

Supplementary Information for

On the Tunneling Instability of a Hypercoordinated Carbocation

Sebastian Kozuch

Chemistry Department, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel

Complete tables of rate constants with (SCT) and without (CVT) tunneling correction, and the tunneling corrected KIEs:

TS1				¹³ C Central				¹³ C Equatorial			
Default				T(K)	CVT	SCT	KIE	T(K)	CVT	SCT	KIE
T(K)				6	3.69E-73	9.89E+04	1.20	6	2.20E-73	1.17E+05	1.02
6				8	3.83E-52	9.89E+04	1.20	8	2.59E-52	1.17E+05	1.02
8				10	1.64E-39	9.89E+04	1.20	10	1.20E-39	1.17E+05	1.02
10				20	3.83E-14	9.90E+04	1.20	20	3.28E-14	1.18E+05	1.01
20				30	1.31E-05	1.02E+05	1.21	30	1.18E-05	1.21E+05	1.02
30				40	2.69E-01	1.20E+05	1.20	40	2.49E-01	1.42E+05	1.01
40				50	1.12E+02	1.88E+05	1.16	50	1.05E+02	2.16E+05	1.01
50				75	4.15E+05	3.55E+06	1.03	75	3.98E+05	3.64E+06	1.00
75				100	2.93E+07	8.76E+07	0.99	100	2.84E+07	8.66E+07	1.00
100				125	4.09E+08	8.41E+08	0.98	125	3.99E+08	8.27E+08	1.00
125				150	2.50E+09	4.23E+09	0.98	150	2.45E+09	4.16E+09	1.00
150				175	9.42E+09	1.41E+10	0.99	175	9.28E+09	1.39E+10	1.00
175				200	2.61E+10	3.60E+10	0.99	200	2.58E+10	3.55E+10	1.00
200				225	5.85E+10	7.61E+10	0.99	225	5.80E+10	7.52E+10	1.00
225				250	1.13E+11	1.40E+11	0.99	250	1.12E+11	1.39E+11	1.00
250				275	1.96E+11	2.34E+11	0.99	275	1.95E+11	2.32E+11	1.00
275				300	3.11E+11	3.60E+11	0.99	300	3.11E+11	3.58E+11	1.00
300				325	4.64E+11	5.22E+11	0.99	325	4.64E+11	5.19E+11	1.00
325				350	6.57E+11	7.20E+11	1.00	350	6.57E+11	7.18E+11	1.00
350				375	8.91E+11	9.55E+11	1.00	375	8.93E+11	9.54E+11	1.00
375				400	1.17E+12	1.23E+12	0.99	400	1.17E+12	1.23E+12	0.99
400				¹³ C Lower Axial				¹³ C all			
¹³ C Upper Axial				T(K)	CVT	SCT	KIE	T(K)	CVT	SCT	KIE
T(K)				6	5.56E-73	1.26E+05	0.94	6	1.69E-73	5.85E+04	2.03
6				8	5.20E-52	1.26E+05	0.94	8	2.13E-52	5.85E+04	2.03
8				10	2.09E-39	1.26E+05	0.94	10	1.02E-39	5.85E+04	2.03
10				20	4.33E-14	1.26E+05	0.94	20	3.03E-14	5.86E+04	2.03
20				30	1.42E-05	1.30E+05	0.95	30	1.12E-05	6.07E+04	2.03
30				40	2.86E-01	1.52E+05	0.95	40	2.40E-01	7.28E+04	1.98
40				50	1.17E+02	2.32E+05	0.94	50	1.02E+02	1.20E+05	1.82
50				75	4.29E+05	3.89E+06	0.94	75	3.92E+05	2.95E+06	1.24
75				100	3.00E+07	9.19E+07	0.94	100	2.81E+07	7.95E+07	1.09
100				125	4.17E+08	8.71E+08	0.95	125	3.96E+08	7.85E+08	1.05
125				150	2.54E+09	4.35E+09	0.95	150	2.43E+09	4.00E+09	1.04
150				175	9.55E+09	1.45E+10	0.96	175	9.20E+09	1.35E+10	1.03
175				200	2.64E+10	3.68E+10	0.96	200	2.55E+10	3.45E+10	1.03
200				225	5.92E+10	7.76E+10	0.97	225	5.73E+10	7.31E+10	1.03
225				250	1.14E+11	1.43E+11	0.97	250	1.11E+11	1.35E+11	1.03
250				275	1.98E+11	2.38E+11	0.97	275	1.92E+11	2.25E+11	1.03
275				300	3.15E+11	3.66E+11	0.98	300	3.05E+11	3.48E+11	1.03
300				325	4.69E+11	5.30E+11	0.98	325	4.55E+11	5.05E+11	1.03
325				350	6.64E+11	7.32E+11	0.98	350	6.44E+11	6.97E+11	1.03
350				375	9.01E+11	9.70E+11	0.98	375	8.74E+11	9.25E+11	1.03
375				400	1.18E+12	1.25E+12	0.98	400	1.14E+12	1.19E+12	1.03
400											
6											
8											
10											
20											
30											
40											
50											
75											
100											
125											
150											
175											
200											
225											
250											
275											
300											
325											
350											
375											
400											

Deuterium (all hydrogens)

T(K)	CVT	SCT	KIE
6	4.90E-98	1.94E+02	613.4
8	8.40E-71	1.94E+02	613.4
10	1.94E-54	1.94E+02	613.4
20	1.32E-21	1.96E+02	607.1
30	1.42E-10	2.19E+02	561.6
40	5.24E-05	3.06E+02	470.6
50	1.25E-01	6.07E+02	359.1
75	4.81E+03	3.95E+04	92.41
100	1.10E+06	2.85E+06	30.35
125	3.13E+07	5.43E+07	15.19
150	3.09E+08	4.40E+08	9.43
175	1.65E+09	2.09E+09	6.65
200	5.94E+09	6.99E+09	5.08
225	1.64E+10	1.83E+10	4.10
250	3.73E+10	4.00E+10	3.48
275	7.39E+10	7.67E+10	3.01
300	1.31E+11	1.33E+11	2.68
325	2.15E+11	2.12E+11	2.45
350	3.29E+11	3.18E+11	2.25
375	4.76E+11	4.52E+11	2.11
400	6.60E+11	6.16E+11	1.98

D (in Lower Axial Carbon)

T(K)	CVT	SCT	KIE
6	2.28E-75	7.40E+04	1.61
8	8.43E-54	7.40E+04	1.61
10	7.73E-41	7.40E+04	1.61
20	8.33E-15	7.40E+04	1.61
30	4.75E-06	7.64E+04	1.61
40	1.26E-01	8.99E+04	1.60
50	6.08E+01	1.38E+05	1.58
75	2.77E+05	2.50E+06	1.46
100	2.17E+07	6.29E+07	1.38
125	3.24E+08	6.26E+08	1.32
150	2.07E+09	3.26E+09	1.27
175	8.06E+09	1.12E+10	1.24
200	2.29E+10	2.94E+10	1.21
225	5.24E+10	6.35E+10	1.18
250	1.03E+11	1.19E+11	1.17
275	1.81E+11	2.02E+11	1.14
300	2.91E+11	3.16E+11	1.13
325	4.37E+11	4.63E+11	1.12
350	6.24E+11	6.47E+11	1.11
375	8.52E+11	8.66E+11	1.10
400	1.12E+12	1.12E+12	1.09

D (Lower H in Equatorial Carbon)

T(K)	CVT	SCT	KIE
6	5.33E-75	7.88E+04	1.51
8	1.59E-53	7.88E+04	1.51
10	1.29E-40	7.88E+04	1.51
20	1.07E-14	7.89E+04	1.51
30	5.63E-06	8.19E+04	1.50
40	1.43E-01	9.78E+04	1.47
50	6.77E+01	1.53E+05	1.42
75	2.99E+05	2.61E+06	1.40
100	2.30E+07	5.96E+07	1.45
125	3.38E+08	5.70E+08	1.45
150	2.14E+09	2.93E+09	1.42
175	8.29E+09	1.01E+10	1.38
200	2.34E+10	2.65E+10	1.34
225	5.34E+10	5.76E+10	1.30
250	1.05E+11	1.09E+11	1.28
275	1.83E+11	1.86E+11	1.24
300	2.94E+11	2.92E+11	1.22
325	4.42E+11	4.31E+11	1.20
350	6.31E+11	6.04E+11	1.19
375	8.62E+11	8.14E+11	1.17
400	1.14E+12	1.06E+12	1.15

D (in Upper Axial Carbon)

T(K)	CVT	SCT	KIE
6	3.30E-77	5.46E+04	2.18
8	3.52E-55	5.46E+04	2.18
10	6.09E-42	5.46E+04	2.18
20	2.34E-15	5.47E+04	2.18
30	2.04E-06	5.64E+04	2.18
40	6.67E-02	6.61E+04	2.18
50	3.67E+01	1.01E+05	2.16
75	1.99E+05	1.82E+06	2.01
100	1.70E+07	4.73E+07	1.83
125	2.66E+08	4.87E+08	1.69
150	1.76E+09	2.62E+09	1.58
175	7.05E+09	9.25E+09	1.50
200	2.04E+10	2.48E+10	1.43
225	4.76E+10	5.46E+10	1.38
250	9.47E+10	1.04E+11	1.34
275	1.68E+11	1.79E+11	1.29
300	2.73E+11	2.84E+11	1.26
325	4.15E+11	4.21E+11	1.23
350	5.96E+11	5.93E+11	1.21
375	8.19E+11	8.00E+11	1.19
400	1.09E+12	1.04E+12	1.17

D (Equatorial H in Equatorial Carbon)

T(K)	CVT	SCT	KIE
6	1.08E-73	1.05E+05	1.13
8	1.52E-52	1.05E+05	1.13
10	7.84E-40	1.05E+05	1.13
20	2.65E-14	1.06E+05	1.12
30	1.03E-05	1.10E+05	1.12
40	2.25E-01	1.31E+05	1.10
50	9.74E+01	2.05E+05	1.06
75	3.82E+05	3.33E+06	1.10
100	2.77E+07	7.22E+07	1.20
125	3.92E+08	6.66E+08	1.24
150	2.42E+09	3.34E+09	1.24
175	9.20E+09	1.13E+10	1.23
200	2.56E+10	2.92E+10	1.22
225	5.77E+10	6.27E+10	1.20
250	1.12E+11	1.17E+11	1.19
275	1.95E+11	1.99E+11	1.16
300	3.11E+11	3.10E+11	1.15
325	4.65E+11	4.55E+11	1.14
350	6.60E+11	6.35E+11	1.13
375	8.99E+11	8.52E+11	1.12
400	1.18E+12	1.10E+12	1.11

D (Upper H in Equatorial Carbon)

T(K)	CVT	SCT	KIE
6	2.70E-74	8.50E+04	1.40
8	5.38E-53	8.50E+04	1.40
10	3.40E-40	8.50E+04	1.40
20	1.75E-14	8.52E+04	1.40
30	7.78E-06	8.84E+04	1.39
40	1.82E-01	1.06E+05	1.36
50	8.22E+01	1.65E+05	1.32
75	3.40E+05	2.89E+06	1.26
100	2.53E+07	6.60E+07	1.31
125	3.65E+08	6.25E+08	1.32
150	2.28E+09	3.18E+09	1.31
175	8.73E+09	1.08E+10	1.29
200	2.44E+10	2.82E+10	1.26
225	5.54E+10	6.07E+10	1.24
250	1.08E+11	1.14E+11	1.22
275	1.88E+11	1.93E+11	1.20
300	3.01E+11	3.02E+11	1.18
325	4.51E+11	4.43E+11	1.17
350	6.41E+11	6.19E+11	1.16
375	8.74E+11	8.31E+11	1.15
400	1.15E+12	1.08E+12	1.13

Tritium (all hydrogens)

T(K)	CVT	SCT	KIE
6	1.97-109	3.50E+00	34000
8	2.38E-79	3.50E+00	34000
10	2.81E-61	3.50E+00	34000
20	5.06E-25	3.61E+00	32964
30	7.65E-13	4.44E+00	27703
40	1.08E-06	7.37E+00	19539
50	5.73E-03	1.96E+01	11122
75	6.46E+02	4.16E+03	877.4
100	2.54E+05	5.50E+05	157.3
125	1.01E+07	1.49E+07	55.37
150	1.24E+08	1.54E+08	26.95
175	7.79E+08	8.75E+08	15.89
200	3.17E+09	3.34E+09	10.63
225	9.59E+09	9.69E+09	7.75
250	2.35E+10	2.30E+10	6.04
275	4.94E+10	4.70E+10	4.91
300	9.20E+10	8.58E+10	4.16
325	1.56E+11	1.43E+11	3.63
350	2.47E+11	2.22E+11	3.23
375	3.67E+11	3.26E+11	2.92
400	5.21E+11	4.55E+11	2.68

¹³C Upper Axial

T(K)	CVT	SCT	KIE
6	2.45E-68	3.84E+03	1.34
8	1.56E-48	3.84E+03	1.34
10	1.26E-36	3.84E+03	1.34
20	1.04E-12	3.89E+03	1.34
30	1.21E-04	5.21E+03	1.32
40	1.48E+00	1.98E+04	1.24
50	4.58E+02	1.57E+05	1.18
75	1.17E+06	1.22E+07	1.12
100	6.91E+07	2.12E+08	1.10
125	8.68E+08	1.55E+09	1.08
150	4.94E+09	6.76E+09	1.07
175	1.77E+10	2.09E+10	1.06
200	4.71E+10	5.12E+10	1.05
225	1.03E+11	1.06E+11	1.04
250	1.93E+11	1.92E+11	1.04
275	3.27E+11	3.18E+11	1.03
300	5.10E+11	4.88E+11	1.03
325	7.47E+11	7.08E+11	1.03
350	1.04E+12	9.78E+11	1.02
375	1.39E+12	1.30E+12	1.02
400	1.80E+12	1.68E+12	1.02

¹³C Lower Axial

T(K)	CVT	SCT	KIE
6	1.56E-67	5.07E+03	1.01
8	6.26E-48	5.07E+03	1.01
10	3.81E-36	5.07E+03	1.01
20	1.82E-12	5.14E+03	1.02
30	1.75E-04	6.83E+03	1.00
40	1.95E+00	2.54E+04	0.97
50	5.72E+02	1.96E+05	0.95
75	1.36E+06	1.45E+07	0.94
100	7.70E+07	2.46E+08	0.95
125	9.46E+08	1.76E+09	0.95
150	5.30E+09	7.51E+09	0.96
175	1.88E+10	2.29E+10	0.97
200	4.96E+10	5.53E+10	0.97
225	1.07E+11	1.13E+11	0.97
250	2.01E+11	2.04E+11	0.98
275	3.38E+11	3.35E+11	0.98
300	5.26E+11	5.11E+11	0.98
325	7.69E+11	7.37E+11	0.99
350	1.07E+12	1.02E+12	0.98
375	1.43E+12	1.35E+12	0.99
400	1.84E+12	1.73E+12	0.99

TS2

Default

T(K)	CVT	SCT
6	6.63E-68	5.14E+03
8	3.30E-48	5.14E+03
10	2.28E-36	5.14E+03
20	1.41E-12	5.22E+03
30	1.47E-04	6.86E+03
40	1.72E+00	2.46E+04
50	5.16E+02	1.86E+05
75	1.27E+06	1.37E+07
100	7.32E+07	2.33E+08
125	9.08E+08	1.68E+09
150	5.13E+09	7.20E+09
175	1.83E+10	2.21E+10
200	4.84E+10	5.36E+10
225	1.05E+11	1.10E+11
250	1.97E+11	1.99E+11
275	3.33E+11	3.28E+11
300	5.19E+11	5.02E+11
325	7.60E+11	7.26E+11
350	1.06E+12	1.00E+12
375	1.41E+12	1.33E+12
400	1.83E+12	1.71E+12

¹³C Central

T(K)	CVT	SCT	KIE
6	8.17E-68	4.12E+03	1.25
8	3.86E-48	4.12E+03	1.25
10	2.59E-36	4.12E+03	1.25
20	1.50E-12	4.18E+03	1.25
30	1.54E-04	5.56E+03	1.23
40	1.77E+00	2.10E+04	1.17
50	5.30E+02	1.67E+05	1.11
75	1.29E+06	1.30E+07	1.05
100	7.43E+07	2.26E+08	1.03
125	9.20E+08	1.65E+09	1.02
150	5.18E+09	7.14E+09	1.01
175	1.84E+10	2.20E+10	1.00
200	4.88E+10	5.34E+10	1.00
225	1.06E+11	1.10E+11	1.00
250	1.98E+11	1.99E+11	1.00
275	3.34E+11	3.27E+11	1.00
300	5.20E+11	5.01E+11	1.00
325	7.59E+11	7.23E+11	1.00
350	1.06E+12	9.97E+11	1.00
375	1.41E+12	1.32E+12	1.01
400	1.82E+12	1.70E+12	1.01

¹³C Equatorial (a)

T(K)	CVT	SCT	KIE
6	1.57E-68	3.94E+03	1.30
8	1.12E-48	3.94E+03	1.30
10	9.61E-37	3.94E+03	1.30
20	9.14E-13	4.00E+03	1.31
30	1.11E-04	5.36E+03	1.28
40	1.38E+00	2.02E+04	1.22
50	4.34E+02	1.58E+05	1.18
75	1.13E+06	1.20E+07	1.14
100	6.73E+07	2.08E+08	1.12
125	8.50E+08	1.52E+09	1.11
150	4.86E+09	6.65E+09	1.08
175	1.75E+10	2.06E+10	1.07
200	4.66E+10	5.05E+10	1.06
225	1.02E+11	1.04E+11	1.06
250	1.91E+11	1.90E+11	1.05
275	3.24E+11	3.15E+11	1.04
300	5.07E+11	4.85E+11	1.04
325	7.43E+11	7.03E+11	1.03
350	1.04E+12	9.73E+11	1.03
375	1.39E+12	1.29E+12	1.03
400	1.80E+12	1.67E+12	1.02

¹³C Equatorial (b,c)

T(K)	CVT	SCT	KIE
6	9.47E-68	5.00E+03	1.03
8	4.31E-48	5.00E+03	1.03
10	2.82E-36	5.00E+03	1.03
20	1.57E-12	5.07E+03	1.03
30	1.58E-04	6.66E+03	1.03
40	1.81E+00	2.42E+04	1.02
50	5.39E+02	1.87E+05	0.99
75	1.31E+06	1.40E+07	0.98
100	7.48E+07	2.37E+08	0.98
125	9.24E+08	1.71E+09	0.98
150	5.21E+09	7.33E+09	0.98
175	1.85E+10	2.24E+10	0.99
200	4.90E+10	5.43E+10	0.99
225	1.06E+11	1.11E+11	0.99
250	1.99E+11	2.01E+11	0.99
275	3.36E+11	3.31E+11	0.99
300	5.23E+11	5.06E+11	0.99
325	7.64E+11	7.31E+11	0.99
350	1.06E+12	1.01E+12	0.99
375	1.42E+12	1.34E+12	0.99
400	1.84E+12	1.72E+12	0.99

¹³C all

T(K)	CVT	SCT	KIE
6	3.56E-68	2.94E+03	1.75
8	2.07E-48	2.94E+03	1.75
10	1.57E-36	2.94E+03	1.75
20	1.17E-12	2.98E+03	1.75
30	1.30E-04	3.98E+03	1.72
40	1.57E+00	1.55E+04	1.59
50	4.81E+02	1.30E+05	1.43
75	1.21E+06	1.11E+07	1.23
100	7.09E+07	2.02E+08	1.15
125	8.87E+08	1.52E+09	1.11
150	5.03E+09	6.68E+09	1.08
175	1.80E+10	2.08E+10	1.06
200	4.77E+10	5.11E+10	1.05
225	1.03E+11	1.05E+11	1.05
250	1.94E+11	1.92E+11	1.04
275	3.28E+11	3.17E+11	1.03
300	5.10E+11	4.86E+11	1.03
325	7.46E+11	7.04E+11	1.03
350	1.04E+12	9.72E+11	1.03
375	1.39E+12	1.29E+12	1.03
400	1.79E+12	1.66E+12	1.03

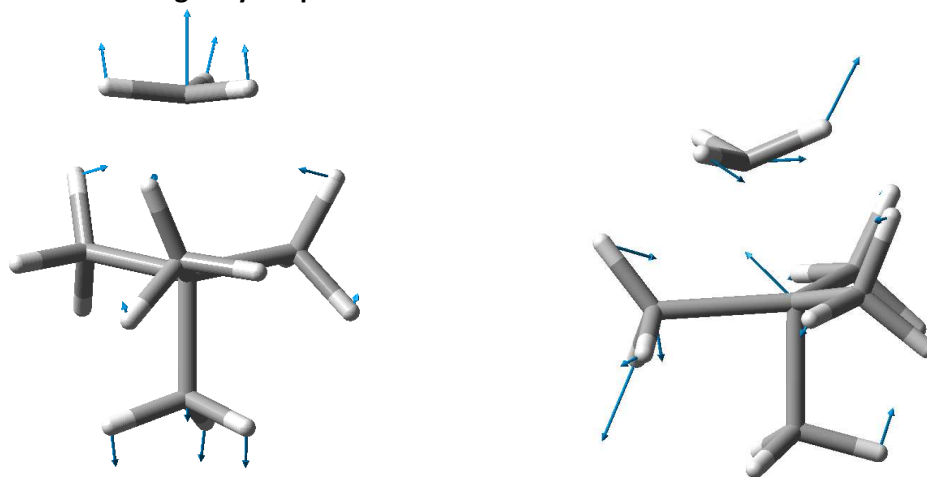
Deuterium (all hydrogens)

T(K)	CVT	SCT	KIE
6	2.73E-77	3.83E+00	1342
8	3.01E-55	3.83E+00	1342
10	5.33E-42	3.83E+00	1342
20	2.20E-15	4.37E+00	1195
30	2.08E-06	1.95E+01	351.8
40	7.43E-02	5.87E+02	41.91
50	4.39E+01	1.31E+04	14.20
75	2.64E+05	2.58E+06	5.31
100	2.36E+07	7.30E+07	3.19
125	3.79E+08	7.19E+08	2.34
150	2.53E+09	3.76E+09	1.91
175	1.01E+10	1.31E+10	1.69
200	2.93E+10	3.47E+10	1.54
225	6.77E+10	7.57E+10	1.45
250	1.34E+11	1.44E+11	1.38
275	2.34E+11	2.45E+11	1.34
300	3.77E+11	3.86E+11	1.30
325	5.65E+11	5.70E+11	1.27
350	8.02E+11	8.00E+11	1.25
375	1.09E+12	1.08E+12	1.23
400	1.43E+12	1.40E+12	1.22

Tritium (all hydrogens)

T(K)	CVT	SCT	KIE
6	1.21E-81	1.65E-02	311515
8	1.64E-58	1.65E-02	311515
10	1.30E-44	1.66E-02	309639
20	1.11E-16	2.52E-02	207143
30	2.97E-07	7.24E-01	9475
40	1.79E-02	8.17E+01	301.1
50	1.45E+01	2.87E+03	64.81
75	1.31E+05	9.83E+05	13.94
100	1.43E+07	3.69E+07	6.31
125	2.58E+08	4.29E+08	3.92
150	1.86E+09	2.49E+09	2.89
175	7.84E+09	9.34E+09	2.37
200	2.35E+10	2.60E+10	2.06
225	5.58E+10	5.91E+10	1.86
250	1.12E+11	1.15E+11	1.73
275	2.00E+11	2.02E+11	1.62
300	3.26E+11	3.23E+11	1.55
325	4.94E+11	4.84E+11	1.50
350	7.07E+11	6.87E+11	1.46
375	9.67E+11	9.34E+11	1.42
400	1.28E+12	1.23E+12	1.39

Displacement vectors of the imaginary frequencies of TS1 and TS2:



Absolute energies and E+ZPE of the reactant, transition states and products:

		Reac	TS1	TS2	Prod1	Prod2
E	$\text{C}(\text{CH}_3)_5^+$	-237.116053	-237.108604	-237.110966	-237.236190	-237.230131
E+ZPE	$\text{C}(\text{CH}_3)_5^+$	-236.913350	-236.909727	-236.909915	-237.040717	-237.035090
	$\text{C}(\text{CD}_3)_5^+$	-236.964216	-236.959450	-236.960377	-237.088946	-237.083103
	$\text{C}(\text{CT}_3)_5^+$	-236.986267	-236.980991	-236.982241	-237.109805	-237.103864
	$\text{C}(\text{CH}_3)_5^+ (^{13}\text{C})$	-236.914418	-236.910793	-236.910970	-237.041850	-237.036234

XYZ geometries of the reactant, transition states and products:

Reactant (C3h)

```
C -0.000628 1.620650 0.000000
C 1.403838 -0.809782 0.000000
C -1.403211 -0.810869 0.000000
C 0.000000 0.000000 0.000000
H -0.491600 2.039973 0.876456
H 2.012468 -0.594248 0.876456
H -1.520868 -1.445724 0.876456
H -0.491600 2.039973 -0.876456
H 2.012468 -0.594248 -0.876456
H -1.520868 -1.445724 -0.876456
H 1.048105 1.931422 0.000000
H 1.148608 -1.873396 0.000000
H -2.196713 -0.058025 0.000000
C 0.000000 0.000000 1.745662
C 0.000000 0.000000 -1.745662
H 0.170991 -1.031275 2.042971
H -0.978606 0.367555 2.042971
H 0.807615 0.663720 2.042971
H 0.170991 -1.031275 -2.042971
H -0.978606 0.367555 -2.042971
H 0.807615 0.663720 -2.042971
```

TS2

```
C -0.190579 -1.009252 -1.277239
C -0.186673 -0.840147 1.387385
C 0.404418 1.602996 -0.068628
C -0.133972 -0.115966 0.004820
H 0.563216 -1.797171 -1.301378
H 0.616677 -1.558670 1.552302
H 1.433148 1.906913 -0.211058
H -0.069034 -0.388713 -2.170486
H -1.127136 -1.387137 1.471851
H 0.053910 1.963904 0.895472
H -1.165965 -1.494350 -1.339783
H -0.156670 -0.104291 2.196865
H -0.178882 1.981038 -0.902961
C 1.762188 -0.134521 -0.012340
C -1.664792 0.465854 -0.037792
H 2.152635 0.368025 0.867305
H 2.133114 0.224234 -0.967160
H 1.810851 -1.212209 0.070952
H -1.842254 1.160559 0.781855
H -1.866182 0.934186 -1.000277
H -2.300967 -0.410102 0.079258
```

Prod TS2

```
C -1.372329 -0.882184 -1.171363
C -0.772599 -0.750063 1.280842
C 1.911420 0.810765 -0.257457
C -1.300015 -0.115538 0.072997
H -0.749019 -1.777574 -1.176400
H 0.289461 -0.974439 1.078788
H 2.442773 1.634848 -0.739411
H -1.208502 -0.254751 -2.052967
H -1.237444 -1.737975 1.412192
H 1.491937 1.199894 0.679053
H -2.431783 -1.201578 -1.233013
H -0.863819 -0.146465 2.182896
H 1.087989 0.533583 -0.931544
C 2.847549 -0.367878 -0.002708
C -1.759202 1.271551 0.105757
H 3.672871 -0.069274 0.647456
H 3.273829 -0.739068 -0.937195
H 2.343625 -1.211644 0.486121
H -0.829198 1.869372 0.176059
H -2.302109 1.582375 -0.787115
H -2.309553 1.492780 1.026672
```

TS1

```
C 0.000000 1.564242 -0.003105
C 1.354674 -0.782121 -0.003105
C -1.354674 -0.782121 -0.003105
C 0.000000 0.000000 0.248677
H -0.628776 2.031683 0.757806
H 2.073877 -0.471305 0.757806
H -1.445101 -1.560378 0.757806
H -0.366444 1.953473 -0.954283
H 1.874979 -0.659386 -0.954283
H -1.508535 -1.294087 -0.954283
H 1.021780 1.932302 0.133973
H 1.162533 -1.851038 0.133973
H -2.184312 -0.081264 0.133973
C 0.000000 0.000000 1.844240
C 0.000000 0.000000 -2.063420
H 0.170642 -1.018263 2.200587
H -0.967162 0.361351 2.200587
H 0.796520 0.656912 2.200587
H 0.166943 -1.064619 -2.178448
H -1.005458 0.387733 -2.178448
H 0.838515 0.676886 -2.178448
```

Prod TS1

```
C 0.740040 -0.922838 -0.272483
C -0.047798 0.816715 1.401983
C 0.034127 1.370241 -1.066732
C 0.217333 0.403676 0.019126
H 0.590894 -1.208337 -1.316307
H -0.040848 -0.005208 2.117764
H 0.045520 2.411495 -0.739716
H -2.934104 0.292910 -0.061938
H -0.990738 1.376648 1.450671
H -0.983741 1.151014 -1.444071
H 0.342751 -1.679666 0.407673
H 0.728682 1.552531 1.672484
H 0.710221 1.190057 -1.907286
C 2.284680 -0.769271 0.000450
C -2.767505 -0.787210 -0.090452
H 2.733921 0.000428 -0.630436
H 2.735706 -1.731156 -0.250370
H 2.484425 -0.550374 1.050637
H -3.737683 -1.283271 -0.132253
H -2.200675 -1.068448 -0.982497
H -2.249589 -1.116503 0.814295
```

Example of Polyrate input file for the deuterated TS1:

*GENERAL		SLM -2.2
	*PROD1	END
TITLE	STATUS 0	
CMe5+		SIGN reactant
END	INITGEO hooks	
		COORD curv3
ATOMS	GEOM	
1 C	1	IDIRECT 1
2 C	2	
3 C	3	PRPATH
4 C	4	coord 4 15
5 H 2.014	5	xmol
6 H 2.014	6	freq 57
7 H 2.014	7	END
8 H 2.014	8	
9 H 2.014	9	INTDEF
10 H 2.014	10	1-4
11 H 2.014	11	1-5
12 H 2.014	12	1-8
13 H 2.014	13	1-11
14 C	14	1-15
15 C	15	1-20
16 H 2.014	16	1-21
17 H 2.014	17	2-4
18 H 2.014	18	2-6
19 H 2.014	19	2-9
20 H 2.014	20	2-12
21 H 2.014	21	2-15
END	END	2-19
		2-21
NOSUPERMOL	SPECIES nonlinrp	3-4
		3-7
*SECOND	*START	3-10
	STATUS 0	3-13
HESSCAL hhook		3-15
	INITGEO hooks	3-19
FPRINT		3-20
	GEOM	4-14
*OPTIMIZATION	1	4-15
	2	4-19
PRINT	3	4-20
	4	4-21
OPTMIN ohook	5	8-15
OPTTS ohook	6	9-15
	7	10-15
*REACT1	8	14-16
STATUS 0	9	14-17
	10	14-18
INITGEO hooks	11	15-19
	12	15-20
GEOM	13	15-21
1	14	4-1-5
2	15	4-1-8
3	16	4-1-11
4	17	5-1-8
5	18	5-1-11
6	19	5-1-15
7	20	5-1-20
8	21	5-1-21
9	END	8-1-11
10		8-1-20
11	SPECIES nonlints	8-1-21
12		11-1-15
13	PROJECT	11-1-20
14		11-1-21
15	*PATH	20-1-21
16	SCALEMASS 1.00	4-2-6
17	INTMU 3	4-2-9
18	SSTEP 0.001	4-2-12
19	INH 10	6-2-9
20		6-2-12
21	RPM pagem	6-2-15
END		6-2-19
	SRANGE	6-2-21
SPECIES nonlinrp	SLP 12.	9-2-12

9-2-19	5-1-4-19	13-3-15-21
9-2-21	8-1-4-2	7-3-19-2
12-2-15	8-1-4-3	10-3-19-2
12-2-19	8-1-4-14	13-3-19-2
12-2-21	8-1-4-19	20-3-19-2
19-2-21	11-1-4-2	7-3-20-1
4-3-7	11-1-4-3	10-3-20-1
4-3-10	11-1-4-14	13-3-20-1
4-3-13	11-1-4-19	19-3-20-1
7-3-10	5-1-15-2	1-4-14-16
7-3-13	5-1-15-3	1-4-14-17
7-3-15	5-1-15-9	1-4-14-18
7-3-19	5-1-15-10	2-4-14-16
7-3-20	5-1-15-19	2-4-14-17
10-3-13	11-1-15-2	2-4-14-18
10-3-19	11-1-15-3	3-4-14-16
10-3-20	11-1-15-9	3-4-14-17
13-3-15	11-1-15-10	3-4-14-18
13-3-19	11-1-15-19	19-4-14-16
13-3-20	5-1-20-3	19-4-14-17
19-3-20	8-1-20-3	19-4-14-18
1-4-2	11-1-20-3	20-4-14-16
1-4-3	21-1-20-3	20-4-14-17
1-4-14	5-1-21-2	20-4-14-18
1-4-19	8-1-21-2	21-4-14-16
2-4-3	11-1-21-2	21-4-14-17
2-4-14	20-1-21-2	21-4-14-18
2-4-20	6-2-4-1	16-14-15-8
3-4-14	6-2-4-3	16-14-15-9
3-4-21	6-2-4-14	16-14-15-10
14-4-19	6-2-4-20	17-14-15-8
14-4-20	9-2-4-1	17-14-15-9
14-4-21	9-2-4-3	17-14-15-10
19-4-20	9-2-4-14	18-14-15-8
19-4-21	9-2-4-20	18-14-15-9
20-4-21	12-2-4-1	18-14-15-10
4-14-16	12-2-4-3	END
4-14-17	12-2-4-14	
4-14-18	12-2-4-20	*TUNNEL
16-14-17	6-2-15-1	
16-14-18	6-2-15-3	ZCT
17-14-18	6-2-15-8	SCT
1-15-2	6-2-15-10	
1-15-3	6-2-15-20	QRST
1-15-9	12-2-15-1	harmonic
1-15-10	12-2-15-3	mode 57
1-15-19	12-2-15-8	states all
2-15-3	12-2-15-10	END
2-15-8	12-2-15-20	
2-15-10	6-2-19-3	*RATE
2-15-20	9-2-19-3	
3-15-8	12-2-19-3	FORWARDK
3-15-9	21-2-19-3	
3-15-21	6-2-21-1	SIGMAF 1
4-15-8	9-2-21-1	
4-15-9	12-2-21-1	TST
4-15-10	19-2-21-1	CVT
8-15-9	7-3-4-1	
8-15-10	7-3-4-2	
8-15-19	7-3-4-14	PRDELG
8-15-20	7-3-4-21	PRPART rtp
8-15-21	10-3-4-1	
9-15-10	10-3-4-2	TEMP
9-15-19	10-3-4-14	6
9-15-20	10-3-4-21	8
9-15-21	13-3-4-1	10
10-15-19	13-3-4-2	20
10-15-20	13-3-4-14	30
10-15-21	13-3-4-21	40
19-15-20	7-3-15-1	50
19-15-21	7-3-15-2	75
20-15-21	7-3-15-8	100
2-19-3	7-3-15-9	125
1-20-3	7-3-15-21	150
1-21-2	13-3-15-1	175
5-1-4-2	13-3-15-2	200
5-1-4-3	13-3-15-8	225
5-1-4-14	13-3-15-9	250
		275

300
325
350
375
400
END

ANALYSIS

6
8
10
20
30
40
50
75
100
125
150
175
200
225
250
275
300
325
350
375
400
END

EACT

6. 10.
10. 20.
20. 50.
50. 100.
200. 225.
300. 325.
END

GTLOG

V_{mep} and V_a^G complete table for the root reaction of TS1:

s	V _{mep}	V _a ^G	-1.9464	1.4868	127.4932	-0.4346	4.4352	129.464	1.0771	3.3716	127.4034
(bohr)	(kcal)	(kcal)	-1.9275	1.528	127.5236	-0.4157	4.4551	129.4717	1.096	3.3307	127.3428
-3.4015	-0.0001	125.8411	-1.9086	1.5695	127.5541	-0.3968	4.4743	129.4787	1.1149	3.2893	127.2807
-3.3826	0	126.9488	-1.8897	1.6111	127.5847	-0.3779	4.4926	129.4849	1.1338	3.2475	127.217
-3.3637	0.0002	126.9789	-1.8708	1.6528	127.6154	-0.359	4.5101	129.4904	1.1527	3.2052	127.1515
-3.3448	0.0007	126.9837	-1.8519	1.6947	127.6462	-0.3402	4.5269	129.4951	1.1716	3.1625	127.0835
-3.3259	0.0013	126.9854	-1.833	1.7368	127.6771	-0.3213	4.5427	129.4991	1.1905	3.1194	127.0121
-3.307	0.0022	126.9863	-1.8141	1.7789	127.7081	-0.3024	4.5578	129.5022	1.2094	3.0758	126.9344
-3.2881	0.0033	126.9871	-1.7952	1.8212	127.7391	-0.2835	4.572	129.5045	1.2283	3.0318	126.8414
-3.2692	0.0045	126.9878	-1.7763	1.8635	127.7702	-0.2646	4.5853	129.5061	1.2472	2.9874	126.7724
-3.2503	0.006	126.9885	-1.7574	1.9059	127.8012	-0.2457	4.5978	129.5068	1.2661	2.9426	126.6887
-3.2314	0.0076	126.9893	-1.7385	1.9484	127.8323	-0.2268	4.6094	129.5066	1.285	2.8974	126.6343
-3.2125	0.0094	126.9902	-1.7197	1.991	127.8634	-0.2079	4.6201	129.5057	1.3039	2.8517	126.5794
-3.1936	0.0115	126.9911	-1.7008	2.0336	127.8945	-0.189	4.6299	129.5039	1.3228	2.8057	126.5241
-3.1747	0.0137	126.9922	-1.6819	2.0762	127.9256	-0.1701	4.6388	129.5012	1.3417	2.7592	126.4683
-3.1558	0.0161	126.9934	-1.663	2.1188	127.9566	-0.1512	4.6467	129.4977	1.3606	2.7124	126.4121
-3.1369	0.0188	126.9946	-1.6441	2.1615	127.9877	-0.1323	4.6538	129.4933	1.3795	2.6652	126.3554
-3.118	0.0216	126.9958	-1.6252	2.2041	128.0186	-0.1134	4.6599	129.488	1.3984	2.6175	126.2983
-3.0992	0.0246	126.997	-1.6063	2.2468	128.0495	-0.0945	4.665	129.4818	1.4173	2.5695	126.2407
-3.0803	0.0278	126.9979	-1.5874	2.2894	128.0803	-0.0756	4.6692	129.4747	1.4362	2.5211	126.1828
-3.0614	0.0312	126.9982	-1.5685	2.332	128.1111	-0.0567	4.6725	129.4666	1.4551	2.4723	126.1244
-3.0425	0.0348	126.9975	-1.5496	2.3746	128.1417	-0.0378	4.6748	129.4569	1.474	2.4231	126.0655
-3.0236	0.0386	126.9949	-1.5307	2.4171	128.1723	-0.0189	4.6762	129.441	1.4929	2.3736	126.0063
-3.0047	0.0427	126.9894	-1.5118	2.4595	128.2028	0	4.6767	129.4395	1.5118	2.3236	125.9467
-2.9858	0.047	126.9793	-1.4929	2.5019	128.2331	0.0189	4.6762	129.421	1.5307	2.2733	125.8866
-2.9669	0.0516	126.9629	-1.474	2.5442	128.2633	0.0378	4.6749	129.4149	1.5496	2.2226	125.8262
-2.948	0.0565	126.9394	-1.4551	2.5864	128.2934	0.0567	4.6726	129.4025	1.5685	2.1716	125.7653
-2.9291	0.0619	126.909	-1.4362	2.6285	128.3233	0.0756	4.6694	129.3886	1.5874	2.1201	125.7041
-2.9102	0.0679	126.8741	-1.4173	2.6705	128.3531	0.0945	4.6652	129.3737	1.6063	2.0683	125.6426
-2.8913	0.0745	126.8377	-1.3984	2.7124	128.3828	0.1134	4.66	129.3578	1.6252	2.0161	125.5806
-2.8724	0.082	126.8031	-1.3795	2.7541	128.4122	0.1323	4.6539	129.341	1.6441	1.9635	125.5183
-2.8535	0.0904	126.772	-1.3606	2.7958	128.4415	0.1512	4.6469	129.3232	1.663	1.9106	125.4556
-2.8346	0.0997	126.7454	-1.3417	2.8372	128.4706	0.1701	4.639	129.3046	1.6819	1.8572	125.3926
-2.8157	0.11	126.7235	-1.3228	2.8785	128.4995	0.189	4.6302	129.285	1.7008	1.8035	125.3293
-2.7968	0.1215	126.706	-1.3039	2.9197	128.5282	0.2079	4.6204	129.2645	1.7197	1.7495	125.2656
-2.7779	0.134	126.6925	-1.285	2.9606	128.5567	0.2268	4.6097	129.2431	1.7385	1.695	125.2016
-2.759	0.1475	126.6825	-1.2661	3.0014	128.585	0.2457	4.5982	129.2208	1.7574	1.6402	125.1372
-2.7401	0.1622	126.6757	-1.2472	3.042	128.613	0.2646	4.5858	129.1975	1.7763	1.5851	125.0726
-2.7212	0.178	126.6716	-1.2283	3.0823	128.6409	0.2835	4.5725	129.1734	1.7952	1.5295	125.0076
-2.7023	0.1949	126.6701	-1.2094	3.1225	128.6684	0.3024	4.5583	129.1483	1.8141	1.4736	124.9423
-2.6834	0.2128	126.6708	-1.1905	3.1624	128.6957	0.3213	4.5433	129.1224	1.833	1.4174	124.8767
-2.6645	0.2318	126.6735	-1.1716	3.2021	128.7228	0.3402	4.5275	129.0955	1.8519	1.3608	124.8108
-2.6456	0.2518	126.678	-1.1527	3.2415	128.7496	0.359	4.5108	129.0678	1.8708	1.3038	124.7445
-2.6267	0.2728	126.6843	-1.1338	3.2806	128.7761	0.3779	4.4933	129.0391	1.8897	1.2464	124.678
-2.6078	0.2948	126.6921	-1.1149	3.3195	128.8023	0.3968	4.4751	129.0096	1.9086	1.1888	124.6112
-2.5889	0.3177	126.7014	-1.096	3.3581	128.8282	0.4157	4.456	128.9792	1.9275	1.1307	124.5441
-2.57	0.3416	126.712	-1.0771	3.3964	128.8538	0.4346	4.4362	128.9479	1.9464	1.0723	124.4768
-2.5511	0.3663	126.7239	-1.0582	3.4345	128.8791	0.4535	4.4156	128.9158	1.9653	1.0136	124.4091
-2.5322	0.392	126.737	-1.0393	3.4722	128.9041	0.4724	4.3942	128.8828	1.9842	0.9545	124.3412
-2.5133	0.4185	126.7513	-1.0205	3.5095	128.9287	0.4913	4.3721	128.8489	2.0031	0.8951	124.273
-2.4944	0.4458	126.7666	-1.0016	3.5465	128.953	0.5102	4.3493	128.8143	2.022	0.8354	124.2045
-2.4755	0.4739	126.7829	-0.9827	3.5832	128.9769	0.5291	4.3257	128.7787	2.0409	0.7753	124.1358
-2.4566	0.5028	126.8002	-0.9638	3.6195	129.0005	0.548	4.3014	128.7424	2.0598	0.7149	124.0668
-2.4377	0.5324	126.8184	-0.9449	3.6555	129.0237	0.5669	4.2765	128.7052	2.0787	0.6542	123.9976
-2.4188	0.5627	126.8375	-0.926	3.691	129.0465	0.5858	4.2508	128.6672	2.0976	0.5931	123.9281
-2.4	0.5938	126.8574	-0.9071	3.7262	129.0689	0.6047	4.2245	128.6285	2.1165	0.5318	123.8584
-2.3811	0.6255	126.878	-0.8882	3.7609	129.0908	0.6236	4.1975	128.5889	2.1354	0.4701	123.7885
-2.3622	0.6578	126.8994	-0.8693	3.7952	129.1124	0.6425	4.1698	128.5485	2.1543	0.4081	123.7183
-2.3433	0.6908	126.9215	-0.8504	3.8291	129.1335	0.6614	4.1415	128.5074	2.1732	0.3459	123.6479
-2.3244	0.7243	126.9442	-0.8315	3.8625	129.1542	0.6803	4.1125	128.4655	2.1921	0.2833	123.5773
-2.3055	0.7584	126.9676	-0.8126	3.8955	129.1744	0.6992	4.0829	128.4228	2.211	0.2205	123.5065
-2.2866	0.7931	126.9915	-0.7937	3.928	129.1942	0.7181	4.0527	128.3794	2.2299	0.1573	123.4354
-2.2677	0.8283	127.0161	-0.7748	3.96	129.2135	0.737	4.0219	128.3352	2.2488	0.0939	123.3642
-2.2488	0.864	127.0411	-0.7559	3.9914	129.2323	0.7559	3.9904	128.2902	2.2677	0.0302	123.2927
-2.2299	0.9001	127.0667	-0.737	4.0224	129.2506	0.7748	3.9584	128.2445	2.2866	-0.0338	123.2211
-2.211	0.9367	127.0927	-0.7181	4.0528	129.2683	0.7937	3.9258	128.198	2.3055	-0.098	123.1492
-2.1921	0.9738	127.1192	-0.6992	4.0827	129.2856	0.8126	3.8926	128.1507	2.3244	-0.1625	123.0772
-2.1732	1.0113	127.1461	-0.6803	4.112	129.3023	0.8315	3.8588	128.1027	2.3433	-0.2272	123.005
-2.1543	1.0491	127.1733	-0.6614	4.1408	129.3184	0.8504	3.8245	128.0539	2.3622	-0.2922	122.9325
-2.1354	1.0874	127.201	-0.6425	4.1689	129.334	0.8693	3.7896	128.0044	2.3811	-0.3575	122.8599
-2.1165	1.126	127.229	-0.6236	4.1964	129.349	0.8882	3.7542	127.954	2.4	-0.4229	122.7871
-2.0976	1.1649	127.2573	-0.6047	4.2233	129.3634	0.9071	3.7182	127.9029	2.4188	-0.4887	122.714
-2.0787	1.2042	127.286	-0.5858	4.2496	129.3772	0.926	3.6817	127.851	2.4377	-0.5546	122.6408
-2.0598	1.2438	127.3149	-0.5669	4.2753	129.3904	0.9449	3.6447	127.7982	2.4566	-0.6208	122.5674
-2.0409	1.2837	127.3441	-0.548	4.3002	129.4029	0.9638	3.6071	127.7446	2.4755	-0.6872	122.4938
-2.022	1.3238	127.3735	-0.5291	4.3245	129.4148	0.9827	3.5691	127.6901	2.4944	-0.7538	122.42
-2.0031	1.3642	127.4031	-0.5102	4.3481	129.426	1.0016	3.5306	127.6348	2.5133	-0.8206	122.346
-1.9842	1.4048	127.433	-0.4913	4.371	129.4365	1.0205	3.4916	127.5785	2.5322	-0.8876	122.2718
-1.9653	1.4457	127.463	-0.4724	4.3931	129.4464	1.0393	3.452	127.5212	2.5511	-0.9548	122.1975
			-0.4535	4.4145	129.4556	1.0582	3.4121	127.4629	2.57	-1.0222	122.1229

2.5889	-1.0898	122.0481	4.1385	-6.8393	115.7626	5.6881	-11.185	110.8789	7.2377	-12.9228	108.8129
2.6078	-1.1577	121.9731	4.1574	-6.9055	115.6903	5.707	-11.2221	110.8367	7.2565	-12.9316	108.8053
2.6267	-1.2256	121.898	4.1763	-6.9714	115.6183	5.7259	-11.2587	110.7949	7.2754	-12.9406	108.7977
2.6456	-1.2938	121.8227	4.1952	-7.037	115.5466	5.7448	-11.295	110.7537	7.2943	-12.9498	108.8094
2.6645	-1.3622	121.7471	4.2141	-7.1024	115.4751	5.7637	-11.3308	110.713	7.3132	-12.9592	108.8708
2.6834	-1.4307	121.6714	4.233	-7.1676	115.4039	5.7826	-11.3662	110.6729	7.3321	-12.9689	108.8956
2.7023	-1.4994	121.5956	4.2519	-7.2325	115.333	5.8015	-11.4012	110.6332	7.351	-12.979	108.9105
2.7212	-1.5683	121.5195	4.2708	-7.2972	115.2624	5.8204	-11.4359	110.594	7.3699	-12.9895	108.9195
2.7401	-1.6373	121.4433	4.2897	-7.3616	115.1921	5.8393	-11.4701	110.5553	7.3888	-13.0004	108.9242
2.759	-1.7065	121.367	4.3086	-7.4258	115.1221	5.8582	-11.5039	110.5171	7.4077	-13.0117	108.9255
2.7779	-1.7759	121.2905	4.3275	-7.4897	115.0525	5.877	-11.5372	110.4793	7.4266	-13.0236	108.9239
2.7968	-1.8454	121.2138	4.3464	-7.5533	114.9831	5.8959	-11.5702	110.442	7.4455	-13.036	108.9198
2.8157	-1.9151	121.137	4.3653	-7.6167	114.9141	5.9148	-11.6028	110.4051	7.4644	-13.049	108.9135
2.8346	-1.9849	121.0601	4.3842	-7.6798	114.8454	5.9337	-11.635	110.3687	7.4833	-13.0625	108.9052
2.8535	-2.0549	120.983	4.4031	-7.7426	114.777	5.9526	-11.6667	110.3327	7.5022	-13.0767	108.8951
2.8724	-2.125	120.9058	4.422	-7.8051	114.7089	5.9715	-11.6981	110.2971	7.5211	-13.0916	108.8833
2.8913	-2.1953	120.8286	4.4409	-7.8674	114.6412	5.9904	-11.729	110.2619	7.54	-13.1072	108.8699
2.9102	-2.2657	120.7512	4.4598	-7.9293	114.5738	6.0093	-11.7595	110.2271	7.5589	-13.1234	108.8549
2.9291	-2.3362	120.6737	4.4787	-7.991	114.5068	6.0282	-11.7896	110.1927	7.5778	-13.1404	108.8385
2.948	-2.4068	120.5961	4.4975	-8.0524	114.4401	6.0471	-11.8193	110.1587	7.5967	-13.1581	108.8207
2.9669	-2.4776	120.5184	4.5164	-8.1134	114.3737	6.066	-11.8487	110.1251	7.6156	-13.1766	108.8015
2.9858	-2.5485	120.4407	4.5353	-8.1742	114.3077	6.0849	-11.8775	110.0919	7.6345	-13.196	108.7809
3.0047	-2.6194	120.3629	4.5542	-8.2346	114.2419	6.1038	-11.906	110.0591	7.6534	-13.2161	108.759
3.0236	-2.6905	120.285	4.5731	-8.2948	114.1765	6.1227	-11.9341	110.0266	7.6723	-13.2371	108.7357
3.0425	-2.7617	120.2071	4.592	-8.3546	114.1115	6.1416	-11.9618	109.9945	7.6912	-13.2589	108.7111
3.0614	-2.833	120.1291	4.6109	-8.4141	114.0467	6.1605	-11.989	109.9628	7.7101	-13.2816	108.6852
3.0803	-2.9043	120.051	4.6298	-8.4732	113.9822	6.1794	-12.0159	109.9315	7.729	-13.3053	108.658
3.0992	-2.9757	119.9729	4.6487	-8.5321	113.918	6.1983	-12.0423	109.9005	7.7479	-13.3298	108.6294
3.118	-3.0472	119.8948	4.6676	-8.5906	113.8541	6.2172	-12.0684	109.87	7.7668	-13.3553	108.5996
3.1369	-3.1188	119.8166	4.6865	-8.6487	113.7905	6.2361	-12.094	109.8397	7.7857	-13.3818	108.5684
3.1558	-3.1904	119.7384	4.7054	-8.7066	113.7272	6.255	-12.1193	109.8099	7.8046	-13.4093	108.5678
3.1747	-3.2621	119.6602	4.7243	-8.764	113.6641	6.2739	-12.1441	109.7804	7.8235	-13.4378	108.5581
3.1936	-3.3338	119.5819	4.7432	-8.8211	113.6013	6.2928	-12.1685	109.7513	7.8424	-13.4673	108.5392
3.2125	-3.4056	119.5036	4.7621	-8.8779	113.5387	6.3117	-12.1925	109.7226	7.8613	-13.4979	108.5157
3.2314	-3.4774	119.4253	4.781	-8.9343	113.4764	6.3306	-12.2162	109.6942	7.8802	-13.5295	108.4889
3.2503	-3.5492	119.347	4.7999	-8.9904	113.4143	6.3495	-12.2394	109.6662	7.8991	-13.5623	108.4594
3.2692	-3.621	119.2687	4.8188	-9.0461	113.3524	6.3684	-12.2622	109.6385	7.918	-13.5962	108.4275
3.2881	-3.6929	119.1904	4.8377	-9.1014	113.2908	6.3873	-12.2846	109.6112	7.9369	-13.6312	108.3933
3.307	-3.7647	119.112	4.8566	-9.1563	113.2293	6.4062	-12.3067	109.5843	7.9557	-13.6674	108.3572
3.3259	-3.8366	119.0337	4.8755	-9.2109	113.1681	6.4251	-12.3283	109.5577	7.9746	-13.7047	108.319
3.3448	-3.9084	118.9554	4.8944	-9.2651	113.1072	6.444	-12.3495	109.5314	7.9935	-13.7433	108.2789
3.3637	-3.9803	118.8771	4.9133	-9.319	113.0464	6.4629	-12.3704	109.5055	8.0124	-13.7831	108.2369
3.3826	-4.0521	118.7989	4.9322	-9.3724	112.9859	6.4818	-12.3908	109.4799	8.0313	-13.8241	108.1931
3.4015	-4.1239	118.7206	4.9511	-9.4255	112.9256	6.5007	-12.4109	109.4547	8.0502	-13.8664	108.1475
3.4204	-4.1957	118.6424	4.97	-9.4781	112.8656	6.5196	-12.4305	109.4298	8.0691	-13.91	108.1001
3.4393	-4.2674	118.5643	4.9889	-9.5304	112.8058	6.5385	-12.4498	109.4053	8.088	-13.9549	108.051
3.4582	-4.3391	118.4862	5.0078	-9.5823	112.7462	6.5574	-12.4687	109.381	8.1069	-14.0011	108.0001
3.4771	-4.4107	118.4082	5.0267	-9.6338	112.687	6.5762	-12.4872	109.3572	8.1258	-14.0487	107.9475
3.496	-4.4823	118.3302	5.0456	-9.685	112.628	6.5951	-12.5053	109.3337	8.1447	-14.0976	107.8932
3.5149	-4.5538	118.2524	5.0645	-9.7357	112.5692	6.614	-12.5231	109.3105	8.1636	-14.1479	107.8371
3.5338	-4.6252	118.1746	5.0834	-9.786	112.5108	6.6329	-12.5405	109.2877	8.1825	-14.1996	107.7792
3.5527	-4.6966	118.0969	5.1023	-9.836	112.4527	6.6518	-12.5574	109.2653	8.2014	-14.2527	107.7196
3.5716	-4.7679	118.0194	5.1212	-9.8855	112.395	6.6707	-12.574	109.2432	8.2203	-14.3073	107.6581
3.5905	-4.839	117.9419	5.1401	-9.9346	112.3376	6.6896	-12.5903	109.2216	8.2392	-14.3633	107.5947
3.6094	-4.9101	117.8646	5.159	-9.9834	112.2805	6.7085	-12.6062	109.2003	8.2581	-14.4208	107.5295
3.6283	-4.9811	117.7874	5.1779	-10.0317	112.2239	6.7274	-12.6217	109.1795	8.277	-14.4798	107.4622
3.6472	-5.0519	117.7103	5.1967	-10.0797	112.1676	6.7463	-12.6368	109.159	8.2959	-14.5403	107.393
3.6661	-5.1227	117.6333	5.2156	-10.1272	112.1118	6.7652	-12.6516	109.1391	8.3148	-14.6023	107.3218
3.685	-5.1933	117.5565	5.2345	-10.1744	112.0564	6.7841	-12.666	109.1195	8.3337	-14.6659	107.2485
3.7039	-5.2638	117.4798	5.2534	-10.2211	112.0014	6.803	-12.68	109.1005	8.3526	-14.7311	107.1732
3.7228	-5.3342	117.4033	5.2723	-10.2674	111.9469	6.8219	-12.6937	109.082	8.3715	-14.7979	107.0957
3.7417	-5.4044	117.327	5.2912	-10.3134	111.8928	6.8408	-12.7071	109.0639	8.3904	-14.8663	107.0162
3.7606	-5.4745	117.2507	5.3101	-10.3589	111.8393	6.8597	-12.7201	109.0464	8.4093	-14.9364	106.9345
3.7795	-5.5444	117.1747	5.329	-10.4041	111.7862	6.8786	-12.7328	109.0295	8.4282	-15.0081	106.8508
3.7984	-5.6142	117.0987	5.3479	-10.4488	111.7336	6.8975	-12.7451	109.0131	8.4471	-15.0815	106.7649
3.8172	-5.6838	117.023	5.3668	-10.4931	111.6815	6.9164	-12.7571	108.9972	8.466	-15.1567	106.6771
3.8361	-5.7533	116.9474	5.3857	-10.5371	111.63	6.9353	-12.7688	108.982	8.4849	-15.2336	106.5871
3.855	-5.8225	116.872	5.4046	-10.5806	111.5789	6.9542	-12.7802	108.9673	8.5038	-15.3123	106.4952
3.8739	-5.8917	116.7967	5.4235	-10.6237	111.5284	6.9731	-12.7913	108.9533	8.5227	-15.3929	106.4012
3.8928	-5.9606	116.7216	5.4424	-10.6664	111.4784	6.992	-12.8021	108.9398	8.5416	-15.4752	106.3052
3.9117	-6.0294	116.6467	5.4613	-10.7087	111.429	7.0109	-12.8125	108.927	8.5605	-15.5594	106.2072
3.9306	-6.098	116.5719	5.4802	-10.7507	111.3801	7.0298	-12.8227	108.9148	8.5794	-15.6455	106.1071
3.9495	-6.1664	116.4974	5.4991	-10.7922	111.3318	7.0487	-12.8327	108.9031	8.5983	-15.7335	106.005
3.9684	-6.2346	116.423	5.518	-10.8333	111.284	7.0676	-12.8424	108.8921	8.6172	-15.8235	105.9008
3.9873	-6.3026	116.3488	5.5369	-10.874	111.2368	7.0865	-12.8519	108.8816	8.6361	-15.9154	105.7943
4.0062	-6.3704	116.2748	5.5558	-10.9143	111.1901	7.1054	-12.8611	108.8716	8.6549	-16.0094	105.6856
4.0251	-6.438	116.2009	5.5747	-10.9542	111.144	7.1243	-12.8702	108.8621	8.6738	-16.1053	105.5745
4.044	-6.5054	116.1273	5.5936	-10.9936	111.0984	7.1432	-12.8792	108.8531	8.6927	-16.2034	105.461
4.0629	-6.5727	116.0539	5.6125	-11.0327	111.0534	7.1621	-12.888	108.8445	8.7116	-16.3035	105.3449
4.0818	-6.6397	115.9807	5.6314	-11.0714	111.009	7.181	-12.8967	108.8363	8.7305	-16.4058	105.2262
4.1007	-6.7064	115.9078	5.6503	-11.1097	110.9651	7.1999	-12.9054	108.8283	8.7494	-16.5102	105.1047
4.1196	-6.773	115.835	5.6692	-11.1475	110.9217	7.2188	-12.9141	108.8206	8.7683	-16.6168	104.9804

8.7872	-16.7257	104.8531	10.3368	-36.4	84.3691	11.8864	-45.6552	77.0275	13.436	-50.5911	72.4394
8.8061	-16.8368	104.7229	10.3557	-36.721	84.0704	11.9053	-45.7103	76.9694	13.4549	-50.6635	72.3599
8.825	-16.9502	104.5895	10.3746	-37.0361	83.7809	11.9242	-45.7653	76.9114	13.4738	-50.7363	72.2808
8.8439	-17.0659	104.4529	10.3935	-37.3448	83.5012	11.9431	-45.8203	76.8535	13.4926	-50.8095	72.2019
8.8628	-17.184	104.313	10.4124	-37.6463	83.2317	11.962	-45.8752	76.7958	13.5115	-50.8831	72.1231
8.8817	-17.3046	104.1695	10.4313	-37.9399	82.9728	11.9809	-45.9301	76.7383	13.5304	-50.9572	72.0444
8.9006	-17.4275	104.0224	10.4502	-38.2251	82.7252	11.9998	-45.985	76.6809	13.5493	-51.0317	71.9658
8.9195	-17.553	103.8713	10.4691	-38.5013	82.4898	12.0187	-46.0398	76.6237	13.5682	-51.1066	71.887
8.9384	-17.6811	103.7158	10.488	-38.7681	82.2673	12.0376	-46.0946	76.5666	13.5871	-51.182	71.8082
8.9573	-17.8117	103.555	10.5069	-39.0251	82.0585	12.0565	-46.1494	76.5097	13.606	-51.2578	71.7293
8.9762	-17.945	103.3859	10.5258	-39.2721	81.8641	12.0754	-46.2041	76.4529	13.6249	-51.3341	71.6502
8.9951	-18.081	103.2027	10.5447	-39.509	81.6844	12.0942	-46.2589	76.3963	13.6438	-51.4108	71.5711
9.014	-18.2197	103.0452	10.5636	-39.7357	81.5188	12.1131	-46.3137	76.3397	13.6627	-51.4879	71.4918
9.0329	-18.3612	102.8847	10.5825	-39.9522	81.3667	12.132	-46.3685	76.2832	13.6816	-51.5655	71.4123
9.0518	-18.5056	102.7211	10.6014	-40.1587	81.2269	12.1509	-46.4234	76.2269	13.7005	-51.6436	71.3328
9.0707	-18.6529	102.5545	10.6203	-40.3554	81.098	12.1698	-46.4783	76.1706	13.7194	-51.7221	71.253
9.0896	-18.8031	102.3847	10.6392	-40.5427	80.9787	12.1887	-46.5332	76.1144	13.7383	-51.801	71.1732
9.1085	-18.9564	102.2117	10.6581	-40.7207	80.8681	12.2076	-46.5882	76.0584	13.7572	-51.8805	71.0932
9.1274	-19.1128	102.0354	10.677	-40.8899	80.7653	12.2265	-46.6432	76.0024	13.7761	-51.9603	71.0132
9.1463	-19.2723	101.8559	10.6959	-41.0507	80.6699	12.2454	-46.6983	75.9467	13.795	-52.0406	70.933
9.1652	-19.435	101.6729	10.7147	-41.2034	80.5817	12.2643	-46.7535	75.891	13.8139	-52.1214	70.8527
9.1841	-19.601	101.4866	10.7336	-41.3483	80.5005	12.2832	-46.8088	75.8356	13.8328	-52.2026	70.7723
9.203	-19.7702	101.2969	10.7525	-41.4858	80.4263	12.3021	-46.8641	75.7804	13.8517	-52.2843	70.6917
9.2219	-19.9429	101.1039	10.7714	-41.6162	80.3589	12.321	-46.9196	75.7253	13.8706	-52.3664	70.6111
9.2408	-20.119	100.9077	10.7903	-41.7399	80.2981	12.3399	-46.9751	75.6705	13.8895	-52.449	70.5303
9.2597	-20.2987	100.7083	10.8092	-41.8574	80.2434	12.3588	-47.0308	75.6157	13.9084	-52.532	70.4494
9.2786	-20.4819	100.5057	10.8281	-41.9688	80.1942	12.3777	-47.0866	75.5611	13.9273	-52.6155	70.3684
9.2975	-20.6687	100.3	10.847	-42.0748	80.1495	12.3966	-47.1425	75.5064	13.9462	-52.6994	70.2872
9.3164	-20.8592	100.0911	10.8659	-42.1757	80.1084	12.4155	-47.1985	75.4518	13.9651	-52.7838	70.2059
9.3352	-21.0535	99.8789	10.8848	-42.272	80.0695	12.4344	-47.2547	75.3969	13.984	-52.8686	70.1243
9.3541	-21.2515	99.663	10.9037	-42.3641	80.0318	12.4533	-47.311	75.3419	14.0029	-52.9538	70.0426
9.373	-21.4533	99.4432	10.9226	-42.4524	79.994	12.4722	-47.3675	75.2865	14.0218	-53.0395	69.9607
9.3919	-21.659	99.2191	10.9415	-42.5374	79.9551	12.4911	-47.4241	75.2307	14.0407	-53.1256	69.8786
9.4108	-21.8687	98.9903	10.9604	-42.6195	79.9143	12.51	-47.4809	75.1744	14.0596	-53.2122	69.7962
9.4297	-22.0822	98.756	10.9793	-42.699	79.871	12.5289	-47.5379	75.1175	14.0785	-53.2992	69.7135
9.4486	-22.2998	98.5156	10.9982	-42.7764	79.825	12.5478	-47.595	75.0598	14.0974	-53.3866	69.6306
9.4675	-22.5213	98.2679	11.0171	-42.8517	79.7762	12.5667	-47.6523	75.0014	14.1163	-53.4745	69.5474
9.4864	-22.7468	98.0107	11.036	-42.9255	79.7247	12.5856	-47.7098	74.9421	14.1352	-53.5627	69.4639
9.5053	-22.9764	97.7373	11.0549	-42.9977	79.6708	12.6045	-47.7676	74.882	14.1541	-53.6514	69.38
9.5242	-23.2101	97.4419	11.0738	-43.0688	79.6148	12.6234	-47.8255	74.821	14.1729	-53.7406	69.2958
9.5431	-23.4478	97.1938	11.0927	-43.1387	79.5572	12.6423	-47.8836	74.759	14.1918	-53.8301	69.2112
9.562	-23.6896	96.9423	11.1116	-43.2076	79.4982	12.6612	-47.9419	74.6962	14.2107	-53.92	69.1262
9.5809	-23.9355	96.6877	11.1305	-43.2756	79.4382	12.6801	-48.0005	74.6327	14.2296	-54.0104	69.0408
9.5998	-24.1855	96.4302	11.1494	-43.3429	79.3775	12.699	-48.0593	74.5686	14.2485	-54.1011	68.9549
9.6187	-24.4395	96.17	11.1683	-43.4094	79.3163	12.7179	-48.1183	74.5041	14.2674	-54.1923	68.8686
9.6376	-24.6977	95.907	11.1872	-43.4753	79.2549	12.7368	-48.1776	74.4397	14.2863	-54.2838	68.7818
9.6565	-24.9598	95.6412	11.2061	-43.5406	79.1933	12.7557	-48.2371	74.376	14.3052	-54.3757	68.6945
9.6754	-25.226	95.3725	11.225	-43.6053	79.1317	12.7746	-48.2969	74.3136	14.3241	-54.4681	68.6066
9.6943	-25.4961	95.101	11.2439	-43.6694	79.07	12.7934	-48.357	74.2534	14.343	-54.5607	68.5183
9.7132	-25.7703	94.8264	11.2628	-43.7331	79.0083	12.8123	-48.4173	74.1962	14.3619	-54.6538	68.4295
9.7321	-26.0483	94.5487	11.2817	-43.7963	78.9467	12.8312	-48.4778	74.1432	14.3808	-54.7472	68.3401
9.751	-26.3302	94.2679	11.3006	-43.859	78.885	12.8501	-48.5387	74.0952	14.3997	-54.841	68.2502
9.7699	-26.616	93.984	11.3195	-43.9213	78.8233	12.869	-48.5998	74.0532	14.4186	-54.9352	68.1598
9.7888	-26.9056	93.6968	11.3384	-43.9832	78.7615	12.8879	-48.6613	74.0187	14.4375	-55.0297	68.0689
9.8077	-27.1989	93.4063	11.3573	-44.0446	78.6996	12.9068	-48.723	73.9941	14.4564	-55.1245	67.9775
9.8266	-27.4958	93.1125	11.3762	-44.1057	78.6377	12.9257	-48.785	73.9841	14.4753	-55.2197	67.8856
9.8455	-27.7964	92.8152	11.3951	-44.1664	78.5757	12.9446	-48.8473	73.9985	14.4942	-55.3152	67.7932
9.8644	-28.1006	92.5143	11.4139	-44.2268	78.5137	12.9635	-48.91	74.0567	14.5131	-55.4111	67.7003
9.8833	-28.4083	92.2097	11.4328	-44.2868	78.4517	12.9824	-48.9729	74.1956	14.532	-55.5072	67.607
9.9022	-28.7194	91.9014	11.4517	-44.3465	78.3898	13.0013	-49.0362	74.4766	14.5509	-55.6037	67.5132
9.9211	-29.0338	91.5895	11.4706	-44.4059	78.328	13.0202	-49.0998	74.9812	14.5698	-55.7005	67.419
9.94	-29.3515	91.274	11.4895	-44.465	78.2664	13.0391	-49.1638	75.7367	14.5887	-55.7976	67.3244
9.9589	-29.6723	90.9553	11.5084	-44.5237	78.205	13.058	-49.228	76.4129	14.6076	-55.895	67.2294
9.9778	-29.9962	90.6337	11.5273	-44.5822	78.1439	13.0769	-49.2927	76.2926	14.6265	-55.9927	67.134
9.9967	-30.323	90.3093	11.5462	-44.6405	78.0831	13.0958	-49.3576	75.5698	14.6454	-56.0906	67.0382
10.0156	-30.6525	89.9825	11.5651	-44.6985	78.0227	13.1147	-49.4229	74.9097	14.6643	-56.1889	66.9421
10.0344	-30.9845	89.6535	11.584	-44.7562	77.9627	13.1336	-49.4886	74.4532	14.6832	-56.2874	66.8456
10.0533	-31.319	89.3225	11.6029	-44.8137	77.9031	13.1525	-49.5546	74.1394	14.7021	-56.3861	66.7489
10.0722	-31.6556	88.9898	11.6218	-44.871	77.8438	13.1714	-49.621	73.9083	14.721	-56.4852	66.6518
10.0911	-31.9941	88.6555	11.6407	-44.9281	77.7848	13.1903	-49.6878	73.7259	14.7399	-56.5844	66.5545
10.11	-32.3343	88.32	11.6596	-44.9849	77.7261	13.2092	-49.7549	73.5743	14.7588	-56.684	66.4568
10.1289	-32.6759	87.9836	11.6785	-45.0416	77.6676	13.2281	-49.8224	73.4433	14.7777	-56.7837	66.3589
10.1478	-33.0185	87.6467	11.6974	-45.0981	77.6093	13.247	-49.8903	73.3265	14.7966	-56.8837	66.2608
10.1667	-33.3618	87.3096	11.7163	-45.1544	77.5511	13.2659	-49.9586	73.2198	14.8155	-56.9839	66.1624
10.1856	-33.7054	86.9728	11.7352	-45.2106	77.493	13.2848	-50.0273	73.1205	14.8344	-57.0843	66.0638
10.2045	-34.0487	86.6366	11.7541	-45.2666	77.4348	13.3037	-50.0964	73.0265	14.8533	-57.1849	65.965
10.2234	-34.3914	86.3016	11.773	-45.3225	77.3767	13.3226	-50.1658	72.9365	14.8721	-57.2857	65.866
10.2423	-34.7328	85.9686	11.7919	-45.3782	77.3185	13.3415	-50.2357	72.8495	14.891	-57.3867	65.7667
10.2612	-35.0723	85.6384	11.8108	-45.4338	77.2603	13.3604	-50.3059	72.7648	14.9099	-57.4878	65.6673
10.2801	-35.4095	85.3122	11.8297	-45.4893	77.2021	13.3793	-50.3766	72.6818	14.9288	-57.5892	65.5677
10.299	-35.7436	84.9911	11.8486	-45.5447	77.1438	13.3982	-50.4477	72.6001	14.9477	-57.6907	65.4679
10.3179	-36.074	84.6763	11.8675	-45.6	77.0856	13.4171	-50.5192	72.5194	14.9666	-57.7924	65.368

14.9855	-57.8942	65.268	15.0233	-58.0983	65.0675	15.0611	-58.303	64.8666	15.0989	-58.508	64.6656
15.0044	-57.9962	65.1678	15.0422	-58.2006	64.9671	15.08	-58.4054	64.7661	15.1178	-58.6108	64.5651

