	41.66	95.66
-0.18	-118.04659	0.08606	-117.96053	42.06	96.06
-0.16	-118.04601	0.08606	-117.95995	42.42	96.43
-0.14	-118.04549	0.08606	-117.95943	42.75	96.76
-0.12	-118.04503	0.08606	-117.95897	43.04	97.04
-0.10	-118.04464	0.08606	-117.95857	43.29	97.29
-0.08	-118.04431	0.08607	-117.95824	43.49	97.50
-0.06	-118.04405	0.08607	-117.95799	43.65	97.66
-0.04	-118.04387	0.08607	-117.95780	43.77	97.78
-0.02	-118.04375	0.08607	-117.95769	43.84	97.85
0.00	-118.04371	0.08594	-117.95777	43.87	97.85
0.02	-118.04375	0.08607	-117.95769	43.84	97.85
0.04	-118.04387	0.08607	-117.95780	43.77	97.78
0.06	-118.04405	0.08607	-117.95799	43.65	97.66
0.08	-118.04431	0.08607	-117.95824	43.49	97.50
0.10	-118.04464	0.08606	-117.95857	43.29	97.29
0.12	-118.04503	0.08606	-117.95897	43.04	97.04
0.14	-118.04549	0.08606	-117.95943	42.75	96.76
0.16	-118.04601	0.08606	-117.95995	42.42	96.43
0.18	-118.04659	0.08606	-117.96053	42.06	96.06

0.20	-118.04723	0.08606	-117.96117	41.66	95.66
0.22	-118.04792	0.08606	-117.96186	41.23	95.23
0.24	-118.04866	0.08606	-117.96260	40.76	94.77
0.26	-118.04944	0.08606	-117.96338	40.27	94.28
0.28	-118.05026	0.08606	-117.96420	39.76	93.76
0.30	-118.05111	0.08606	-117.96506	39.22	93.22
0.32	-118.05200	0.08606	-117.96594	38.66	92.67
0.34	-118.05292	0.08606	-117.96686	38.09	92.09
0.36	-118.05386	0.08606	-117.96780	37.50	91.50
0.38	-118.05481	0.08606	-117.96875	36.90	90.90
0.40	-118.05578	0.08606	-117.96972	36.29	90.30
0.42	-118.05676	0.08605	-117.97071	35.68	89.68
0.44	-118.05775	0.08604	-117.97171	35.06	89.05
0.46	-118.05874	0.08598	-117.97276	34.44	88.39
0.48	-118.05973	0.08599	-117.97374	33.82	87.77
0.50	-118.06071	0.08602	-117.97469	33.20	87.18
0.52	-118.06169	0.08606	-117.97563	32.58	86.59
0.54	-118.06266	0.08609	-117.97657	31.98	86.00
0.56	-118.06361	0.08611	-117.97751	31.38	85.41
0.58	-118.06455	0.08606	-117.97850	30.79	84.79
0.60	-118.06548	0.08618	-117.97930	30.21	84.29
0.62	-118.06638	0.08630	-117.98008	29.64	83.80
0.64	-118.06727	0.08643	-117.98084	29.08	83.32
0.66	-118.06814	0.08657	-117.98157	28.54	82.86
0.68	-118.06898	0.08670	-117.98228	28.01	82.41
0.70	-118.06981	0.08684	-117.98297	27.49	81.98
0.72	-118.07062	0.08697	-117.98365	26.98	81.56
0.74	-118.07141	0.08710	-117.98430	26.49	81.15
0.76	-118.07218	0.08723	-117.98495	26.01	80.74
0.78	-118.07293	0.08735	-117.98558	25.53	80.34
0.80	-118.07366	0.08746	-117.98620	25.07	79.95
0.82	-118.07438	0.08756	-117.98682	24.62	79.57
0.84	-118.07509	0.08766	-117.98743	24.18	79.19
0.86	-118.07578	0.08775	-117.98803	23.74	78.81
0.88	-118.07646	0.08783	-117.98863	23.32	78.43
0.90	-118.07712	0.08790	-117.98922	22.90	78.06
0.92	-118.07777	0.08797	-117.98980	22.50	77.70
0.94	-118.07841	0.08803	-117.99038	22.10	77.33
0.96	-118.07903	0.08808	-117.99095	21.70	76.97
0.98	-118.07965	0.08812	-117.99152	21.32	76.62
1.00	-118.08025	0.08817	-117.99208	20.94	76.27
1.02	-118.08084	0.08820	-117.99263	20.57	75.92
1.04	-118.08141	0.08824	-117.99318	20.21	75.58
1.06	-118.08198	0.08827	-117.99371	19.85	75.24
1.08	-118.08254	0.08830	-117.99424	19.50	74.91
1.10	-118.08308	0.08833	-117.99476	19.16	74.59
1.12	-118.08362	0.08835	-117.99527	18.83	74.27
1.14	-118.08414	0.08837	-117.99577	18.50	73.95
1.16	-118.08465	0.08839	-117.99626	18.17	73.64
1.18	-118.08516	0.08841	-117.99675	17.86	73.34
1.20	-118.08565	0.08843	-117.99723	17.55	73.04

1.22	-118.08614	0.08844	-117.99769	17.25	72.74
1.24	-118.08661	0.08846	-117.99815	16.95	72.45
1.26	-118.08708	0.08847	-117.99861	16.66	72.17
1.28	-118.08753	0.08848	-117.99905	16.37	71.89
1.30	-118.08798	0.08849	-117.99949	16.09	71.62
1.32	-118.08842	0.08850	-117.99992	15.81	71.35
1.34	-118.08885	0.08851	-118.00034	15.54	71.08
1.36	-118.08928	0.08852	-118.00076	15.28	70.82
1.38	-118.08969	0.08853	-118.00116	15.01	70.57
1.40	-118.09010	0.08854	-118.00156	14.76	70.31
1.42	-118.09050	0.08854	-118.00196	14.51	70.07
1.44	-118.09089	0.08855	-118.00235	14.26	69.82
1.46	-118.09128	0.08855	-118.00273	14.02	69.58
1.48	-118.09166	0.08856	-118.00310	13.78	69.35
1.50	-118.09203	0.08856	-118.00347	13.54	69.12

SI Table 20: Potential energy data along the MEP for reaction CCCC.= C.CCC. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction CCCC. = C.CCC

$E_{CCCC.}$ = -157.31174 hartree $ZPE_{CCCC.}$ = 0.1200698 hartree

Reaction coordinate ($amu^{1/2}$ bohr)	V_C (Hartree)	ZPE (Hartree)	V_{ag} (Hartree)	$V_c - E_{CCCC.}$ (kcal/mol)	$V_{ag}-E_{CCCC.}$ (kcal/mol)
-1.500	-157.2972	0.11921	-157.17800	9.12	83.92
-1.490	-157.2971	0.11921	-157.17787	9.20	84.00
-1.480	-157.2970	0.11921	-157.17778	9.26	84.06
-1.470	-157.2969	0.11921	-157.17765	9.34	84.14
-1.460	-157.2967	0.11921	-157.17754	9.41	84.21
-1.450	-157.2966	0.11921	-157.17742	9.48	84.28
-1.440	-157.2965	0.11921	-157.17730	9.56	84.36
-1.430	-157.2964	0.11921	-157.17719	9.63	84.43
-1.420	-157.2963	0.11921	-157.17706	9.71	84.51
-1.410	-157.2961	0.11921	-157.17693	9.79	84.59
-1.400	-157.2960	0.11921	-157.17682	9.86	84.66
-1.390	-157.2959	0.11920	-157.17669	9.94	84.74
-1.380	-157.2958	0.11920	-157.17657	10.02	84.82
-1.370	-157.2957	0.11920	-157.17645	10.09	84.89
-1.360	-157.2955	0.11920	-157.17633	10.17	84.97
-1.350	-157.2954	0.11920	-157.17622	10.24	85.04
-1.340	-157.2953	0.11920	-157.17607	10.33	85.13

-1.330	-157.2951	0.11920	-157.17595	10.41	85.21
-1.320	-157.2950	0.11920	-157.17582	10.49	85.29
-1.310	-157.2949	0.11920	-157.17569	10.57	85.37
-1.300	-157.2948	0.11920	-157.17555	10.66	85.46
-1.290	-157.2946	0.11920	-157.17544	10.73	85.53
-1.280	-157.2945	0.11920	-157.17530	10.82	85.62
-1.270	-157.2944	0.11920	-157.17516	10.91	85.71
-1.260	-157.2942	0.11919	-157.17503	10.99	85.79
-1.250	-157.2941	0.11919	-157.17490	11.07	85.86
-1.240	-157.2940	0.11919	-157.17476	11.16	85.95
-1.230	-157.2938	0.11919	-157.17464	11.24	86.03
-1.220	-157.2937	0.11919	-157.17449	11.33	86.12
-1.210	-157.2936	0.11919	-157.17437	11.41	86.20
-1.200	-157.2934	0.11918	-157.17421	11.51	86.30
-1.190	-157.2933	0.11918	-157.17409	11.59	86.38
-1.180	-157.2931	0.11918	-157.17395	11.68	86.47
-1.170	-157.2930	0.11918	-157.17380	11.77	86.55
-1.160	-157.2928	0.11917	-157.17365	11.87	86.65
-1.150	-157.2927	0.11917	-157.17351	11.96	86.74
-1.140	-157.2925	0.11917	-157.17337	12.05	86.83
-1.130	-157.2924	0.11917	-157.17323	12.14	86.92
-1.120	-157.2922	0.11916	-157.17309	12.23	87.01
-1.110	-157.2921	0.11916	-157.17295	12.32	87.09
-1.100	-157.2919	0.11916	-157.17279	12.42	87.19
-1.090	-157.2918	0.11915	-157.17263	12.52	87.29
-1.080	-157.2916	0.11915	-157.17249	12.61	87.38
-1.070	-157.2915	0.11915	-157.17232	12.72	87.48
-1.060	-157.2913	0.11914	-157.17218	12.81	87.57
-1.050	-157.2912	0.11914	-157.17203	12.91	87.67
-1.040	-157.2910	0.11913	-157.17189	13.00	87.76
-1.030	-157.2908	0.11913	-157.17172	13.11	87.86
-1.020	-157.2907	0.11912	-157.17158	13.20	87.95
-1.010	-157.2905	0.11912	-157.17141	13.31	88.06
-1.000	-157.2904	0.11911	-157.17126	13.41	88.15
-0.990	-157.2902	0.11910	-157.17111	13.51	88.25
-0.980	-157.2900	0.11910	-157.17094	13.62	88.35
-0.970	-157.2899	0.11909	-157.17078	13.72	88.45
-0.960	-157.2897	0.11908	-157.17061	13.83	88.56
-0.950	-157.2895	0.11908	-157.17046	13.93	88.65
-0.940	-157.2894	0.11907	-157.17030	14.04	88.76
-0.930	-157.2892	0.11906	-157.17013	14.15	88.86
-0.920	-157.2890	0.11905	-157.16996	14.26	88.97
-0.910	-157.2888	0.11904	-157.16978	14.38	89.08
-0.900	-157.2887	0.11903	-157.16963	14.48	89.17
-0.890	-157.2885	0.11902	-157.16947	14.59	89.28
-0.880	-157.2883	0.11901	-157.16928	14.71	89.39
-0.870	-157.2881	0.11900	-157.16914	14.81	89.48
-0.860	-157.2879	0.11899	-157.16896	14.93	89.60
-0.850	-157.2878	0.11898	-157.16879	15.04	89.70
-0.840	-157.2876	0.11896	-157.16862	15.16	89.81
-0.830	-157.2874	0.11895	-157.16844	15.28	89.92

-0.820	-157.2872	0.11893	-157.16826	15.40	90.03
-0.810	-157.2870	0.11892	-157.16810	15.51	90.13
-0.800	-157.2868	0.11890	-157.16793	15.63	90.24
-0.790	-157.2866	0.11888	-157.16774	15.76	90.36
-0.780	-157.2864	0.11886	-157.16757	15.88	90.47
-0.770	-157.2862	0.11884	-157.16740	16.00	90.58
-0.760	-157.2860	0.11882	-157.16721	16.13	90.69
-0.750	-157.2858	0.11880	-157.16704	16.25	90.80
-0.740	-157.2856	0.11877	-157.16686	16.38	90.91
-0.730	-157.2854	0.11874	-157.16670	16.50	91.01
-0.720	-157.2852	0.11871	-157.16652	16.63	91.12
-0.710	-157.2850	0.11868	-157.16635	16.76	91.23
-0.700	-157.2848	0.11865	-157.16619	16.88	91.33
-0.690	-157.2846	0.11861	-157.16601	17.02	91.45
-0.680	-157.2844	0.11857	-157.16584	17.15	91.55
-0.670	-157.2842	0.11852	-157.16570	17.27	91.64
-0.660	-157.2840	0.11847	-157.16552	17.41	91.75
-0.650	-157.2838	0.11842	-157.16537	17.54	91.85
-0.640	-157.2836	0.11836	-157.16522	17.67	91.94
-0.630	-157.2834	0.11830	-157.16506	17.81	92.04
-0.620	-157.2831	0.11823	-157.16490	17.95	92.14
-0.610	-157.2829	0.11816	-157.16475	18.09	92.24
-0.600	-157.2827	0.11817	-157.16452	18.23	92.38
-0.590	-157.2824	0.11815	-157.16430	18.38	92.52
-0.580	-157.2822	0.11811	-157.16411	18.52	92.64
-0.570	-157.2820	0.11807	-157.16394	18.66	92.75
-0.560	-157.2818	0.11801	-157.16375	18.81	92.86
-0.550	-157.2815	0.11795	-157.16357	18.96	92.97
-0.540	-157.2813	0.11789	-157.16340	19.11	93.09
-0.530	-157.2810	0.11782	-157.16321	19.27	93.21
-0.520	-157.2808	0.11776	-157.16301	19.43	93.33
-0.510	-157.2805	0.11769	-157.16284	19.58	93.43
-0.500	-157.2803	0.11763	-157.16265	19.74	93.55
-0.490	-157.2800	0.11757	-157.16244	19.91	93.69
-0.480	-157.2797	0.11751	-157.16223	20.08	93.82
-0.470	-157.2795	0.11745	-157.16202	20.25	93.95
-0.460	-157.2792	0.11739	-157.16180	20.42	94.09
-0.450	-157.2789	0.11734	-157.16157	20.60	94.23
-0.440	-157.2786	0.11729	-157.16133	20.78	94.38
-0.430	-157.2783	0.11724	-157.16109	20.96	94.53
-0.420	-157.2780	0.11720	-157.16083	21.15	94.69
-0.410	-157.2777	0.11716	-157.16057	21.34	94.86
-0.400	-157.2774	0.11712	-157.16032	21.52	95.01
-0.390	-157.2772	0.11709	-157.16007	21.70	95.17
-0.380	-157.2768	0.11705	-157.15979	21.90	95.35
-0.370	-157.2765	0.11702	-157.15951	22.09	95.52
-0.360	-157.2762	0.11700	-157.15924	22.28	95.70
-0.350	-157.2759	0.11697	-157.15893	22.49	95.89
-0.340	-157.2756	0.11695	-157.15866	22.67	96.06
-0.330	-157.2753	0.11693	-157.15836	22.87	96.24
-0.320	-157.2750	0.11691	-157.15808	23.06	96.42

-0.310	-157.2747	0.11690	-157.15779	23.25	96.60
-0.300	-157.2744	0.11688	-157.15750	23.44	96.78
-0.290	-157.2741	0.11687	-157.15721	23.63	96.97
-0.280	-157.2738	0.11686	-157.15694	23.81	97.14
-0.270	-157.2735	0.11685	-157.15666	23.99	97.31
-0.260	-157.2732	0.11684	-157.15637	24.18	97.50
-0.250	-157.2729	0.11683	-157.15610	24.35	97.66
-0.240	-157.2726	0.11682	-157.15582	24.53	97.84
-0.230	-157.2724	0.11682	-157.15556	24.70	98.00
-0.220	-157.2721	0.11681	-157.15529	24.87	98.17
-0.210	-157.2719	0.11681	-157.15504	25.03	98.33
-0.200	-157.2716	0.11680	-157.15481	25.18	98.48
-0.190	-157.2714	0.11680	-157.15456	25.34	98.63
-0.180	-157.2711	0.11680	-157.15434	25.48	98.77
-0.170	-157.2709	0.11679	-157.15410	25.63	98.92
-0.160	-157.2707	0.11679	-157.15389	25.76	99.05
-0.150	-157.2705	0.11679	-157.15370	25.88	99.17
-0.140	-157.2703	0.11679	-157.15351	26.00	99.29
-0.130	-157.2701	0.11679	-157.15334	26.11	99.40
-0.120	-157.2700	0.11679	-157.15316	26.22	99.51
-0.110	-157.2698	0.11679	-157.15301	26.32	99.61
-0.100	-157.2697	0.11679	-157.15286	26.41	99.70
-0.090	-157.2695	0.11679	-157.15273	26.49	99.78
-0.080	-157.2694	0.11679	-157.15261	26.57	99.86
-0.070	-157.2693	0.11679	-157.15251	26.63	99.92
-0.060	-157.2692	0.11679	-157.15241	26.69	99.98
-0.050	-157.2691	0.11679	-157.15234	26.74	100.03
-0.040	-157.2691	0.11679	-157.15227	26.78	100.07
-0.030	-157.2690	0.11679	-157.15222	26.81	100.10
-0.020	-157.2690	0.11679	-157.15219	26.83	100.12
-0.010	-157.2689	0.11678	-157.15217	26.85	100.13
0.000	-157.2689	0.11678	-157.15207	26.91	100.19
0.010	-157.2689	0.11678	-157.15217	26.85	100.13
0.020	-157.2690	0.11679	-157.15219	26.83	100.12
0.030	-157.2690	0.11679	-157.15222	26.81	100.10
0.040	-157.2691	0.11679	-157.15227	26.78	100.07
0.050	-157.2691	0.11679	-157.15235	26.73	100.02
0.060	-157.2692	0.11679	-157.15241	26.69	99.98
0.070	-157.2693	0.11679	-157.15251	26.63	99.92
0.080	-157.2694	0.11679	-157.15262	26.56	99.85
0.090	-157.2695	0.11679	-157.15273	26.49	99.78
0.100	-157.2697	0.11679	-157.15286	26.41	99.70
0.110	-157.2698	0.11679	-157.15302	26.31	99.60
0.120	-157.2700	0.11679	-157.15316	26.22	99.51
0.130	-157.2701	0.11679	-157.15334	26.11	99.40
0.140	-157.2703	0.11679	-157.15351	26.00	99.29
0.150	-157.2705	0.11679	-157.15370	25.88	99.17
0.160	-157.2707	0.11679	-157.15391	25.75	99.04
0.170	-157.2709	0.11679	-157.15413	25.61	98.90
0.180	-157.2711	0.11680	-157.15434	25.48	98.77

0.190	-157.2714	0.11680	-157.15457	25.33	98.62
0.200	-157.2716	0.11680	-157.15481	25.18	98.48
0.210	-157.2719	0.11681	-157.15506	25.02	98.32
0.220	-157.2721	0.11681	-157.15531	24.86	98.16
0.230	-157.2724	0.11682	-157.15556	24.70	98.00
0.240	-157.2727	0.11682	-157.15584	24.52	97.83
0.250	-157.2729	0.11683	-157.15610	24.35	97.66
0.260	-157.2732	0.11684	-157.15640	24.16	97.48
0.270	-157.2735	0.11685	-157.15666	23.99	97.31
0.280	-157.2738	0.11686	-157.15694	23.81	97.14
0.290	-157.2741	0.11687	-157.15721	23.63	96.97
0.300	-157.2744	0.11688	-157.15752	23.43	96.77
0.310	-157.2747	0.11690	-157.15781	23.24	96.59
0.320	-157.2750	0.11691	-157.15809	23.05	96.41
0.330	-157.2753	0.11693	-157.15838	22.86	96.24
0.340	-157.2756	0.11695	-157.15868	22.66	96.05
0.350	-157.2759	0.11697	-157.15896	22.47	95.87
0.360	-157.2762	0.11700	-157.15923	22.28	95.70
0.370	-157.2765	0.11703	-157.15951	22.09	95.52
0.380	-157.2768	0.11705	-157.15978	21.90	95.35
0.390	-157.2772	0.11709	-157.16007	21.70	95.17
0.400	-157.2774	0.11712	-157.16032	21.52	95.02
0.410	-157.2778	0.11716	-157.16060	21.32	94.84
0.420	-157.2780	0.11720	-157.16085	21.14	94.68
0.430	-157.2783	0.11725	-157.16109	20.96	94.53
0.440	-157.2786	0.11729	-157.16133	20.78	94.38
0.450	-157.2789	0.11734	-157.16158	20.59	94.22
0.460	-157.2792	0.11739	-157.16180	20.42	94.09
0.470	-157.2795	0.11745	-157.16202	20.25	93.95
0.480	-157.2797	0.11751	-157.16223	20.08	93.82
0.490	-157.2800	0.11757	-157.16244	19.91	93.69
0.500	-157.2803	0.11763	-157.16265	19.74	93.56
0.510	-157.2805	0.11770	-157.16284	19.58	93.44
0.520	-157.2808	0.11776	-157.16303	19.42	93.32
0.530	-157.2810	0.11783	-157.16320	19.27	93.21
0.540	-157.2813	0.11789	-157.16341	19.10	93.08
0.550	-157.2815	0.11795	-157.16357	18.96	92.98
0.560	-157.2818	0.11801	-157.16375	18.81	92.86
0.570	-157.2820	0.11807	-157.16395	18.65	92.74
0.580	-157.2822	0.11812	-157.16412	18.51	92.63
0.590	-157.2825	0.11815	-157.16431	18.37	92.51
0.600	-157.2827	0.11817	-157.16453	18.22	92.37
0.610	-157.2829	0.11817	-157.16474	18.09	92.24
0.620	-157.2831	0.11824	-157.16490	17.95	92.14
0.630	-157.2834	0.11830	-157.16505	17.81	92.05
0.640	-157.2836	0.11836	-157.16522	17.67	91.94
0.650	-157.2838	0.11842	-157.16537	17.54	91.85
0.660	-157.2840	0.11847	-157.16552	17.41	91.75
0.670	-157.2842	0.11852	-157.16569	17.27	91.64
0.680	-157.2844	0.11857	-157.16586	17.14	91.54
0.690	-157.2846	0.11861	-157.16601	17.02	91.45

0.700	-157.2848	0.11865	-157.16619	16.88	91.33
0.710	-157.2850	0.11868	-157.16635	16.76	91.23
0.720	-157.2852	0.11871	-157.16652	16.63	91.12
0.730	-157.2854	0.11875	-157.16670	16.50	91.01
0.740	-157.2856	0.11877	-157.16686	16.38	90.91
0.750	-157.2858	0.11880	-157.16704	16.25	90.80
0.760	-157.2860	0.11882	-157.16721	16.13	90.69
0.770	-157.2862	0.11884	-157.16740	16.00	90.58
0.780	-157.2864	0.11886	-157.16757	15.88	90.47
0.790	-157.2866	0.11888	-157.16776	15.75	90.35
0.800	-157.2868	0.11890	-157.16793	15.63	90.24
0.810	-157.2870	0.11892	-157.16810	15.51	90.13
0.820	-157.2872	0.11893	-157.16826	15.40	90.03
0.830	-157.2874	0.11895	-157.16845	15.27	89.91
0.840	-157.2876	0.11896	-157.16862	15.16	89.81
0.850	-157.2878	0.11898	-157.16879	15.04	89.70
0.860	-157.2879	0.11899	-157.16896	14.93	89.60
0.870	-157.2881	0.11900	-157.16914	14.81	89.48
0.880	-157.2883	0.11901	-157.16930	14.70	89.38
0.890	-157.2885	0.11902	-157.16947	14.59	89.28
0.900	-157.2887	0.11903	-157.16963	14.48	89.17
0.910	-157.2889	0.11904	-157.16981	14.36	89.06
0.920	-157.2890	0.11905	-157.16996	14.26	88.97
0.930	-157.2892	0.11906	-157.17014	14.14	88.85
0.940	-157.2894	0.11907	-157.17030	14.04	88.76
0.950	-157.2895	0.11908	-157.17046	13.93	88.65
0.960	-157.2897	0.11908	-157.17062	13.83	88.56
0.970	-157.2899	0.11909	-157.17078	13.72	88.45
0.980	-157.2900	0.11910	-157.17094	13.62	88.36
0.990	-157.2902	0.11910	-157.17110	13.51	88.25
1.000	-157.2904	0.11911	-157.17126	13.41	88.15
1.010	-157.2905	0.11912	-157.17141	13.31	88.06
1.020	-157.2907	0.11912	-157.17158	13.20	87.95
1.030	-157.2909	0.11913	-157.17174	13.10	87.85
1.040	-157.2910	0.11913	-157.17189	13.00	87.76
1.050	-157.2912	0.11914	-157.17203	12.91	87.67
1.060	-157.2913	0.11914	-157.17218	12.81	87.57
1.070	-157.2915	0.11915	-157.17235	12.70	87.46
1.080	-157.2916	0.11915	-157.17249	12.61	87.38
1.090	-157.2918	0.11915	-157.17263	12.52	87.29
1.100	-157.2919	0.11916	-157.17279	12.42	87.19
1.110	-157.2921	0.11916	-157.17294	12.32	87.09
1.120	-157.2922	0.11916	-157.17308	12.23	87.01
1.130	-157.2924	0.11917	-157.17323	12.14	86.92
1.140	-157.2925	0.11917	-157.17337	12.05	86.83
1.150	-157.2927	0.11917	-157.17352	11.95	86.73
1.160	-157.2928	0.11918	-157.17365	11.87	86.65
1.170	-157.2930	0.11918	-157.17380	11.77	86.56
1.180	-157.2931	0.11918	-157.17394	11.68	86.47
1.190	-157.2933	0.11918	-157.17409	11.59	86.38
1.200	-157.2934	0.11918	-157.17421	11.51	86.30

1.210	-157.2936	0.11919	-157.17437	11.41	86.20
1.220	-157.2937	0.11919	-157.17449	11.33	86.12
1.230	-157.2938	0.11919	-157.17464	11.24	86.03
1.240	-157.2940	0.11919	-157.17476	11.16	85.95
1.250	-157.2941	0.11919	-157.17490	11.07	85.86
1.260	-157.2942	0.11920	-157.17503	10.99	85.79
1.270	-157.2944	0.11920	-157.17516	10.91	85.71
1.280	-157.2945	0.11920	-157.17530	10.82	85.62
1.290	-157.2946	0.11920	-157.17544	10.73	85.53
1.300	-157.2948	0.11920	-157.17555	10.66	85.46
1.310	-157.2949	0.11920	-157.17569	10.57	85.37
1.320	-157.2950	0.11920	-157.17582	10.49	85.29
1.330	-157.2951	0.11920	-157.17595	10.41	85.21
1.340	-157.2953	0.11920	-157.17607	10.33	85.13
1.350	-157.2954	0.11920	-157.17622	10.24	85.04
1.360	-157.2955	0.11920	-157.17633	10.17	84.97
1.370	-157.2957	0.11921	-157.17645	10.09	84.89
1.380	-157.2958	0.11921	-157.17657	10.02	84.82
1.390	-157.2959	0.11921	-157.17669	9.94	84.74
1.400	-157.2960	0.11921	-157.17682	9.86	84.66
1.410	-157.2961	0.11921	-157.17693	9.79	84.59
1.420	-157.2963	0.11921	-157.17706	9.71	84.51
1.430	-157.2964	0.11921	-157.17718	9.63	84.43
1.440	-157.2965	0.11921	-157.17730	9.56	84.36
1.450	-157.2966	0.11921	-157.17742	9.48	84.28
1.460	-157.2967	0.11921	-157.17754	9.41	84.21
1.470	-157.2969	0.11921	-157.17765	9.34	84.14
1.480	-157.2970	0.11921	-157.17777	9.26	84.06
1.490	-157.2971	0.11921	-157.17790	9.18	83.98
1.500	-157.2972	0.11921	-157.17800	9.12	83.92

SI Table 21: Potential energy data along the MEP for reaction CCCCC.= C.CCCC. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction CCCCC. = C.CCCC

$E_{CCCCC.}$ = -196.50766 hartree $ZPE_{CCCCC.}$ = 0.149565 hartree

Reaction coordinate ($amu^{1/2}$ bohr)	V_C (Hartree)	ZPE (Hartree)	V_{ag} (Hartree)	$V_c - E_{CCCCC.}$ (kcal/mol)	$V_{ag}-E_{CCCCC.}$ (kcal/mol)
-1.51	-196.4978	0.14902	-196.3488	6.17	99.68

-1.49	-196.4977	0.14902	-196.3487	6.27	99.78
-1.47	-196.4975	0.14902	-196.3485	6.38	99.89
-1.45	-196.4973	0.14902	-196.3483	6.48	100.00
-1.43	-196.4972	0.14902	-196.3481	6.59	100.10
-1.41	-196.4970	0.14902	-196.3480	6.70	100.21
-1.39	-196.4968	0.14902	-196.3478	6.81	100.32
-1.37	-196.4966	0.14901	-196.3476	6.93	100.43
-1.35	-196.4964	0.14901	-196.3474	7.04	100.55
-1.33	-196.4963	0.14901	-196.3473	7.16	100.66
-1.31	-196.4961	0.14901	-196.3471	7.27	100.78
-1.29	-196.4959	0.14900	-196.3469	7.39	100.89
-1.27	-196.4957	0.14900	-196.3467	7.51	101.01
-1.25	-196.4955	0.14900	-196.3465	7.63	101.13
-1.23	-196.4953	0.14899	-196.3463	7.75	101.25
-1.21	-196.4951	0.14899	-196.3461	7.87	101.37
-1.19	-196.4949	0.14898	-196.3459	8.00	101.49
-1.17	-196.4947	0.14898	-196.3457	8.12	101.61
-1.15	-196.4945	0.14897	-196.3455	8.25	101.73
-1.13	-196.4943	0.14897	-196.3453	8.38	101.86
-1.11	-196.4941	0.14896	-196.3451	8.51	101.99
-1.09	-196.4939	0.14896	-196.3449	8.64	102.11
-1.07	-196.4937	0.14895	-196.3447	8.78	102.24
-1.05	-196.4935	0.14894	-196.3445	8.91	102.37
-1.03	-196.4932	0.14893	-196.3443	9.05	102.50
-1.01	-196.4930	0.14892	-196.3441	9.19	102.63
-0.99	-196.4928	0.14891	-196.3439	9.33	102.77
-0.97	-196.4926	0.14890	-196.3437	9.47	102.90
-0.95	-196.4924	0.14889	-196.3435	9.61	103.04
-0.93	-196.4921	0.14888	-196.3432	9.75	103.18
-0.91	-196.4919	0.14886	-196.3430	9.90	103.31
-0.89	-196.4917	0.14885	-196.3428	10.05	103.45
-0.87	-196.4914	0.14883	-196.3426	10.20	103.59
-0.85	-196.4912	0.14882	-196.3424	10.35	103.73
-0.83	-196.4909	0.14880	-196.3421	10.51	103.88
-0.81	-196.4907	0.14878	-196.3419	10.66	104.02
-0.79	-196.4904	0.14876	-196.3417	10.82	104.16
-0.77	-196.4902	0.14873	-196.3414	10.98	104.31
-0.75	-196.4899	0.14871	-196.3412	11.14	104.46
-0.73	-196.4897	0.14868	-196.3410	11.30	104.60
-0.71	-196.4894	0.14865	-196.3407	11.47	104.75
-0.69	-196.4891	0.14862	-196.3405	11.64	104.90
-0.67	-196.4889	0.14858	-196.3403	11.80	105.04
-0.65	-196.4886	0.14854	-196.3400	11.98	105.19
-0.63	-196.4883	0.14849	-196.3398	12.15	105.33
-0.61	-196.4880	0.14844	-196.3396	12.32	105.47
-0.59	-196.4878	0.14837	-196.3394	12.50	105.60
-0.57	-196.4875	0.14829	-196.3392	12.67	105.72
-0.55	-196.4872	0.14818	-196.3390	12.85	105.83
-0.53	-196.4869	0.14805	-196.3389	13.02	105.93
-0.51	-196.4866	0.14790	-196.3387	13.20	106.01
-0.49	-196.4863	0.14772	-196.3386	13.38	106.08

-0.47	-196.4860	0.14763	-196.3384	13.57	106.21
-0.45	-196.4857	0.14745	-196.3383	13.76	106.29
-0.43	-196.4854	0.14726	-196.3382	13.96	106.37
-0.41	-196.4851	0.14708	-196.3380	14.17	106.46
-0.39	-196.4847	0.14691	-196.3378	14.39	106.58
-0.37	-196.4844	0.14676	-196.3376	14.63	106.72
-0.35	-196.4840	0.14664	-196.3373	14.87	106.89
-0.33	-196.4836	0.14654	-196.3370	15.12	107.08
-0.31	-196.4831	0.14646	-196.3367	15.39	107.29
-0.29	-196.4827	0.14640	-196.3363	15.65	107.52
-0.27	-196.4823	0.14635	-196.3359	15.92	107.76
-0.25	-196.4819	0.14631	-196.3356	16.19	108.00
-0.23	-196.4814	0.14629	-196.3352	16.45	108.25
-0.21	-196.4810	0.14627	-196.3348	16.71	108.50
-0.19	-196.4806	0.14626	-196.3344	16.96	108.74
-0.17	-196.4803	0.14625	-196.3340	17.19	108.97
-0.15	-196.4799	0.14625	-196.3337	17.41	109.19
-0.13	-196.4796	0.14625	-196.3333	17.61	109.38
-0.11	-196.4793	0.14625	-196.3331	17.79	109.56
-0.09	-196.4791	0.14625	-196.3328	17.94	109.72
-0.07	-196.4789	0.14626	-196.3326	18.07	109.85
-0.05	-196.4787	0.14626	-196.3324	18.18	109.96
-0.03	-196.4786	0.14626	-196.3323	18.25	110.03
-0.01	-196.4785	0.14626	-196.3322	18.30	110.08
0.01	-196.4785	0.14626	-196.3322	18.30	110.08
0.03	-196.4786	0.14626	-196.3323	18.25	110.03
0.05	-196.4787	0.14626	-196.3324	18.18	109.96
0.07	-196.4789	0.14626	-196.3326	18.07	109.85
0.09	-196.4791	0.14625	-196.3328	17.94	109.72
0.11	-196.4793	0.14625	-196.3331	17.79	109.56
0.13	-196.4796	0.14625	-196.3333	17.61	109.38
0.15	-196.4799	0.14625	-196.3337	17.41	109.19
0.17	-196.4803	0.14625	-196.3340	17.19	108.97
0.19	-196.4806	0.14626	-196.3344	16.96	108.74
0.21	-196.4810	0.14627	-196.3348	16.71	108.50
0.23	-196.4814	0.14629	-196.3352	16.45	108.25
0.25	-196.4819	0.14631	-196.3356	16.19	108.00
0.27	-196.4823	0.14635	-196.3359	15.92	107.76
0.29	-196.4827	0.14640	-196.3363	15.65	107.52
0.31	-196.4831	0.14646	-196.3367	15.39	107.29
0.33	-196.4836	0.14654	-196.3370	15.12	107.08
0.35	-196.4840	0.14664	-196.3373	14.87	106.89
0.37	-196.4844	0.14676	-196.3376	14.63	106.72
0.39	-196.4847	0.14691	-196.3378	14.39	106.58
0.41	-196.4851	0.14708	-196.3380	14.17	106.46
0.43	-196.4854	0.14726	-196.3382	13.96	106.37
0.45	-196.4857	0.14745	-196.3383	13.76	106.29
0.47	-196.4860	0.14763	-196.3384	13.57	106.21
0.49	-196.4863	0.14772	-196.3386	13.38	106.08
0.51	-196.4866	0.14790	-196.3387	13.20	106.01
0.53	-196.4869	0.14805	-196.3389	13.02	105.93

0.55	-196.4872	0.14818	-196.3390	12.85	105.83
0.57	-196.4875	0.14829	-196.3392	12.67	105.72
0.59	-196.4878	0.14837	-196.3394	12.50	105.60
0.61	-196.4880	0.14844	-196.3396	12.32	105.47
0.63	-196.4883	0.14849	-196.3398	12.15	105.33
0.65	-196.4886	0.14854	-196.3400	11.98	105.19
0.67	-196.4889	0.14858	-196.3403	11.80	105.04
0.69	-196.4891	0.14862	-196.3405	11.64	104.90
0.71	-196.4894	0.14865	-196.3407	11.47	104.75
0.73	-196.4897	0.14868	-196.3410	11.30	104.60
0.75	-196.4899	0.14871	-196.3412	11.14	104.46
0.77	-196.4902	0.14873	-196.3414	10.98	104.31
0.79	-196.4904	0.14876	-196.3417	10.82	104.16
0.81	-196.4907	0.14878	-196.3419	10.66	104.02
0.83	-196.4909	0.14880	-196.3421	10.51	103.88
0.85	-196.4912	0.14882	-196.3424	10.35	103.73
0.87	-196.4914	0.14883	-196.3426	10.20	103.59
0.89	-196.4917	0.14885	-196.3428	10.05	103.45
0.91	-196.4919	0.14886	-196.3430	9.90	103.31
0.93	-196.4921	0.14888	-196.3432	9.75	103.18
0.95	-196.4924	0.14889	-196.3435	9.61	103.04
0.97	-196.4926	0.14890	-196.3437	9.47	102.90
0.99	-196.4928	0.14891	-196.3439	9.33	102.77
1.01	-196.4930	0.14892	-196.3441	9.19	102.63
1.03	-196.4932	0.14893	-196.3443	9.05	102.50
1.05	-196.4935	0.14894	-196.3445	8.91	102.37
1.07	-196.4937	0.14895	-196.3447	8.78	102.24
1.09	-196.4939	0.14896	-196.3449	8.64	102.11
1.11	-196.4941	0.14896	-196.3451	8.51	101.99
1.13	-196.4943	0.14897	-196.3453	8.38	101.86
1.15	-196.4945	0.14897	-196.3455	8.25	101.73
1.17	-196.4947	0.14898	-196.3457	8.12	101.61
1.19	-196.4949	0.14898	-196.3459	8.00	101.49
1.21	-196.4951	0.14899	-196.3461	7.87	101.37
1.23	-196.4953	0.14899	-196.3463	7.75	101.25
1.25	-196.4955	0.14900	-196.3465	7.63	101.13
1.27	-196.4957	0.14900	-196.3467	7.51	101.01
1.29	-196.4959	0.14900	-196.3469	7.39	100.89
1.31	-196.4961	0.14901	-196.3471	7.27	100.78
1.33	-196.4963	0.14901	-196.3473	7.16	100.66
1.35	-196.4964	0.14901	-196.3474	7.04	100.55
1.37	-196.4966	0.14901	-196.3476	6.93	100.43
1.39	-196.4968	0.14902	-196.3478	6.81	100.32
1.41	-196.4970	0.14902	-196.3480	6.70	100.21
1.43	-196.4972	0.14902	-196.3481	6.59	100.10
1.45	-196.4973	0.14902	-196.3483	6.48	100.00
1.47	-196.4975	0.14902	-196.3485	6.38	99.89
1.49	-196.4977	0.14902	-196.3487	6.27	99.78
1.51	-196.4978	0.14902	-196.3488	6.17	99.68

SI Table 22: Potential energy data along the MEP for reaction CCCCCC.= C.CCCCC. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction CCCCCC. = C.CCCCC

$E_{CCCCCC.}$ = -235.7019505 Hartree $ZPE_{CCCCCC.}$ = 0.17895 Hartree

Reaction coordinate ($amu^{1/2}$ bohr)	V_C (Hartree)	ZPE (Hartree)	V_{ag} (Hartree)	$V_c - E_{CCCCCC.}$ (kcal/mol)	$V_{ag}-E_{CCCCCC.}$ (kcal/mol)
-1.50	-235.6933	0.178566	-235.5147	5.42	117.47
-1.48	-235.6932	0.178564	-235.5146	5.51	117.56
-1.46	-235.6930	0.178562	-235.5145	5.59	117.64
-1.44	-235.6929	0.178560	-235.5143	5.68	117.73
-1.42	-235.6928	0.178558	-235.5142	5.77	117.81
-1.40	-235.6926	0.178555	-235.5141	5.85	117.90
-1.38	-235.6925	0.178552	-235.5139	5.94	117.99
-1.36	-235.6923	0.178550	-235.5138	6.03	118.08
-1.34	-235.6922	0.178546	-235.5136	6.12	118.16
-1.32	-235.6920	0.178543	-235.5135	6.22	118.25
-1.30	-235.6919	0.178540	-235.5134	6.31	118.35
-1.28	-235.6917	0.178536	-235.5132	6.40	118.44
-1.26	-235.6916	0.178532	-235.5131	6.50	118.53
-1.24	-235.6914	0.178528	-235.5129	6.60	118.63
-1.22	-235.6913	0.178523	-235.5128	6.70	118.72
-1.20	-235.6911	0.178518	-235.5126	6.79	118.82
-1.18	-235.6910	0.178513	-235.5125	6.89	118.91
-1.16	-235.6908	0.178508	-235.5123	7.00	119.01
-1.14	-235.6906	0.178502	-235.5121	7.10	119.11
-1.12	-235.6905	0.178496	-235.5120	7.20	119.21
-1.10	-235.6903	0.178490	-235.5118	7.31	119.31
-1.08	-235.6901	0.178483	-235.5117	7.41	119.41
-1.06	-235.6900	0.178475	-235.5115	7.52	119.51
-1.04	-235.6898	0.178468	-235.5113	7.63	119.62
-1.02	-235.6896	0.178459	-235.5112	7.74	119.72
-1.00	-235.6894	0.178450	-235.5110	7.85	119.83
-0.98	-235.6893	0.178441	-235.5108	7.96	119.93
-0.96	-235.6891	0.178431	-235.5107	8.07	120.04
-0.94	-235.6889	0.178420	-235.5105	8.19	120.15
-0.92	-235.6887	0.178409	-235.5103	8.30	120.25
-0.90	-235.6885	0.178397	-235.5101	8.42	120.36
-0.88	-235.6883	0.178384	-235.5100	8.54	120.47
-0.86	-235.6882	0.178370	-235.5098	8.66	120.58
-0.84	-235.6880	0.178355	-235.5096	8.78	120.70

-0.82	-235.6878	0.178339	-235.5094	8.90	120.81
-0.80	-235.6876	0.178321	-235.5093	9.02	120.92
-0.78	-235.6874	0.178303	-235.5091	9.15	121.03
-0.76	-235.6872	0.178283	-235.5089	9.27	121.15
-0.74	-235.6870	0.178262	-235.5087	9.40	121.26
-0.72	-235.6868	0.178239	-235.5085	9.53	121.38
-0.70	-235.6866	0.178214	-235.5083	9.66	121.49
-0.68	-235.6863	0.178187	-235.5082	9.79	121.61
-0.66	-235.6861	0.178157	-235.5080	9.93	121.72
-0.64	-235.6859	0.178125	-235.5078	10.06	121.84
-0.62	-235.6857	0.178089	-235.5076	10.20	121.95
-0.60	-235.6855	0.178049	-235.5074	10.34	122.06
-0.58	-235.6853	0.178000	-235.5073	10.47	122.17
-0.56	-235.6850	0.177941	-235.5071	10.61	122.27
-0.54	-235.6848	0.177865	-235.5070	10.75	122.36
-0.52	-235.6846	0.177763	-235.5068	10.89	122.44
-0.50	-235.6844	0.177626	-235.5068	11.03	122.49
-0.48	-235.6842	0.177445	-235.5067	11.16	122.51
-0.46	-235.6839	0.177222	-235.5067	11.30	122.51
-0.44	-235.6837	0.176967	-235.5067	11.45	122.50
-0.42	-235.6835	0.176700	-235.5068	11.60	122.48
-0.40	-235.6832	0.176525	-235.5067	11.76	122.53
-0.38	-235.6829	0.176332	-235.5066	11.94	122.59
-0.36	-235.6826	0.176167	-235.5065	12.13	122.67
-0.34	-235.6823	0.176035	-235.5063	12.33	122.79
-0.32	-235.6820	0.175934	-235.5060	12.54	122.94
-0.30	-235.6816	0.175859	-235.5058	12.76	123.12
-0.28	-235.6812	0.175805	-235.5054	12.99	123.31
-0.26	-235.6809	0.175768	-235.5051	13.23	123.52
-0.24	-235.6805	0.175744	-235.5048	13.46	123.74
-0.22	-235.6801	0.175730	-235.5044	13.69	123.96
-0.20	-235.6798	0.175724	-235.5041	13.91	124.18
-0.18	-235.6794	0.175722	-235.5037	14.13	124.39
-0.16	-235.6791	0.175725	-235.5034	14.33	124.59
-0.14	-235.6788	0.175729	-235.5031	14.51	124.78
-0.12	-235.6786	0.175734	-235.5028	14.68	124.95
-0.10	-235.6783	0.175740	-235.5026	14.82	125.10
-0.08	-235.6781	0.175746	-235.5024	14.94	125.22
-0.06	-235.6780	0.175751	-235.5022	15.04	125.32
-0.04	-235.6779	0.175754	-235.5021	15.11	125.40
-0.02	-235.6778	0.175748	-235.5021	15.15	125.44
0.00	-235.6778	0.175853	-235.5019	15.17	125.52
0.02	-235.6778	0.175748	-235.5021	15.15	125.44
0.04	-235.6779	0.175754	-235.5021	15.11	125.40
0.06	-235.6780	0.175751	-235.5022	15.04	125.32
0.08	-235.6781	0.175746	-235.5024	14.94	125.22
0.10	-235.6783	0.175740	-235.5026	14.82	125.10
0.12	-235.6786	0.175734	-235.5028	14.68	124.95
0.14	-235.6788	0.175729	-235.5031	14.51	124.78
0.16	-235.6791	0.175725	-235.5034	14.33	124.59
0.18	-235.6794	0.175722	-235.5037	14.13	124.39

0.20	-235.6798	0.175724	-235.5041	13.91	124.18
0.22	-235.6801	0.175730	-235.5044	13.69	123.96
0.24	-235.6805	0.175744	-235.5048	13.46	123.74
0.26	-235.6809	0.175768	-235.5051	13.23	123.52
0.28	-235.6812	0.175805	-235.5054	12.99	123.31
0.30	-235.6816	0.175859	-235.5058	12.76	123.12
0.32	-235.6820	0.175934	-235.5060	12.54	122.94
0.34	-235.6823	0.176035	-235.5063	12.33	122.79
0.36	-235.6826	0.176167	-235.5065	12.13	122.67
0.38	-235.6829	0.176332	-235.5066	11.94	122.59
0.40	-235.6832	0.176525	-235.5067	11.76	122.53
0.42	-235.6835	0.176700	-235.5068	11.60	122.48
0.44	-235.6837	0.176967	-235.5067	11.45	122.50
0.46	-235.6839	0.177222	-235.5067	11.30	122.51
0.48	-235.6842	0.177445	-235.5067	11.16	122.51
0.50	-235.6844	0.177626	-235.5068	11.03	122.49
0.52	-235.6846	0.177763	-235.5068	10.89	122.44
0.54	-235.6848	0.177865	-235.5070	10.75	122.36
0.56	-235.6850	0.177941	-235.5071	10.61	122.27
0.58	-235.6853	0.178000	-235.5073	10.47	122.17
0.60	-235.6855	0.178049	-235.5074	10.34	122.06
0.62	-235.6857	0.178089	-235.5076	10.20	121.95
0.64	-235.6859	0.178125	-235.5078	10.06	121.84
0.66	-235.6861	0.178157	-235.5080	9.93	121.72
0.68	-235.6863	0.178187	-235.5082	9.79	121.61
0.70	-235.6866	0.178214	-235.5083	9.66	121.49
0.72	-235.6868	0.178239	-235.5085	9.53	121.38
0.74	-235.6870	0.178262	-235.5087	9.40	121.26
0.76	-235.6872	0.178283	-235.5089	9.27	121.15
0.78	-235.6874	0.178303	-235.5091	9.15	121.03
0.80	-235.6876	0.178321	-235.5093	9.02	120.92
0.82	-235.6878	0.178339	-235.5094	8.90	120.81
0.84	-235.6880	0.178355	-235.5096	8.78	120.70
0.86	-235.6882	0.178370	-235.5098	8.66	120.58
0.88	-235.6883	0.178384	-235.5100	8.54	120.47
0.90	-235.6885	0.178397	-235.5101	8.42	120.36
0.92	-235.6887	0.178409	-235.5103	8.30	120.25
0.94	-235.6889	0.178420	-235.5105	8.19	120.15
0.96	-235.6891	0.178431	-235.5107	8.07	120.04
0.98	-235.6893	0.178441	-235.5108	7.96	119.93
1.00	-235.6894	0.178450	-235.5110	7.85	119.83
1.02	-235.6896	0.178459	-235.5112	7.74	119.72
1.04	-235.6898	0.178468	-235.5113	7.63	119.62
1.06	-235.6900	0.178475	-235.5115	7.52	119.51
1.08	-235.6901	0.178483	-235.5117	7.41	119.41
1.10	-235.6903	0.178490	-235.5118	7.31	119.31
1.12	-235.6905	0.178496	-235.5120	7.20	119.21
1.14	-235.6906	0.178502	-235.5121	7.10	119.11
1.16	-235.6908	0.178508	-235.5123	7.00	119.01
1.18	-235.6910	0.178513	-235.5125	6.89	118.91
1.20	-235.6911	0.178518	-235.5126	6.79	118.82

1.22	-235.6913	0.178523	-235.5128	6.70	118.72
1.24	-235.6914	0.178528	-235.5129	6.60	118.63
1.26	-235.6916	0.178532	-235.5131	6.50	118.53
1.28	-235.6917	0.178536	-235.5132	6.40	118.44
1.30	-235.6919	0.178540	-235.5134	6.31	118.35
1.32	-235.6920	0.178543	-235.5135	6.22	118.25
1.34	-235.6922	0.178546	-235.5136	6.12	118.16
1.36	-235.6923	0.178550	-235.5138	6.03	118.08
1.38	-235.6925	0.178552	-235.5139	5.94	117.99
1.40	-235.6926	0.178555	-235.5141	5.85	117.90
1.42	-235.6928	0.178558	-235.5142	5.77	117.81
1.44	-235.6929	0.178560	-235.5143	5.68	117.73
1.46	-235.6930	0.178562	-235.5145	5.59	117.64
1.48	-235.6932	0.178564	-235.5146	5.51	117.56
1.50	-235.6933	0.178566	-235.5147	5.42	117.47

SI Tables 23-26: Calculated high pressure limits of rate constants for reactions R1-R4. Units are s^{-1}.

SI Table 23: Calculated high-pressure rates for reaction R1: CCC. = C.CC

T(K)	1000/T (1/K)	High pressure limit of the rate constants (s^{-1})				
		This Study TST/HR	This study TST/Eckart/HR	This study CVT/HR	This study CVT/SCT/HR	Matheu et al. ref. 11
300	3.33	9.42E-18	4.40E-12	8.43E-18	8.43E-18	2.00E-18
400	2.50	3.26E-10	5.50E-07	2.90E-10	2.90E-10	2.85E-11
500	2.00	1.15E-05	8.95E-04	1.02E-05	1.02E-05	5.78E-07
600	1.67	1.29E-02	1.57E-01	1.14E-02	1.14E-02	4.40E-04
700	1.43	2.03E+00	7.42E+00	1.77E+00	1.77E+00	5.11E-02
800	1.25	9.21E+01	1.52E+02	8.02E+01	8.02E+01	1.83E+00
900	1.11	1.83E+03	1.75E+03	1.59E+03	1.59E+03	2.98E+01
1000	1.00	2.04E+04	1.34E+04	1.76E+04	1.76E+04	2.81E+02
1100	0.91	1.48E+05	7.52E+04	1.28E+05	1.28E+05	1.77E+03
1200	0.83	7.85E+05	3.35E+05	6.73E+05	6.73E+05	8.22E+03
1300	0.77	3.24E+06	1.24E+06	2.77E+06	2.77E+06	3.03E+04
1400	0.71	1.10E+07	3.95E+06	9.39E+06	9.39E+06	9.33E+04
1500	0.67	3.20E+07	1.12E+07	2.72E+07	2.72E+07	2.48E+05
1600	0.63	8.18E+07	2.85E+07	6.94E+07	6.94E+07	5.84E+05
1700	0.59	1.88E+08	6.70E+07	1.59E+08	1.59E+08	1.25E+06
1800	0.56	3.96E+08	1.46E+08	3.34E+08	3.34E+08	2.45E+06
1900	0.53	7.75E+08	3.00E+08	6.52E+08	6.52E+08	4.50E+06
2000	0.50	1.42E+09	5.85E+08	1.19E+09	1.19E+09	7.79E+06
2100	0.48	2.47E+09	1.09E+09	2.07E+09	2.07E+09	1.28E+07
2200	0.45	4.08E+09	1.94E+09	3.42E+09	3.42E+09	2.02E+07
2300	0.43	6.48E+09	3.33E+09	5.41E+09	5.41E+09	3.06E+07
2400	0.42	9.92E+09	5.54E+09	8.28E+09	8.28E+09	4.48E+07
2500	0.40	1.47E+10	8.96E+09	1.22E+10	1.22E+10	6.38E+07
2600	0.38	2.12E+10	1.41E+10	1.76E+10	1.76E+10	8.85E+07
2700	0.37	2.98E+10	2.17E+10	2.47E+10	2.47E+10	1.20E+08
2800	0.36	4.09E+10	3.27E+10	3.39E+10	3.39E+10	1.59E+08
2900	0.34	5.50E+10	4.82E+10	4.55E+10	4.55E+10	2.07E+08
3000	0.33	7.26E+10	6.99E+10	6.01E+10	6.01E+10	2.65E+08

SI Table 24: Calculated high-pressure rate constants for reaction R2: CCCC. = C.CCC

T(K)	1000/T (1/K)	High pressure limit of rate constants (s^{-1})				
		This Study TST/HR	This study TST/Eckart/HR	This study CVT/HR	This study CVT/SCT/HR	Matheu et al. ref. 11
300	3.33	2.88E-06	1.21E-02	2.83E-06	1.03E-03	5.86E-06
400	2.50	8.95E-02	2.92E+00	8.84E-02	1.92E+00	9.13E-02
500	2.00	4.59E+01	3.12E+02	4.54E+01	2.96E+02	2.97E+01
600	1.67	3.04E+03	1.09E+04	3.02E+03	1.06E+04	1.40E+03
700	1.43	6.27E+04	1.62E+05	6.21E+04	1.54E+05	2.19E+04
800	1.25	6.20E+05	1.31E+06	6.16E+05	1.22E+06	1.72E+05
900	1.11	3.76E+06	6.98E+06	3.74E+06	6.39E+06	8.52E+05
1000	1.00	1.62E+07	2.74E+07	1.61E+07	2.47E+07	3.06E+06
1100	0.91	5.40E+07	8.53E+07	5.37E+07	7.65E+07	8.71E+06
1200	0.83	1.49E+08	2.23E+08	1.48E+08	1.99E+08	2.08E+07
1300	0.77	3.56E+08	5.11E+08	3.53E+08	4.54E+08	4.34E+07
1400	0.71	7.54E+08	1.05E+09	7.48E+08	9.29E+08	8.15E+07
1500	0.67	1.46E+09	1.97E+09	1.44E+09	1.74E+09	1.41E+08
1600	0.63	2.60E+09	3.42E+09	2.58E+09	3.05E+09	2.26E+08
1700	0.59	4.37E+09	5.64E+09	4.33E+09	5.01E+09	3.45E+08
1800	0.56	6.95E+09	8.81E+09	6.89E+09	7.85E+09	5.00E+08
1900	0.53	1.06E+10	1.32E+10	1.05E+10	1.18E+10	6.98E+08
2000	0.50	1.54E+10	1.90E+10	1.53E+10	1.70E+10	9.43E+08
2100	0.48	2.18E+10	2.65E+10	2.17E+10	2.38E+10	1.24E+09
2200	0.45	3.00E+10	3.61E+10	2.98E+10	3.25E+10	1.58E+09
2300	0.43	4.02E+10	4.80E+10	3.99E+10	4.32E+10	1.98E+09
2400	0.42	5.27E+10	6.23E+10	5.22E+10	5.62E+10	2.43E+09
2500	0.40	6.77E+10	7.94E+10	6.71E+10	7.18E+10	2.93E+09
2600	0.38	8.54E+10	9.95E+10	8.47E+10	9.01E+10	3.49E+09
2700	0.37	1.06E+11	1.23E+11	1.05E+11	1.11E+11	4.10E+09
2800	0.36	1.30E+11	1.50E+11	1.29E+11	1.36E+11	4.76E+09
2900	0.34	1.57E+11	1.80E+11	1.56E+11	1.64E+11	5.47E+09
3000	0.33	1.88E+11	2.14E+11	1.87E+11	1.96E+11	6.23E+09

SI Table 25: Calculated high-pressure rate constants for reaction R3: CCCCC. = C.CCCC

T(K)	1000/T (1/K)	High pressure limit of rate constants (s^{-1})				
		This Study TST/HR	This study TST/Eckart/HR	This study CVT/HR	This study CVT/SCT/HR	Matheu et al. ref. 11
300	3.33	2.93E+00	6.54E+02	2.74E+00	2.54E+02	2.58E+01
400	2.50	2.16E+03	2.79E+04	2.06E+03	3.30E+04	1.33E+04
500	2.00	1.12E+05	5.25E+05	1.08E+05	7.01E+05	5.48E+05
600	1.67	1.58E+06	4.65E+06	1.53E+06	5.84E+06	6.40E+06
700	1.43	1.06E+07	2.41E+07	1.03E+07	2.80E+07	3.65E+07
800	1.25	4.46E+07	8.65E+07	4.38E+07	9.50E+07	1.33E+08
900	1.11	1.39E+08	2.42E+08	1.36E+08	2.52E+08	3.63E+08
1000	1.00	3.47E+08	5.57E+08	3.41E+08	5.61E+08	8.01E+08
1100	0.91	7.41E+08	1.12E+09	7.30E+08	1.10E+09	1.52E+09
1200	0.83	1.41E+09	2.04E+09	1.39E+09	1.95E+09	2.59E+09
1300	0.77	2.44E+09	3.40E+09	2.41E+09	3.22E+09	4.05E+09
1400	0.71	3.93E+09	5.31E+09	3.88E+09	4.97E+09	5.91E+09
1500	0.67	5.98E+09	7.88E+09	5.91E+09	7.32E+09	8.19E+09
1600	0.63	8.67E+09	1.12E+10	8.56E+09	1.03E+10	1.09E+10
1700	0.59	1.21E+10	1.53E+10	1.19E+10	1.41E+10	1.39E+10
1800	0.56	1.63E+10	2.03E+10	1.61E+10	1.86E+10	1.73E+10
1900	0.53	2.14E+10	2.63E+10	2.11E+10	2.40E+10	2.09E+10
2000	0.50	2.73E+10	3.31E+10	2.70E+10	3.03E+10	2.49E+10
2100	0.48	3.42E+10	4.10E+10	3.38E+10	3.75E+10	2.90E+10
2200	0.45	4.21E+10	5.01E+10	4.16E+10	4.56E+10	3.33E+10
2300	0.43	5.10E+10	6.01E+10	5.04E+10	5.47E+10	3.78E+10
2400	0.42	6.09E+10	7.12E+10	6.01E+10	6.49E+10	4.24E+10
2500	0.40	7.18E+10	8.34E+10	7.09E+10	7.60E+10	4.70E+10
2600	0.38	8.37E+10	9.65E+10	8.27E+10	8.81E+10	5.17E+10
2700	0.37	9.67E+10	1.11E+11	9.55E+10	1.01E+11	5.64E+10
2800	0.36	1.11E+11	1.27E+11	1.09E+11	1.15E+11	6.11E+10
2900	0.34	1.26E+11	1.43E+11	1.24E+11	1.30E+11	6.58E+10
3000	0.33	1.42E+11	1.60E+11	1.40E+11	1.46E+11	7.04E+10

SI Table 26: Calculated high-pressure rate constants for reaction R4: CCCCCC. = C.CCCCC

T(K)	1000/T (1/K)	High pressure limit of rate constants (s^{-1})				
		This Study TST/HR	This study TST/Eckart/HR	This study CVT/HR	This study CVT/SCT/HR	
300	3.33	3.63E+02	4.34E+04	3.63E+02	7.38E+03	
400	2.50	7.53E+04	9.17E+05	7.53E+04	4.22E+05	
500	2.00	1.86E+06	9.48E+06	1.86E+06	5.63E+06	
600	1.67	1.60E+07	5.34E+07	1.60E+07	3.46E+07	
700	1.43	7.59E+07	1.99E+08	7.59E+07	1.33E+08	
800	1.25	2.47E+08	5.55E+08	2.47E+08	3.81E+08	
900	1.11	6.28E+08	1.26E+09	6.28E+08	8.83E+08	
1000	1.00	1.34E+09	2.47E+09	1.34E+09	1.76E+09	
1100	0.91	2.50E+09	4.36E+09	2.50E+09	3.15E+09	
1200	0.83	4.26E+09	7.05E+09	4.26E+09	5.15E+09	
1300	0.77	6.71E+09	1.07E+10	6.71E+09	7.89E+09	
1400	0.71	9.95E+09	1.53E+10	9.95E+09	1.15E+10	
1500	0.67	1.41E+10	2.11E+10	1.41E+10	1.59E+10	
1600	0.63	1.91E+10	2.79E+10	1.91E+10	2.13E+10	
1700	0.59	2.51E+10	3.60E+10	2.51E+10	2.77E+10	
1800	0.56	3.22E+10	4.53E+10	3.22E+10	3.50E+10	
1900	0.53	4.02E+10	5.57E+10	4.02E+10	4.33E+10	
2000	0.50	4.92E+10	6.72E+10	4.92E+10	5.27E+10	
2100	0.48	5.91E+10	7.98E+10	5.91E+10	6.30E+10	
2200	0.45	7.01E+10	9.35E+10	7.01E+10	7.42E+10	
2300	0.43	8.19E+10	1.08E+11	8.19E+10	8.63E+10	
2400	0.42	9.47E+10	1.24E+11	9.46E+10	9.93E+10	
2500	0.40	1.08E+11	1.40E+11	1.08E+11	1.13E+11	
2600	0.38	1.23E+11	1.58E+11	1.23E+11	1.28E+11	
2700	0.37	1.38E+11	1.76E+11	1.38E+11	1.43E+11	
2800	0.36	1.54E+11	1.96E+11	1.54E+11	1.59E+11	
2900	0.34	1.70E+11	2.15E+11	1.70E+11	1.76E+11	
3000	0.33	1.87E+11	2.36E+11	1.87E+11	1.93E+11	

SI Table 27: Calculation of the RC-TST rate constants for the reaction R5: 1-hexyl = 2-hexyl.

R5: 1-hexyl = 2-hexyl		Delta V for R5 = 19.997 kcal/mol						
T	$k_r(T)$	FACTORS					k(T)	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	2.54E+02	0.67	0.92	0.44	5.90E-02	1.00	4.05E+00	0.61
400	3.30E+04	0.67	0.99	0.33	1.20E-01	0.93	7.84E+02	2.89
500	7.01E+05	0.67	1.00	0.26	1.83E-01	0.87	1.90E+04	4.28
600	5.84E+06	0.67	1.00	0.21	2.43E-01	0.83	1.65E+05	5.22
700	2.80E+07	0.67	1.00	0.18	2.97E-01	0.80	7.95E+05	5.90
800	9.50E+07	0.67	1.00	0.15	3.46E-01	0.79	2.66E+06	6.42
900	2.52E+08	0.67	1.00	0.14	3.89E-01	0.77	6.89E+06	6.84
1000	5.61E+08	0.67	1.00	0.12	4.28E-01	0.77	1.49E+07	7.17
1100	1.10E+09	0.67	1.00	0.11	4.62E-01	0.76	2.82E+07	7.45
1200	1.95E+09	0.67	1.00	0.10	4.93E-01	0.75	4.82E+07	7.68
1300	3.22E+09	0.67	1.00	0.09	5.20E-01	0.75	7.67E+07	7.88
1400	4.97E+09	0.67	1.00	0.08	5.45E-01	0.74	1.14E+08	8.06
1500	7.32E+09	0.67	1.00	0.08	5.68E-01	0.74	1.61E+08	8.21
1600	1.03E+10	0.67	1.00	0.07	5.88E-01	0.73	2.17E+08	8.34
1700	1.41E+10	0.67	1.00	0.07	6.07E-01	0.73	2.85E+08	8.45
1800	1.86E+10	0.67	1.00	0.06	6.24E-01	0.72	3.60E+08	8.56
1900	2.40E+10	0.67	1.00	0.06	6.40E-01	0.72	4.45E+08	8.65
2000	3.03E+10	0.67	1.00	0.06	6.54E-01	0.71	5.39E+08	8.73
2100	3.75E+10	0.67	1.00	0.05	6.67E-01	0.70	6.39E+08	8.81
2200	4.56E+10	0.67	1.00	0.05	6.80E-01	0.69	7.46E+08	8.87
2300	5.47E+10	0.67	1.00	0.05	6.91E-01	0.69	8.57E+08	8.93
2400	6.49E+10	0.67	1.00	0.05	7.02E-01	0.68	9.75E+08	8.99
2500	7.60E+10	0.67	1.00	0.05	7.12E-01	0.67	1.10E+09	9.04
2600	8.81E+10	0.67	1.00	0.04	7.21E-01	0.66	1.22E+09	9.09
2700	1.01E+11	0.67	1.00	0.04	7.30E-01	0.66	1.34E+09	9.13
2800	1.15E+11	0.67	1.00	0.04	7.38E-01	0.65	1.47E+09	9.17
2900	1.30E+11	0.67	1.00	0.04	7.46E-01	0.64	1.60E+09	9.20
3000	1.46E+11	0.67	1.00	0.04	7.54E-01	0.63	1.72E+09	9.24

SI Table 28: Calculation of the RC-TST rate constants for the reaction R6: 1-hexyl = 3-hexyl.

R6:1-hexyl = 3-hexyl RC-TST			Delta V = 25.43 kcal/mol						
T	1000/T	$k_r(T)$	FACTORS					k(T)	log k(T)
			Symmetry	Tunnelling	Partition	Energy	HR		
300	3.33	1.03E-03	0.67	1.66	0.85	1.16E+01	0.97	1.13E-02	-1.95
400	2.50	1.92E+00	0.67	1.14	0.63	6.28E+00	1.07	5.79E+00	0.76
500	2.00	2.96E+02	0.67	1.04	0.50	4.35E+00	1.17	4.45E+02	2.65
600	1.67	1.06E+04	0.67	1.02	0.41	3.40E+00	1.26	1.01E+04	4.00
700	1.43	1.54E+05	0.67	1.01	0.35	2.86E+00	1.36	1.04E+05	5.02
800	1.25	1.22E+06	0.67	1.01	0.30	2.51E+00	1.46	6.23E+05	5.79
900	1.11	6.39E+06	0.67	1.00	0.27	2.26E+00	1.57	2.60E+06	6.41
1000	1.00	2.47E+07	0.67	1.00	0.24	2.08E+00	1.68	8.28E+06	6.92
1100	0.91	7.65E+07	0.67	1.00	0.22	1.95E+00	1.79	2.17E+07	7.34
1200	0.83	1.99E+08	0.67	1.00	0.20	1.84E+00	1.90	4.86E+07	7.69
1300	0.77	4.54E+08	0.67	1.00	0.18	1.76E+00	2.02	9.72E+07	7.99
1400	0.71	9.29E+08	0.67	1.00	0.17	1.69E+00	2.13	1.77E+08	8.25
1500	0.67	1.74E+09	0.67	1.00	0.16	1.63E+00	2.24	2.97E+08	8.47
1600	0.63	3.05E+09	0.67	1.00	0.15	1.58E+00	2.34	4.72E+08	8.67
1700	0.59	5.01E+09	0.67	1.00	0.14	1.54E+00	2.45	7.08E+08	8.85
1800	0.56	7.85E+09	0.67	1.00	0.13	1.50E+00	2.55	1.02E+09	9.01
1900	0.53	1.18E+10	0.67	1.00	0.12	1.47E+00	2.65	1.42E+09	9.15
2000	0.50	1.70E+10	0.67	1.00	0.12	1.44E+00	2.75	1.90E+09	9.28
2100	0.48	2.38E+10	0.67	1.00	0.11	1.42E+00	2.84	2.48E+09	9.39
2200	0.45	3.25E+10	0.67	1.00	0.10	1.40E+00	2.93	3.17E+09	9.50
2300	0.43	4.32E+10	0.67	1.00	0.10	1.38E+00	3.02	3.96E+09	9.60
2400	0.42	5.62E+10	0.67	1.00	0.10	1.36E+00	3.10	4.87E+09	9.69
2500	0.40	7.18E+10	0.67	1.00	0.09	1.34E+00	3.19	5.89E+09	9.77
2600	0.38	9.01E+10	0.67	1.00	0.09	1.33E+00	3.27	7.00E+09	9.85
2700	0.37	1.11E+11	0.67	1.00	0.08	1.31E+00	3.34	8.21E+09	9.91
2800	0.36	1.36E+11	0.67	1.00	0.08	1.30E+00	3.42	9.58E+09	9.98
2900	0.34	1.64E+11	0.67	1.00	0.08	1.29E+00	3.48	1.10E+10	10.04
3000	0.33	1.96E+11	0.67	1.00	0.08	1.28E+00	3.56	1.26E+10	10.10

SI Table 29: Calculation of the RC-TST/LER rate constants for the reaction R6: 1-hexyl = 3-hexyl.

R6:1-hexyl = 3-hexyl RC-TST/LER			Delta E= -3.441 kcal/mol Delta V_{LER} = 24.47 kcal/mol						
T	1000/T	$k_r(T)$	FACTORS					k(T)	log k(T)
			Symmetry	Tunnelling	Partition	Energy	HR		
300	3.33	1.03E-03	0.67	0.78	0.83	5.89E+01	0.93	2.61E-02	-1.58
400	2.50	1.92E+00	0.67	0.97	0.61	2.13E+01	0.97	1.60E+01	1.20
500	2.00	2.96E+02	0.67	1.00	0.48	1.15E+01	1.01	1.09E+03	3.04
600	1.67	1.06E+04	0.67	1.00	0.40	7.68E+00	1.04	2.16E+04	4.33
700	1.43	1.54E+05	0.67	1.00	0.34	5.74E+00	1.08	1.99E+05	5.30
800	1.25	1.22E+06	0.67	1.00	0.29	4.61E+00	1.12	1.10E+06	6.04
900	1.11	6.39E+06	0.67	1.00	0.26	3.89E+00	1.15	4.29E+06	6.63
1000	1.00	2.47E+07	0.67	1.00	0.23	3.40E+00	1.19	1.29E+07	7.11
1100	0.91	7.65E+07	0.67	1.00	0.21	3.04E+00	1.23	3.24E+07	7.51
1200	0.83	1.99E+08	0.67	1.00	0.19	2.77E+00	1.26	7.01E+07	7.85
1300	0.77	4.54E+08	0.67	1.00	0.17	2.56E+00	1.30	1.36E+08	8.13
1400	0.71	9.29E+08	0.67	1.00	0.16	2.40E+00	1.34	2.40E+08	8.38
1500	0.67	1.74E+09	0.67	1.00	0.15	2.26E+00	1.38	3.94E+08	8.60
1600	0.63	3.05E+09	0.67	1.00	0.14	2.15E+00	1.41	6.13E+08	8.79
1700	0.59	5.01E+09	0.67	1.00	0.13	2.05E+00	1.45	9.03E+08	8.96
1800	0.56	7.85E+09	0.67	1.00	0.12	1.97E+00	1.49	1.28E+09	9.11
1900	0.53	1.18E+10	0.67	1.00	0.12	1.90E+00	1.52	1.75E+09	9.24
2000	0.50	1.70E+10	0.67	1.00	0.11	1.84E+00	1.56	2.32E+09	9.36
2100	0.48	2.38E+10	0.67	1.00	0.11	1.79E+00	1.60	2.99E+09	9.48
2200	0.45	3.25E+10	0.67	1.00	0.10	1.74E+00	1.63	3.79E+09	9.58
2300	0.43	4.32E+10	0.67	1.00	0.10	1.70E+00	1.67	4.68E+09	9.67
2400	0.42	5.62E+10	0.67	1.00	0.09	1.66E+00	1.71	5.70E+09	9.76
2500	0.40	7.18E+10	0.67	1.00	0.09	1.63E+00	1.75	6.84E+09	9.83
2600	0.38	9.01E+10	0.67	1.00	0.08	1.60E+00	1.78	8.07E+09	9.91
2700	0.37	1.11E+11	0.67	1.00	0.08	1.57E+00	1.82	9.40E+09	9.97
2800	0.36	1.36E+11	0.67	1.00	0.08	1.55E+00	1.86	1.09E+10	10.04
2900	0.34	1.64E+11	0.67	1.00	0.07	1.52E+00	1.89	1.25E+10	10.10
3000	0.33	1.96E+11	0.67	1.00	0.07	1.50E+00	1.93	1.42E+10	10.15

SI Table 30: Calculation of the RC-TST rate constants for the reaction R7: 1-octyl = 3-octyl.

R7: 1-octyl=3-octyl RC-TST			Delta V = 20.02 kcal/mol						
T	1000/T	$k_r(T)$	FACTORS					k(T)	log k(T)
			Symmetry	Tunnelling	Partition	Energy	HR		
300	3.33	7.38E+03	0.67	2.96	0.74	2.88E-04	1.14	3.09E+00	0.49
400	2.50	4.22E+05	0.67	1.27	0.58	2.21E-03	1.18	4.56E+02	2.66
500	2.00	5.63E+06	0.67	1.07	0.44	7.51E-03	1.22	1.33E+04	4.12
600	1.67	3.46E+07	0.67	1.02	0.36	1.70E-02	1.24	1.46E+05	5.16
700	1.43	1.33E+08	0.67	1.01	0.28	3.04E-02	1.27	7.60E+05	5.88
800	1.25	3.81E+08	0.67	1.00	0.23	4.70E-02	1.29	2.74E+06	6.44
900	1.11	8.83E+08	0.67	1.00	0.18	6.60E-02	1.31	7.17E+06	6.86
1000	1.00	1.76E+09	0.67	1.00	0.17	8.67E-02	1.33	1.70E+07	7.23
1100	0.91	3.15E+09	0.67	1.00	0.14	1.08E-01	1.35	3.09E+07	7.49
1200	0.83	5.15E+09	0.67	1.00	0.12	1.30E-01	1.37	5.39E+07	7.73
1300	0.77	7.89E+09	0.67	1.00	0.12	1.52E-01	1.39	9.53E+07	7.98
1400	0.71	1.15E+10	0.67	1.00	0.10	1.74E-01	1.40	1.34E+08	8.13
1500	0.67	1.59E+10	0.67	1.00	0.10	1.96E-01	1.41	2.09E+08	8.32
1600	0.63	2.13E+10	0.67	1.00	0.10	2.17E-01	1.43	3.03E+08	8.48
1700	0.59	2.77E+10	0.67	1.00	0.10	2.37E-01	1.44	4.15E+08	8.62
1800	0.56	3.50E+10	0.67	1.00	0.09	2.57E-01	1.45	5.52E+08	8.74
1900	0.53	4.33E+10	0.67	1.00	0.09	2.76E-01	1.46	7.16E+08	8.85
2000	0.50	5.27E+10	0.67	1.00	0.09	2.94E-01	1.46	9.14E+08	8.96
2100	0.48	6.30E+10	0.67	1.00	0.09	3.12E-01	1.47	1.14E+09	9.06
2200	0.45	7.42E+10	0.67	1.00	0.09	3.29E-01	1.48	1.40E+09	9.15
2300	0.43	8.63E+10	0.67	1.00	0.09	3.45E-01	1.48	1.70E+09	9.23
2400	0.42	9.93E+10	0.67	1.00	0.09	3.61E-01	1.48	2.03E+09	9.31
2500	0.40	1.13E+11	0.67	1.00	0.08	3.76E-01	1.48	2.40E+09	9.38
2600	0.38	1.28E+11	0.67	1.00	0.08	3.90E-01	1.49	2.81E+09	9.45
2700	0.37	1.43E+11	0.67	1.00	0.08	4.04E-01	1.49	3.25E+09	9.51
2800	0.36	1.59E+11	0.67	1.00	0.08	4.18E-01	1.49	3.72E+09	9.57
2900	0.34	1.76E+11	0.67	1.00	0.08	4.30E-01	1.49	4.24E+09	9.63
3000	0.33	1.93E+11	0.67	1.00	0.08	4.43E-01	1.49	4.78E+09	9.68

SI Table 31: Calculation of the RC-TST rate constants for the reaction R8: 1-octyl = 4-octyl.

R8: 1-octyl=4-octyl RC-TST		Delta V = 20.585 kcal/mol						
T	$k_r(T)$	FACTORS					k(T)	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	2.54E+02	0.67	2.00	0.70	0.02	1.01	5.33E+00	0.73
400	3.30E+04	0.67	1.17	0.55	0.06	1.11	8.99E+02	2.95
500	7.01E+05	0.67	1.05	0.43	0.10	1.22	2.61E+04	4.42
600	5.84E+06	0.67	1.02	0.34	0.15	1.33	2.69E+05	5.43
700	2.80E+07	0.67	1.01	0.28	0.20	1.44	1.48E+06	6.17
800	9.50E+07	0.67	1.00	0.23	0.24	1.56	5.50E+06	6.74
900	2.52E+08	0.67	1.00	0.19	0.28	1.68	1.55E+07	7.19
1000	5.61E+08	0.67	1.00	0.17	0.32	1.81	3.61E+07	7.56
1100	1.10E+09	0.67	1.00	0.15	0.35	1.93	7.34E+07	7.87
1200	1.95E+09	0.67	1.00	0.13	0.39	2.05	1.35E+08	8.13
1300	3.22E+09	0.67	1.00	0.12	0.42	2.17	2.31E+08	8.36
1400	4.97E+09	0.67	1.00	0.11	0.44	2.29	3.70E+08	8.57
1500	7.32E+09	0.67	1.00	0.10	0.47	2.40	5.66E+08	8.75
1600	1.03E+10	0.67	1.00	0.10	0.49	2.51	8.32E+08	8.92
1700	1.41E+10	0.67	1.00	0.10	0.51	2.60	1.19E+09	9.07
1800	1.86E+10	0.67	1.00	0.09	0.53	2.70	1.64E+09	9.21
1900	2.40E+10	0.67	1.00	0.09	0.55	2.79	2.21E+09	9.34
2000	3.03E+10	0.67	1.00	0.09	0.56	2.88	2.91E+09	9.46
2100	3.75E+10	0.67	1.00	0.09	0.58	2.96	3.76E+09	9.57
2200	4.56E+10	0.67	1.00	0.09	0.59	3.04	4.75E+09	9.68
2300	5.47E+10	0.67	1.00	0.09	0.61	3.12	5.93E+09	9.77
2400	6.49E+10	0.67	1.00	0.09	0.62	3.18	7.28E+09	9.86
2500	7.60E+10	0.67	1.00	0.08	0.63	3.24	8.83E+09	9.95
2600	8.81E+10	0.67	1.00	0.08	0.64	3.31	1.06E+10	10.03
2700	1.01E+11	0.67	1.00	0.08	0.66	3.36	1.25E+10	10.10
2800	1.15E+11	0.67	1.00	0.08	0.67	3.42	1.47E+10	10.17
2900	1.30E+11	0.67	1.00	0.08	0.67	3.47	1.70E+10	10.23
3000	1.46E+11	0.67	1.00	0.08	0.68	3.52	1.97E+10	10.29