Supplementary Information for:

Kinetics of the C-C Bond Beta Scission Reactions in Alkyl Radicals

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SI Table 1: Energies, zero point energies, moments of inertia values for reactants, products and transition states of the reactions R1-R12. 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
CCC.	-118.393126	-118.111295	57.32811 202.93896 225.51944	0.090663
C=C	-78.535203	-78.352596	12.30874 59.33805 71.64680	0.052487
C.	-39.811568	-39.715156	6.32926 6.32928 12.65854	0.030235
TS R1	-118.3359319	-118.0585036	64.84996 284.95692 313.03142	0.086357
CCCC.	-1.576823	-157.311775	72.96050 474.18892 501.34894	0.120044
CC.	-79.105029	-78.9158971	17.44815 79.05434 85.30820	0.060750
TS R2	-157.628309	-157.259228	91.96298 578.31617 622.50737	0.116293
CCC.C	-157.6880079	-157.313452	67.60139 492.78849 524.19216	0.119855

SI Table 1 cont.: Energies, zero point energies, moments of inertia values for reactants, products and transition states of the reactions R1-R12. 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
C=CC	-117.8260564	-117.5509873	38.60719 193.76571 221.17905	0.081406
TS R3	-157.629911	-157.2608033	137.93027 491.11307 555.33596	0.115401
CC(C.)C	-157.683173	-157.3111560	212.90727 226.17460 387.71724	0.119552
TS R4	-157.626381	-157.25862916	227.25657 305.45438 465.33096	0.115565
C.CCCCC	-236.260089		119.09412 1533.08096 1584.2665	0.1787319
TS R5	-236.2057292		142.0351 1740.0218 1812.1858	0.1752405
CC.CCCC	-236.2658779		112.6570 1570.3021 1623.6570	0.1784701
TS R6	-236.2104516		185.0610 1646.2317 1714.3834	0.1748826
CCC.CCC	-236.2655834		120.5044 1563.3609 1620.4529	0.1786369

SI Table 1 cont.: Energies, zero point energies, moments of inertia values for reactants, products and transition states of the reactions R1-R12. 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
TS R7	-236.2105258		171.1500 1623.1412 1669.0686	0.1748226
C=CCC	-157.1145840		61.2909 450.0574 489.1062	0.1110103
C.CCCCCCC	-314.8378788		163.1718 3579.3801 3652.5462	0.2373327
TS R8	-314.7819211		190.4557 3881.6939 3980.1776	0.2338345
CC.CCCCCC	-314.8436626		156.5424 3634.4237 3708.7747	0.2370665
TS R9	-314.789179		235.0984 3776.2607 3844.6045	0.2334470
C.CCCC	-196.9711964		100.8923 894.1817 938.2075	0.1494508
CCC.CCCCC	-314.8433621		168.9410 3621.4785 3702.4130	0.2372145
TS R10	-314.7851800		249.6236 3551.8279 3668.0918	0.2327849

SI Table 1 cont.: Energies, zero point energies, moments of inertia values for reactants, products and transition states of the reactions R1-R12. 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
C=CCCCCC	-274.9814980		126.2333 2359.3765 2430.2125	0.1989689
CCCC.CCCC	-314.8434515		168.5369 3637.2375 3713.0985	0.2371799
TS R11	-314.7883822		235.0619 3776.2781 3844.6706	0.2334470
C=CCCC	-196.4037150		82.7803 870.7818 920.2680	0.1403662
TS R12	-314.7884598		250.3183 3618.1065 3693.5221	0.2334003
C=CCCCC	-235.6925920		105.2947 1491.8224 1552.7708	0.1696574

SI Tables 2-33: Optimized geometries and frequencies for reactants, products and transition states of the reactions R1-R12. All data calculated with GAUSSIAN 03 program at the BH&HLYP/cc-pVDZ level of theory.

SI Table 2: 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: TS R1				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-0.0001	0.0001	0.0001
2	C	-0.0003	-0.0002	2.2954
3	H	1.0838	-0.0008	2.2661
4	H	-0.4789	-0.973	2.266
5	C	-0.6747	1.0839	2.7478
6	H	-1.7487	1.0579	2.9025
7	H	-0.1767	2.0358	2.9025
8	H	0.5677	-0.909	-0.1761
9	H	0.502	0.9378	-0.2135
10	H	-1.0629	-0.0394	-0.2141
Frequencies (cm^{-1})				
105	230	365	517	538
817	840	888	975	1039
1270	1327	1440	1445	1490
1619	3170	3228	3240	3316
3341	3342	3350	-465i	

SI Table 4: C=C

Optimized geometry (Angstrom)

Atom number	Atom Symbol	X	Y	Z
1	C	-0.0036	0	0.0023
2	H	-0.0029	0	1.0883
3	C	1.1224	0	-0.6926
4	H	1.1216	0	-1.7787
5	H	2.0928	0	-0.2049
6	H	-0.974	0	-0.4855

Frequencies (cm^{-1})

852	1014	1015	1095	1272
1413	1497	1766	3223	3243
3309	3335			

SI Table 5: C.				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	0	0	0
2	H	0	0	1.0828
3	H	0.9377	0	-0.5414
4	H	-0.9377	0.0007	-0.5414
Frequencies (cm^{-1})				
457	1424	1424	3190	3387
3387				

SI Table 6: CCCC.

Optimized geometry (Angstrom)

Atom number	Atom Symbol	X	Y	Z
1	C	-0.0015	0.0008	-0.0013
2	H	0.0001	0.0016	1.0951
3	H	1.0512	0.0016	-0.3076
4	C	-0.6705	1.2889	-0.5027
5	H	-1.7231	1.2738	-0.1927
6	H	-0.6694	1.273	-1.6
7	C	-0.0172	2.5323	-0.0144
8	H	0.8462	2.9438	-0.5272
9	H	-0.2698	2.9485	0.9555
10	C	-0.6877	-1.2546	-0.5155
11	H	-0.1952	-2.1588	-0.1464
12	H	-1.7349	-1.2923	-0.1968
13	H	-0.6757	-1.2923	-1.6101

Frequencies (cm^{-1})

69	131	252	262	405
532	759	821	907	970
1076	1116	1129	1230	1318
1331	1365	1416	1450	1493
1517	1520	1522	1535	3097
3112	3115	3132	3155	3187
3192	3225	3334		

SI Table 7. CC.

Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	0.0023	0.0009	0.0017
2	H	0.0027	-0.0042	1.0964
3	H	1.0426	-0.0043	-0.339
4	H	-0.4365	-0.9588	-0.3161
5	C	-0.7505	1.1574	-0.5438
6	H	-0.5433	1.5346	-1.5395
7	H	-1.6336	1.5328	-0.0378
Frequencies (cm^{-1})				
132	466	826	1004	1104
1223	1431	1492	1507	1511
3056	3143	3190	3232	3341

SI Table 8: TS R2				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-0.0013	-0.0014	0.0005
2	C	-0.002	-0.0011	2.2763
3	H	1.0825	-0.0043	2.2439
4	H	-0.4805	-0.9743	2.2448
5	C	-0.6696	1.075	2.762
6	H	-1.7415	1.0473	2.9296
7	H	-0.1688	2.0233	2.9286
8	H	0.4701	0.9631	-0.1694
9	H	-1.0749	-0.0073	-0.1698
10	C	0.7664	-1.2235	-0.379
11	H	0.835	-1.3323	-1.4715
12	H	1.7927	-1.1932	0.0014
13	H	0.2935	-2.135	0.0011
Frequencies (cm^{-1})				
58	162	166	262	385
582	797	837	846	871
926	1037	1064	1105	1247
1269	1321	1434	1488	1499
1512	1513	1615	3077	3147
3185	3209	3224	3236	3305
3313	3338	-469i		

SI Table 9: CCC.C

Optimized geometry (Angstrom)

Atom number	Atom Symbol	X	Y	Z
1	C	-0.0028	-0.0038	0.0061
2	H	-0.0135	-0.0119	1.1108
3	H	1.0628	0.0043	-0.2634
4	C	-0.6475	1.2425	-0.4917
5	H	-1.7048	1.2058	-0.7458
6	C	-0.6576	-1.2784	-0.5062
7	H	-0.1625	-2.1692	-0.1096
8	H	-1.7111	-1.3238	-0.2111
9	H	-0.618	-1.3283	-1.5987
10	C	-0.01	2.5697	-0.2895
11	H	-0.4774	3.3457	-0.9018
12	H	-0.0809	2.9025	0.7595
13	H	1.0593	2.5427	-0.5317

Frequencies (cm^{-1})

66	119	251	265	413
442	791	878	996	1013
1072	1103	1170	1217	1307
1345	1434	1450	1469	1497
1502	1511	1522	1530	3022
3046	3097	3117	3130	3189
3190	3197	3240		

SI Table 10: C=CC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	C	0.1334	-0.4522
2	H	H	0.1673	-1.5411
3	C	C	1.2754	0.2202
4	H	H	1.2936	1.307
5	H	H	2.2333	-0.2892
6	C	C	-1.2281	0.1617
7	H	H	-1.8014	-0.1541
8	H	H	-1.8014	-0.1541
9	H	H	-1.1756	1.2535
Frequencies (cm^{-1})				
216	435	611	963	970
984	1063	1105	1226	1361
1440	1482	1504	1518	1797
3109	3168	3200	3224	3235

SI Table 11: TS R3				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-0.0003	-0.0003	-0.0001
2	C	-0.0001	0.0003	2.2928
3	H	1.085	0.0002	2.2651
4	H	-0.481	-0.9708	2.2786
5	C	-0.6711	1.09	2.7425
6	H	-1.7467	1.0158	2.8918
7	H	0.5669	-0.9091	-0.1799
8	H	0.5028	0.9361	-0.2192
9	H	-1.0621	-0.04	-0.2205
10	C	-0.0573	2.4334	2.9494
11	H	-0.2578	2.8121	3.9585
12	H	1.0267	2.4047	2.8077
13	H	-0.4692	3.174	2.2518
Frequencies (cm^{-1})				
98	121	156	268	428
508	521	688	813	941
956	970	1020	1073	1223
1319	1434	1441	1445	1471
1501	1516	1637	3097	3151
3168	3193	3230	3238	3330
3337	3345	-474i		

SI Table 12: CC(C.)C				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	0.0045	0.0074	0.0029
2	H	0.0041	-0.007	1.0881
3	H	0.9645	-0.005	-0.5033
4	C	-1.1658	0.3597	-2.1727
5	H	-2.0717	0.14	-2.7456
6	H	-1.0387	1.4472	-2.1453
7	H	-0.3148	-0.0629	-2.7155
8	C	-2.4678	0.3442	-0.0117
9	H	-3.3964	0.1235	-0.5468
10	H	-2.5469	-0.0888	0.9901
11	H	-2.3917	1.4312	0.0986
12	C	-1.2579	-0.2099	-0.7594
13	H	-1.4092	-1.3001	-0.8586
Frequencies (cm^{-1})				
137	239	269	369	381
411	534	849	930	966
1003	1020	1122	1222	1243
1368	1380	1437	1449	1492
1511	1516	1526	1537	3009
3111	3115	3186	3190	3191
3194	3221	3331		

SI Table 13: TS R4				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	0.0003	-0.0005	0.0002
2	C	0	0.0003	2.2773
3	H	1.0852	0.0006	2.2148
4	C	-0.614	1.1654	2.617
5	H	-1.6798	1.1993	2.824
6	H	0.6857	-0.8226	-0.1867
7	H	0.3613	0.9922	-0.2483
8	H	-1.0491	-0.1923	-0.2015
9	C	-0.6449	-1.3393	2.4963
10	H	-1.733	-1.2721	2.4088
11	H	-0.2911	-2.0899	1.7864
12	H	-0.4147	-1.7073	3.503
13	H	-0.0786	2.1084	2.6089
Frequencies (cm^{-1})				
122	177	220	287	424
531	547	564	839	874
948	965	1017	1078	1218
1310	1435	1441	1446	1474
1510	1520	1618	3115	3165
3182	3209	3227	3246	3327
3333	3342	-510i		

SI Table 14. C.CCCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-3.1264	0.2109	0
2	H	-3.2126	0.8533	-0.8829
3	H	-3.9827	-0.4698	0
4	H	-3.2126	0.8533	0.8829
5	C	-1.8094	-0.5492	0
6	H	-1.7667	-1.2087	-0.876
7	H	-1.7667	-1.2087	0.876
8	C	-0.5906	0.3623	0
9	H	-0.6322	1.0227	-0.8766
10	H	-0.6322	1.0227	0.8765
11	C	0.7315	-0.391	0
12	H	0.7799	-1.0489	0.8766
13	H	0.7799	-1.0489	-0.8766
14	C	1.9537	0.5381	0
15	H	1.8911	1.1921	0.8789
16	H	1.8911	1.1921	-0.8789
17	C	3.2539	-0.1842	0
18	H	3.6935	-0.5357	-0.928
Frequencies (cm^{-1})				
67	83	116	137	162
259	296	381	438	547
758	768	824	923	933
1027	1032	1074	1115	1117
1164	1233	1281	1286	1344
1364	1365	1374	1419	1451
1462	1494	1515	1517	1520
1523	1531	1540	3091	3098
3101	3109	3112	3117	3130
3142	3160	3185	3191	3224
3333				

SI Table 15: TS R5				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	0.5126	0.7182	0
2	C	2.33	-0.6552	-0.0001
3	H	1.958	-1.0941	-0.9197
4	H	1.9579	-1.0943	0.9195
5	C	3.4798	0.0639	0
6	H	3.9393	0.3961	-0.9254
7	H	0.7165	1.2739	-0.9124
8	H	0.7165	1.2739	0.9124
9	C	-0.6657	-0.2017	0
10	H	-0.6264	-0.8595	-0.8781
11	H	-0.6264	-0.8593	0.8782
12	H	3.9392	0.3959	0.9255
13	C	-2.0118	0.5297	0
14	H	-2.0632	1.187	0.8762
15	H	-2.0632	1.1869	-0.8763
16	C	-3.1991	-0.4205	0
17	H	-4.1475	0.1245	0
18	H	-3.1877	-1.0684	-0.883
Frequencies (cm^{-1})				
42	64	93	134	234
257	303	381	428	577
762	800	832	838	878
917	978	985	1038	1075
1112	1146	1241	1269	1321
1325	1338	1369	1423	1453
1488	1499	1516	1520	1523
1536	1615	3094	3111	3114
3127	3152	3187	3192	3200
3225	3237	3296	3313	3339
-442i				

SI Table 16: CC.CCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-3.1595	0.2338	-0.0662
2	H	-3.2182	0.7925	-1.0064
3	H	-4.0214	-0.4384	-0.0253
4	H	-3.262	0.9556	0.7511
5	C	-1.8497	-0.5311	0.0372
6	H	-1.791	-1.2686	-0.7733
7	H	-1.834	-1.1077	0.9708
8	C	-0.6244	0.3691	-0.016
9	H	-0.6348	0.9462	-0.9493
10	H	-0.6801	1.106	0.7962
11	C	0.6925	-0.3888	0.0875
12	H	0.6912	-0.9796	1.0219
13	H	0.7526	-1.1378	-0.7158
14	C	1.8986	0.4825	0.0438
15	H	1.8029	1.5088	0.3908
16	C	3.2598	-0.0969	-0.098
17	H	3.2873	-0.8729	-0.8724
18	H	4.0036	0.6632	-0.3522
Frequencies (cm^{-1})				
51	98	123	128	149
258	306	377	409	479
758	806	930	938	943
1010	1071	1095	1117	1134
1177	1209	1269	1299	1343
1366	1373	1430	1449	1459
1476	1496	1502	1511	1516
1523	1525	1538	3013	3046
3087	3097	3104	3113	3125
3130	3149	3185	3189	3191
3242				

SI Table 17: TS R6				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-0.7566	-0.3398	0.402
2	C	1.0606	0.8969	-0.1897
3	H	0.5873	1.7699	0.2451
4	H	0.8233	0.6918	-1.2293
5	C	2.1904	0.3861	0.3641
6	H	2.4847	0.7239	1.356
7	H	-0.4481	-1.3082	0.0132
8	C	-1.9144	0.3305	-0.2673
9	H	-1.9834	1.3729	0.0674
10	H	-1.7463	0.3666	-1.3507
11	C	3.0112	-0.7007	-0.2443
12	H	2.6611	-0.952	-1.2495
13	H	4.0666	-0.4124	-0.3155
14	H	2.9794	-1.6157	0.3614
15	H	-0.6882	-0.256	1.4846
16	C	-3.2503	-0.3643	0.0021
17	H	-3.4744	-0.386	1.0732
18	H	-4.0727	0.1529	-0.5032
Frequencies (cm^{-1})				
38	66	95	147	159
264	279	378	434	558
687	774	806	927	932
940	952	973	1019	1072
1087	1144	1222	1244	1315
1354	1381	1433	1441	1469
1499	1502	1512	1516	1520
1533	1631	3095	3103	3112
3140	3148	3186	3191	3194
3194	3223	3237	3290	3323
-457i				

SI Table 18: CCC.CCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	3.184	-0.1292	0.0904
2	H	3.2491	-0.7926	0.9595
3	H	3.361	-0.7392	-0.8019
4	C	1.8313	0.5605	0.0258
5	H	1.6922	1.1879	0.9141
6	H	1.8064	1.2418	-0.8337
7	C	0.6655	-0.4148	-0.0806
8	H	0.8183	-1.0553	-0.9686
9	H	0.6867	-1.1097	0.7717
10	C	-0.6682	0.2412	-0.1556
11	H	-0.7265	1.2412	-0.5828
12	C	-1.9272	-0.5419	-0.0231
13	H	-1.841	-1.231	0.8286
14	H	-2.0514	-1.1974	-0.9033
15	C	-3.1715	0.3205	0.1326
16	H	-3.2982	0.9852	-0.7282
17	H	-4.0738	-0.2917	0.2157
18	H	-3.1053	0.9475	1.0271
Frequencies (cm^{-1})				
43	55	118	152	252
256	302	385	406	481
758	794	884	933	941
1063	1071	1097	1114	1133
1175	1207	1282	1292	1310
1358	1375	1432	1451	1457
1484	1493	1504	1519	1522
1523	1530	1535	3012	3024
3088	3099	3109	3113	3117
3145	3185	3190	3192	3196
3227				

SI Table 19: TS R7				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-2.047	-0.564	0.4163
2	C	-0.3485	0.8351	-0.1491
3	H	-0.9226	1.6634	0.2505
4	H	-0.5294	0.586	-1.1905
5	C	0.8096	0.4541	0.4496
6	H	1.0399	0.841	1.4415
7	H	-1.6208	-1.5042	0.0749
8	C	-3.2338	-0.0379	-0.3205
9	H	-3.47	0.9905	-0.0276
10	H	-3.0769	-0.05	-1.4042
11	C	1.7638	-0.5519	-0.1086
12	H	1.4286	-0.8587	-1.1057
13	H	1.7458	-1.4583	0.5139
14	H	-2.0292	-0.4355	1.4957
15	H	-4.1331	-0.6399	-0.1224
16	C	3.1991	-0.0388	-0.1784
17	H	3.5591	0.2587	0.8121
18	H	3.8764	-0.8081	-0.561
Frequencies (cm^{-1})				
41	58	91	169	178
224	245	386	448	566
725	797	815	847	879
919	975	1038	1062	1068
1104	1117	1234	1247	1307
1328	1376	1434	1447	1474
1500	1508	1512	1513	1521
1532	1627	3076	3081	3116
3142	3145	3183	3190	3196
3205	3220	3227	3300	3321
-483i				

SI Table 20: C=CCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	0.718	-0.3007	0.3299
2	H	0.6673	-1.2374	0.8856
3	C	1.8521	0.0229	-0.2749
4	H	1.9485	0.9449	-0.8424
5	H	2.7262	-0.6178	-0.2237
6	C	-0.5377	0.5132	0.3101
7	H	-0.7902	0.8039	1.3382
8	H	-0.3619	1.442	-0.2428
9	C	-1.7191	-0.2399	-0.2934
10	H	-1.9196	-1.166	0.2556
11	H	-2.6289	0.3667	-0.2653
12	H	-1.5214	-0.5088	-1.3353
Frequencies (cm^{-1})				
112	243	325	446	677
819	892	987	1014	1065
1077	1132	1236	1327	1353
1390	1448	1487	1510	1521
1534	1794	3103	3117	3152
3192	3199	3216	3230	3320

SI Table 21: C.CCCCCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-3.2431	0.5293	0
2	C	-4.522	-0.2299	0
3	H	-3.1992	1.1848	0.8788
4	H	-3.1992	1.1848	-0.8788
5	H	-4.9507	-0.5944	-0.928
6	H	-4.9507	-0.5944	0.928
7	C	-1.9948	-0.3645	0
8	H	-2.0242	-1.0235	0.8766
9	H	-2.0242	-1.0235	-0.8766
10	C	-0.6951	0.4271	0
11	H	-0.6735	1.0884	-0.8763
12	H	-0.6735	1.0884	0.8763
13	C	0.5493	-0.4489	0
14	H	0.5268	-1.1103	0.8762
15	H	0.5268	-1.1103	-0.8762
16	C	1.8502	0.3404	0
17	H	1.8736	1.002	-0.8763
18	H	1.8736	1.002	0.8763
19	C	3.0949	-0.5355	0
20	H	3.071	-1.1961	0.8759
21	H	3.071	-1.1961	-0.8759
22	C	4.3894	0.2618	0
23	H	5.2651	-0.3937	0
24	H	4.4571	0.9066	-0.8828
25	H	4.4571	0.9066	0.8828
Frequencies (cm^{-1})				
52	65	81	83	122
152	173	200	258	284
336	447	486	548	759
760	776	824	898	933
981	1018	1059	1073	1075
1111	1118	1120	1175	1234
1264	1267	1313	1325	1354
1361	1374	1377	1377	1418
1447	1458	1470	1494	1515
1515	1518	1520	1523	1528
1536	1542	3090	3092	3096
3099	3104	3108	3112	3113
3119	3129	3137	3150	3162
3185	3191	3224	3334	

SI Table 22: TS R8				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	-1.8388	0.7107	0.0001
2	C	-3.6168	-0.7134	-0.0001
3	H	-3.2322	-1.1416	0.9195
4	H	-3.2322	-1.1414	-0.9197
5	C	-4.7868	-0.0277	0
6	H	-5.2556	0.2911	-0.9255
7	H	-5.2557	0.2909	0.9254
8	H	-2.058	1.2606	0.9124
9	H	-2.0579	1.2606	-0.9123
10	C	-0.6351	-0.1761	0.0001
11	H	-0.6568	-0.8344	0.8781
12	H	-0.6569	-0.8345	-0.8778
13	C	0.6892	0.5934	0
14	H	0.7234	1.2525	-0.8766
15	H	0.7234	1.2527	0.8765
16	C	1.9105	-0.315	0.0001
17	H	1.8717	-0.9757	-0.8764
18	H	1.8718	-0.9755	0.8767
19	C	3.2312	0.4414	-0.0001
20	H	3.2689	1.1013	0.8757
21	H	3.2688	1.1011	-0.8761
22	C	4.4456	-0.4735	0
23	H	4.4526	-1.1219	-0.8828
24	H	5.3785	0.0975	-0.0001
25	H	4.4527	-1.1216	0.8829
Frequencies (cm^{-1})				
37	46	64	87	124
162	163	230	260	304
381	399	479	576	759
771	802	830	837	878
932	933	970	1037	1039
1050	1074	1111	1116	1170
1240	1269	1287	1290	1322
1346	1367	1367	1375	1423
1454	1462	1488	1500	1514
1517	1520	1524	1532	1540
1615	3091	3096	3100	3107
3113	3117	3126	3140	3158
3185	3191	3200	3225	3237
3296	3313	3339	-440i	

SI Table 23: CC.CCCCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	-1.876	0.3468	-0.0255
2	H	-1.8845	0.9444	-0.9469
3	H	-1.9104	1.0691	0.8012
4	C	-0.5777	-0.4428	0.05
5	H	-0.545	-1.1655	-0.7761
6	H	-0.5694	-1.0396	0.9718
7	C	0.6683	0.4286	0.0041
8	H	0.6656	1.0237	-0.9176
9	H	0.638	1.1504	0.8306
10	C	1.9673	-0.3633	0.0821
11	H	1.9589	-0.9712	1.0053
12	H	2.0025	-1.0982	-0.7354
13	C	3.1937	0.4794	0.0442
14	H	3.1265	1.4995	0.4157
15	C	-3.123	-0.5245	0.0183
16	H	-3.1142	-1.1209	0.9395
17	H	-3.088	-1.246	-0.8077
18	C	-4.4152	0.2731	-0.0584
19	H	-4.4678	0.8526	-0.9863
20	H	-5.2926	-0.3792	-0.0243
21	H	-4.494	0.9799	0.7745
22	C	4.5391	-0.129	-0.1239
23	H	4.539	-0.893	-0.9106
24	H	5.2973	0.6177	-0.3756
25	H	4.8789	-0.6331	0.7962
Frequencies (cm^{-1})				
42	69	79	87	121
152	158	204	259	287
345	411	485	487	758
765	811	904	926	944
995	1029	1052	1071	1109
1116	1121	1148	1178	1206
1255	1279	1309	1330	1352
1367	1374	1385	1428	1445
1456	1468	1477	1496	1503
1511	1515	1516	1523	1523
1533	1541	3013	3046	3087
3091	3092	3101	3105	3112
3114	3124	3130	3141	3155
3185	3189	3191	3242	

SI Table 24: TS R9				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	0.7582	-0.797	0.0728
2	C	2.7036	0.2542	-0.3834
3	H	2.4147	0.212	-1.431
4	C	2.6326	1.4631	0.2403
5	H	3.0376	1.6045	1.2384
6	H	0.8772	-1.6061	-0.6465
7	H	0.968	-1.0861	1.101
8	C	3.6382	-0.8272	0.0816
9	H	3.7855	-0.7816	1.1644
10	H	3.2754	-1.8262	-0.171
11	H	4.6196	-0.7073	-0.3916
12	H	2.0963	2.2959	-0.2008
13	C	-0.3735	0.1519	-0.1507
14	H	-0.2555	1.0209	0.5074
15	H	-0.3367	0.5373	-1.1782
16	C	-1.7514	-0.4692	0.0901
17	H	-1.8812	-1.3358	-0.571
18	H	-1.798	-0.8605	1.1146
19	C	-2.8966	0.5098	-0.1296
20	H	-2.8434	0.9031	-1.1526
21	H	-2.7635	1.3741	0.5331
22	C	-4.2658	-0.1073	0.1076
23	H	-5.0674	0.6187	-0.057
24	H	-4.4405	-0.9534	-0.5655
25	H	-4.3599	-0.4792	1.1334
Frequencies (cm^{-1})				
42	49	75	126	135
175	195	226	260	290
404	427	437	565	579
760	791	825	857	891
930	949	965	1014	1018
1046	1076	1107	1118	1163
1216	1242	1302	1304	1312
1362	1366	1394	1435	1445
1456	1473	1499	1510	1514
1515	1521	1523	1527	1538
1613	3096	3098	3106	3113
3115	3123	3137	3156	3180
3184	3186	3190	3206	3226
3238	3281	3327	-488i	

SI Table 25: C.CCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-2.4751	-0.3175	0
2	H	-2.5271	-0.9633	-0.8829
3	H	-2.5271	-0.9633	0.8829
4	C	-1.2004	0.5113	0
5	H	-1.1919	1.1719	-0.8761
6	H	-1.1919	1.1719	0.8761
7	C	0.0638	-0.3361	0
8	H	0.0639	-0.9959	0.8768
9	H	0.0639	-0.9959	-0.8768
10	C	1.349	0.5033	0
11	H	1.3325	1.16	0.8789
12	H	1.3325	1.16	-0.8789
13	C	2.5952	-0.3082	0
14	H	3.008	-0.6897	-0.9283
15	H	3.008	-0.6897	0.9283
16	H	-3.3659	0.3173	0
Frequencies (cm^{-1})				
71	122	128	184	258
372	412	531	759	784
879	933	1008	1027	1105
1116	1153	1232	1296	1303
1362	1367	1389	1442	1456
1493	1516	1517	1523	1527
1539	3097	3101	3108	3113
3125	3136	3158	3186	3191
3224	3334			

SI Table 26: 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 27: TS R10				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	-4.4885	0.9187	-0.0978
2	C	-2.9833	-0.6933	0.5234
3	H	-3.7552	-1.4425	0.3917
4	H	-2.9291	-0.2256	1.5013
5	C	-1.915	-0.6557	-0.3117
6	H	-1.9423	-1.2503	-1.2238
7	H	-5.2542	0.7492	0.6538
8	H	-4.7292	0.6163	-1.1118
9	H	-3.8971	1.8225	0.0081
10	C	-0.7209	0.223	-0.1272
11	H	-0.6934	0.9764	-0.9284
12	H	-0.8155	0.7786	0.8132
13	C	0.6007	-0.543	-0.141
14	H	0.5939	-1.2845	0.6672
15	H	0.6764	-1.1145	-1.0754
16	C	1.8198	0.356	0.0001
17	H	1.822	1.0953	-0.8122
18	H	1.7402	0.9327	0.9314
19	C	3.1392	-0.4025	-0.0082
20	H	3.2176	-0.9796	-0.9383
21	H	3.1363	-1.1397	0.8045
22	C	4.3523	0.5032	0.1314
23	H	4.3189	1.0679	1.0693
24	H	5.2842	-0.0695	0.1221
25	H	4.4004	1.2294	-0.6871
Frequencies (cm^{-1})				
39	60	62	98	119
133	149	215	259	329
342	451	471	511	531
730	760	784	815	869
926	952	967	992	1016
1056	1083	1096	1117	1168
1232	1270	1288	1314	1333
1363	1366	1370	1424	1441
1445	1453	1464	1479	1508
1516	1518	1523	1531	1540
1633	3075	3091	3099	3106
3113	3117	3129	3141	3157
3168	3185	3191	3224	3232
3328	3337	3345	-476i	

SI Table 28: C=CCCCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	-2.6876	0.2126	0.3299
2	H	-2.7804	0.9885	1.0899
3	C	-3.7021	0.0051	-0.4976
4	H	-3.6549	-0.7557	-1.2723
5	H	-4.6174	0.5838	-0.4304
6	C	-1.3878	-0.5278	0.3094
7	H	-1.2545	-1.0452	1.2693
8	H	-1.4205	-1.3053	-0.4619
9	C	-0.1846	0.3831	0.0759
10	H	-0.1722	1.1702	0.8413
11	H	-0.3064	0.8975	-0.8852
12	C	1.1435	-0.3586	0.0944
13	H	1.2592	-0.8731	1.0578
14	H	1.1287	-1.1486	-0.6684
15	C	2.3466	0.5432	-0.1409
16	H	2.2293	1.0569	-1.1034
17	H	2.3609	1.3319	0.6218
18	C	3.6696	-0.2058	-0.1223
19	H	4.5143	0.4675	-0.2938
20	H	3.8302	-0.7018	0.8409
21	H	3.6979	-0.9785	-0.8979
Frequencies (cm^{-1})				
62	73	118	137	155
259	283	342	448	470
679	761	786	873	928
974	986	997	1057	1068
1088	1098	1118	1172	1234
1272	1290	1332	1352	1366
1370	1374	1428	1454	1465
1487	1510	1516	1519	1523
1531	1540	1794	3090	3095
3099	3106	3112	3117	3132
3144	3160	3185	3191	3217
3230	3320			

SI Table 29: 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 30: TS R11				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	0.5657	-0.387	0.4876
2	C	2.3549	0.8926	-0.0928
3	H	1.9206	1.7205	0.456
4	H	2.05	0.794	-1.1302
5	C	3.512	0.3234	0.3333
6	H	3.8731	0.5586	1.3326
7	H	0.8449	-1.316	-0.0051
8	C	-0.6226	0.3448	-0.0496
9	H	-0.6652	1.3532	0.382
10	H	-0.5176	0.4803	-1.1339
11	C	4.2794	-0.7013	-0.4323
12	H	3.8626	-0.849	-1.4327
13	H	5.3314	-0.4127	-0.5431
14	H	4.2761	-1.6722	0.08
15	H	0.698	-0.4023	1.5672
16	C	-1.9538	-0.3602	0.226
17	H	-2.0732	-0.4971	1.3084
18	H	-1.9246	-1.3688	-0.2057
19	C	-3.1571	0.3921	-0.3253
20	H	-3.0314	0.5306	-1.4066
21	H	-3.1812	1.4004	0.1071
22	C	-4.4781	-0.3098	-0.0528
23	H	-4.647	-0.4316	1.0224
24	H	-5.3232	0.253	-0.4598
25	H	-4.4959	-1.308	-0.5029
Frequencies (cm^{-1})				
27	42	65	110	125
134	157	206	259	268
399	424	438	556	687
759	788	806	890	922
943	954	975	1017	1020
1044	1072	1107	1109	1162
1222	1241	1302	1306	1316
1363	1367	1394	1433	1444
1456	1469	1500	1501	1512
1515	1517	1523	1526	1538
1631	3092	3095	3098	3105
3113	3121	3131	3148	3154
3186	3190	3191	3196	3223
3238	3291	3323	-456i	

SI Table 31: C=CCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	**X**	**Y**	**Z**
1	C	-1.4091	0.3408	0.2653
2	H	-1.4897	1.3614	0.6399
3	C	-2.4707	-0.2176	-0.2988
4	H	-2.4377	-1.2317	-0.6884
5	H	-3.4118	0.3146	-0.3894
6	C	-0.0718	-0.3095	0.4279
7	H	0.1695	-0.3729	1.498
8	H	-0.1164	-1.3399	0.0569
9	C	1.0513	0.446	-0.2795
10	H	1.0747	1.4808	0.0846
11	H	0.8213	0.5059	-1.3496
12	C	2.4141	-0.1964	-0.0781
13	H	3.1994	0.3623	-0.5953
14	H	2.6795	-0.2384	0.9836
15	H	2.4286	-1.2221	-0.4614
16	C	-1.4091	0.3408	0.2653
Frequencies (cm^{-1})				
101	108	237	260	397
447	668	775	901	921
987	990	1057	1075	1102
1155	1234	1302	1331	1358
1369	1432	1455	1487	1511
1520	1523	1536	1794	3092
3109	3113	3136	3155	3186
3193	3217	3230	3320	

SI Table 32: TS R12				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	-3.2872	-0.4937	0.5208
2	C	-1.6733	0.8253	-0.3828
3	H	-2.349	1.6703	-0.3124
4	H	-1.7414	0.2331	-1.2904
5	C	-0.5433	0.7893	0.3699
6	H	-0.4351	1.5006	1.1875
7	H	-3.3791	-0.0182	1.4942
8	H	-2.7514	-1.4396	0.5386
9	C	-4.4432	-0.3747	-0.4161
10	H	-5.3008	-0.9763	-0.08
11	H	-4.7942	0.6593	-0.4981
12	H	-4.1873	-0.7225	-1.4225
13	C	0.5388	-0.2315	0.229
14	H	0.3166	-0.8864	-0.6218
15	H	0.5526	-0.8789	1.1188
16	C	1.9286	0.3784	0.0577
17	H	2.1379	1.0444	0.9053
18	H	1.9342	1.0153	-0.8356
19	C	3.0343	-0.6615	-0.0498
20	H	3.0208	-1.2966	0.8451
21	H	2.8217	-1.3278	-0.8953
22	C	4.4161	-0.0504	-0.2193
23	H	5.1894	-0.8206	-0.2927
24	H	4.4697	0.5617	-1.1258
25	H	4.6698	0.5954	0.6281
Frequencies (cm^{-1})				
32	39	66	99	129
149	172	178	255	264
374	410	471	566	724
762	801	819	847	904
935	943	964	1014	1062
1069	1079	1105	1112	1160
1232	1247	1280	1302	1313
1351	1367	1392	1435	1447
1458	1476	1499	1508	1512
1513	1516	1523	1526	1538
1627	3071	3076	3098	3104
3113	3123	3133	3145	3154
3183	3185	3191	3205	3220
3228	3300	3321	-483i	

SI Table 33: C=CCCCC				
Optimized geometry (Angstrom)				
Atom number	Atom Symbol	X	Y	Z
1	C	2.0304	-0.2131	0.3813
2	H	2.0704	-0.886	1.238
3	C	3.0698	-0.1626	-0.4397
4	H	3.075	0.4913	-1.3078
5	H	3.9544	-0.7687	-0.2741
6	C	0.7688	0.5768	0.2311
7	H	0.642	1.221	1.1119
8	H	0.8547	1.2445	-0.6335
9	C	-0.4726	-0.3002	0.0865
10	H	-0.5394	-0.9797	0.9466
11	H	-0.3583	-0.9406	-0.797
12	C	-1.7632	0.4982	-0.0251
13	H	-1.8699	1.1375	0.8605
14	H	-1.6926	1.1798	-0.8821
15	C	-2.997	-0.3777	-0.1724
16	H	-3.9078	0.2227	-0.2511
17	H	-2.9331	-1.0037	-1.0688
18	H	-3.1129	-1.0463	0.6873
Frequencies (cm^{-1})				
77	96	135	179	258
365	370	471	674	764
823	936	953	974	988
1064	1072	1085	1113	1166
1234	1283	1306	1351	1357
1370	1399	1449	1459	1487
1511	1516	1523	1527	1539
1794	3093	3098	3105	3113
3125	3139	3158	3186	3192
3217	3230	3320		

SI Table 34: Potential energy data along the MEP for reaction CCC•→ C• + C=C. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction CCC•→ C• + C=C					
$E_{CCC.}$ = -118.393126 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)
-3.0791	-118.10905	0.08818	-118.02087	2.6740	1.1146
-3.0591	-118.10879	0.08816	-118.02063	2.8363	1.2663
-3.0391	-118.10852	0.08815	-118.02038	3.0033	1.4232
-3.0191	-118.10825	0.08813	-118.02012	3.1757	1.5856
-2.9991	-118.10797	0.08811	-118.01985	3.3528	1.7526
-2.9791	-118.10768	0.08810	-118.01958	3.5344	1.9248
-2.9591	-118.10738	0.08808	-118.01930	3.7208	2.1019
-2.9391	-118.10708	0.08807	-118.01901	3.9117	2.2840
-2.9191	-118.10677	0.08806	-118.01871	4.1070	2.4705
-2.8991	-118.10645	0.08804	-118.01840	4.3069	2.6622
-2.8791	-118.10612	0.08803	-118.01809	4.5108	2.8573
-2.8591	-118.10579	0.08802	-118.01778	4.7183	3.0567
-2.8391	-118.10545	0.08800	-118.01745	4.9309	3.2610
-2.8191	-118.10511	0.08799	-118.01712	5.1467	3.4693
-2.7991	-118.10476	0.08798	-118.01678	5.3663	3.6808
-2.7791	-118.10440	0.08797	-118.01644	5.5894	3.8964
-2.7591	-118.10404	0.08795	-118.01609	5.8163	4.1158
-2.7391	-118.10367	0.08794	-118.01573	6.0467	4.3387
-2.7191	-118.10330	0.08793	-118.01537	6.2803	4.5647
-2.6991	-118.10292	0.08792	-118.01501	6.5172	4.7947
-2.6791	-118.10254	0.08791	-118.01463	6.7579	5.0279
-2.6591	-118.10215	0.08790	-118.01426	7.0011	5.2642
-2.6391	-118.10176	0.08788	-118.01388	7.2469	5.5024
-2.6191	-118.10136	0.08787	-118.01349	7.4968	5.7454
-2.5991	-118.10096	0.08786	-118.01310	7.7484	5.9901
-2.5791	-118.10056	0.08785	-118.01271	8.0028	6.2383
-2.5591	-118.10015	0.08784	-118.01231	8.2605	6.4890
-2.5391	-118.09973	0.08783	-118.01190	8.5201	6.7418
-2.5191	-118.09931	0.08782	-118.01150	8.7821	6.9975
-2.4991	-118.09889	0.08781	-118.01108	9.0468	7.2553

-2.4791	-118.09847	0.08780	-118.01067	9.3133	7.5155
-2.4591	-118.09804	0.08779	-118.01025	9.5825	7.7778
-2.4391	-118.09761	0.08778	-118.00983	9.8534	8.0424
-2.4191	-118.09717	0.08777	-118.00941	10.1262	8.3089
-2.3991	-118.09673	0.08776	-118.00898	10.4012	8.5776
-2.3791	-118.09629	0.08775	-118.00855	10.6778	8.8480
-2.3591	-118.09585	0.08774	-118.00811	10.9566	9.1205
-2.3391	-118.09540	0.08773	-118.00768	11.2368	9.3944
-2.3191	-118.09495	0.08772	-118.00724	11.5183	9.6703
-2.29911	-118.09450	0.08771	-118.00680	11.8012	9.9469
-2.27911	-118.09405	0.08770	-118.00635	12.0860	10.2255
-2.25911	-118.09359	0.08769	-118.00591	12.3717	10.5055
-2.23911	-118.09314	0.08768	-118.00546	12.6592	10.7868
-2.21911	-118.09268	0.08767	-118.00501	12.9471	11.0690
-2.19911	-118.09222	0.08766	-118.00456	13.2365	11.3528
-2.17911	-118.09175	0.08765	-118.00410	13.5267	11.6366
-2.15911	-118.09129	0.08764	-118.00365	13.8185	11.9228
-2.13911	-118.09082	0.08763	-118.00319	14.1110	12.2096
-2.11911	-118.09036	0.08762	-118.00273	14.4041	12.4971
-2.09911	-118.08989	0.08761	-118.00227	14.6978	12.7845
-2.07911	-118.08942	0.08761	-118.00181	14.9919	13.0730
-2.05911	-118.08895	0.08760	-118.00135	15.2872	13.3632
-2.03911	-118.08848	0.08759	-118.00089	15.5828	13.6526
-2.01911	-118.08801	0.08758	-118.00043	15.8787	13.9428
-1.99911	-118.08753	0.08757	-117.99996	16.1749	14.2334
-1.97911	-118.08706	0.08756	-117.99950	16.4720	14.5254
-1.95911	-118.08659	0.08755	-117.99904	16.7685	14.8164
-1.93911	-118.08611	0.08754	-117.99857	17.0655	15.1077
-1.91911	-118.08564	0.08753	-117.99811	17.3628	15.3993
-1.89911	-118.08517	0.08753	-117.99764	17.6599	15.6914
-1.87911	-118.08469	0.08752	-117.99718	17.9574	15.9832
-1.85911	-118.08422	0.08751	-117.99671	18.2541	16.2744
-1.83911	-118.08375	0.08750	-117.99625	18.5511	16.5656
-1.81911	-118.08328	0.08749	-117.99579	18.8471	16.8560
-1.79911	-118.08280	0.08748	-117.99532	19.1434	17.1473
-1.77911	-118.08233	0.08747	-117.99486	19.4392	17.4375
-1.75911	-118.08186	0.08746	-117.99440	19.7345	17.7271
-1.73911	-118.08139	0.08746	-117.99394	20.0295	18.0165
-1.71911	-118.08092	0.08745	-117.99348	20.3235	18.3048
-1.69911	-118.08046	0.08744	-117.99302	20.6165	18.5922
-1.67911	-118.07999	0.08743	-117.99256	20.9091	18.8791
-1.65911	-118.07953	0.08742	-117.99211	21.2003	19.1647
-1.63911	-118.07906	0.08741	-117.99165	21.4911	19.4499
-1.61911	-118.07860	0.08740	-117.99120	21.7800	19.7330
-1.59911	-118.07814	0.08739	-117.99075	22.0687	20.0161
-1.57911	-118.07768	0.08738	-117.99030	22.3556	20.2974

-1.55911	-118.07723	0.08737	-117.98985	22.6414	20.5775
-1.53911	-118.07678	0.08736	-117.98941	22.9258	20.8557
-1.51911	-118.07633	0.08736	-117.98897	23.2079	21.1321
-1.49911	-118.07588	0.08735	-117.98853	23.4890	21.4075
-1.47911	-118.07543	0.08734	-117.98810	23.7685	21.6808
-1.45911	-118.07499	0.08733	-117.98766	24.0458	21.9518
-1.43911	-118.07455	0.08732	-117.98723	24.3212	22.2216
-1.41911	-118.07412	0.08731	-117.98681	24.5949	22.4889
-1.39911	-118.07368	0.08730	-117.98639	24.8663	22.7541
-1.37911	-118.07325	0.08729	-117.98597	25.1354	23.0163
-1.35911	-118.07283	0.08728	-117.98555	25.4027	23.2774
-1.33911	-118.07241	0.08727	-117.98514	25.6670	23.5353
-1.31911	-118.07199	0.08726	-117.98474	25.9286	23.7901
-1.29911	-118.07158	0.08725	-117.98433	26.1878	24.0430
-1.27911	-118.07117	0.08723	-117.98393	26.4441	24.2923
-1.25911	-118.07076	0.08722	-117.98354	26.6976	24.5389
-1.23911	-118.07037	0.08721	-117.98315	26.9479	24.7823
-1.21911	-118.06997	0.08720	-117.98277	27.1954	25.0230
-1.19911	-118.06958	0.08719	-117.98239	27.4397	25.2597
-1.17911	-118.06920	0.08718	-117.98202	27.6810	25.4941
-1.15911	-118.06882	0.08717	-117.98165	27.9186	25.7242
-1.13911	-118.06845	0.08715	-117.98129	28.1525	25.9506
-1.11911	-118.06808	0.08714	-117.98094	28.3833	26.1738
-1.09911	-118.06772	0.08713	-117.98059	28.6100	26.3930
-1.07911	-118.06736	0.08712	-117.98024	28.8331	26.6086
-1.05911	-118.06701	0.08711	-117.97991	29.0523	26.8202
-1.03911	-118.06667	0.08709	-117.97958	29.2682	27.0279
-1.01911	-118.06633	0.08708	-117.97925	29.4792	27.2309
-0.99911	-118.06600	0.08707	-117.97893	29.6865	27.4300
-0.97911	-118.06568	0.08706	-117.97862	29.8892	27.6252
-0.95911	-118.06536	0.08704	-117.97832	30.0883	27.8155
-0.93911	-118.06505	0.08703	-117.97802	30.2828	28.0018
-0.91911	-118.06475	0.08702	-117.97773	30.4726	28.1835
-0.89911	-118.06445	0.08700	-117.97745	30.6582	28.3609
-0.87911	-118.06416	0.08699	-117.97718	30.8392	28.5331
-0.85911	-118.06388	0.08697	-117.97691	31.0157	28.7008
-0.83911	-118.06361	0.08696	-117.97665	31.1878	28.8648
-0.81911	-118.06334	0.08695	-117.97640	31.3550	29.0232
-0.79911	-118.06308	0.08693	-117.97615	31.5173	29.1767
-0.77911	-118.06283	0.08692	-117.97591	31.6754	29.3260
-0.75911	-118.06259	0.08691	-117.97568	31.8285	29.4703
-0.73911	-118.06235	0.08689	-117.97546	31.9769	29.6100
-0.71911	-118.06212	0.08688	-117.97525	32.1205	29.7448
-0.69911	-118.06190	0.08686	-117.97504	32.2595	29.8743
-0.67911	-118.06169	0.08685	-117.97484	32.3931	29.9991
-0.65911	-118.06148	0.08683	-117.97465	32.5226	30.1198

-0.63911	-118.06128	0.08682	-117.97446	32.6471	30.2356
-0.61911	-118.06109	0.08681	-117.97429	32.7667	30.3458
-0.59911	-118.06091	0.08679	-117.97412	32.8815	30.4518
-0.57911	-118.06073	0.08678	-117.97396	32.9919	30.5534
-0.55911	-118.06057	0.08676	-117.97380	33.0971	30.6492
-0.53911	-118.06041	0.08675	-117.97366	33.1981	30.7414
-0.51911	-118.06025	0.08673	-117.97352	33.2948	30.8293
-0.49911	-118.06011	0.08672	-117.97339	33.3863	30.9114
-0.47911	-118.05997	0.08671	-117.97326	33.4728	30.9897
-0.45911	-118.05984	0.08669	-117.97314	33.5558	31.0633
-0.43911	-118.05971	0.08668	-117.97303	33.6336	31.1323
-0.41911	-118.05959	0.08666	-117.97293	33.7079	31.1978
-0.39911	-118.05948	0.08665	-117.97283	33.7769	31.2581
-0.37911	-118.05938	0.08663	-117.97274	33.8434	31.3151
-0.35911	-118.05928	0.08662	-117.97266	33.9041	31.3677
-0.33911	-118.05919	0.08661	-117.97258	33.9616	31.4164
-0.31911	-118.05910	0.08659	-117.97251	34.0145	31.4606
-0.29911	-118.05902	0.08658	-117.97245	34.0654	31.5001
-0.27911	-118.05895	0.08657	-117.97239	34.1093	31.5378
-0.25912	-118.05889	0.08655	-117.97234	34.1520	31.5704
-0.23912	-118.05883	0.08654	-117.97229	34.1891	31.6000
-0.21912	-118.05877	0.08652	-117.97225	34.2243	31.6257
-0.19912	-118.05872	0.08651	-117.97222	34.2531	31.6458
-0.17913	-118.05868	0.08650	-117.97218	34.2825	31.6677
-0.15913	-118.05864	0.08648	-117.97216	34.3063	31.6827
-0.13913	-118.05860	0.08647	-117.97214	34.3287	31.6944
-0.11914	-118.05858	0.08645	-117.97213	34.3445	31.7002
-0.09917	-118.05855	0.08641	-117.97214	34.3632	31.7048
-0.07926	-118.05854	0.08636	-117.97218	34.3699	31.7055
-0.05948	-118.05851	0.08622	-117.97229	34.3862	31.7086
-0.03985	-118.05851	0.08640	-117.97211	34.3876	31.7106
-0.01986	-118.05850	0.08639	-117.97212	34.3919	31.7131
0	-118.05850	0.08449	-117.97401	34.3800	31.6772
0.01984	-118.05852	0.08632	-117.97220	34.3706	31.6391
0.03984	-118.05854	0.08631	-117.97223	34.3652	31.5480
0.05934	-118.05855	0.08603	-117.97252	34.3450	31.5337
0.07904	-118.05858	0.08618	-117.97239	34.3356	31.5432
0.0989	-118.05859	0.08621	-117.97238	34.3148	31.5418
0.11885	-118.05863	0.08624	-117.97238	34.2987	31.5201
0.13883	-118.05865	0.08624	-117.97242	34.2768	31.4944
0.15882	-118.05869	0.08623	-117.97246	34.2556	31.4645
0.17882	-118.05872	0.08622	-117.97251	34.2288	31.4151
0.19877	-118.05876	0.08618	-117.97258	34.2077	31.3933
0.21874	-118.05880	0.08618	-117.97262	34.1797	31.3622
0.23874	-118.05884	0.08617	-117.97267	34.1519	31.3250
0.25874	-118.05889	0.08616	-117.97273	34.1207	31.2819

0.27872	-118.05894	0.08614	-117.97280	34.0923	31.2453
0.29871	-118.05898	0.08613	-117.97285	34.0599	31.2054
0.31871	-118.05903	0.08611	-117.97292	34.0281	31.1573
0.3387	-118.05908	0.08609	-117.97299	33.9922	31.1189
0.35869	-118.05914	0.08608	-117.97306	33.9577	31.0749
0.37869	-118.05919	0.08607	-117.97313	33.9200	31.0265
0.39868	-118.05926	0.08605	-117.97320	33.8842	30.9819
0.41868	-118.05931	0.08604	-117.97327	33.8461	30.9344
0.43868	-118.05937	0.08602	-117.97335	33.8071	30.8848
0.45868	-118.05943	0.08601	-117.97343	33.7672	30.8361
0.47868	-118.05950	0.08599	-117.97351	33.7270	30.7827
0.49867	-118.05956	0.08597	-117.97359	33.6854	30.7348
0.51867	-118.05963	0.08596	-117.97367	33.6437	30.6832
0.53867	-118.05970	0.08595	-117.97375	33.6011	30.6298
0.55867	-118.05976	0.08593	-117.97384	33.5581	30.5774
0.57867	-118.05983	0.08591	-117.97392	33.5137	30.5224
0.59866	-118.05990	0.08590	-117.97401	33.4698	30.4684
0.61866	-118.05997	0.08588	-117.97409	33.4252	30.4144
0.63866	-118.06004	0.08587	-117.97418	33.3797	30.3583
0.65866	-118.06012	0.08585	-117.97427	33.3343	30.3015
0.67866	-118.06019	0.08583	-117.97436	33.2883	30.2461
0.69866	-118.06026	0.08582	-117.97445	33.2422	30.1893
0.71866	-118.06034	0.08580	-117.97454	33.1950	30.1321
0.73866	-118.06041	0.08578	-117.97463	33.1481	30.0739
0.75866	-118.06049	0.08576	-117.97472	33.1008	30.0172
0.77866	-118.06056	0.08575	-117.97481	33.0530	29.9575
0.79865	-118.06064	0.08573	-117.97491	33.0057	29.9001
0.81865	-118.06071	0.08571	-117.97500	32.9574	29.8418
0.83865	-118.06079	0.08570	-117.97509	32.9093	29.7830
0.85865	-118.06087	0.08568	-117.97518	32.8609	29.7233
0.87865	-118.06094	0.08566	-117.97528	32.8124	29.6648
0.89865	-118.06102	0.08565	-117.97537	32.7635	29.6040
0.91865	-118.06110	0.08563	-117.97547	32.7149	29.5460
0.93865	-118.06118	0.08561	-117.97556	32.6662	29.4847
0.95864	-118.06125	0.08559	-117.97566	32.6173	29.4270
0.97864	-118.06133	0.08558	-117.97575	32.5684	29.3668
0.99864	-118.06141	0.08556	-117.97585	32.5194	29.3071
1.01864	-118.06149	0.08554	-117.97594	32.4706	29.2471
1.03864	-118.06156	0.08553	-117.97604	32.4216	29.1880
1.05864	-118.06164	0.08551	-117.97613	32.3723	29.1275
1.07864	-118.06172	0.08549	-117.97623	32.3237	29.0682
1.09864	-118.06180	0.08548	-117.97632	32.2743	29.0075
1.11864	-118.06188	0.08546	-117.97642	32.2258	28.9495
1.13863	-118.06195	0.08544	-117.97651	32.1771	28.8902
1.15863	-118.06203	0.08543	-117.97661	32.1283	28.8308
1.17863	-118.06211	0.08541	-117.97670	32.0796	28.7707

1.19863	-118.06219	0.08539	-117.97680	32.0314	28.7125
1.21863	-118.06226	0.08537	-117.97689	31.9827	28.6525
1.23863	-118.06234	0.08536	-117.97699	31.9347	28.5945
1.25863	-118.06242	0.08534	-117.97708	31.8867	28.5352
1.27863	-118.06250	0.08532	-117.97717	31.8382	28.4773
1.29863	-118.06257	0.08531	-117.97727	31.7911	28.4194
1.31863	-118.06265	0.08529	-117.97736	31.7430	28.3607
1.33863	-118.06272	0.08527	-117.97745	31.6957	28.3028
1.35863	-118.06280	0.08526	-117.97754	31.6485	28.2455
1.37863	-118.06287	0.08524	-117.97763	31.6010	28.1874
1.39862	-118.06295	0.08522	-117.97773	31.5544	28.1307
1.41862	-118.06302	0.08521	-117.97782	31.5075	28.0726
1.43862	-118.06310	0.08519	-117.97791	31.4610	28.0172
1.45862	-118.06317	0.08518	-117.97800	31.4145	27.9607
1.47862	-118.06325	0.08516	-117.97809	31.3684	27.9040
1.49862	-118.06332	0.08514	-117.97818	31.3225	27.8474
1.51862	-118.06339	0.08513	-117.97827	31.2771	27.7925
1.53862	-118.06347	0.08511	-117.97836	31.2318	27.7359
1.55861	-118.06354	0.08509	-117.97845	31.1864	27.6824
1.57861	-118.06361	0.08508	-117.97853	31.1415	27.6275
1.59861	-118.06368	0.08506	-117.97862	31.0970	27.5735
1.61861	-118.06375	0.08505	-117.97871	31.0526	27.5178
1.63861	-118.06382	0.08503	-117.97879	31.0083	27.4653
1.65861	-118.06390	0.08502	-117.97888	30.9645	27.4102
1.67861	-118.06396	0.08500	-117.97897	30.9207	27.3577
1.69861	-118.06403	0.08499	-117.97905	30.8775	27.3057
1.71861	-118.06410	0.08497	-117.97913	30.8340	27.2522
1.73861	-118.06417	0.08496	-117.97922	30.7911	27.1986
1.7586	-118.06424	0.08494	-117.97930	30.7487	27.1481
1.7786	-118.06431	0.08493	-117.97938	30.7065	27.0964
1.7986	-118.06438	0.08491	-117.97947	30.6643	27.0455
1.8186	-118.06444	0.08490	-117.97955	30.6227	26.9932
1.8386	-118.06451	0.08488	-117.97963	30.5812	26.9435
1.8586	-118.06458	0.08487	-117.97971	30.5397	26.8932
1.8786	-118.06464	0.08485	-117.97979	30.4990	26.8432
1.8986	-118.06471	0.08484	-117.97987	30.4584	26.7925
1.91859	-118.06477	0.08482	-117.97995	30.4180	26.7446
1.93859	-118.06484	0.08481	-117.98003	30.3780	26.6952
1.95859	-118.06490	0.08479	-117.98011	30.3383	26.6473
1.97859	-118.06496	0.08478	-117.98018	30.2988	26.5972
1.99859	-118.06503	0.08476	-117.98026	30.2597	26.5511
2.01858	-118.06509	0.08475	-117.98034	30.2207	26.5033
2.03858	-118.06515	0.08474	-117.98041	30.1826	26.4565
2.05858	-118.06521	0.08473	-117.98049	30.1443	26.4100
2.07858	-118.06527	0.08471	-117.98056	30.1060	26.3623
2.09858	-118.06533	0.08470	-117.98064	30.0685	26.3172

2.11858	-118.06539	0.08469	-117.98071	30.0312	26.2712
2.13858	-118.06545	0.08467	-117.98078	29.9939	26.2257
2.15858	-118.06551	0.08466	-117.98085	29.9576	26.1813
2.17858	-118.06557	0.08465	-117.98092	29.9210	26.1352
2.19857	-118.06563	0.08463	-117.98100	29.8848	26.0921
2.21857	-118.06569	0.08462	-117.98107	29.8491	26.0482
2.23857	-118.06574	0.08461	-117.98114	29.8136	26.0040
2.25857	-118.06580	0.08459	-117.98121	29.7779	25.9614
2.27857	-118.06586	0.08458	-117.98127	29.7432	25.9166
2.29856	-118.06591	0.08457	-117.98135	29.7087	25.8759
2.31856	-118.06597	0.08456	-117.98141	29.6743	25.8340
2.33856	-118.06602	0.08454	-117.98148	29.6401	25.7916
2.35856	-118.06608	0.08453	-117.98155	29.6063	25.7503
2.37856	-118.06613	0.08452	-117.98161	29.5728	25.7049
2.39855	-118.06618	0.08450	-117.98168	29.5397	25.6673
2.41854	-118.06624	0.08449	-117.98174	29.5069	25.6276
2.43854	-118.06629	0.08448	-117.98181	29.4743	25.5863
2.45854	-118.06634	0.08447	-117.98187	29.4422	25.5479
2.47853	-118.06639	0.08446	-117.98193	29.4100	25.5088
2.49853	-118.06644	0.08445	-117.98200	29.3785	25.4685
2.51853	-118.06649	0.08443	-117.98206	29.3471	25.4308
2.53853	-118.06654	0.08442	-117.98212	29.3163	25.3931
2.55853	-118.06659	0.08441	-117.98218	29.2853	25.3539
2.57853	-118.06664	0.08440	-117.98224	29.2548	25.3172
2.59852	-118.06669	0.08439	-117.98230	29.2244	25.2799
2.61852	-118.06674	0.08438	-117.98236	29.1945	25.2418
2.63852	-118.06679	0.08436	-117.98242	29.1647	25.2058
2.65852	-118.06683	0.08435	-117.98248	29.1356	25.1698
2.67852	-118.06688	0.08434	-117.98254	29.1064	25.1337
2.69852	-118.06693	0.08433	-117.98259	29.0779	25.0983
2.71852	-118.06697	0.08432	-117.98265	29.0494	25.0635
2.73852	-118.06702	0.08431	-117.98271	29.0211	25.0276
2.75852	-118.06706	0.08430	-117.98276	28.9931	24.9939
2.77851	-118.06711	0.08429	-117.98282	28.9655	24.9595
2.79851	-118.06715	0.08428	-117.98287	28.9383	24.9248
2.81851	-118.06719	0.08427	-117.98293	28.9111	24.8919
2.83851	-118.06724	0.08426	-117.98298	28.8840	24.8585
2.85851	-118.06728	0.08425	-117.98303	28.8579	24.8243
2.8785	-118.06732	0.08424	-117.98309	28.8314	24.7934
2.8985	-118.06736	0.08423	-117.98314	28.8052	24.7610
2.9185	-118.06741	0.08422	-117.98319	28.7795	24.7264
2.93849	-118.06745	0.08420	-117.98324	28.7541	24.6966
2.95849	-118.06749	0.08420	-117.98329	28.7290	24.6658
2.97849	-118.06753	0.08419	-117.98334	28.7040	24.6296
2.99847	-118.06757	0.08417	-117.98340	28.6794	24.6031
3.01846	-118.06761	0.08417	-117.98344	28.6550	24.5731

3.03846	-118.06765	0.08416	-117.98349	28.6309	24.5433
3.05846	-118.06768	0.08415	-117.98353	28.6070	24.5119
3.07846	-118.06772	0.08414	-117.98358	28.5830	24.4829
3.09845	-118.06776	0.08413	-117.98363	28.5598	24.4546
3.11845	-118.06780	0.08412	-117.98368	28.5368	24.4184
3.13843	-118.06783	0.08410	-117.98373	28.5138	24.3954
3.15842	-118.06787	0.08410	-117.98377	28.4912	24.3679
3.17842	-118.06791	0.08409	-117.98381	28.4686	24.3396
3.19842	-118.06794	0.08408	-117.98386	28.4465	24.3081
3.21841	-118.06798	0.08407	-117.98391	28.4245	24.2842
3.2384	-118.06801	0.08407	-117.98395	28.4029	24.2576
3.2584	-118.06805	0.08406	-117.98399	28.3815	24.2305
3.2784	-118.06808	0.08405	-117.98403	28.3599	24.1989
3.29838	-118.06812	0.08403	-117.98408	28.3393	24.1758
3.31838	-118.06815	0.08403	-117.98412	28.3184	24.1511
3.33838	-118.06818	0.08402	-117.98416	28.2978	24.1242
3.35838	-118.06821	0.08401	-117.98420	28.2774	24.0944
3.37836	-118.06825	0.08400	-117.98425	28.2577	24.0716
3.39835	-118.06828	0.08399	-117.98429	28.2378	24.0479
3.41835	-118.06831	0.08399	-117.98432	28.2181	24.0226
3.43835	-118.06834	0.08398	-117.98436	28.1983	23.9928
3.45833	-118.06837	0.08396	-117.98441	28.1795	23.9714
3.47832	-118.06840	0.08396	-117.98445	28.1602	23.9490
3.49832	-118.06843	0.08395	-117.98448	28.1416	23.9241
3.51832	-118.06846	0.08394	-117.98452	28.1227	23.8889
3.53828	-118.06849	0.08392	-117.98458	28.1047	23.8740
3.55826	-118.06852	0.08392	-117.98460	28.0864	23.8532
3.57825	-118.06855	0.08392	-117.98463	28.0686	23.8304
3.59825	-118.06858	0.08391	-117.98467	28.0509	23.8070
3.61825	-118.06861	0.08390	-117.98471	28.0333	23.7763
3.63822	-118.06864	0.08388	-117.98476	28.0159	23.7595
3.65821	-118.06866	0.08388	-117.98478	27.9989	23.7394
3.6782	-118.06869	0.08388	-117.98482	27.9815	23.7176
3.6982	-118.06872	0.08387	-117.98485	27.9648	23.6953
3.7182	-118.06875	0.08386	-117.98489	27.9484	23.6644
3.73818	-118.06877	0.08384	-117.98494	27.9321	23.6494
3.75816	-118.06880	0.08384	-117.98496	27.9160	23.6307
3.77815	-118.06882	0.08383	-117.98499	27.8997	23.6094
3.79815	-118.06885	0.08383	-117.98502	27.8840	23.5881
3.81815	-118.06887	0.08382	-117.98506	27.8683	23.5548
3.83811	-118.06890	0.08379	-117.98511	27.8527	23.5423
3.85809	-118.06892	0.08379	-117.98513	27.8374	23.5258
3.87808	-118.06895	0.08379	-117.98516	27.8225	23.5058

SI Table 35: Potential energy data along the MEP for reaction C•CCC→ CC• + C=C. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction C•CCC→ C•C+C=C					
$E_{C.CCC}$ = -157.311776 hartree		$ZPE_{C.CCC}$ = 0.120044 hartree			
Reaction coordinate (amu$^{1/2}$ bohr)	V_C (Hartree)	ZPE (Hartree)	V_{ag} (Hartree)	V_c - $E_{C.CCC}$ (kcal/mol)	V_{ag}-$E_{C.CCC}$ (kcal/mol)
-3.080	-157.30757	0.11762	-157.18994	2.64	1.12
-3.060	-157.30735	0.11760	-157.18974	2.78	1.25
-3.059	-157.30748	0.11762	-157.18987	2.70	1.17
-3.040	-157.30712	0.11758	-157.18954	2.92	1.38
-3.029	-157.30714	0.11758	-157.18956	2.91	1.36
-3.020	-157.30688	0.11756	-157.18932	3.07	1.51
-3.000	-157.30664	0.11754	-157.18910	3.22	1.65
-2.999	-157.30679	0.11755	-157.18924	3.13	1.56
-2.980	-157.30640	0.11752	-157.18887	3.38	1.79
-2.969	-157.30642	0.11752	-157.18890	3.36	1.78
-2.960	-157.30614	0.11750	-157.18864	3.54	1.94
-2.940	-157.30588	0.11749	-157.18839	3.70	2.09
-2.939	-157.30604	0.11750	-157.18854	3.60	2.00
-2.920	-157.30561	0.11747	-157.18814	3.87	2.25
-2.909	-157.30564	0.11747	-157.18817	3.85	2.24
-2.900	-157.30534	0.11745	-157.18788	4.04	2.41
-2.880	-157.30505	0.11744	-157.18762	4.22	2.58
-2.879	-157.30523	0.11745	-157.18778	4.11	2.48
-2.860	-157.30477	0.11742	-157.18735	4.40	2.75
-2.849	-157.30480	0.11742	-157.18738	4.38	2.73
-2.840	-157.30448	0.11741	-157.18707	4.58	2.93
-2.820	-157.30418	0.11739	-157.18679	4.77	3.10
-2.819	-157.30436	0.11740	-157.18696	4.66	3.00
-2.800	-157.30387	0.11738	-157.18649	4.96	3.29
-2.789	-157.30390	0.11738	-157.18652	4.94	3.27
-2.780	-157.30356	0.11736	-157.18620	5.16	3.47
-2.760	-157.30324	0.11735	-157.18589	5.35	3.66
-2.759	-157.30343	0.11736	-157.18608	5.23	3.55
-2.740	-157.30292	0.11734	-157.18559	5.56	3.86

-2.729	-157.30295	0.11734	-157.18562	5.54	3.84
-2.720	-157.30259	0.11732	-157.18527	5.76	4.06
-2.700	-157.30226	0.11731	-157.18495	5.97	4.26
-2.699	-157.30246	0.11732	-157.18514	5.85	4.13
-2.680	-157.30192	0.11730	-157.18462	6.18	4.46
-2.669	-157.30196	0.11730	-157.18466	6.16	4.44
-2.660	-157.30158	0.11729	-157.18429	6.40	4.67
-2.640	-157.30123	0.11728	-157.18396	6.62	4.88
-2.639	-157.30144	0.11728	-157.18416	6.48	4.75
-2.620	-157.30088	0.11727	-157.18362	6.84	5.09
-2.609	-157.30092	0.11727	-157.18365	6.82	5.07
-2.600	-157.30052	0.11725	-157.18327	7.06	5.31
-2.580	-157.30016	0.11724	-157.18292	7.29	5.53
-2.579	-157.30038	0.11725	-157.18313	7.15	5.40
-2.560	-157.29980	0.11723	-157.18256	7.52	5.75
-2.549	-157.29983	0.11723	-157.18260	7.50	5.73
-2.540	-157.29942	0.11722	-157.18220	7.75	5.98
-2.520	-157.29905	0.11721	-157.18184	7.99	6.21
-2.519	-157.29928	0.11722	-157.18206	7.84	6.07
-2.500	-157.29867	0.11720	-157.18147	8.22	6.44
-2.489	-157.29871	0.11720	-157.18151	8.20	6.42
-2.480	-157.29829	0.11719	-157.18110	8.46	6.67
-2.460	-157.29790	0.11718	-157.18072	8.70	6.91
-2.459	-157.29814	0.11719	-157.18095	8.56	6.77
-2.440	-157.29752	0.11717	-157.18034	8.95	7.15
-2.429	-157.29755	0.11718	-157.18038	8.92	7.12
-2.420	-157.29712	0.11716	-157.17996	9.20	7.39
-2.400	-157.29672	0.11716	-157.17957	9.44	7.63
-2.399	-157.29696	0.11716	-157.17980	9.30	7.49
-2.380	-157.29633	0.11715	-157.17918	9.70	7.88
-2.369	-157.29637	0.11715	-157.17922	9.67	7.85
-2.360	-157.29592	0.11714	-157.17878	9.95	8.12
-2.340	-157.29552	0.11713	-157.17839	10.20	8.37
-2.339	-157.29576	0.11713	-157.17863	10.05	8.22
-2.320	-157.29511	0.11712	-157.17799	10.46	8.62
-2.309	-157.29515	0.11712	-157.17803	10.43	8.60
-2.300	-157.29470	0.11711	-157.17759	10.72	8.88
-2.280	-157.29428	0.11710	-157.17718	10.98	9.13
-2.279	-157.29453	0.11711	-157.17742	10.82	8.98
-2.260	-157.29387	0.11710	-157.17677	11.24	9.39
-2.249	-157.29391	0.11710	-157.17681	11.21	9.36
-2.240	-157.29345	0.11709	-157.17636	11.50	9.65
-2.220	-157.29302	0.11708	-157.17595	11.77	9.91
-2.219	-157.29328	0.11708	-157.17619	11.61	9.75
-2.200	-157.29260	0.11707	-157.17553	12.03	10.17
-2.189	-157.29264	0.11707	-157.17557	12.01	10.14

-2.180	-157.29218	0.11706	-157.17511	12.30	10.43
-2.160	-157.29175	0.11706	-157.17469	12.57	10.69
-2.159	-157.29200	0.11706	-157.17494	12.41	10.54
-2.140	-157.29132	0.11705	-157.17427	12.84	10.96
-2.129	-157.29136	0.11705	-157.17431	12.81	10.93
-2.120	-157.29089	0.11704	-157.17385	13.11	11.22
-2.100	-157.29045	0.11703	-157.17342	13.38	11.49
-2.099	-157.29071	0.11704	-157.17367	13.22	11.33
-2.080	-157.29002	0.11703	-157.17299	13.65	11.76
-2.069	-157.29006	0.11703	-157.17303	13.63	11.73
-2.060	-157.28958	0.11702	-157.17256	13.93	12.03
-2.040	-157.28914	0.11701	-157.17213	14.20	12.30
-2.039	-157.28940	0.11702	-157.17239	14.04	12.14
-2.020	-157.28870	0.11700	-157.17170	14.48	12.57
-2.009	-157.28875	0.11700	-157.17174	14.45	12.54
-2.000	-157.28826	0.11700	-157.17127	14.75	12.84
-1.980	-157.28782	0.11699	-157.17084	15.03	13.11
-1.979	-157.28809	0.11699	-157.17110	14.86	12.95
-1.960	-157.28738	0.11698	-157.17040	15.31	13.39
-1.949	-157.28742	0.11698	-157.17044	15.28	13.36
-1.940	-157.28694	0.11697	-157.16997	15.59	13.66
-1.920	-157.28650	0.11697	-157.16953	15.86	13.93
-1.919	-157.28676	0.11697	-157.16979	15.70	13.77
-1.900	-157.28605	0.11696	-157.16909	16.14	14.21
-1.889	-157.28609	0.11696	-157.16913	16.12	14.18
-1.880	-157.28561	0.11695	-157.16866	16.42	14.48
-1.860	-157.28516	0.11695	-157.16822	16.70	14.76
-1.859	-157.28543	0.11695	-157.16848	16.53	14.59
-1.840	-157.28472	0.11694	-157.16778	16.98	15.03
-1.829	-157.28476	0.11694	-157.16782	16.95	15.00
-1.820	-157.28427	0.11693	-157.16734	17.26	15.31
-1.800	-157.28383	0.11692	-157.16690	17.54	15.58
-1.799	-157.28409	0.11693	-157.16716	17.37	15.42
-1.780	-157.28338	0.11692	-157.16646	17.82	15.86
-1.769	-157.28342	0.11692	-157.16650	17.79	15.83
-1.760	-157.28294	0.11691	-157.16603	18.10	16.13
-1.740	-157.28249	0.11690	-157.16559	18.38	16.41
-1.739	-157.28276	0.11691	-157.16585	18.21	16.24
-1.720	-157.28205	0.11690	-157.16515	18.66	16.68
-1.709	-157.28209	0.11690	-157.16519	18.63	16.65
-1.700	-157.28160	0.11689	-157.16471	18.93	16.95
-1.680	-157.28116	0.11688	-157.16428	19.21	17.23
-1.679	-157.28142	0.11689	-157.16454	19.05	17.07
-1.660	-157.28072	0.11688	-157.16384	19.49	17.50
-1.649	-157.28076	0.11688	-157.16388	19.46	17.48
-1.640	-157.28027	0.11687	-157.16341	19.77	17.77

-1.620	-157.27983	0.11686	-157.16297	20.04	18.05
-1.619	-157.28010	0.11687	-157.16323	19.88	17.89
-1.600	-157.27939	0.11685	-157.16254	20.32	18.32
-1.589	-157.27943	0.11686	-157.16258	20.29	18.29
-1.580	-157.27895	0.11685	-157.16211	20.60	18.59
-1.560	-157.27852	0.11684	-157.16168	20.87	18.86
-1.559	-157.27878	0.11685	-157.16193	20.71	18.70
-1.540	-157.27808	0.11683	-157.16125	21.14	19.13
-1.529	-157.27812	0.11683	-157.16129	21.12	19.10
-1.520	-157.27765	0.11683	-157.16082	21.42	19.40
-1.500	-157.27722	0.11682	-157.16040	21.69	19.66
-1.499	-157.27747	0.11682	-157.16065	21.53	19.51
-1.480	-157.27679	0.11681	-157.15997	21.96	19.93
-1.469	-157.27683	0.11681	-157.16001	21.93	19.90
-1.460	-157.27636	0.11681	-157.15955	22.23	20.19
-1.440	-157.27593	0.11680	-157.15913	22.49	20.46
-1.439	-157.27618	0.11680	-157.15938	22.33	20.30
-1.420	-157.27551	0.11679	-157.15872	22.76	20.72
-1.409	-157.27555	0.11679	-157.15875	22.73	20.69
-1.400	-157.27509	0.11679	-157.15830	23.02	20.98
-1.380	-157.27467	0.11678	-157.15789	23.28	21.24
-1.379	-157.27492	0.11678	-157.15814	23.13	21.08
-1.360	-157.27425	0.11677	-157.15748	23.55	21.49
-1.349	-157.27429	0.11677	-157.15752	23.52	21.47
-1.340	-157.27384	0.11677	-157.15708	23.80	21.75
-1.320	-157.27343	0.11676	-157.15667	24.06	22.00
-1.319	-157.27368	0.11676	-157.15691	23.91	21.85
-1.300	-157.27303	0.11675	-157.15628	24.32	22.25
-1.289	-157.27307	0.11675	-157.15631	24.29	22.23
-1.280	-157.27262	0.11675	-157.15588	24.57	22.50
-1.260	-157.27223	0.11674	-157.15549	24.82	22.74
-1.259	-157.27246	0.11674	-157.15572	24.67	22.60
-1.240	-157.27183	0.11673	-157.15510	25.07	22.99
-1.229	-157.27187	0.11673	-157.15514	25.04	22.96
-1.220	-157.27144	0.11673	-157.15472	25.31	23.23
-1.200	-157.27106	0.11672	-157.15434	25.55	23.47
-1.199	-157.27128	0.11672	-157.15456	25.41	23.32
-1.180	-157.27067	0.11671	-157.15396	25.79	23.70
-1.169	-157.27071	0.11671	-157.15400	25.77	23.68
-1.160	-157.27030	0.11671	-157.15359	26.03	23.93
-1.140	-157.26992	0.11670	-157.15322	26.26	24.16
-1.139	-157.27014	0.11670	-157.15344	26.12	24.03
-1.120	-157.26956	0.11669	-157.15286	26.49	24.39
-1.109	-157.26959	0.11669	-157.15290	26.47	24.37
-1.100	-157.26919	0.11669	-157.15251	26.72	24.61
-1.080	-157.26884	0.11668	-157.15216	26.95	24.83

-1.079	-157.26905	0.11668	-157.15236	26.81	24.70
-1.060	-157.26848	0.11667	-157.15181	27.17	25.05
-1.049	-157.26852	0.11667	-157.15184	27.15	25.03
-1.040	-157.26814	0.11667	-157.15147	27.38	25.26
-1.020	-157.26780	0.11666	-157.15114	27.60	25.47
-1.019	-157.26800	0.11666	-157.15133	27.47	25.35
-1.000	-157.26746	0.11665	-157.15081	27.81	25.68
-0.989	-157.26749	0.11665	-157.15084	27.79	25.66
-0.980	-157.26713	0.11665	-157.15048	28.02	25.88
-0.960	-157.26681	0.11664	-157.15017	28.22	26.08
-0.959	-157.26700	0.11664	-157.15036	28.10	25.96
-0.940	-157.26649	0.11663	-157.14986	28.42	26.28
-0.929	-157.26652	0.11664	-157.14989	28.40	26.26
-0.920	-157.26618	0.11663	-157.14955	28.61	26.47
-0.900	-157.26587	0.11662	-157.14925	28.80	26.66
-0.899	-157.26606	0.11663	-157.14943	28.69	26.54
-0.880	-157.26558	0.11662	-157.14896	28.99	26.84
-0.869	-157.26561	0.11662	-157.14899	28.97	26.82
-0.860	-157.26529	0.11661	-157.14868	29.17	27.02
-0.840	-157.26500	0.11660	-157.14840	29.35	27.19
-0.839	-157.26517	0.11661	-157.14856	29.25	27.09
-0.820	-157.26472	0.11660	-157.14813	29.53	27.36
-0.809	-157.26475	0.11660	-157.14815	29.51	27.35
-0.800	-157.26445	0.11659	-157.14786	29.70	27.53
-0.780	-157.26419	0.11658	-157.14761	29.86	27.69
-0.779	-157.26435	0.11659	-157.14776	29.76	27.59
-0.760	-157.26393	0.11658	-157.14736	30.02	27.85
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-0.720	-157.26344	0.11656	-157.14688	30.33	28.15
-0.719	-157.26358	0.11657	-157.14702	30.24	28.06
-0.700	-157.26321	0.11656	-157.14665	30.48	28.29
-0.689	-157.26323	0.11656	-157.14667	30.46	28.28
-0.680	-157.26298	0.11655	-157.14643	30.62	28.43
-0.660	-157.26276	0.11654	-157.14621	30.76	28.56
-0.659	-157.26289	0.11655	-157.14634	30.68	28.48
-0.640	-157.26254	0.11654	-157.14601	30.89	28.69
-0.629	-157.26256	0.11654	-157.14603	30.88	28.68
-0.620	-157.26234	0.11653	-157.14581	31.02	28.82
-0.600	-157.26214	0.11652	-157.14561	31.15	28.94
-0.599	-157.26226	0.11653	-157.14573	31.07	28.87
-0.580	-157.26195	0.11652	-157.14543	31.27	29.06
-0.569	-157.26196	0.11652	-157.14545	31.26	29.04
-0.560	-157.26176	0.11651	-157.14525	31.38	29.17
-0.540	-157.26159	0.11650	-157.14508	31.50	29.27
-0.539	-157.26169	0.11651	-157.14518	31.43	29.21

-0.520	-157.26142	0.11650	-157.14492	31.60	29.38
-0.509	-157.26143	0.11650	-157.14493	31.59	29.37
-0.500	-157.26125	0.11649	-157.14476	31.70	29.47
-0.480	-157.26110	0.11648	-157.14461	31.80	29.57
-0.479	-157.26119	0.11649	-157.14470	31.74	29.51
-0.460	-157.26095	0.11648	-157.14447	31.89	29.66
-0.449	-157.26096	0.11648	-157.14449	31.89	29.65
-0.440	-157.26081	0.11647	-157.14434	31.98	29.74
-0.420	-157.26067	0.11646	-157.14421	32.07	29.82
-0.419	-157.26075	0.11647	-157.14428	32.02	29.77
-0.400	-157.26054	0.11646	-157.14409	32.15	29.90
-0.389	-157.26056	0.11646	-157.14410	32.14	29.89
-0.380	-157.26042	0.11645	-157.14397	32.22	29.97
-0.360	-157.26031	0.11644	-157.14387	32.30	30.04
-0.359	-157.26038	0.11645	-157.14393	32.25	30.00
-0.340	-157.26020	0.11644	-157.14376	32.36	30.10
-0.329	-157.26021	0.11644	-157.14377	32.36	30.09
-0.320	-157.26010	0.11643	-157.14367	32.43	30.16
-0.300	-157.26000	0.11642	-157.14358	32.49	30.21
-0.299	-157.26006	0.11642	-157.14364	32.45	30.18
-0.280	-157.25991	0.11641	-157.14350	32.54	30.27
-0.269	-157.25992	0.11642	-157.14351	32.54	30.26
-0.260	-157.25983	0.11641	-157.14342	32.60	30.31
-0.240	-157.25975	0.11640	-157.14335	32.65	30.36
-0.239	-157.25980	0.11640	-157.14340	32.62	30.33
-0.220	-157.25968	0.11639	-157.14329	32.69	30.40
-0.209	-157.25969	0.11639	-157.14330	32.69	30.39
-0.200	-157.25962	0.11639	-157.14323	32.73	30.43
-0.180	-157.25956	0.11638	-157.14318	32.77	30.47
-0.179	-157.25959	0.11636	-157.14323	32.75	30.44
-0.160	-157.25950	0.11637	-157.14313	32.80	30.50
-0.150	-157.25951	0.11632	-157.14319	32.80	30.46
-0.140	-157.25945	0.11636	-157.14310	32.83	30.52
-0.120	-157.25943	0.11636	-157.14308	32.84	30.53
-0.120	-157.25941	0.11631	-157.14310	32.86	30.52
-0.100	-157.25937	0.11635	-157.14302	32.89	30.57
-0.090	-157.25937	0.11635	-157.14303	32.88	30.56
-0.080	-157.25933	0.11633	-157.14300	32.91	30.58
-0.060	-157.25930	0.11633	-157.14298	32.93	30.59
-0.060	-157.25932	0.11632	-157.14300	32.91	30.58
-0.040	-157.25928	0.11630	-157.14299	32.94	30.59
-0.030	-157.25928	0.11632	-157.14296	32.94	30.60
-0.020	-157.25926	0.11631	-157.14295	32.95	30.61
0.000	-157.25923	0.11040	-157.14883	32.97	30.72
0.020	-157.25922	0.11627	-157.14295	32.97	30.61
0.030	-157.25922	0.11626	-157.14296	32.97	30.58

0.040	-157.25922	0.11623	-157.14299	32.97	30.58
0.060	-157.25923	0.11623	-157.14300	32.97	30.60
0.060	-157.2592233	0.11626	-157.14297	32.96	30.59
0.080	-157.2592318	0.11624	-157.14299	32.96	30.58
0.090	-157.2592439	0.11624	-157.14301	32.96	30.58
0.100	-157.2592431	0.11624	-157.14300	32.95	30.51
0.120	-157.2592591	0.11614	-157.14312	32.95	30.55
0.120	-157.2592687	0.11622	-157.14305	32.94	30.54
0.140	-157.259275	0.11620	-157.14307	32.93	30.45
0.149	-157.2592974	0.11609	-157.14321	32.93	30.52
0.160	-157.2592967	0.11620	-157.14309	32.91	30.46
0.179	-157.2593359	0.11614	-157.14319	32.92	30.51
0.180	-157.2593204	0.11620	-157.14312	32.90	30.48
0.200	-157.2593467	0.11619	-157.14315	32.88	30.45
0.209	-157.2593779	0.11617	-157.14321	32.88	30.45
0.219	-157.2593758	0.11616	-157.14321	32.85	30.41
0.239	-157.259427	0.11616	-157.14327	32.86	30.43
0.239	-157.259408	0.11617	-157.14324	32.84	30.40
0.259	-157.2594419	0.11616	-157.14328	32.82	30.37
0.269	-157.2594813	0.11615	-157.14333	32.82	30.38
0.279	-157.2594785	0.11615	-157.14333	32.78	30.33
0.299	-157.2595406	0.11614	-157.14340	32.79	30.34
0.299	-157.2595168	0.11614	-157.14338	32.77	30.31
0.319	-157.2595585	0.11613	-157.14343	32.74	30.26
0.329	-157.2596034	0.11610	-157.14350	32.74	30.28
0.339	-157.2596004	0.11612	-157.14348	32.70	30.22
0.359	-157.2596725	0.11610	-157.14357	32.71	30.24
0.359	-157.2596459	0.11611	-157.14354	32.68	30.21
0.379	-157.259692	0.11610	-157.14359	32.65	30.17
0.389	-157.2597439	0.11609	-157.14365	32.65	30.17
0.399	-157.2597406	0.11609	-157.14365	32.60	30.11
0.419	-157.2598202	0.11607	-157.14375	32.62	30.13
0.419	-157.2597906	0.11608	-157.14371	32.59	30.09
0.439	-157.2598425	0.11607	-157.14377	32.55	30.04
0.449	-157.2598994	0.11605	-157.14385	32.56	30.05
0.459	-157.2598961	0.11605	-157.14384	32.50	29.99
0.479	-157.2599831	0.11604	-157.14395	32.52	30.01
0.479	-157.2599513	0.11605	-157.14391	32.49	29.97
0.499	-157.260007	0.11604	-157.14397	32.45	29.92
0.509	-157.260068	0.11602	-157.14405	32.45	29.93
0.519	-157.2600652	0.11602	-157.14404	32.39	29.84
0.539	-157.2601586	0.11599	-157.14417	32.41	29.88
0.539	-157.2601229	0.11601	-157.14411	32.37	29.84
0.559	-157.2601838	0.11600	-157.14419	32.33	29.79
0.569	-157.2602482	0.11599	-157.14426	32.34	29.79
0.579	-157.2602441	0.11599	-157.14426	32.28	29.72

0.599	-157.2603419	0.11597	-157.14437	32.30	29.75
0.599	-157.2603062	0.11598	-157.14433	32.26	29.70
0.619	-157.2603695	0.11596	-157.14441	32.22	29.65
0.629	-157.2604377	0.11595	-157.14449	32.22	29.65
0.639	-157.2604338	0.11595	-157.14448	32.15	29.57
0.659	-157.2605359	0.11593	-157.14461	32.18	29.60
0.659	-157.2604981	0.11594	-157.14456	32.14	29.55
0.679	-157.260564	0.11593	-157.14464	32.09	29.50
0.689	-157.2606353	0.11591	-157.14472	32.09	29.50
0.699	-157.2606305	0.11591	-157.14472	32.03	29.42
0.719	-157.260736	0.11589	-157.14484	32.05	29.45
0.719	-157.2606977	0.11590	-157.14480	32.01	29.40
0.739	-157.2607657	0.11589	-157.14488	31.96	29.35
0.749	-157.2608386	0.11587	-157.14497	31.97	29.35
0.759	-157.2608349	0.11587	-157.14496	31.90	29.27
0.779	-157.2609427	0.11585	-157.14509	31.92	29.30
0.779	-157.2609034	0.11586	-157.14504	31.88	29.25
0.799	-157.2609726	0.11585	-157.14512	31.83	29.19
0.809	-157.2610474	0.11583	-157.14521	31.84	29.19
0.819	-157.2610432	0.11584	-157.14521	31.77	29.11
0.839	-157.2611542	0.11581	-157.14534	31.79	29.14
0.839	-157.2611136	0.11582	-157.14529	31.75	29.09
0.859	-157.2611842	0.11581	-157.14538	31.70	29.03
0.869	-157.2612606	0.11579	-157.14547	31.70	29.03
0.879	-157.2612561	0.11579	-157.14546	31.63	28.95
0.899	-157.2613686	0.11577	-157.14560	31.66	28.98
0.899	-157.2613275	0.11578	-157.14555	31.61	28.93
0.919	-157.2613999	0.11577	-157.14563	31.56	28.87
0.929	-157.261476	0.11575	-157.14573	31.57	28.87
0.939	-157.2614715	0.11575	-157.14572	31.50	28.79
0.959	-157.2615855	0.11573	-157.14586	31.52	28.82
0.959	-157.2615449	0.11574	-157.14581	31.48	28.76
0.979	-157.2616171	0.11572	-157.14589	31.43	28.70
0.989	-157.2616951	0.11571	-157.14599	31.43	28.71
0.999	-157.2616902	0.11571	-157.14598	31.36	28.62
1.019	-157.261804	0.11568	-157.14612	31.38	28.65
1.019	-157.2617635	0.11569	-157.14607	31.34	28.60
1.039	-157.2618365	0.11568	-157.14616	31.29	28.54
1.049	-157.2619143	0.11566	-157.14625	31.29	28.54
1.059	-157.2619088	0.11566	-157.14625	31.22	28.45
1.079	-157.2620239	0.11564	-157.14639	31.25	28.49
1.079	-157.2619826	0.11565	-157.14633	31.20	28.43
1.099	-157.2620558	0.11563	-157.14642	31.15	28.37
1.109	-157.2621344	0.11562	-157.14652	31.15	28.37
1.119	-157.2621297	0.11562	-157.14651	31.08	28.29
1.139	-157.2622438	0.11559	-157.14665	31.11	28.32

1.139	-157.2622026	0.11560	-157.14660	31.06	28.26
1.159	-157.2622764	0.11558	-157.14669	31.01	28.20
1.169	-157.2623546	0.11557	-157.14679	31.02	28.21
1.179	-157.262349	0.11557	-157.14678	30.94	28.11
1.199	-157.2624636	0.11553	-157.14693	30.97	28.15
1.199	-157.2624224	0.11555	-157.14688	30.92	28.09
1.219	-157.2624955	0.11552	-157.14697	30.87	28.03
1.229	-157.262574	0.11550	-157.14707	30.88	28.03
1.239	-157.2625688	0.11551	-157.14706	30.81	27.95
1.259	-157.2626821	0.11549	-157.14720	30.83	27.98
1.259	-157.2626413	0.11549	-157.14715	30.79	27.92
1.279	-157.2627145	0.11548	-157.14723	30.74	27.87
1.289	-157.2627914	0.11547	-157.14732	30.74	27.87
1.299	-157.2627869	0.11547	-157.14732	30.67	27.78
1.319	-157.2629003	0.11544	-157.14746	30.70	27.82
1.319	-157.2628596	0.11545	-157.14741	30.65	27.76
1.339	-157.2629312	0.11544	-157.14749	30.60	27.70
1.349	-157.2630083	0.11543	-157.14758	30.61	27.71
1.359	-157.2630038	0.11542	-157.14758	30.54	27.62
1.379	-157.2631153	0.11541	-157.14771	30.56	27.65
1.379	-157.2630759	0.11541	-157.14766	30.52	27.60
1.399	-157.2631467	0.11540	-157.14775	30.47	27.54
1.409	-157.2632231	0.11539	-157.14784	30.47	27.55
1.419	-157.2632185	0.11539	-157.14783	30.40	27.46
1.439	-157.2633295	0.11537	-157.14796	30.43	27.49
1.439	-157.2632895	0.11537	-157.14792	30.38	27.44
1.459	-157.26336	0.11536	-157.14800	30.33	27.39
1.469	-157.2634351	0.11534	-157.14809	30.34	27.39
1.479	-157.2634306	0.11534	-157.14809	30.27	27.31
1.499	-157.2635405	0.11532	-157.14822	30.29	27.34
1.499	-157.2635009	0.11533	-157.14817	30.25	27.28
1.519	-157.2635709	0.11532	-157.14826	30.20	27.23
1.529	-157.2636448	0.11530	-157.14834	30.21	27.23
1.539	-157.2636404	0.11530	-157.14834	30.14	27.15
1.559	-157.2637488	0.11528	-157.14847	30.16	27.18
1.559	-157.26371	0.11529	-157.14842	30.12	27.13
1.579	-157.2637786	0.11528	-157.14850	30.07	27.07
1.589	-157.2638516	0.11526	-157.14859	30.08	27.07
1.599	-157.2638475	0.11526	-157.14859	30.01	27.00
1.619	-157.2639534	0.11524	-157.14871	30.03	27.02
1.619	-157.2639153	0.11525	-157.14867	29.99	26.97
1.639	-157.2639843	0.11523	-157.14875	29.95	26.92
1.649	-157.2640555	0.11522	-157.14884	29.95	26.92
1.659	-157.2640514	0.11522	-157.14883	29.88	26.84
1.679	-157.2641562	0.11520	-157.14896	29.91	26.87
1.679	-157.264119	0.11521	-157.14891	29.86	26.82

1.699	-157.2641854	0.11520	-157.14899	29.82	26.77
1.709	-157.2642564	0.11518	-157.14908	29.82	26.77
1.719	-157.2642516	0.11518	-157.14907	29.76	26.69
1.739	-157.2643549	0.11516	-157.14920	29.78	26.72
1.739	-157.264318	0.11517	-157.14915	29.74	26.67
1.759	-157.2643837	0.11515	-157.14923	29.70	26.62
1.769	-157.2644528	0.11514	-157.14931	29.70	26.62
1.779	-157.2644492	0.11514	-157.14931	29.63	26.54
1.799	-157.2645497	0.11512	-157.14943	29.66	26.57
1.799	-157.2645142	0.11512	-157.14939	29.62	26.52
1.819	-157.2645783	0.11511	-157.14946	29.57	26.47
1.829	-157.2646465	0.11510	-157.14955	29.58	26.47
1.839	-157.2646421	0.11510	-157.14954	29.51	26.40
1.859	-157.2647418	0.11508	-157.14966	29.54	26.43
1.859	-157.2647065	0.11509	-157.14962	29.50	26.38
1.879	-157.2647699	0.11507	-157.14970	29.46	26.33
1.889	-157.2648359	0.11506	-157.14978	29.46	26.33
1.899	-157.2648325	0.11506	-157.14977	29.40	26.25
1.919	-157.2649295	0.11504	-157.14989	29.42	26.28
1.919	-157.2648949	0.11505	-157.14985	29.38	26.24
1.939	-157.2649569	0.11503	-157.14992	29.34	26.19
1.949	-157.2650224	0.11502	-157.15000	29.34	26.19
1.959	-157.2650186	0.11502	-157.15000	29.28	26.12
1.979	-157.2651134	0.11500	-157.15011	29.30	26.14
1.979	-157.2650796	0.11501	-157.15007	29.26	26.10
1.999	-157.2651404	0.11500	-157.15014	29.22	26.04
2.009	-157.2652051	0.11498	-157.15023	29.23	26.05
2.019	-157.2652005	0.11498	-157.15022	29.17	25.98
2.039	-157.2652935	0.11496	-157.15033	29.19	26.00
2.039	-157.2652603	0.11497	-157.15029	29.15	25.96
2.059	-157.2653194	0.11496	-157.15036	29.11	25.91
2.069	-157.2653828	0.11494	-157.15044	29.11	25.91
2.079	-157.2653789	0.11495	-157.15043	29.06	25.84
2.099	-157.2654697	0.11492	-157.15055	29.08	25.87
2.099	-157.2654377	0.11493	-157.15051	29.04	25.82
2.119	-157.2654955	0.11492	-157.15058	29.00	25.78
2.129	-157.2655564	0.11491	-157.15065	29.01	25.78
2.139	-157.2655534	0.11491	-157.15065	28.95	25.71
2.159	-157.2656427	0.11489	-157.15075	28.97	25.74
2.159	-157.2656106	0.11490	-157.15071	28.93	25.70
2.179	-157.2656671	0.11488	-157.15078	28.90	25.65
2.189	-157.2657267	0.11487	-157.15086	28.90	25.65
2.199	-157.2657239	0.11487	-157.15085	28.84	25.58
2.219	-157.2658102	0.11485	-157.15096	28.86	25.61
2.219	-157.2657796	0.11486	-157.15092	28.83	25.57
2.239	-157.2658349	0.11485	-157.15099	28.79	25.52

2.249	-157.2658931	0.11483	-157.15106	28.79	25.52
2.259	-157.2658904	0.11484	-157.15106	28.74	25.46
2.279	-157.2659749	0.11482	-157.15116	28.76	25.48
2.279	-157.2659447	0.11482	-157.15112	28.73	25.44
2.299	-157.2659988	0.11481	-157.15119	28.69	25.40
2.308	-157.266056	0.11480	-157.15126	28.69	25.40
2.319	-157.2660526	0.11480	-157.15125	28.64	25.34
2.338	-157.2661348	0.11478	-157.15135	28.66	25.36
2.339	-157.2661056	0.11479	-157.15132	28.63	25.32
2.359	-157.2661583	0.11478	-157.15138	28.59	25.28
2.368	-157.2662138	0.11477	-157.15145	28.59	25.28
2.379	-157.2662105	0.11477	-157.15145	28.54	25.21
2.398	-157.2662914	0.11474	-157.15156	28.56	25.24
2.399	-157.2662628	0.11475	-157.15151	28.53	25.20
2.419	-157.2663138	0.11474	-157.15157	28.49	25.16
2.428	-157.2663686	0.11473	-157.15164	28.50	25.16
2.439	-157.2663652	0.11473	-157.15163	28.45	25.10
2.458	-157.2664437	0.11471	-157.15173	28.46	25.12
2.459	-157.2664158	0.11472	-157.15169	28.43	25.08
2.479	-157.266466	0.11471	-157.15176	28.40	25.04
2.488	-157.2665185	0.11470	-157.15182	28.40	25.05
2.499	-157.2665157	0.11470	-157.15182	28.35	24.98
2.518	-157.2665918	0.11467	-157.15192	28.37	25.01
2.519	-157.2665648	0.11469	-157.15188	28.34	24.97
2.539	-157.2666141	0.11468	-157.15194	28.31	24.93
2.548	-157.2666653	0.11466	-157.15200	28.31	24.93
2.559	-157.2666625	0.11467	-157.15200	28.26	24.88
2.578	-157.2667364	0.11465	-157.15209	28.28	24.90
2.579	-157.2667108	0.11465	-157.15206	28.25	24.86
2.599	-157.2667577	0.11465	-157.15211	28.22	24.82
2.608	-157.2668069	0.11463	-157.15217	28.22	24.83
2.619	-157.2668053	0.11464	-157.15217	28.17	24.77
2.638	-157.2668767	0.11461	-157.15227	28.19	24.79
2.639	-157.2668514	0.11462	-157.15223	28.16	24.75
2.659	-157.2668977	0.11461	-157.15228	28.13	24.72
2.668	-157.2669461	0.11460	-157.15235	28.13	24.72
2.679	-157.2669435	0.11460	-157.15234	28.09	24.66
2.698	-157.2670137	0.11459	-157.15243	28.10	24.68
2.699	-157.266989	0.11459	-157.15240	28.08	24.65
2.719	-157.2670342	0.11458	-157.15245	28.05	24.61
2.728	-157.2670812	0.11457	-157.15251	28.05	24.61
2.739	-157.2670787	0.11457	-157.15251	28.01	24.56
2.758	-157.2671465	0.11455	-157.15260	28.02	24.58
2.759	-157.2671229	0.11456	-157.15256	27.99	24.55
2.779	-157.2671667	0.11455	-157.15261	27.96	24.51
2.788	-157.2672122	0.11454	-157.15267	27.97	24.51

2.799	-157.2672107	0.11454	-157.15267	27.92	24.46
2.818	-157.2672756	0.11453	-157.15275	27.94	24.48
2.819	-157.2672529	0.11453	-157.15272	27.91	24.45
2.839	-157.2672951	0.11452	-157.15277	27.88	24.41
2.848	-157.2673399	0.11451	-157.15283	27.89	24.41
2.859	-157.2673374	0.11451	-157.15283	27.85	24.36
2.878	-157.2674016	0.11448	-157.15292	27.86	24.38
2.879	-157.267379	0.11450	-157.15288	27.83	24.35
2.899	-157.2674204	0.11449	-157.15293	27.81	24.32
2.908	-157.2674635	0.11448	-157.15298	27.81	24.31
2.919	-157.2674616	0.11448	-157.15298	27.77	24.27
2.938	-157.2675233	0.11447	-157.15306	27.78	24.29
2.939	-157.2675017	0.11447	-157.15303	27.76	24.26
2.959	-157.2675422	0.11447	-157.15308	27.73	24.22
2.968	-157.2675834	0.11446	-157.15313	27.73	24.22
2.979	-157.2675815	0.11445	-157.15314	27.69	24.18
2.998	-157.2676421	0.11444	-157.15320	27.71	24.19
2.999	-157.2676212	0.11445	-157.15318	27.68	24.17
3.019	-157.2676596	0.11444	-157.15322	27.66	24.13
3.028	-157.267701	0.11442	-157.15328	27.66	24.14
3.039	-157.2676984	0.11443	-157.15327	27.62	24.09
3.058	-157.267757	0.11441	-157.15335	27.64	24.10
3.059	-157.2677365	0.11442	-157.15332	27.61	24.08
3.079	-157.2677743	0.11441	-157.15336	27.59	24.04
3.088	-157.2678139	0.11440	-157.15341	27.59	24.05
3.099	-157.2678121	0.11440	-157.15341	27.55	24.00

SI Table 36: Potential energy data along the MEP for reaction CC•CC → C• + C=CC. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction CC•CC→ C• + C=CC					
$E_{CC.CC}$ = -157.3092267 hartree $ZPE_{CC.CC}$ = 0.119855 hartree					
Reaction coordinate ($amu^{1/2}$ bohr)	V_C (Hartree)	ZPE (Hartree)	V_{ag} (Hartree)	V_c - $E_{CC.CC}$ (kcal/mol)	V_{ag}-$E_{CC.CC}$ (kcal/mol)
-1.950	-157.29426	0.11700	-157.17726	9.39	7.60
-1.940	-157.29395	0.11699	-157.17696	9.59	7.79
-1.930	-157.29364	0.11698	-157.17666	9.78	7.98
-1.920	-157.29333	0.11697	-157.17635	9.98	8.17
-1.910	-157.29301	0.11697	-157.17605	10.17	8.36
-1.900	-157.29270	0.11696	-157.17574	10.37	8.55
-1.890	-157.29238	0.11695	-157.17543	10.57	8.75
-1.880	-157.29206	0.11694	-157.17513	10.77	8.94
-1.870	-157.29175	0.11693	-157.17482	10.97	9.13
-1.860	-157.29143	0.11692	-157.17451	11.17	9.33
-1.850	-157.29111	0.11691	-157.17420	11.37	9.52
-1.840	-157.29079	0.11690	-157.17389	11.57	9.72
-1.830	-157.29048	0.11690	-157.17358	11.77	9.91
-1.820	-157.29016	0.11689	-157.17327	11.97	10.11
-1.810	-157.28984	0.11688	-157.17296	12.17	10.30
-1.800	-157.28952	0.11687	-157.17265	12.37	10.50
-1.790	-157.28920	0.11686	-157.17234	12.57	10.69
-1.780	-157.28888	0.11685	-157.17202	12.77	10.89
-1.770	-157.28856	0.11685	-157.17171	12.97	11.08
-1.760	-157.28824	0.11684	-157.17140	13.17	11.28
-1.750	-157.28792	0.11683	-157.17109	13.37	11.47
-1.740	-157.28760	0.11682	-157.17078	13.57	11.67
-1.730	-157.28728	0.11681	-157.17047	13.77	11.86
-1.720	-157.28696	0.11680	-157.17016	13.97	12.06
-1.710	-157.28664	0.11679	-157.16985	14.17	12.25
-1.700	-157.28632	0.11679	-157.16954	14.37	12.45
-1.690	-157.28601	0.11678	-157.16923	14.57	12.64
-1.680	-157.28569	0.11677	-157.16892	14.77	12.83
-1.670	-157.28537	0.11676	-157.16861	14.97	13.03
-1.660	-157.28506	0.11675	-157.16830	15.17	13.22
-1.650	-157.28474	0.11674	-157.16800	15.37	13.41

-1.640	-157.28443	0.11673	-157.16769	15.56	13.61
-1.630	-157.28411	0.11673	-157.16739	15.76	13.80
-1.620	-157.28380	0.11672	-157.16708	15.96	13.99
-1.610	-157.28349	0.11671	-157.16678	16.15	14.18
-1.600	-157.28318	0.11670	-157.16648	16.35	14.37
-1.590	-157.28287	0.11669	-157.16617	16.54	14.56
-1.580	-157.28256	0.11668	-157.16587	16.73	14.74
-1.570	-157.28225	0.11668	-157.16558	16.93	14.93
-1.560	-157.28195	0.11667	-157.16528	17.12	15.12
-1.550	-157.28164	0.11666	-157.16498	17.31	15.30
-1.540	-157.28134	0.11665	-157.16469	17.50	15.49
-1.530	-157.28104	0.11664	-157.16439	17.69	15.67
-1.520	-157.28074	0.11663	-157.16410	17.88	15.86
-1.510	-157.28044	0.11662	-157.16381	18.07	16.04
-1.500	-157.28014	0.11662	-157.16352	18.25	16.22
-1.490	-157.27984	0.11661	-157.16324	18.44	16.40
-1.480	-157.27955	0.11660	-157.16295	18.62	16.58
-1.470	-157.27926	0.11659	-157.16267	18.80	16.76
-1.460	-157.27897	0.11658	-157.16239	18.99	16.93
-1.450	-157.27868	0.11658	-157.16211	19.17	17.11
-1.440	-157.27840	0.11657	-157.16183	19.35	17.28
-1.430	-157.27811	0.11656	-157.16155	19.52	17.46
-1.420	-157.27783	0.11655	-157.16128	19.70	17.63
-1.410	-157.27755	0.11654	-157.16101	19.88	17.80
-1.400	-157.27727	0.11653	-157.16074	20.05	17.97
-1.390	-157.27700	0.11652	-157.16047	20.22	18.13
-1.380	-157.27672	0.11652	-157.16021	20.40	18.30
-1.370	-157.27645	0.11651	-157.15995	20.57	18.46
-1.360	-157.27619	0.11650	-157.15969	20.73	18.63
-1.350	-157.27592	0.11649	-157.15943	20.90	18.79
-1.340	-157.27566	0.11648	-157.15917	21.07	18.95
-1.330	-157.27539	0.11647	-157.15892	21.23	19.11
-1.320	-157.27514	0.11647	-157.15867	21.39	19.27
-1.310	-157.27488	0.11646	-157.15842	21.55	19.42
-1.300	-157.27463	0.11645	-157.15818	21.71	19.57
-1.290	-157.27438	0.11644	-157.15794	21.87	19.73
-1.280	-157.27413	0.11643	-157.15770	22.03	19.88
-1.270	-157.27388	0.11642	-157.15746	22.18	20.03
-1.260	-157.27364	0.11641	-157.15722	22.33	20.17
-1.250	-157.27340	0.11641	-157.15699	22.48	20.32
-1.240	-157.27316	0.11640	-157.15676	22.63	20.46
-1.230	-157.27293	0.11639	-157.15654	22.78	20.60
-1.220	-157.27270	0.11638	-157.15632	22.92	20.74
-1.210	-157.27247	0.11637	-157.15609	23.07	20.88
-1.200	-157.27224	0.11636	-157.15588	23.21	21.02
-1.190	-157.27202	0.11636	-157.15566	23.35	21.15

-1.180	-157.27180	0.11635	-157.15545	23.49	21.29
-1.170	-157.27158	0.11634	-157.15524	23.62	21.42
-1.160	-157.27136	0.11633	-157.15503	23.76	21.55
-1.150	-157.27115	0.11632	-157.15483	23.89	21.67
-1.140	-157.27094	0.11631	-157.15463	24.02	21.80
-1.130	-157.27074	0.11630	-157.15443	24.15	21.92
-1.120	-157.27053	0.11630	-157.15424	24.28	22.05
-1.110	-157.27033	0.11629	-157.15405	24.41	22.17
-1.100	-157.27014	0.11628	-157.15386	24.53	22.29
-1.090	-157.26994	0.11627	-157.15367	24.65	22.40
-1.080	-157.26975	0.11626	-157.15349	24.77	22.52
-1.070	-157.26956	0.11625	-157.15331	24.89	22.63
-1.060	-157.26938	0.11625	-157.15313	25.01	22.74
-1.050	-157.26919	0.11624	-157.15296	25.12	22.85
-1.040	-157.26901	0.11623	-157.15278	25.23	22.96
-1.030	-157.26884	0.11622	-157.15261	25.35	23.07
-1.020	-157.26865	0.11621	-157.15244	25.46	23.17
-1.010	-157.26848	0.11620	-157.15227	25.57	23.28
-1.000	-157.26830	0.11620	-157.15211	25.68	23.38
-0.990	-157.26813	0.11619	-157.15195	25.79	23.48
-0.980	-157.26797	0.11618	-157.15179	25.89	23.58
-0.970	-157.26781	0.11617	-157.15164	25.99	23.68
-0.960	-157.26765	0.11616	-157.15149	26.09	23.77
-0.950	-157.26749	0.11616	-157.15134	26.19	23.87
-0.940	-157.26734	0.11615	-157.15119	26.28	23.96
-0.930	-157.26719	0.11614	-157.15105	26.38	24.05
-0.920	-157.26704	0.11613	-157.15091	26.47	24.13
-0.910	-157.26689	0.11612	-157.15077	26.56	24.22
-0.900	-157.26675	0.11612	-157.15063	26.66	24.31
-0.890	-157.26660	0.11611	-157.15050	26.75	24.39
-0.880	-157.26646	0.11610	-157.15036	26.84	24.48
-0.870	-157.26632	0.11609	-157.15023	26.92	24.56
-0.860	-157.26618	0.11608	-157.15010	27.01	24.64
-0.850	-157.26605	0.11607	-157.14997	27.10	24.72
-0.840	-157.26591	0.11607	-157.14985	27.18	24.80
-0.830	-157.26578	0.11606	-157.14972	27.26	24.88
-0.820	-157.26565	0.11605	-157.14960	27.35	24.96
-0.810	-157.26552	0.11604	-157.14948	27.43	25.03
-0.800	-157.26539	0.11603	-157.14936	27.51	25.11
-0.790	-157.26526	0.11602	-157.14924	27.59	25.18
-0.780	-157.26514	0.11602	-157.14912	27.66	25.26
-0.770	-157.26502	0.11601	-157.14901	27.74	25.33
-0.760	-157.26490	0.11600	-157.14890	27.82	25.40
-0.750	-157.26478	0.11599	-157.14879	27.89	25.47
-0.740	-157.26466	0.11598	-157.14868	27.96	25.53
-0.730	-157.26455	0.11597	-157.14857	28.04	25.60

-0.720	-157.26443	0.11597	-157.14847	28.11	25.67
-0.710	-157.26432	0.11596	-157.14837	28.18	25.73
-0.700	-157.26421	0.11595	-157.14827	28.25	25.79
-0.690	-157.26411	0.11594	-157.14817	28.31	25.86
-0.680	-157.26400	0.11593	-157.14807	28.38	25.92
-0.670	-157.26390	0.11592	-157.14797	28.44	25.98
-0.660	-157.26380	0.11592	-157.14788	28.51	26.04
-0.650	-157.26370	0.11591	-157.14779	28.57	26.09
-0.640	-157.26360	0.11590	-157.14770	28.63	26.15
-0.630	-157.26350	0.11589	-157.14761	28.69	26.20
-0.620	-157.26341	0.11588	-157.14753	28.75	26.26
-0.610	-157.26332	0.11587	-157.14744	28.81	26.31
-0.600	-157.26323	0.11587	-157.14736	28.87	26.36
-0.590	-157.26314	0.11586	-157.14728	28.92	26.41
-0.580	-157.26305	0.11585	-157.14720	28.98	26.46
-0.570	-157.26297	0.11584	-157.14713	29.03	26.51
-0.560	-157.26288	0.11583	-157.14705	29.08	26.56
-0.550	-157.26280	0.11582	-157.14698	29.13	26.60
-0.540	-157.26272	0.11582	-157.14691	29.18	26.65
-0.530	-157.26265	0.11581	-157.14684	29.23	26.69
-0.520	-157.26257	0.11580	-157.14677	29.28	26.73
-0.510	-157.26250	0.11579	-157.14670	29.32	26.77
-0.500	-157.26242	0.11578	-157.14664	29.37	26.81
-0.490	-157.26235	0.11577	-157.14658	29.41	26.85
-0.480	-157.26229	0.11577	-157.14652	29.46	26.89
-0.470	-157.26222	0.11576	-157.14646	29.50	26.93
-0.460	-157.26215	0.11575	-157.14640	29.54	26.96
-0.450	-157.26209	0.11574	-157.14635	29.58	27.00
-0.440	-157.26203	0.11573	-157.14629	29.62	27.03
-0.430	-157.26197	0.11573	-157.14624	29.66	27.06
-0.420	-157.26191	0.11572	-157.14619	29.69	27.10
-0.410	-157.26185	0.11571	-157.14614	29.73	27.13
-0.400	-157.26180	0.11570	-157.14610	29.76	27.16
-0.390	-157.26175	0.11569	-157.14605	29.80	27.18
-0.380	-157.26169	0.11569	-157.14601	29.83	27.21
-0.370	-157.26164	0.11568	-157.14597	29.86	27.24
-0.360	-157.26160	0.11567	-157.14593	29.89	27.26
-0.350	-157.26155	0.11566	-157.14589	29.92	27.29
-0.340	-157.26150	0.11565	-157.14585	29.95	27.31
-0.330	-157.26146	0.11564	-157.14582	29.97	27.33
-0.320	-157.26142	0.11564	-157.14578	30.00	27.35
-0.310	-157.26138	0.11563	-157.14575	30.03	27.37
-0.300	-157.26134	0.11562	-157.14572	30.05	27.39
-0.290	-157.26130	0.11561	-157.14569	30.07	27.41
-0.280	-157.26127	0.11561	-157.14566	30.10	27.43
-0.270	-157.26123	0.11560	-157.14563	30.12	27.45

-0.260	-157.26120	0.11559	-157.14561	30.14	27.46
-0.250	-157.26117	0.11558	-157.14559	30.16	27.48
-0.240	-157.26114	0.11557	-157.14557	30.18	27.49
-0.230	-157.26111	0.11557	-157.14554	30.19	27.50
-0.220	-157.26108	0.11556	-157.14552	30.21	27.52
-0.210	-157.26106	0.11555	-157.14551	30.23	27.53
-0.200	-157.26103	0.11554	-157.14549	30.24	27.54
-0.190	-157.26101	0.11553	-157.14547	30.26	27.55
-0.180	-157.26099	0.11553	-157.14546	30.27	27.55
-0.170	-157.26097	0.11552	-157.14545	30.28	27.56
-0.160	-157.26095	0.11551	-157.14544	30.30	27.57
-0.150	-157.26093	0.11550	-157.14543	30.31	27.58
-0.140	-157.26091	0.11550	-157.14542	30.32	27.58
-0.130	-157.26090	0.11549	-157.14541	30.33	27.59
-0.120	-157.26088	0.11548	-157.14541	30.34	27.59
-0.110	-157.26087	0.11547	-157.14540	30.34	27.59
-0.100	-157.26086	0.11546	-157.14539	30.35	27.60
-0.090	-157.26085	0.11545	-157.14539	30.36	27.60
-0.080	-157.26084	0.11545	-157.14539	30.36	27.60
-0.070	-157.26083	0.11544	-157.14539	30.37	27.60
-0.060	-157.26082	0.11543	-157.14539	30.37	27.60
-0.050	-157.26082	0.11542	-157.14540	30.38	27.60
-0.040	-157.26081	0.11540	-157.14541	30.38	27.59
-0.030	-157.26081	0.11538	-157.14542	30.38	27.58
-0.020	-157.26080	0.11533	-157.14548	30.39	27.54
-0.010	-157.26080	0.11536	-157.14545	30.39	27.56
0.000	-157.26080	0.11141	-157.14939	30.39	27.59
0.010	-157.26081	0.11532	-157.14549	30.38	27.54
0.020	-157.26081	0.11528	-157.14553	30.38	27.51
0.030	-157.26081	0.11532	-157.14549	30.38	27.54
0.040	-157.26082	0.11533	-157.14549	30.38	27.54
0.050	-157.26082	0.11533	-157.14549	30.37	27.53
0.060	-157.26083	0.11532	-157.14550	30.37	27.53
0.070	-157.26084	0.11532	-157.14552	30.36	27.52
0.080	-157.26085	0.11531	-157.14553	30.36	27.51
0.090	-157.26086	0.11530	-157.14555	30.35	27.50
0.100	-157.26086	0.11530	-157.14557	30.35	27.49
0.110	-157.26088	0.11529	-157.14558	30.34	27.48
0.120	-157.26089	0.11528	-157.14561	30.33	27.46
0.130	-157.26090	0.11528	-157.14562	30.33	27.45
0.140	-157.26091	0.11527	-157.14564	30.32	27.44
0.150	-157.26093	0.11526	-157.14567	30.31	27.43
0.160	-157.26094	0.11526	-157.14568	30.30	27.41
0.170	-157.26096	0.11525	-157.14571	30.29	27.40
0.180	-157.26097	0.11524	-157.14573	30.28	27.38
0.190	-157.26099	0.11523	-157.14575	30.27	27.37

0.200	-157.26101	0.11523	-157.14578	30.26	27.35
0.210	-157.26102	0.11522	-157.14580	30.25	27.34
0.220	-157.26104	0.11521	-157.14583	30.24	27.32
0.230	-157.26106	0.11521	-157.14586	30.22	27.31
0.240	-157.26108	0.11520	-157.14588	30.21	27.29
0.250	-157.26110	0.11519	-157.14591	30.20	27.27
0.260	-157.26112	0.11518	-157.14594	30.19	27.25
0.270	-157.26114	0.11518	-157.14597	30.17	27.24
0.280	-157.26117	0.11517	-157.14600	30.16	27.22
0.290	-157.26119	0.11516	-157.14603	30.14	27.20
0.300	-157.26121	0.11515	-157.14606	30.13	27.18
0.310	-157.26124	0.11515	-157.14609	30.11	27.16
0.320	-157.26126	0.11514	-157.14612	30.10	27.14
0.330	-157.26128	0.11513	-157.14615	30.08	27.12
0.340	-157.26131	0.11513	-157.14618	30.07	27.10
0.350	-157.26134	0.11512	-157.14622	30.05	27.08
0.360	-157.26136	0.11511	-157.14625	30.04	27.06
0.370	-157.26139	0.11511	-157.14628	30.02	27.04
0.380	-157.26142	0.11510	-157.14632	30.00	27.02
0.390	-157.26144	0.11509	-157.14635	29.99	27.00
0.400	-157.26147	0.11508	-157.14639	29.97	26.97
0.410	-157.26150	0.11508	-157.14642	29.95	26.95
0.420	-157.26153	0.11507	-157.14646	29.93	26.93
0.430	-157.26156	0.11506	-157.14649	29.91	26.91
0.440	-157.26159	0.11505	-157.14653	29.90	26.88
0.450	-157.26162	0.11505	-157.14657	29.88	26.86
0.460	-157.26165	0.11504	-157.14661	29.86	26.84
0.470	-157.26168	0.11503	-157.14664	29.84	26.81
0.480	-157.26171	0.11502	-157.14668	29.82	26.79
0.490	-157.26174	0.11502	-157.14672	29.80	26.76
0.500	-157.26177	0.11501	-157.14676	29.78	26.74
0.510	-157.26180	0.11500	-157.14680	29.76	26.72
0.520	-157.26183	0.11499	-157.14684	29.74	26.69
0.530	-157.26186	0.11499	-157.14688	29.72	26.67
0.540	-157.26190	0.11498	-157.14692	29.70	26.64
0.550	-157.26193	0.11497	-157.14696	29.68	26.62
0.560	-157.26196	0.11497	-157.14700	29.66	26.59
0.570	-157.26200	0.11496	-157.14704	29.64	26.56
0.580	-157.26203	0.11495	-157.14708	29.62	26.54
0.590	-157.26206	0.11494	-157.14712	29.59	26.51
0.600	-157.26210	0.11493	-157.14716	29.57	26.49
0.610	-157.26213	0.11493	-157.14720	29.55	26.46
0.620	-157.26217	0.11492	-157.14725	29.53	26.43
0.630	-157.26220	0.11491	-157.14729	29.51	26.41
0.640	-157.26224	0.11490	-157.14733	29.49	26.38
0.650	-157.26227	0.11490	-157.14737	29.46	26.35

0.660	-157.2623076	0.11489	-157.14742	29.44	26.33
0.670	-157.2623429	0.11488	-157.14746	29.42	26.30
0.680	-157.2623784	0.11488	-157.14750	29.40	26.27
0.690	-157.2624148	0.11487	-157.14755	29.37	26.25
0.700	-157.2624505	0.11486	-157.14759	29.35	26.22
0.710	-157.262487	0.11485	-157.14764	29.33	26.19
0.720	-157.2625229	0.11485	-157.14768	29.31	26.16
0.730	-157.2625601	0.11484	-157.14772	29.28	26.14
0.740	-157.2625964	0.11483	-157.14777	29.26	26.11
0.750	-157.2626337	0.11482	-157.14781	29.24	26.08
0.760	-157.2626703	0.11481	-157.14786	29.21	26.05
0.770	-157.2627078	0.11481	-157.14790	29.19	26.02
0.780	-157.2627446	0.11480	-157.14795	29.17	26.00
0.790	-157.2627821	0.11479	-157.14799	29.14	25.97
0.800	-157.2628196	0.11478	-157.14804	29.12	25.94
0.810	-157.2628572	0.11478	-157.14808	29.10	25.91
0.820	-157.2628948	0.11477	-157.14813	29.07	25.88
0.830	-157.2629323	0.11476	-157.14817	29.05	25.85
0.840	-157.2629702	0.11475	-157.14822	29.03	25.82
0.850	-157.2630078	0.11475	-157.14826	29.00	25.80
0.860	-157.2630463	0.11474	-157.14831	28.98	25.77
0.870	-157.2630841	0.11473	-157.14835	28.95	25.74
0.880	-157.2631227	0.11472	-157.14840	28.93	25.71
0.890	-157.2631607	0.11471	-157.14845	28.91	25.68
0.900	-157.2631992	0.11471	-157.14849	28.88	25.65
0.910	-157.2632372	0.11470	-157.14854	28.86	25.62
0.920	-157.2632753	0.11469	-157.14858	28.83	25.59
0.930	-157.263314	0.11468	-157.14863	28.81	25.57
0.940	-157.2633524	0.11468	-157.14868	28.79	25.54
0.950	-157.263391	0.11467	-157.14872	28.76	25.51
0.960	-157.2634292	0.11466	-157.14877	28.74	25.48
0.970	-157.2634679	0.11465	-157.14882	28.71	25.45
0.980	-157.2635066	0.11464	-157.14886	28.69	25.42
0.990	-157.2635452	0.11464	-157.14891	28.67	25.39
1.000	-157.2635843	0.11463	-157.14896	28.64	25.36
1.010	-157.263623	0.11462	-157.14900	28.62	25.33
1.020	-157.2636617	0.11461	-157.14905	28.59	25.30
1.030	-157.2637004	0.11460	-157.14910	28.57	25.27
1.040	-157.2637389	0.11460	-157.14914	28.54	25.24
1.050	-157.2637776	0.11459	-157.14919	28.52	25.22
1.060	-157.2638162	0.11458	-157.14923	28.50	25.19
1.070	-157.2638558	0.11457	-157.14928	28.47	25.16
1.080	-157.2638941	0.11457	-157.14933	28.45	25.13
1.090	-157.2639331	0.11456	-157.14937	28.42	25.10
1.100	-157.2639713	0.11455	-157.14942	28.40	25.07
1.110	-157.2640104	0.11454	-157.14947	28.37	25.04

1.120	-157.2640495	0.11454	-157.14951	28.35	25.01
1.130	-157.2640879	0.11453	-157.14956	28.33	24.98
1.140	-157.2641265	0.11452	-157.14961	28.30	24.95
1.150	-157.2641656	0.11451	-157.14965	28.28	24.92
1.160	-157.2642043	0.11450	-157.14970	28.25	24.89
1.170	-157.2642423	0.11450	-157.14975	28.23	24.87
1.180	-157.264281	0.11449	-157.14979	28.20	24.84
1.190	-157.2643196	0.11448	-157.14984	28.18	24.81
1.200	-157.264358	0.11447	-157.14988	28.16	24.78
1.210	-157.2643966	0.11446	-157.14993	28.13	24.75
1.220	-157.2644351	0.11446	-157.14998	28.11	24.72
1.230	-157.264474	0.11445	-157.15002	28.08	24.69
1.240	-157.2645117	0.11444	-157.15007	28.06	24.66
1.250	-157.2645503	0.11443	-157.15012	28.03	24.63
1.260	-157.264589	0.11443	-157.15016	28.01	24.60
1.270	-157.2646269	0.11442	-157.15021	27.99	24.58
1.280	-157.2646651	0.11441	-157.15026	27.96	24.55
1.290	-157.2647034	0.11440	-157.15030	27.94	24.52
1.300	-157.2647415	0.11439	-157.15035	27.91	24.49
1.310	-157.2647794	0.11439	-157.15039	27.89	24.46
1.320	-157.2648174	0.11438	-157.15044	27.87	24.43
1.330	-157.2648555	0.11437	-157.15048	27.84	24.40
1.340	-157.2648929	0.11436	-157.15053	27.82	24.37
1.350	-157.2649308	0.11436	-157.15058	27.80	24.34
1.360	-157.2649687	0.11435	-157.15062	27.77	24.32
1.370	-157.2650057	0.11434	-157.15067	27.75	24.29
1.380	-157.2650437	0.11433	-157.15071	27.73	24.26
1.390	-157.2650819	0.11433	-157.15076	27.70	24.23
1.400	-157.2651192	0.11432	-157.15080	27.68	24.20
1.410	-157.2651562	0.11431	-157.15085	27.65	24.18
1.420	-157.2651937	0.11430	-157.15089	27.63	24.15
1.430	-157.2652307	0.11429	-157.15094	27.61	24.12
1.440	-157.265268	0.11429	-157.15098	27.58	24.09
1.450	-157.2653051	0.11428	-157.15103	27.56	24.06
1.460	-157.2653424	0.11427	-157.15107	27.54	24.03
1.470	-157.265379	0.11426	-157.15112	27.51	24.01
1.480	-157.2654158	0.11426	-157.15116	27.49	23.98
1.490	-157.2654526	0.11425	-157.15120	27.47	23.95
1.500	-157.2654892	0.11424	-157.15125	27.45	23.92
1.510	-157.2655258	0.11423	-157.15129	27.42	23.89
1.520	-157.2655623	0.11423	-157.15134	27.40	23.87
1.530	-157.2655988	0.11422	-157.15138	27.38	23.84
1.540	-157.265635	0.11421	-157.15143	27.35	23.81
1.550	-157.2656712	0.11420	-157.15147	27.33	23.78
1.560	-157.2657077	0.11419	-157.15151	27.31	23.76
1.570	-157.2657436	0.11419	-157.15156	27.29	23.73

1.580	-157.2657796	0.11418	-157.15160	27.26	23.70
1.590	-157.2658157	0.11417	-157.15164	27.24	23.67
1.600	-157.2658511	0.11416	-157.15169	27.22	23.65
1.610	-157.2658869	0.11416	-157.15173	27.20	23.62
1.620	-157.2659226	0.11415	-157.15177	27.17	23.59
1.630	-157.2659578	0.11414	-157.15182	27.15	23.57
1.640	-157.2659936	0.11414	-157.15186	27.13	23.54
1.650	-157.2660289	0.11413	-157.15190	27.11	23.51
1.660	-157.2660636	0.11412	-157.15194	27.09	23.49
1.670	-157.2660988	0.11411	-157.15199	27.06	23.46
1.680	-157.266134	0.11410	-157.15203	27.04	23.43
1.690	-157.266169	0.11410	-157.15207	27.02	23.41
1.700	-157.2662035	0.11409	-157.15211	27.00	23.38
1.710	-157.2662386	0.11408	-157.15215	26.98	23.35
1.720	-157.2662728	0.11408	-157.15220	26.95	23.33
1.730	-157.2663076	0.11407	-157.15224	26.93	23.30
1.740	-157.2663419	0.11406	-157.15228	26.91	23.28
1.750	-157.2663761	0.11405	-157.15232	26.89	23.25
1.760	-157.2664101	0.11405	-157.15236	26.87	23.22
1.770	-157.2664444	0.11404	-157.15240	26.85	23.20
1.780	-157.2664781	0.11403	-157.15244	26.83	23.17
1.790	-157.2665122	0.11403	-157.15249	26.80	23.15
1.800	-157.2665459	0.11402	-157.15253	26.78	23.12
1.810	-157.2665797	0.11401	-157.15257	26.76	23.10
1.820	-157.2666129	0.11401	-157.15261	26.74	23.07
1.830	-157.2666459	0.11400	-157.15265	26.72	23.04
1.840	-157.2666797	0.11399	-157.15269	26.70	23.02
1.850	-157.2667126	0.11398	-157.15273	26.68	22.99
1.860	-157.2667455	0.11398	-157.15277	26.66	22.97
1.870	-157.2667787	0.11397	-157.15281	26.64	22.94
1.880	-157.2668114	0.11396	-157.15285	26.62	22.92
1.890	-157.2668443	0.11396	-157.15289	26.60	22.89
1.900	-157.2668769	0.11395	-157.15293	26.57	22.87
1.910	-157.2669095	0.11394	-157.15297	26.55	22.84
1.920	-157.2669415	0.11394	-157.15301	26.53	22.82
1.930	-157.2669739	0.11393	-157.15304	26.51	22.80
1.940	-157.2670062	0.11392	-157.15308	26.49	22.77
1.950	-157.267038	0.11392	-157.15312	26.47	22.75

SI Table 37: Potential energy data along the MEP for reaction C•C(C)C → C• + C=CC. All data calculated with GAUSSIAN 03 program at the CCSD(T)/cc-pVDZ//BH&HLYP/cc-pVDZ level of theory.

Reaction C•C(C)C→ C• + C=CC					
$E_{C.C(C)C}$ = -157.683173 hartree		$ZPE_{CC.CC}$ = 0.119552 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)
-5.840	-157.63967	0.11289	-157.52679	27.296556	23.11
-5.810	-157.63964	0.11289	-157.52675	27.31626	23.14
-5.780	-157.63961	0.11290	-157.52671	27.336293	23.16
-5.750	-157.63958	0.11290	-157.52668	27.356625	23.18
-5.720	-157.63954	0.11290	-157.52664	27.377253	23.20
-5.690	-157.63951	0.11290	-157.52661	27.398214	23.23
-5.660	-157.63948	0.11289	-157.52659	27.419491	23.24
-5.630	-157.63944	0.11287	-157.52657	27.441024	23.25
-5.601	-157.63941	0.11285	-157.52656	27.462738	23.26
-5.571	-157.63937	0.11294	-157.52644	27.484824	23.33
-5.541	-157.63934	0.11294	-157.52640	27.507495	23.36
-5.511	-157.63930	0.11295	-157.52636	27.530554	23.38
-5.481	-157.63926	0.11295	-157.52632	27.553944	23.41
-5.451	-157.63923	0.11295	-157.52627	27.577667	23.44
-5.421	-157.63919	0.11295	-157.52624	27.601757	23.46
-5.391	-157.63915	0.11295	-157.52620	27.626189	23.48
-5.361	-157.63911	0.11299	-157.52612	27.650995	23.53
-5.331	-157.63907	0.11300	-157.52607	27.676253	23.56
-5.301	-157.63903	0.11300	-157.52603	27.701893	23.59
-5.271	-157.63899	0.11302	-157.52597	27.727942	23.63
-5.241	-157.63894	0.11302	-157.52592	27.754343	23.66
-5.211	-157.63890	0.11302	-157.52589	27.781157	23.68
-5.181	-157.63886	0.11304	-157.52582	27.808311	23.72
-5.151	-157.63881	0.11305	-157.52576	27.835872	23.76
-5.121	-157.63877	0.11306	-157.52571	27.863914	23.79
-5.091	-157.63872	0.11308	-157.52565	27.892372	23.83
-5.061	-157.63868	0.11309	-157.52559	27.921269	23.87
-5.031	-157.63863	0.11310	-157.52553	27.950588	23.90
-5.001	-157.63858	0.11311	-157.52548	27.980351	23.94
-4.971	-157.63854	0.11312	-157.52542	28.010601	23.97
-4.941	-157.63849	0.11313	-157.52536	28.041192	24.01

-4.911	-157.63844	0.11314	-157.52530	28.072277	24.05
-4.881	-157.63839	0.11315	-157.52524	28.103822	24.09
-4.851	-157.63834	0.11316	-157.52518	28.135755	24.12
-4.821	-157.63828	0.11316	-157.52513	28.168158	24.16
-4.791	-157.63823	0.11317	-157.52506	28.200988	24.20
-4.761	-157.63818	0.11319	-157.52499	28.234208	24.24
-4.731	-157.63813	0.11321	-157.52492	28.268032	24.29
-4.701	-157.63807	0.11321	-157.52486	28.302327	24.32
-4.671	-157.63802	0.11322	-157.52479	28.337032	24.37
-4.641	-157.63796	0.11324	-157.52472	28.372192	24.41
-4.611	-157.63790	0.11325	-157.52465	28.407891	24.45
-4.581	-157.63784	0.11326	-157.52459	28.444069	24.50
-4.551	-157.63779	0.11327	-157.52452	28.480661	24.54
-4.521	-157.63773	0.11326	-157.52446	28.517729	24.57
-4.491	-157.63767	0.11328	-157.52439	28.555164	24.62
-4.462	-157.63761	0.11329	-157.52431	28.593165	24.67
-4.432	-157.63755	0.11331	-157.52424	28.631631	24.71
-4.402	-157.63748	0.11332	-157.52416	28.670656	24.76
-4.372	-157.63742	0.11333	-157.52409	28.710152	24.81
-4.342	-157.63736	0.11334	-157.52401	28.75013	24.85
-4.312	-157.63729	0.11336	-157.52394	28.790651	24.90
-4.282	-157.63723	0.11337	-157.52386	28.831653	24.95
-4.252	-157.63716	0.11338	-157.52378	28.873125	25.00
-4.222	-157.63709	0.11339	-157.52371	28.91515	25.05
-4.192	-157.63703	0.11340	-157.52363	28.957642	25.10
-4.162	-157.63696	0.11341	-157.52355	29.000612	25.14
-4.132	-157.63689	0.11342	-157.52347	29.044125	25.20
-4.102	-157.63682	0.11343	-157.52339	29.088111	25.25
-4.072	-157.63675	0.11344	-157.52331	29.132638	25.30
-4.042	-157.63668	0.11345	-157.52323	29.177635	25.35
-4.012	-157.63660	0.11346	-157.52314	29.223171	25.40
-3.982	-157.63653	0.11347	-157.52306	29.269168	25.45
-3.952	-157.63646	0.11348	-157.52298	29.315626	25.50
-3.922	-157.63638	0.11349	-157.52289	29.362622	25.56
-3.892	-157.63631	0.11350	-157.52281	29.410155	25.61
-3.862	-157.63623	0.11351	-157.52272	29.458142	25.67
-3.832	-157.63615	0.11352	-157.52263	29.506665	25.72
-3.802	-157.63607	0.11353	-157.52255	29.555717	25.77
-3.772	-157.63599	0.11354	-157.52246	29.605214	25.83
-3.742	-157.63591	0.11355	-157.52237	29.655246	25.89
-3.712	-157.63583	0.11355	-157.52228	29.705801	25.94
-3.682	-157.63575	0.11357	-157.52219	29.756798	26.00
-3.652	-157.63567	0.11357	-157.52210	29.808321	26.05
-3.622	-157.63559	0.11359	-157.52200	29.860304	26.12
-3.592	-157.63550	0.11360	-157.52191	29.912972	26.18
-3.562	-157.63542	0.11361	-157.52181	29.965982	26.24

-3.532	-157.63533	0.11362	-157.52172	30.019603	26.29
-3.502	-157.63525	0.11363	-157.52162	30.073743	26.36
-3.472	-157.63516	0.11364	-157.52153	30.128407	26.42
-3.442	-157.63507	0.11365	-157.52143	30.183493	26.48
-3.412	-157.63498	0.11365	-157.52133	30.239097	26.54
-3.382	-157.63489	0.11366	-157.52123	30.295318	26.60
-3.352	-157.63480	0.11368	-157.52113	30.35191	26.66
-3.322	-157.63471	0.11369	-157.52103	30.409168	26.73
-3.292	-157.63462	0.11370	-157.52093	30.466844	26.79
-3.262	-157.63453	0.11371	-157.52082	30.52513	26.86
-3.232	-157.63443	0.11372	-157.52072	30.583831	26.92
-3.202	-157.63434	0.11373	-157.52061	30.643142	26.99
-3.172	-157.63424	0.11373	-157.52051	30.702973	27.05
-3.142	-157.63415	0.11375	-157.52040	30.763262	27.12
-3.112	-157.63405	0.11376	-157.52030	30.824111	27.19
-3.082	-157.63395	0.11377	-157.52019	30.885464	27.25
-3.052	-157.63386	0.11377	-157.52008	30.947331	27.32
-3.022	-157.63376	0.11379	-157.51997	31.009685	27.39
-2.992	-157.63366	0.11379	-157.51987	31.072668	27.46
-2.962	-157.63355	0.11381	-157.51975	31.136099	27.53
-2.932	-157.63345	0.11381	-157.51964	31.200079	27.60
-2.902	-157.63335	0.11383	-157.51952	31.264547	27.67
-2.872	-157.63325	0.11383	-157.51941	31.329515	27.74
-2.842	-157.63314	0.11385	-157.51930	31.395048	27.81
-2.812	-157.63304	0.11385	-157.51918	31.461113	27.89
-2.782	-157.63293	0.11387	-157.51907	31.527658	27.96
-2.752	-157.63282	0.11387	-157.51895	31.594689	28.03
-2.722	-157.63272	0.11389	-157.51883	31.662308	28.11
-2.692	-157.63261	0.11390	-157.51871	31.730378	28.18
-2.662	-157.63250	0.11391	-157.51859	31.798962	28.26
-2.632	-157.63239	0.11392	-157.51847	31.868125	28.33
-2.602	-157.63228	0.11393	-157.51835	31.937625	28.41
-2.572	-157.63217	0.11394	-157.51823	32.007688	28.49
-2.542	-157.63205	0.11395	-157.51810	32.078367	28.56
-2.512	-157.63194	0.11396	-157.51798	32.149362	28.64
-2.482	-157.63183	0.11397	-157.51785	32.220933	28.72
-2.452	-157.63171	0.11399	-157.51772	32.293047	28.80
-2.422	-157.63160	0.11400	-157.51760	32.365498	28.88
-2.392	-157.63148	0.11401	-157.51747	32.438511	28.96
-2.362	-157.63136	0.11402	-157.51734	32.511911	29.04
-2.332	-157.63124	0.11404	-157.51721	32.5859	29.13
-2.302	-157.63113	0.11405	-157.51708	32.66016	29.21
-2.272	-157.63101	0.11406	-157.51695	32.73497	29.29
-2.242	-157.63089	0.11408	-157.51681	32.810257	29.37
-2.212	-157.63077	0.11409	-157.51668	32.885853	29.46
-2.182	-157.63064	0.11410	-157.51654	32.961951	29.54

-2.152	-157.63052	0.11411	-157.51641	33.038527	29.63
-2.122	-157.63040	0.11413	-157.51627	33.115368	29.71
-2.092	-157.63028	0.11414	-157.51614	33.192547	29.80
-2.062	-157.63015	0.11415	-157.51600	33.270208	29.88
-2.032	-157.63003	0.11416	-157.51587	33.348153	29.96
-2.002	-157.62990	0.11416	-157.51574	33.426461	30.04
-1.972	-157.62978	0.11417	-157.51561	33.505203	30.13
-1.942	-157.62965	0.11419	-157.51546	33.584036	30.22
-1.912	-157.62953	0.11421	-157.51531	33.663345	30.31
-1.882	-157.62940	0.11423	-157.51517	33.742891	30.40
-1.852	-157.62927	0.11425	-157.51502	33.822624	30.50
-1.822	-157.62915	0.11427	-157.51487	33.902492	30.59
-1.792	-157.62902	0.11429	-157.51473	33.982708	30.68
-1.762	-157.62889	0.11431	-157.51458	34.063017	30.78
-1.732	-157.62876	0.11433	-157.51443	34.143409	30.87
-1.702	-157.62863	0.11435	-157.51428	34.224059	30.96
-1.672	-157.62851	0.11437	-157.51413	34.304603	31.05
-1.642	-157.62838	0.11439	-157.51399	34.385301	31.15
-1.612	-157.62825	0.11441	-157.51384	34.466049	31.24
-1.582	-157.62812	0.11443	-157.51369	34.546703	31.33
-1.552	-157.62799	0.11445	-157.51354	34.627168	31.42
-1.522	-157.62786	0.11447	-157.51340	34.707582	31.52
-1.492	-157.62774	0.11449	-157.51325	34.787942	31.61
-1.462	-157.62761	0.11450	-157.51310	34.867874	31.70
-1.432	-157.62748	0.11452	-157.51296	34.947646	31.79
-1.402	-157.62735	0.11454	-157.51281	35.027085	31.88
-1.372	-157.62723	0.11456	-157.51267	35.106164	31.97
-1.342	-157.62710	0.11457	-157.51253	35.184831	32.06
-1.312	-157.62698	0.11459	-157.51239	35.26288	32.15
-1.282	-157.62685	0.11461	-157.51225	35.340473	32.24
-1.252	-157.62673	0.11462	-157.51211	35.417399	32.32
-1.222	-157.62661	0.11464	-157.51198	35.493639	32.41
-1.192	-157.62649	0.11465	-157.51184	35.56904	32.49
-1.162	-157.62637	0.11467	-157.51171	35.64376	32.58
-1.132	-157.62625	0.11468	-157.51157	35.717436	32.66
-1.102	-157.62614	0.11469	-157.51144	35.790245	32.74
-1.072	-157.62602	0.11471	-157.51132	35.862015	32.82
-1.042	-157.62591	0.11472	-157.51119	35.932569	32.90
-1.012	-157.62580	0.11473	-157.51107	36.002128	32.98
-0.982	-157.62569	0.11474	-157.51095	36.070272	33.05
-0.952	-157.62558	0.11476	-157.51083	36.137322	33.13
-0.922	-157.62548	0.11477	-157.51071	36.203014	33.20
-0.892	-157.62538	0.11478	-157.51060	36.267302	33.27
-0.862	-157.62528	0.11479	-157.51049	36.330275	33.34
-0.832	-157.62518	0.11479	-157.51039	36.391844	33.41
-0.802	-157.62508	0.11481	-157.51028	36.45203	33.47

-0.772	-157.62499	0.11482	-157.51017	36.510932	33.54
-0.742	-157.62490	0.11483	-157.51007	36.568562	33.60
-0.712	-157.62481	0.11484	-157.50997	36.624993	33.67
-0.682	-157.62472	0.11484	-157.50988	36.680409	33.72
-0.652	-157.62463	0.11484	-157.50979	36.734872	33.78
-0.622	-157.62455	0.11486	-157.50969	36.788732	33.84
-0.592	-157.62446	0.11486	-157.50960	36.841992	33.90
-0.562	-157.62438	0.11486	-157.50952	36.895097	33.95
-0.532	-157.62429	0.11487	-157.50943	36.948207	34.01
-0.502	-157.62421	0.11486	-157.50935	37.001657	34.06
-0.472	-157.62412	0.11486	-157.50926	37.055808	34.11
-0.442	-157.62403	0.11485	-157.50919	37.110949	34.16
-0.412	-157.62394	0.11483	-157.50911	37.167408	34.21
-0.382	-157.62385	0.11481	-157.50904	37.22551	34.25
-0.352	-157.62375	0.11477	-157.50899	37.286002	34.28
-0.322	-157.62365	0.11471	-157.50894	37.349537	34.31
-0.292	-157.62355	0.11464	-157.50891	37.416974	34.33
-0.262	-157.62343	0.11453	-157.50890	37.489586	34.34
-0.232	-157.62330	0.11439	-157.50892	37.568995	34.33
-0.202	-157.62316	0.11420	-157.50896	37.65779	34.30
-0.173	-157.62300	0.11398	-157.50902	37.759229	34.26
-0.143	-157.62281	0.11373	-157.50908	37.877404	34.22
-0.113	-157.62259	0.11331	-157.50928	38.017768	34.10
-0.083	-157.62230	0.11200	-157.51031	38.195826	33.45
-0.053	-157.62188	0.11053	-157.51135	38.463288	32.80
-0.023	-157.62120	0.10959	-157.51162	38.886161	32.63
0.000	-157.62639	0.11543	-157.51096	35.632943	33.05
0.004	-157.62638	0.11554	-157.51085	35.636867	33.12
0.024	-157.62639	0.11555	-157.51084	35.629812	33.12
0.044	-157.62641	0.11549	-157.51092	35.62015	33.07
0.064	-157.62643	0.11556	-157.51087	35.607762	33.10
0.084	-157.62645	0.11560	-157.51086	35.592419	33.11
0.104	-157.62648	0.11563	-157.51086	35.574103	33.11
0.124	-157.62652	0.11564	-157.51088	35.552787	33.10
0.144	-157.62656	0.11566	-157.51090	35.528388	33.08
0.164	-157.62660	0.11567	-157.51093	35.500845	33.06
0.184	-157.62665	0.11568	-157.51096	35.470067	33.04
0.204	-157.62670	0.11570	-157.51100	35.436001	33.02
0.224	-157.62676	0.11571	-157.51105	35.398571	32.99
0.244	-157.62683	0.11573	-157.51110	35.357706	32.96
0.264	-157.62690	0.11574	-157.51116	35.313335	32.92
0.284	-157.62697	0.11575	-157.51122	35.265391	32.88
0.304	-157.62706	0.11577	-157.51129	35.213801	32.84
0.324	-157.62714	0.11578	-157.51136	35.1585	32.79
0.344	-157.62724	0.11579	-157.51145	35.099426	32.74
0.364	-157.62734	0.11581	-157.51153	35.03651	32.69

0.384	-157.62745	0.11582	-157.51163	34.969872	32.63
0.404	-157.62756	0.11583	-157.51173	34.899103	32.56
0.424	-157.62768	0.11585	-157.51183	34.824329	32.50
0.444	-157.62780	0.11586	-157.51195	34.745459	32.43
0.464	-157.62794	0.11587	-157.51207	34.662474	32.35
0.484	-157.62807	0.11588	-157.51219	34.5755	32.27
0.504	-157.62822	0.11590	-157.51232	34.484109	32.19
0.524	-157.62837	0.11591	-157.51246	34.388438	32.10
0.544	-157.62853	0.11592	-157.51261	34.288673	32.01
0.564	-157.62870	0.11593	-157.51277	34.184316	31.91
0.584	-157.62887	0.11594	-157.51293	34.075831	31.81
0.604	-157.62905	0.11596	-157.51310	33.962625	31.71
0.624	-157.62924	0.11597	-157.51327	33.845275	31.60
0.644	-157.62943	0.11598	-157.51345	33.723415	31.48
0.664	-157.62963	0.11599	-157.51364	33.596772	31.36
0.684	-157.62984	0.11600	-157.51384	33.465908	31.24
0.704	-157.63006	0.11601	-157.51405	33.330189	31.11
0.724	-157.63028	0.11602	-157.51426	33.190237	30.98
0.744	-157.63051	0.11603	-157.51448	33.045716	30.84
0.764	-157.63075	0.11604	-157.51471	32.896627	30.70
0.784	-157.63099	0.11606	-157.51494	32.743023	30.55
0.804	-157.63125	0.11607	-157.51518	32.584485	30.40
0.824	-157.63151	0.11608	-157.51543	32.42174	30.24
0.844	-157.63177	0.11609	-157.51569	32.254519	30.08
0.864	-157.63205	0.11610	-157.51595	32.082782	29.91
0.884	-157.63233	0.11611	-157.51622	31.90655	29.74
0.904	-157.63261	0.11612	-157.51650	31.72585	29.57
0.924	-157.63291	0.11613	-157.51678	31.540784	29.39
0.944	-157.63321	0.11614	-157.51708	31.35131	29.21
0.964	-157.63352	0.11614	-157.51738	31.157483	29.02
0.984	-157.63384	0.11615	-157.51768	30.959352	28.83
1.004	-157.63416	0.11616	-157.51800	30.757016	28.63
1.024	-157.63449	0.11617	-157.51832	30.550977	28.43
1.044	-157.63482	0.11618	-157.51864	30.340365	28.23
1.064	-157.63516	0.11619	-157.51897	30.125604	28.02
1.084	-157.63551	0.11620	-157.51931	29.906924	27.80
1.104	-157.63587	0.11621	-157.51966	29.684256	27.59
1.124	-157.63623	0.11622	-157.52001	29.458327	27.36
1.144	-157.63660	0.11622	-157.52037	29.228072	27.14
1.164	-157.63697	0.11623	-157.52074	28.994125	26.91
1.184	-157.63735	0.11624	-157.52110	28.757128	26.68
1.204	-157.63773	0.11625	-157.52148	28.516024	26.44
1.224	-157.63812	0.11626	-157.52186	28.272085	26.21
1.244	-157.63851	0.11627	-157.52225	28.024206	25.96
1.264	-157.63891	0.11627	-157.52264	27.773682	25.72
1.284	-157.63932	0.11628	-157.52304	27.519385	25.47

1.304	-157.63973	0.11629	-157.52344	27.262627	25.22
1.324	-157.64014	0.11630	-157.52384	27.002265	24.96
1.344	-157.64056	0.11631	-157.52426	26.739679	24.70
1.364	-157.64098	0.11631	-157.52467	26.47434	24.44
1.384	-157.64141	0.11632	-157.52509	26.20627	24.18
1.404	-157.64184	0.11633	-157.52551	25.935026	23.91
1.424	-157.64228	0.11634	-157.52594	25.661891	23.64
1.444	-157.64272	0.11634	-157.52637	25.386382	23.37
1.464	-157.64316	0.11635	-157.52681	25.108607	23.10
1.484	-157.64361	0.11636	-157.52725	24.829321	22.83
1.504	-157.64405	0.11637	-157.52769	24.54724	22.55
1.524	-157.64451	0.11638	-157.52813	24.263199	22.27
1.544	-157.64496	0.11638	-157.52858	23.977922	21.99
1.564	-157.64542	0.11639	-157.52903	23.690194	21.71
1.584	-157.64588	0.11640	-157.52948	23.401396	21.42
1.604	-157.64634	0.11641	-157.52994	23.11101	21.14
1.624	-157.64681	0.11641	-157.53040	22.818392	20.85
1.644	-157.64728	0.11642	-157.53086	22.525069	20.56
1.664	-157.64775	0.11643	-157.53132	22.231094	20.27
1.684	-157.64822	0.11644	-157.53178	21.935181	19.98
1.704	-157.64869	0.11644	-157.53225	21.638062	19.69
1.724	-157.64916	0.11645	-157.53271	21.340626	19.39
1.744	-157.64964	0.11646	-157.53318	21.041478	19.10
1.764	-157.65012	0.11647	-157.53365	20.742113	18.81
1.784	-157.65060	0.11647	-157.53412	20.441998	18.51
1.804	-157.65108	0.11648	-157.53459	20.14183	18.21
1.824	-157.65156	0.11649	-157.53507	19.840314	17.92
1.844	-157.65204	0.11650	-157.53554	19.538931	17.62
1.864	-157.65252	0.11650	-157.53601	19.236339	17.32
1.884	-157.65300	0.11651	-157.53649	18.934855	17.03
1.904	-157.65348	0.11652	-157.53696	18.632246	16.73
1.924	-157.65396	0.11653	-157.53744	18.329404	16.43
1.944	-157.65445	0.11653	-157.53791	18.027103	16.13
1.964	-157.65493	0.11654	-157.53838	17.724772	15.84
1.984	-157.65541	0.11655	-157.53886	17.422402	15.54
2.004	-157.65589	0.11656	-157.53933	17.120038	15.24
2.024	-157.65637	0.11657	-157.53981	16.818625	14.94
2.044	-157.65685	0.11657	-157.54028	16.517366	14.65
2.064	-157.65733	0.11658	-157.54075	16.216435	14.35
2.084	-157.65781	0.11659	-157.54122	15.91657	14.06
2.104	-157.65829	0.11660	-157.54169	15.617125	13.76
2.124	-157.65876	0.11660	-157.54216	15.318182	13.47
2.144	-157.65924	0.11661	-157.54263	15.019855	13.17
2.164	-157.65971	0.11662	-157.54309	14.722895	12.88
2.184	-157.66018	0.11663	-157.54356	14.42667	12.59
2.204	-157.66065	0.11663	-157.54402	14.131149	12.30

2.224	-157.66112	0.11664	-157.54448	13.837305	12.01
2.244	-157.66159	0.11665	-157.54494	13.544431	11.72
2.264	-157.66205	0.11666	-157.54540	13.25326	11.44
2.284	-157.66252	0.11667	-157.54585	12.963136	11.15
2.304	-157.66298	0.11667	-157.54630	12.674193	10.87
2.324	-157.66343	0.11668	-157.54675	12.387205	10.59
2.344	-157.66389	0.11669	-157.54720	12.101553	10.30
2.364	-157.66434	0.11670	-157.54764	11.81715	10.03
2.384	-157.66479	0.11671	-157.54808	11.535048	9.75
2.404	-157.66524	0.11672	-157.54852	11.254333	9.47
2.424	-157.66568	0.11672	-157.54896	10.97601	9.20
2.444	-157.66612	0.11673	-157.54939	10.700065	8.93
2.464	-157.66656	0.11674	-157.54982	10.425011	8.66
2.484	-157.66699	0.11675	-157.55024	10.153267	8.39
2.504	-157.66742	0.11676	-157.55067	9.8827524	8.13
2.524	-157.66785	0.11677	-157.55108	9.6155008	7.87
2.544	-157.66827	0.11678	-157.55150	9.3502734	7.61
2.564	-157.66869	0.11679	-157.55190	9.0870811	7.35
2.584	-157.66911	0.11680	-157.55231	8.8268462	7.10
2.604	-157.66952	0.11681	-157.55271	8.5695286	6.85
2.624	-157.66992	0.11682	-157.55311	8.3144402	6.60
2.644	-157.67032	0.11683	-157.55350	8.0624567	6.35
2.664	-157.67072	0.11684	-157.55388	7.813555	6.11
2.684	-157.67111	0.11685	-157.55426	7.5673313	5.87
2.704	-157.67150	0.11686	-157.55464	7.3242499	5.64
2.724	-157.67188	0.11687	-157.55501	7.0844781	5.40
2.744	-157.67226	0.11688	-157.55538	6.8475175	5.17
2.764	-157.67263	0.11690	-157.55574	6.6146492	4.95
2.784	-157.67300	0.11691	-157.55609	6.3846554	4.73
2.804	-157.67336	0.11692	-157.55644	6.1583655	4.51
2.824	-157.67371	0.11694	-157.55678	5.9356159	4.29
2.844	-157.67406	0.11695	-157.55712	5.7166034	4.08
2.864	-157.67441	0.11696	-157.55744	5.5015073	3.88
2.884	-157.67474	0.11698	-157.55777	5.2901618	3.67
2.904	-157.67507	0.11699	-157.55808	5.0832642	3.48
2.924	-157.67540	0.11701	-157.55839	4.879942	3.28
2.944	-157.67571	0.11702	-157.55869	4.681087	3.09
2.964	-157.67602	0.11704	-157.55899	4.4858284	2.91
2.984	-157.67633	0.11706	-157.55927	4.2957597	2.73
3.004	-157.67662	0.11707	-157.55955	4.109941	2.55
3.024	-157.67691	0.11709	-157.55982	3.928292	2.38
3.044	-157.67719	0.11711	-157.56008	3.7515754	2.22
3.064	-157.67747	0.11713	-157.56034	3.5790611	2.06
3.084	-157.67774	0.11715	-157.56059	3.4119726	1.90
3.104	-157.67800	0.11717	-157.56082	3.2493401	1.76
3.124	-157.67825	0.11719	-157.56105	3.0919336	1.61

3.144	-157.67849	0.11722	-157.56127	2.9395612	1.47
3.164	-157.67872	0.11724	-157.56148	2.7920113	1.34
3.184	-157.67895	0.11727	-157.56168	2.6498523	1.22
3.204	-157.67917	0.11729	-157.56188	2.5129351	1.10
3.224	-157.67938	0.11732	-157.56206	2.381359	0.98
3.244	-157.67958	0.11735	-157.56223	2.2548883	0.87
3.264	-157.67977	0.11738	-157.56239	2.1342306	0.77
3.284	-157.67996	0.11742	-157.56254	2.0186587	0.68
3.304	-157.68013	0.11745	-157.56268	1.9086822	0.59
3.324	-157.68030	0.11749	-157.56281	1.8039504	0.51
3.344	-157.68046	0.11753	-157.56292	1.7049062	0.44
3.364	-157.68061	0.11758	-157.56303	1.6112453	0.37
3.384	-157.68075	0.11763	-157.56312	1.5227999	0.31
3.404	-157.68088	0.11768	-157.56320	1.4398099	0.26
3.424	-157.68100	0.11773	-157.56327	1.3617433	0.22
3.444	-157.68112	0.11779	-157.56333	1.2888994	0.19
3.464	-157.68123	0.11786	-157.56337	1.2209627	0.16
3.484	-157.68133	0.11793	-157.56340	1.1576765	0.14
3.504	-157.68142	0.11801	-157.56342	1.0990264	0.13
3.524	-157.68151	0.11809	-157.56342	1.0448508	0.12
3.544	-157.68159	0.11817	-157.56342	0.994706	0.13
3.564	-157.68166	0.11825	-157.56341	0.9486246	0.13
3.584	-157.68173	0.11834	-157.56339	0.9064114	0.14
3.604	-157.68179	0.11842	-157.56337	0.8676654	0.16
3.624	-157.68185	0.11849	-157.56335	0.8322211	0.17
3.644	-157.68190	0.11856	-157.56334	0.7995198	0.18
3.664	-157.68195	0.11862	-157.56333	0.7692608	0.18
3.684	-157.68199	0.11867	-157.56332	0.7407757	0.19
3.704	-157.68204	0.11872	-157.56332	0.7135348	0.19
3.724	-157.68208	0.11875	-157.56333	0.6872124	0.19
3.744	-157.68212	0.11879	-157.56333	0.6614928	0.18
3.764	-157.68216	0.11881	-157.56335	0.6364815	0.17
3.784	-157.68220	0.11884	-157.56336	0.6122708	0.16
3.804	-157.68223	0.11886	-157.56338	0.5891655	0.15
3.824	-157.68227	0.11888	-157.56339	0.5673476	0.14
3.844	-157.68230	0.11890	-157.56340	0.5469329	0.14
3.864	-157.68233	0.11890	-157.56343	0.5279274	0.12
3.883	-157.68236	0.11893	-157.56343	0.5101632	0.12

SI Table 38: Calculated high pressure limits of CVT/SCT rate constants for reactions R1-R4. Units are s^{-1}.

T(K)	1000/T (1/K)	High pressure limit of the rate constants (s^{-1})			
		C•CC → C• + C=C	C•CCC → CC• + C=C	CC•CC→C• + C=CC	C•C(C)C→C• + C=CC
300	3.33	7.28E-10	9.16E-10	4.560E-09	2.43E-09
400	2.50	2.84E-04	3.57E-04	1.580E-03	9.56E-04
500	2.00	7.17E-01	8.89E-01	3.660E+00	2.22E+00
600	1.67	1.31E+02	1.73E+02	6.760E+02	4.13E+02
700	1.43	5.90E+03	7.19E+03	3.000E+04	1.81E+04
800	1.25	1.01E+05	1.26E+05	4.960E+05	3.13E+05
900	1.11	9.23E+05	1.18E+06	4.660E+06	2.80E+06
1000	1.00	5.33E+06	6.65E+06	2.740E+07	1.67E+07
1100	0.91	2.27E+07	2.90E+07	1.120E+08	6.95E+07
1200	0.83	7.80E+07	9.89E+07	3.860E+08	2.37E+08
1300	0.77	2.11E+08	2.70E+08	1.100E+09	6.73E+08
1400	0.71	5.17E+08	6.48E+08	2.620E+09	1.57E+09
1500	0.67	1.09E+09	1.39E+09	5.540E+09	3.42E+09
1600	0.63	2.15E+09	2.63E+09	1.060E+10	6.78E+09
1700	0.59	3.78E+09	4.79E+09	1.880E+10	1.18E+10
1800	0.56	6.44E+09	8.16E+09	3.210E+10	2.02E+10
1900	0.53	1.04E+10	1.32E+10	5.180E+10	3.27E+10
2000	0.50	1.52E+10	1.89E+10	7.480E+10	4.80E+10
2100	0.48	2.22E+10	2.79E+10	1.110E+11	7.13E+10
2200	0.45	3.15E+10	3.97E+10	1.580E+11	1.02E+11
2300	0.43	4.18E+10	5.49E+10	2.180E+11	1.42E+11
2400	0.42	5.55E+10	7.07E+10	2.770E+11	1.82E+11
2500	0.40	7.25E+10	9.28E+10	3.630E+11	2.41E+11
2600	0.38	9.27E+10	1.19E+11	4.680E+11	3.13E+11
2700	0.37	1.15E+11	1.51E+11	5.910E+11	3.98E+11
2800	0.36	1.39E+11	1.87E+11	7.130E+11	4.71E+11
2900	0.34	1.69E+11	2.29E+11	8.720E+11	5.80E+11
3000	0.33	2.03E+11	2.68E+11	1.010E+12	7.06E+11

SI Table 39: Calculated high pressure limits of CVT/SCT rate constants for reactions reverse to R1-R4 (R^{-1} - R^{-4}). Units are s^{-1}.

T(K)	1000/T (1/K)	High pressure limit of the rate constants (s^{-1})			
		C• + C=C → C•CC	CC• + C=C → C•CCC	C• + C=CC → CC•CC	C• + C=CC → C•C(C)C
300	3.33	7.70E-19	4.56E-19	4.79E-19	5.09E-20
400	2.50	1.95E-17	1.16E-17	1.22E-17	1.95E-18
500	2.00	1.57E-16	9.46E-17	9.93E-17	2.02E-17
600	1.67	6.93E-16	4.26E-16	4.47E-16	1.06E-16
700	1.43	2.15E-15	1.35E-15	1.41E-15	3.74E-16
800	1.25	5.31E-15	3.37E-15	3.54E-15	1.01E-15
900	1.11	1.12E-14	7.19E-15	7.55E-15	2.30E-15
1000	1.00	2.10E-14	1.37E-14	1.43E-14	4.59E-15
1100	0.91	3.62E-14	2.37E-14	2.49E-14	8.30E-15
1200	0.83	5.82E-14	3.85E-14	4.05E-14	1.39E-14
1300	0.77	8.88E-14	5.93E-14	6.22E-14	2.20E-14
1400	0.71	1.30E-13	8.72E-14	9.16E-14	3.31E-14
1500	0.67	1.83E-13	1.24E-13	1.30E-13	4.78E-14
1600	0.63	2.50E-13	1.70E-13	1.79E-13	6.69E-14
1700	0.59	3.32E-13	2.28E-13	2.39E-13	9.09E-14
1800	0.56	4.33E-13	2.99E-13	3.14E-13	1.21E-13
1900	0.53	5.54E-13	3.84E-13	4.03E-13	1.57E-13
2000	0.50	6.97E-13	4.86E-13	5.10E-13	2.00E-13
2100	0.48	8.64E-13	6.05E-13	6.35E-13	2.51E-13
2200	0.45	1.06E-12	7.43E-13	7.80E-13	3.11E-13
2300	0.43	1.28E-12	9.03E-13	9.48E-13	3.80E-13
2400	0.42	1.53E-12	1.09E-12	1.14E-12	4.60E-13
2500	0.40	1.81E-12	1.29E-12	1.36E-12	5.50E-13
2600	0.38	2.13E-12	1.53E-12	1.60E-12	6.52E-13
2700	0.37	2.49E-12	1.79E-12	1.88E-12	7.67E-13
2800	0.36	2.88E-12	2.08E-12	2.18E-12	8.95E-13
2900	0.34	3.32E-12	2.40E-12	2.52E-12	1.04E-12
3000	0.33	3.80E-12	2.76E-12	2.89E-12	1.20E-12

SI Table 40: Calculation of the RC-TST rate constants for the reaction R5: C•CCCCC → C•CCC + C=C.

R5		Delta V = 34.112 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	0.98	0.94	19.90	1.00	1.34E-08	-7.87
400	2.84E-04	1.00	0.99	0.93	9.42	0.99	2.43E-03	-2.61
500	7.17E-01	1.00	0.99	0.93	6.02	0.99	3.90E+00	0.59
600	1.31E+02	1.00	0.99	0.94	4.46	0.99	5.35E+02	2.73
700	5.90E+03	1.00	0.99	0.95	3.60	0.99	1.98E+04	4.30
800	1.01E+05	1.00	0.99	0.96	3.07	1.00	2.96E+05	5.47
900	9.23E+05	1.00	1.00	0.98	2.71	1.01	2.45E+06	6.39
1000	5.33E+06	1.00	1.00	0.99	2.45	1.02	1.31E+07	7.12
1100	2.27E+07	1.00	1.00	1.00	2.26	1.03	5.26E+07	7.72
1200	7.80E+07	1.00	1.00	1.00	2.11	1.01	1.67E+08	8.22
1300	2.11E+08	1.00	1.00	1.01	1.99	0.96	4.07E+08	8.61
1400	5.17E+08	1.00	1.00	1.01	1.90	0.95	9.43E+08	8.97
1500	1.09E+09	1.00	1.00	1.02	1.82	0.92	1.85E+09	9.27
1600	2.15E+09	1.00	1.00	1.02	1.75	0.94	3.60E+09	9.56
1700	3.78E+09	1.00	1.00	1.02	1.70	0.88	5.74E+09	9.76
1800	6.44E+09	1.00	1.00	1.02	1.65	0.87	9.38E+09	9.97
1900	1.04E+10	1.00	1.00	1.02	1.60	0.85	1.44E+10	10.16
2000	1.52E+10	1.00	1.00	1.02	1.57	0.86	2.08E+10	10.32
2100	2.22E+10	1.00	1.00	1.01	1.53	0.84	2.89E+10	10.46
2200	3.15E+10	1.00	1.00	1.01	1.50	0.82	3.92E+10	10.59
2300	4.18E+10	1.00	1.00	1.01	1.48	0.80	4.97E+10	10.70
2400	5.55E+10	1.00	1.00	1.01	1.45	0.78	6.31E+10	10.80
2500	7.25E+10	1.00	1.00	1.00	1.43	0.79	8.20E+10	10.91
2600	9.27E+10	1.00	1.00	1.00	1.41	0.77	1.00E+11	11.00
2700	1.15E+11	1.00	1.00	0.99	1.39	0.76	1.21E+11	11.08
2800	1.39E+11	1.00	1.00	0.99	1.38	0.77	1.45E+11	11.16
2900	1.69E+11	1.00	1.00	0.98	1.36	0.75	1.69E+11	11.23
3000	2.03E+11	1.00	1.00	0.98	1.35	0.74	1.98E+11	11.30

SI Table 41: Calculation of the RC-TST rate constants for the reaction R6: CC•CCCC → C•CC + C=CC.

R6		Delta V = 34.781 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	0.99	0.94	6.48	0.95	4.16E-09	-8.38
400	2.84E-04	1.00	1.00	0.99	4.06	1.14	1.29E-03	-2.89
500	7.17E-01	1.00	1.00	1.01	3.07	1.26	2.80E+00	0.45
600	1.31E+02	1.00	1.00	1.03	2.55	1.34	4.61E+02	2.66
700	5.90E+03	1.00	1.00	1.05	2.23	1.40	1.92E+04	4.28
800	1.01E+05	1.00	1.00	1.06	2.02	1.44	3.10E+05	5.49
900	9.23E+05	1.00	1.00	1.07	1.86	1.47	2.70E+06	6.43
1000	5.33E+06	1.00	1.00	1.08	1.75	1.49	1.50E+07	7.18
1100	2.27E+07	1.00	1.00	1.08	1.66	1.51	6.17E+07	7.79
1200	7.80E+07	1.00	1.00	1.09	1.60	1.52	2.06E+08	8.31
1300	2.11E+08	1.00	1.00	1.09	1.54	1.53	5.43E+08	8.73
1400	5.17E+08	1.00	1.00	1.10	1.49	1.54	1.30E+09	9.11
1500	1.09E+09	1.00	1.00	1.10	1.45	1.55	2.69E+09	9.43
1600	2.15E+09	1.00	1.00	1.10	1.42	1.56	5.22E+09	9.72
1700	3.78E+09	1.00	1.00	1.10	1.39	1.56	9.05E+09	9.96
1800	6.44E+09	1.00	1.00	1.10	1.37	1.57	1.52E+10	10.18
1900	1.04E+10	1.00	1.00	1.11	1.34	1.57	2.42E+10	10.38
2000	1.52E+10	1.00	1.00	1.11	1.32	1.57	3.50E+10	10.54
2100	2.22E+10	1.00	1.00	1.11	1.31	1.58	5.06E+10	10.70
2200	3.15E+10	1.00	1.00	1.11	1.29	1.58	7.11E+10	10.85
2300	4.18E+10	1.00	1.00	1.11	1.28	1.58	9.36E+10	10.97
2400	5.55E+10	1.00	1.00	1.11	1.26	1.58	1.23E+11	11.09
2500	7.25E+10	1.00	1.00	1.11	1.25	1.59	1.60E+11	11.20
2600	9.27E+10	1.00	1.00	1.11	1.24	1.59	2.03E+11	11.31
2700	1.15E+11	1.00	1.00	1.11	1.23	1.59	2.50E+11	11.40
2800	1.39E+11	1.00	1.00	1.11	1.22	1.59	3.00E+11	11.48
2900	1.69E+11	1.00	1.00	1.11	1.21	1.59	3.63E+11	11.56
3000	2.03E+11	1.00	1.00	1.11	1.21	1.59	4.33E+11	11.64

SI Table 42: Calculation of the RC-TST rate constants for the reaction R7: CCC•CCC → C•C + C=CCC.

R7		Delta V = 34.549 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	1.02	0.93	9.56	1.25	8.23E-09	-8.08
400	2.84E-04	1.00	1.01	1.08	5.44	1.23	2.08E-03	-2.68
500	7.17E-01	1.00	1.01	1.17	3.88	1.25	4.11E+00	0.61
600	1.31E+02	1.00	1.01	1.23	3.09	1.20	6.03E+02	2.78
700	5.90E+03	1.00	1.01	1.27	2.63	1.21	2.40E+04	4.38
800	1.01E+05	1.00	1.00	1.30	2.33	1.22	3.75E+05	5.57
900	9.23E+05	1.00	1.00	1.32	2.12	1.20	3.11E+06	6.49
1000	5.33E+06	1.00	1.00	1.33	1.97	1.15	1.62E+07	7.21
1100	2.27E+07	1.00	1.00	1.35	1.85	1.18	6.70E+07	7.83
1200	7.80E+07	1.00	1.00	1.35	1.76	1.13	2.11E+08	8.32
1300	2.11E+08	1.00	1.00	1.36	1.68	1.12	5.43E+08	8.74
1400	5.17E+08	1.00	1.00	1.37	1.62	1.10	1.26E+09	9.10
1500	1.09E+09	1.00	1.00	1.37	1.57	1.11	2.60E+09	9.42
1600	2.15E+09	1.00	1.00	1.38	1.53	1.11	5.04E+09	9.70
1700	3.78E+09	1.00	1.00	1.38	1.49	1.12	8.74E+09	9.94
1800	6.44E+09	1.00	1.00	1.38	1.46	1.13	1.47E+10	10.17
1900	1.04E+10	1.00	1.00	1.38	1.43	1.14	2.34E+10	10.37
2000	1.52E+10	1.00	1.00	1.39	1.40	1.14	3.38E+10	10.53
2100	2.22E+10	1.00	1.00	1.39	1.38	1.15	4.91E+10	10.69
2200	3.15E+10	1.00	1.00	1.39	1.36	1.16	6.89E+10	10.84
2300	4.18E+10	1.00	1.00	1.39	1.34	1.16	9.10E+10	10.96
2400	5.55E+10	1.00	1.00	1.39	1.33	1.17	1.20E+11	11.08
2500	7.25E+10	1.00	1.00	1.39	1.31	1.18	1.56E+11	11.19
2600	9.27E+10	1.00	1.00	1.39	1.30	1.18	1.98E+11	11.30
2700	1.15E+11	1.00	1.00	1.39	1.29	1.19	2.44E+11	11.39
2800	1.39E+11	1.00	1.00	1.40	1.27	1.18	2.92E+11	11.46
2900	1.69E+11	1.00	1.00	1.40	1.26	1.17	3.49E+11	11.54
3000	2.03E+11	1.00	1.00	1.40	1.25	1.14	4.05E+11	11.61

SI Table 43: Calculation of the RC-TST rate constants for the reaction R8: C•CCCCCCC → C•CCCCC + C=C.

R8		Delta V = 34.114 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	0.98	0.73	3.71	1.02	1.96E-09	-8.71
400	2.84E-04	1.00	0.99	0.87	2.67	1.01	6.58E-04	-3.18
500	7.17E-01	1.00	0.99	0.95	2.19	1.00	1.48E+00	0.17
600	1.31E+02	1.00	0.99	1.00	1.93	1.00	2.50E+02	2.40
700	5.90E+03	1.00	0.99	1.03	1.75	1.01	1.06E+04	4.03
800	1.01E+05	1.00	0.99	1.04	1.63	1.02	1.74E+05	5.24
900	9.23E+05	1.00	0.99	1.06	1.55	1.03	1.54E+06	6.19
1000	5.33E+06	1.00	1.00	1.07	1.48	1.04	8.71E+06	6.94
1100	2.27E+07	1.00	1.00	1.07	1.43	1.05	3.64E+07	7.56
1200	7.80E+07	1.00	1.00	1.08	1.39	1.06	1.23E+08	8.09
1300	2.11E+08	1.00	1.00	1.08	1.35	1.07	3.31E+08	8.52
1400	5.17E+08	1.00	1.00	1.08	1.32	1.09	8.03E+08	8.90
1500	1.09E+09	1.00	1.00	1.09	1.30	1.10	1.68E+09	9.23
1600	2.15E+09	1.00	1.00	1.09	1.28	1.11	3.31E+09	9.52
1700	3.78E+09	1.00	1.00	1.09	1.26	1.12	5.78E+09	9.76
1800	6.44E+09	1.00	1.00	1.09	1.24	1.13	9.81E+09	9.99
1900	1.04E+10	1.00	1.00	1.09	1.23	1.14	1.58E+10	10.20
2000	1.52E+10	1.00	1.00	1.09	1.22	1.15	2.31E+10	10.36
2100	2.22E+10	1.00	1.00	1.09	1.21	1.15	3.37E+10	10.53
2200	3.15E+10	1.00	1.00	1.09	1.20	1.16	4.77E+10	10.68
2300	4.18E+10	1.00	1.00	1.09	1.19	1.17	6.32E+10	10.80
2400	5.55E+10	1.00	1.00	1.09	1.18	1.18	8.39E+10	10.92
2500	7.25E+10	1.00	1.00	1.09	1.17	1.18	1.09E+11	11.04
2600	9.27E+10	1.00	1.00	1.09	1.16	1.19	1.40E+11	11.15
2700	1.15E+11	1.00	1.00	1.09	1.16	1.19	1.73E+11	11.24
2800	1.39E+11	1.00	1.00	1.09	1.15	1.20	2.10E+11	11.32
2900	1.69E+11	1.00	1.00	1.09	1.15	1.20	2.55E+11	11.41
3000	2.03E+11	1.00	1.00	1.09	1.14	1.21	3.06E+11	11.49

SI Table 44: Calculation of the RC-TST rate constants for the reaction R9: CC•CCCCCC → C•CCCC + C=CC.

R9		Delta V = 36.536 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	1.02	1.16	4.22	1.22	4.46E-09	-8.35
400	2.84E-04	1.00	1.01	1.39	2.95	1.20	1.42E-03	-2.85
500	7.17E-01	1.00	1.01	1.53	2.37	1.24	3.26E+00	0.51
600	1.31E+02	1.00	1.01	1.62	2.06	1.27	5.60E+02	2.75
700	5.90E+03	1.00	1.01	1.69	1.85	1.29	2.40E+04	4.38
800	1.01E+05	1.00	1.01	1.74	1.72	1.30	3.96E+05	5.60
900	9.23E+05	1.00	1.01	1.78	1.62	1.32	3.51E+06	6.54
1000	5.33E+06	1.00	1.00	1.80	1.54	1.32	1.96E+07	7.29
1100	2.27E+07	1.00	1.00	1.82	1.48	1.32	8.15E+07	7.91
1200	7.80E+07	1.00	1.00	1.84	1.43	1.32	2.73E+08	8.44
1300	2.11E+08	1.00	1.00	1.86	1.39	1.32	7.22E+08	8.86
1400	5.17E+08	1.00	1.00	1.87	1.36	1.31	1.73E+09	9.24
1500	1.09E+09	1.00	1.00	1.88	1.33	1.31	3.58E+09	9.55
1600	2.15E+09	1.00	1.00	1.88	1.31	1.30	6.91E+09	9.84
1700	3.78E+09	1.00	1.00	1.89	1.29	1.29	1.19E+10	10.08
1800	6.44E+09	1.00	1.00	1.90	1.27	1.28	2.00E+10	10.30
1900	1.04E+10	1.00	1.00	1.90	1.26	1.27	3.16E+10	10.50
2000	1.52E+10	1.00	1.00	1.90	1.24	1.26	4.55E+10	10.66
2100	2.22E+10	1.00	1.00	1.91	1.23	1.26	6.55E+10	10.82
2200	3.15E+10	1.00	1.00	1.91	1.22	1.24	9.13E+10	10.96
2300	4.18E+10	1.00	1.00	1.91	1.21	1.23	1.19E+11	11.08
2400	5.55E+10	1.00	1.00	1.92	1.20	1.23	1.56E+11	11.19
2500	7.25E+10	1.00	1.00	1.92	1.19	1.21	2.01E+11	11.30
2600	9.27E+10	1.00	1.00	1.92	1.18	1.20	2.54E+11	11.40
2700	1.15E+11	1.00	1.00	1.92	1.17	1.19	3.10E+11	11.49
2800	1.39E+11	1.00	1.00	1.92	1.17	1.18	3.70E+11	11.57
2900	1.69E+11	1.00	1.00	1.92	1.16	1.17	4.43E+11	11.65
3000	2.03E+11	1.00	1.00	1.93	1.15	1.16	5.26E+11	11.72

SI Table 45: Calculation of the RC-TST rate constants for the reaction R10: CC•CCCCCC → C•CCCC + C=CC.

R10		Delta V = 36.510 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	1.01	1.28	0.36	1.25	4.20E-10	-9.38
400	2.84E-04	1.00	1.01	1.31	0.46	1.22	2.11E-04	-3.68
500	7.17E-01	1.00	1.01	1.34	0.54	1.24	6.42E-01	-0.19
600	1.31E+02	1.00	1.00	1.36	0.60	1.26	1.35E+02	2.13
700	5.90E+03	1.00	1.00	1.39	0.64	1.29	6.79E+03	3.83
800	1.01E+05	1.00	1.00	1.41	0.68	1.30	1.26E+05	5.10
900	9.23E+05	1.00	1.00	1.42	0.71	1.36	1.27E+06	6.10
1000	5.33E+06	1.00	1.00	1.43	0.73	1.40	7.87E+06	6.90
1100	2.27E+07	1.00	1.00	1.45	0.75	1.41	3.50E+07	7.54
1200	7.80E+07	1.00	1.00	1.46	0.77	1.42	1.25E+08	8.10
1300	2.11E+08	1.00	1.00	1.46	0.79	1.43	3.49E+08	8.54
1400	5.17E+08	1.00	1.00	1.47	0.80	1.43	8.73E+08	8.94
1500	1.09E+09	1.00	1.00	1.48	0.81	1.44	1.89E+09	9.28
1600	2.15E+09	1.00	1.00	1.48	0.82	1.43	3.75E+09	9.57
1700	3.78E+09	1.00	1.00	1.48	0.83	1.40	6.56E+09	9.82
1800	6.44E+09	1.00	1.00	1.49	0.84	1.35	1.09E+10	10.04
1900	1.04E+10	1.00	1.00	1.49	0.85	1.33	1.75E+10	10.24
2000	1.52E+10	1.00	1.00	1.49	0.86	1.34	2.61E+10	10.42
2100	2.22E+10	1.00	1.00	1.50	0.86	1.32	3.79E+10	10.58
2200	3.15E+10	1.00	1.00	1.50	0.87	1.33	5.46E+10	10.74
2300	4.18E+10	1.00	1.00	1.50	0.87	1.28	7.03E+10	10.85
2400	5.55E+10	1.00	1.00	1.50	0.88	1.27	9.32E+10	10.97
2500	7.25E+10	1.00	1.00	1.50	0.88	1.25	1.21E+11	11.08
2600	9.27E+10	1.00	1.00	1.51	0.89	1.24	1.54E+11	11.19
2700	1.15E+11	1.00	1.00	1.51	0.89	1.23	1.90E+11	11.28
2800	1.39E+11	1.00	1.00	1.51	0.90	1.20	2.25E+11	11.35
2900	1.69E+11	1.00	1.00	1.51	0.90	1.19	2.73E+11	11.44
3000	2.03E+11	1.00	1.00	1.51	0.90	1.17	3.24E+11	11.51

SI Table 46: Calculation of the RC-TST rate constants for the reaction R11: CCCC•CCCC → C•CC + C=CCCC.

R11		Delta V = 34.557 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	0.99	0.97	9.43	1.16	7.65E-09	-8.12
400	2.84E-04	1.00	0.99	1.15	5.38	1.17	2.04E-03	-2.69
500	7.17E-01	1.00	1.00	1.26	3.84	1.18	4.07E+00	0.61
600	1.31E+02	1.00	1.00	1.34	3.07	1.18	6.33E+02	2.80
700	5.90E+03	1.00	1.00	1.39	2.62	1.19	2.54E+04	4.41
800	1.01E+05	1.00	1.00	1.42	2.32	1.19	3.98E+05	5.60
900	9.23E+05	1.00	1.00	1.45	2.11	1.20	3.39E+06	6.53
1000	5.33E+06	1.00	1.00	1.47	1.96	1.23	1.89E+07	7.28
1100	2.27E+07	1.00	1.00	1.49	1.84	1.24	7.69E+07	7.89
1200	7.80E+07	1.00	1.00	1.50	1.75	1.27	2.61E+08	8.42
1300	2.11E+08	1.00	1.00	1.51	1.68	1.32	7.08E+08	8.85
1400	5.17E+08	1.00	1.00	1.52	1.62	1.32	1.68E+09	9.23
1500	1.09E+09	1.00	1.00	1.53	1.57	1.32	3.43E+09	9.54
1600	2.15E+09	1.00	1.00	1.53	1.52	1.31	6.59E+09	9.82
1700	3.78E+09	1.00	1.00	1.54	1.49	1.31	1.13E+10	10.05
1800	6.44E+09	1.00	1.00	1.54	1.45	1.30	1.88E+10	10.27
1900	1.04E+10	1.00	1.00	1.55	1.43	1.29	2.96E+10	10.47
2000	1.52E+10	1.00	1.00	1.55	1.40	1.28	4.23E+10	10.63
2100	2.22E+10	1.00	1.00	1.55	1.38	1.27	6.04E+10	10.78
2200	3.15E+10	1.00	1.00	1.55	1.36	1.26	8.39E+10	10.92
2300	4.18E+10	1.00	1.00	1.56	1.34	1.26	1.09E+11	11.04
2400	5.55E+10	1.00	1.00	1.56	1.32	1.24	1.42E+11	11.15
2500	7.25E+10	1.00	1.00	1.56	1.31	1.23	1.83E+11	11.26
2600	9.27E+10	1.00	1.00	1.56	1.30	1.22	2.29E+11	11.36
2700	1.15E+11	1.00	1.00	1.56	1.28	1.23	2.83E+11	11.45
2800	1.39E+11	1.00	1.00	1.56	1.27	1.11	3.06E+11	11.49
2900	1.69E+11	1.00	1.00	1.56	1.26	1.13	3.76E+11	11.58
3000	2.03E+11	1.00	1.00	1.57	1.25	1.03	4.09E+11	11.61

SI Table 47: Calculation of the RC-TST rate constants for the reaction R12: CCCC•CCCC → C•CC + C=CCCC.

R12		Delta V = 34.508 kcal/mol						
T	$k_r(T)$	FACTORS					Rate Constants	log k(T)
		Symmetry	Tunnelling	Partition	Energy	HR		
300	7.28E-10	1.00	0.98	0.94	10.24	0.77	5.28E-09	-8.28
400	2.84E-04	1.00	0.99	1.10	5.73	0.79	1.40E-03	-2.85
500	7.17E-01	1.00	0.99	1.20	4.04	0.80	2.75E+00	0.44
600	1.31E+02	1.00	0.99	1.27	3.20	0.81	4.26E+02	2.63
700	5.90E+03	1.00	0.99	1.31	2.71	0.82	1.70E+04	4.23
800	1.01E+05	1.00	0.99	1.34	2.39	0.84	2.70E+05	5.43
900	9.23E+05	1.00	0.99	1.36	2.17	0.86	2.33E+06	6.37
1000	5.33E+06	1.00	1.00	1.38	2.01	0.85	1.25E+07	7.10
1100	2.27E+07	1.00	1.00	1.39	1.89	0.86	5.10E+07	7.71
1200	7.80E+07	1.00	1.00	1.40	1.79	0.87	1.69E+08	8.23
1300	2.11E+08	1.00	1.00	1.41	1.71	0.88	4.46E+08	8.65
1400	5.17E+08	1.00	1.00	1.41	1.65	0.88	1.06E+09	9.02
1500	1.09E+09	1.00	1.00	1.42	1.59	0.80	1.96E+09	9.29
1600	2.15E+09	1.00	1.00	1.42	1.55	0.85	4.01E+09	9.60
1700	3.78E+09	1.00	1.00	1.43	1.51	0.81	6.55E+09	9.82
1800	6.44E+09	1.00	1.00	1.43	1.47	0.81	1.09E+10	10.04
1900	1.04E+10	1.00	1.00	1.43	1.44	0.83	1.78E+10	10.25
2000	1.52E+10	1.00	1.00	1.43	1.42	0.83	2.55E+10	10.41
2100	2.22E+10	1.00	1.00	1.44	1.39	0.83	3.66E+10	10.56
2200	3.15E+10	1.00	1.00	1.44	1.37	0.88	5.46E+10	10.74
2300	4.18E+10	1.00	1.00	1.44	1.35	0.89	7.23E+10	10.86
2400	5.55E+10	1.00	1.00	1.44	1.34	0.92	9.81E+10	10.99
2500	7.25E+10	1.00	1.00	1.44	1.32	0.90	1.24E+11	11.09
2600	9.27E+10	1.00	1.00	1.44	1.31	0.94	1.64E+11	11.21
2700	1.15E+11	1.00	1.00	1.44	1.29	1.00	2.14E+11	11.33
2800	1.39E+11	1.00	1.00	1.44	1.28	1.04	2.67E+11	11.43
2900	1.69E+11	1.00	1.00	1.44	1.27	1.20	3.72E+11	11.57
3000	2.03E+11	1.00	1.00	1.44	1.26	1.22	4.51E+11	11.65