Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

Quantum Mechanical Tunnelling:

The Missing Term to Achieve sub-kJ mol^{-1} Barrier Heights

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Details of CCSDT(Q)/CBS Calculations

Valence post-CCSD(T) contributions up to CCSDT(Q) are calculated in conjunction with the cc-pVDZ basis set as well as truncated versions of the cc-pVDZ and cc-pVTZ basis sets.[1] Regular cc-pV*n*Z basis sets are denoted by V*n*Z throughout the text. The truncated basis sets are the VDZ basis set without the p functions on hydrogens (denoted by VDZ(no p on H)), the VDZ basis set without the p functions on hydrogen and d functions on carbon (denoted by VDZ(no d)), and a basis set which combines the sp part of the VTZ basis set with the d function from the VDZ basis set on carbon and the s part of the VTZ basis set with the p function from the VDZ basis set on hydrogen (denoted by VTZ(no f 1d)). Table S1 summarizes the largest basis sets that are used for the post-CCSD(T) calculations for each of the systems. For a detailed discussion of the use of these truncated basis sets in post-CCSD(T) calculations of reaction barrier heights see refs. 2 and 3.

Table S1. Largest basis sets used for the final CCSDT–CCSD(T) (T–(T)) and CCSDT(Q)–CCSDT ((Q)) components.

	T–(T)	(Q)
C_7H_6	VTZ(no f 1d)	VDZ
C_8H_8	VDZ	VDZ
C_9H_{10}	VDZ	VDZ(no p on H)
$C_{10}H_{10}$	VDZ	VDZ(no d)

In order to estimate the accuracy of our best post-CCSD(T) components, it is worthwhile to examine the magnitude of the CCSDT–CCSD(T) (T–(T)) and CCSDT(Q)–CCSDT ((Q)) components obtained with the various basis sets. These results are summarized in Table S2. For the smaller norbornylidene hydrocarbon (C_7H_6) we were able to obtain the higher-order T_3 effects (CCSDT–CCSD(T)) in conjunction with the cc-pVTZ(no f 1d) basis set (as prescribed in the W3lite[4] and W3lite-F12[5] thermochemical protocols). This contribution amounts to as much as –1.74 kJ mol^{-1}. Calculating the T–(T) contribution with the VDZ basis set results in a slightly lower contribution of –1.64 kJ mol^{-1}, and removing the p functions from hydrogens (in the VDZ(no p on H) basis set) has no visible effect. Nevertheless, further omission of the d functions from carbons (in the VDZ(no d) basis set) results in a significantly lower value of –0.91 kJ mol^{-1}. These results indicate that the T–(T)/VDZ level of theory should provide a fairly robust estimation of the higher-order T_3 effects and this is the level of theory used for the larger hydrocarbons in this work.

Table S2. CCSDT–CCSD(T) (T–(T)) and CCSDT(Q)–CCSDT ((Q)) contributions to the reaction barrier heights (in kJ mol^{-1}).

		C_7H_6	C_8H_8	C_9H_{10}	$C_{10}H_{10}$
T–(T)	VDZ(no d)	–0.91	0.47	0.64	0.80
	VDZ(no p on H)	–1.64	1.30	1.55	1.68
	VDZ	–1.64	1.37	1.62	1.74
	VTZ(no f 1d)	–1.74	N/A	N/A	N/A
(Q)	VDZ(no d)	0.19	–0.91	–0.95	–1.12
	VDZ(no p on H)	0.22	–2.20	–2.20	N/A
	VDZ	0.21	–2.32	N/A	N/A
Best post-CCSD(T) cont.[a]		–1.53	–0.95	–0.58	+0.61

[a]Best overall CCSDT(Q) – CCSD(T) contribution.

For two systems (C_7H_6 and C_8H_8) we were able to calculate the quasiperturbative T_4 effects (CCSDT(Q)–CCSDT) in conjunction with the VDZ basis set, as prescribed in the W4lite thermochemical protocol.[6] For C_7H_6 the (Q)/VDZ contribution to the reaction barrier height is fairly small and has a weak basis set dependency, such that the VDZ(no d) and VDZ basis sets give indistinguishable results. However, the (Q) component of the reaction barrier height in C_8H_8 exhibits a much more pronounced basis set dependency. At the (Q)/VDZ level we obtain a fairly large contribution of –2.32 kJ mol^{-1}. Calculating the (Q) contribution with the VDZ(no p on H) basis set results in a slightly lower contribution of –2.20 kJ mol^{-1}. However, removing the d functions from carbons (in the VDZ(no d) basis set), as was done in ref. 7, results in a significantly lower value of –0.91 kJ mol^{-1}. These results indicate that the (Q)/VDZ(no p on H) level of theory should provide a fairly robust estimation of the quasiperturbative T_4 effects. This is the level of theory used for the larger C_9H_{10} hydrocarbon. However, for the $C_{10}H_{10}$ hydrocarbon we were only able to obtain the (Q)/VDZ(no d) component, which suggests that this component is underestimated by 1–2 kJ mol^{-1}.

Overall, we obtain post-CCSD(T) (CCSDT(Q) – CCSD(T)) contributions of –1.53 (C_7H_6), –0.95 (C_8H_8), –0.58 (C_9H_{10}), and +0.61 ($C_{10}H_{10}$) kJ mol^{-1}. However, as discussed above the (Q)/VDZ(no d) contribution in bullvalene likely represents an underestimation and the use of a larger basis set in the (Q) calculation is likely to reduce the overall post-CCSD(T) contribution for $C_{10}H_{10}$ by 1–2 kJ mol^{-1}.

References

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Table S3. B3LYP-D3BJ/Def2-TZVPP optimized geometries (in Å).

NBY reactant (C_7H_6, C_s)
C 0.283648 0.058590 1.144226
C 0.283648 −1.361519 −0.664316
C −0.884125 0.875869 0.683420
C −0.884125 0.875869 −0.683420
C 0.283648 −1.361519 0.664316
H 0.610050 0.271162 2.154487
C 0.283648 0.058590 −1.144226
H 0.610050 0.271162 −2.154487
C 0.832507 0.971393 0.000000
H −1.414568 1.594288 1.290900
H −1.414568 1.594288 −1.290900
H 0.207968 −2.217267 −1.318471
H 0.207968 −2.217267 1.318471

NBY TS (C_7H_6, C_{2v})
H 0.000000 2.141623 0.673912
C 0.000000 1.122880 0.301197
C −1.267934 −0.669138 −0.408862
C 1.267934 −0.669138 −0.408862
C −0.000000 −1.122880 0.301197
C 1.267934 0.669138 −0.408862
C −1.267934 0.669138 −0.408862
H −0.000000 −2.141623 0.673912
H 2.030435 1.327175 −0.797724
H −2.030435 1.327175 −0.797724
H −2.030435 −1.327175 −0.797724
H 2.030435 −1.327175 −0.797724
C 0.000000 0.000000 1.340234

SBV reactant (C_8H_8, C_s)
C 0.629841 1.001437 0.804990
C −0.630881 1.045601 −0.000000
C 0.629841 −0.265023 1.550844
H 1.398718 −0.541433 2.258623
C 0.629841 1.001437 −0.804990
C 0.629841 −0.265023 −1.550844
C −0.394911 −1.043451 −1.178732
H 1.058357 1.896620 −1.233342
H 1.398718 −0.541433 −2.258623
C −0.394911 −1.043451 1.178732
C −1.138254 −0.420630 0.000000
H −0.574511 −2.055398 1.514277
H −0.574511 −2.055398 −1.514277
H 1.058357 1.896620 1.233342
H −2.218547 −0.552777 0.000000
H −1.309010 1.887808 −0.000000

SBV TS (C_8H_8, C_s)
C 0.425144 −1.063442 1.063866
C 1.154417 −0.299030 0.000000
C −0.593858 −0.296207 1.603344
H −1.330449 −0.663598 2.303538
C 0.425144 −1.063442 −1.063866
C −0.593858 −0.296207 −1.603344
C −0.593858 0.979318 −1.063701
H 0.667118 −2.080149 −1.329849
H −1.330449 −0.663598 −2.303538
C −0.593858 0.979318 1.063701
C 0.455609 1.102020 −0.000000
H −1.260391 1.784270 1.329736
H −1.260391 1.784270 −1.329736
H 0.667118 −2.080149 1.329849
H 1.096248 1.980948 −0.000000
H 2.241913 −0.315978 0.000000

BBL reactant (C_9H_{10}, C_s)
C 0.053300 1.403469 0.000000
C −0.752559 0.956918 1.197264
H 0.188263 2.483833 0.000000
H −1.378872 1.672326 1.713500
C −0.752559 −0.338273 1.531549
C 0.060263 −1.306361 0.791943
H −1.378935 −0.704885 2.334678
C 1.231066 −0.796968 0.000000
C −0.752559 0.956918 −1.197264
C −0.752559 −0.338273 −1.531549
H −1.378872 1.672326 −1.713500
C 0.060263 −1.306361 −0.791943
H 2.125857 −1.404904 0.000000
H −1.378935 −0.704885 −2.334678
C 1.427494 0.697661 0.000000
H 1.991143 1.003116 −0.883881
H 1.991143 1.003116 0.883881
H 0.143154 −2.296220 1.217249
H 0.143154 −2.296220 −1.217249

BBL TS (C_9H_{10}, C_{2v})
C 1.242472 −0.000000 0.699967
C 1.208560 1.056543 −0.357176
H 2.162271 −0.000000 1.279876
H 2.143118 1.398968 −0.776926
C 0.000000 1.540671 −0.828396
C −1.208560 1.056543 −0.357176
H 0.000000 2.247865 −1.647877
C −1.242472 0.000000 0.699967
C 1.208560 −1.056543 −0.357176
C −0.000000 −1.540671 −0.828396
H 2.143118 −1.398968 −0.776926
C −1.208560 −1.056543 −0.357176
H −2.143118 −1.398968 −0.776926
H −2.162271 0.000000 1.279876
H −0.000000 −2.247865 −1.647877
H −2.143118 1.398968 −0.776926
C 0.000000 0.000000 1.584878
H 0.000000 −0.883940 2.223911
H 0.000000 0.883940 2.223911

BV reactant ($C_{10}H_{10}$, C_{3v})
C 0.000000 0.000000 1.547026
C 1.245123 −0.718872 1.073250
C 0.000000 1.437744 1.073250
H 0.000000 0.000000 2.635291
H 1.915621 −1.105984 1.830202
H 0.000000 2.211969 1.830202
C −0.000000 1.793889 −0.213058
C −0.000000 0.883563 −1.364343
H −0.000000 2.850185 −0.454919
C 1.553553 −0.896944 −0.213058
C 0.765188 −0.441781 −1.364343
C −1.245123 −0.718872 1.073250
C −1.553553 −0.896944 −0.213058
H −1.915621 −1.105984 1.830202
C −0.765188 −0.441781 −1.364343
H −1.197361 −0.691296 −2.322859
H 2.468333 −1.425092 −0.454919
H 1.197361 −0.691296 −2.322859
H −2.468333 −1.425092 −0.454919
H 0.000000 1.382593 −2.322859

BV TS ($C_{10}H_{10}$, C_{2v})
C 0.000000 1.499619 0.469482
C 0.000000 0.662790 1.711687
C −1.061310 1.241875 −0.561027
H 0.000000 2.551591 0.740440
H 0.000000 1.193917 2.655847
H −1.437610 2.114113 −1.077231
C −1.516777 0.000000 −0.969072
C −1.061310 −1.241875 −0.561027
H −2.233378 0.000000 −1.782079
C −0.000000 −0.662790 1.711687
C −0.000000 −1.499619 0.469482
C 1.061310 1.241875 −0.561027
C 1.516777 −0.000000 −0.969072
H 1.437610 2.114113 −1.077231
C 1.061310 −1.241875 −0.561027
H 1.437610 −2.114113 −1.077231
H −0.000000 −1.193917 2.655847
H −0.000000 −2.551591 0.740440
H 2.233378 −0.000000 −1.782079
H −1.437610 −2.114113 −1.077231

Table S4. Summary of key experimental enthalpic reaction barrier heights (in kJ mol^{-1}).[a]

	Year	Method	Temp (K)	Solvent	$\Delta H^{\ddagger}$	Ref.
Bullvalene	1967	^{1}H-NMR	233–273		45.6±0.4	*b*
	1974	^{13}C-NMR	206–401	$C_2H_2Cl_4$	55.6±0.4	*c*
	1974	^{13}C-NMR	234.1–382.2	$CDCl_3$	58.2±2.9	*d*
	1974	^{1}H,^{13}C-NMR	233–413	CS_2	52.9±0.3	*e*
	1984	^{2}H-NMR	238–388	Liq. cryst.	55.6	*f*
	1992	^{1}H-NMR	340.8–366.6	Gas	55.2±1.3	*g*
	1992	^{1}H-NMR	272.5–341.2	CS_2	52.7±1.3	*g*
Semibullvalene	1974	^{1}H,^{13}C-NMR	103–173	CF_2Cl_2	20.1±0.8	*h*
	1989	^{13}C-NMR	118–206	CF_2CI_2	21.9±0.4	*i*
Barbaralane	1985	^{13}C-NMR	146–305	THF/CS_2	30.7±0.2	*j*

[a]This summary is not intended as an exhaustive review of all available literature.

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Full tunnelling graphs

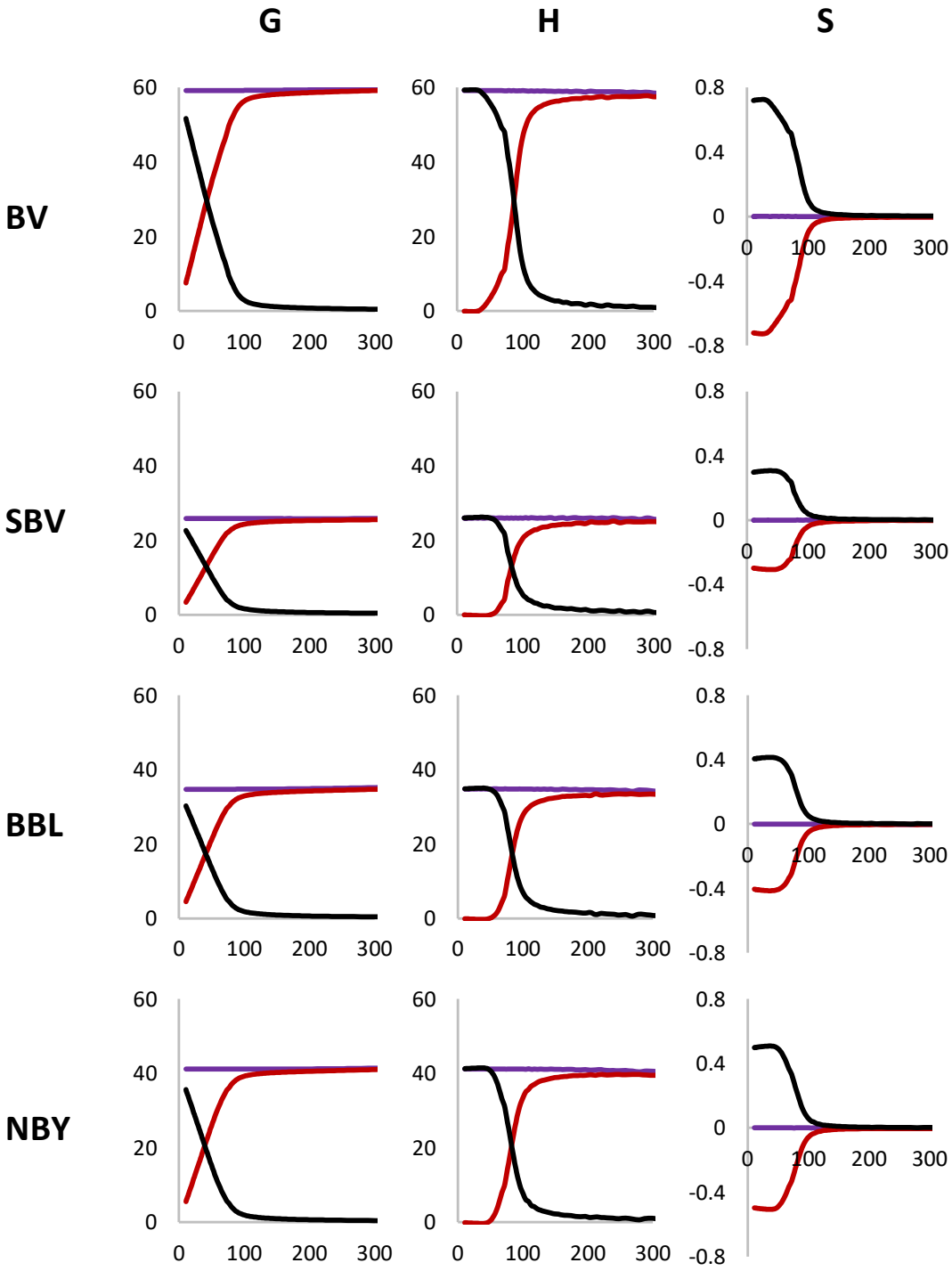

Figure S1. Gibbs energy, enthalpy, and entropy activation parameters as a function of the temperature (in K) for the four systems. In red the QMT included effective values ($\Delta G^{\ddagger}$, $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ from eqs. 2 and 3), in purple the classical values ($\Delta G_C^{\ddagger}$, $\Delta H_C^{\ddagger}$ and $\Delta S_C^{\ddagger}$ from eqs. 5 to 7), and in black the tunnelling corrections (C_f^G, C_f^H and C_f^S). *G* and *H* values in kJ mol^{-1}, *S* in kJ K^{-1} mol^{-1}.

Full QMT and barrier parameters tables

Temperature (in K); classical (CVT) and QMT included (+SCT) rate constants (in s^{-1}); transmission coefficients (κ); classical, QMT included and tunnelling corrections for Gibbs energies, enthalpies, entropies and Arrhenius activation energies (in kJ mol^{-1}, except entropies in J K^{-1} mol^{-1}). E_a, H and S were calculated with the derivative method (eq. 3), and therefore they are shown against the mean temperature between adjacent temperatures.

NBY				$\Delta G^{\ddagger}$		
T	CVT	CVT+SCT	kappa	Class.	QMT	Corr.
10.54	2.08E-193	7.06E-15	3.39E+178	41.169	5.144	36.025
11.28	5.42E-180	7.06E-15	1.30E+165	41.169	5.512	35.657
12.07	1.74E-167	7.06E-15	4.06E+152	41.169	5.904	35.264
12.91	7.31E-156	7.06E-15	9.66E+140	41.168	6.323	34.846
13.82	7.28E-145	7.06E-15	9.70E+129	41.168	6.776	34.392
14.79	1.25E-134	7.06E-15	5.65E+119	41.168	7.260	33.908
15.82	3.92E-125	7.06E-15	1.80E+110	41.168	7.774	33.393
16.93	3.44E-116	7.06E-15	2.05E+101	41.167	8.329	32.837
18.11	6.95E-108	7.06E-15	1.02E+93	41.167	8.920	32.247
19.38	4.50E-100	7.06E-15	1.57E+85	41.166	9.557	31.610
20.74	9.11E-93	7.06E-15	7.75E+77	41.166	10.239	30.927
22.19	5.81E-86	7.06E-15	1.22E+71	41.166	10.967	30.198
23.74	1.32E-79	7.06E-15	5.35E+64	41.165	11.747	29.419
25.41	1.27E-73	7.06E-15	5.56E+58	41.165	12.587	28.578
27.18	4.42E-68	7.06E-15	1.60E+53	41.164	13.479	27.685
29.09	7.41E-63	7.06E-15	9.53E+47	41.164	14.443	26.721
31.12	5.27E-58	7.06E-15	1.34E+43	41.163	15.468	25.694
33.30	1.88E-53	7.07E-15	3.76E+38	41.163	16.570	24.593
35.63	3.37E-49	7.08E-15	2.10E+34	41.162	17.749	23.412
38.13	3.27E-45	7.10E-15	2.17E+30	41.161	19.015	22.145
40.80	1.72E-41	7.18E-15	4.17E+26	41.160	20.366	20.794
43.65	5.08E-38	7.35E-15	1.45E+23	41.159	21.805	19.354
46.71	9.18E-35	7.73E-15	8.42E+19	41.158	23.340	17.818
49.98	1.01E-31	8.57E-15	8.49E+16	41.157	24.959	16.198
53.47	6.95E-29	1.04E-14	1.50E+14	41.157	26.646	14.511
57.22	3.22E-26	1.44E-14	4.47E+11	41.155	28.392	12.763
61.22	9.83E-24	2.39E-14	2.43E+09	41.154	30.154	11.001
65.51	2.10E-21	5.04E-14	2.40E+07	41.153	31.897	9.256
70.09	3.14E-19	1.40E-13	4.46E+05	41.151	33.571	7.580
75.00	3.43E-17	4.83E-13	1.41E+04	41.150	35.193	5.957
78.00	4.51E-16	1.22E-12	2.71E+03	41.150	36.025	5.125
81.12	5.40E-15	3.54E-12	6.56E+02	41.148	36.774	4.374
84.36	5.85E-14	1.18E-11	2.02E+02	41.148	37.426	3.722
87.74	5.84E-13	4.53E-11	7.76E+01	41.147	37.973	3.174
91.25	5.32E-12	1.95E-10	3.67E+01	41.146	38.414	2.732
94.90	4.46E-11	9.16E-10	2.05E+01	41.145	38.761	2.385
98.69	3.44E-10	4.50E-09	1.31E+01	41.145	39.035	2.110
102.64	2.47E-09	2.26E-08	9.15E+00	41.142	39.253	1.889
106.75	1.64E-08	1.14E-07	6.95E+00	41.145	39.424	1.721
111.02	1.02E-07	5.57E-07	5.46E+00	41.139	39.572	1.567
115.46	5.87E-07	2.66E-06	4.53E+00	41.142	39.692	1.451
120.08	3.18E-06	1.22E-05	3.84E+00	41.141	39.798	1.342
124.88	1.61E-05	5.39E-05	3.35E+00	41.142	39.887	1.255
129.88	7.71E-05	2.29E-04	2.97E+00	41.140	39.965	1.176
135.07	3.46E-04	9.25E-04	2.67E+00	41.142	40.038	1.104
140.47	1.47E-03	3.58E-03	2.44E+00	41.143	40.104	1.040
146.09	5.93E-03	1.33E-02	2.24E+00	41.143	40.162	0.981
151.94	2.27E-02	4.74E-02	2.09E+00	41.144	40.214	0.930
158.01	8.24E-02	1.61E-01	1.95E+00	41.146	40.266	0.880
164.33	2.85E-01	5.26E-01	1.85E+00	41.149	40.312	0.837
170.91	9.43E-01	1.65E+00	1.75E+00	41.153	40.358	0.795
177.74	2.98E+00	4.97E+00	1.67E+00	41.155	40.399	0.756
184.85	9.00E+00	1.44E+01	1.60E+00	41.162	40.440	0.722
192.25	2.61E+01	4.02E+01	1.54E+00	41.171	40.481	0.690
199.94	7.28E+01	1.08E+02	1.48E+00	41.178	40.522	0.656
207.94	1.95E+02	2.81E+02	1.44E+00	41.190	40.558	0.632
216.25	5.04E+02	7.03E+02	1.39E+00	41.199	40.601	0.598
224.90	1.26E+03	1.71E+03	1.36E+00	41.207	40.636	0.571
233.90	3.03E+03	4.01E+03	1.32E+00	41.226	40.681	0.545
243.25	7.05E+03	9.13E+03	1.30E+00	41.245	40.722	0.523
252.99	1.59E+04	2.02E+04	1.27E+00	41.269	40.765	0.503
263.10	3.48E+04	4.33E+04	1.24E+00	41.290	40.812	0.478
273.63	7.39E+04	9.05E+04	1.22E+00	41.318	40.857	0.461
284.57	1.52E+05	1.84E+05	1.21E+00	41.357	40.905	0.452
295.96	3.06E+05	3.64E+05	1.19E+00	41.387	40.960	0.427
307.79	5.99E+05	7.01E+05	1.17E+00	41.423	41.020	0.402
320.11	1.14E+06	1.32E+06	1.16E+00	41.472	41.082	0.390
332.91	2.12E+06	2.43E+06	1.15E+00	41.522	41.144	0.378

	E_a			$\Delta H^{\ddagger}$			$\Delta S^{\ddagger}$		
$\bar{T}$	Class.	QMT	Corr.	Class.	QMT	Corr.	Class.	QMT	Corr.
10.91	41.266	0.000	41.266	41.175	-0.091	41.266	5.662E-04	-0.4967	0.4972
11.68	41.265	0.000	41.265	41.168	-0.097	41.265	-9.975E-05	-0.4972	0.4971
12.49	41.280	0.000	41.280	41.176	-0.104	41.280	5.944E-04	-0.4978	0.4984
13.37	41.282	0.000	41.282	41.171	-0.111	41.282	2.438E-04	-0.4983	0.4986
14.31	41.289	0.000	41.289	41.170	-0.119	41.289	1.455E-04	-0.4989	0.4991
15.31	41.300	0.000	41.300	41.172	-0.127	41.300	3.063E-04	-0.4995	0.4998
16.38	41.313	0.000	41.313	41.177	-0.136	41.313	5.956E-04	-0.5000	0.5006
17.52	41.315	0.000	41.315	41.169	-0.146	41.315	1.372E-04	-0.5006	0.5007
18.75	41.327	0.000	41.327	41.172	-0.156	41.327	2.712E-04	-0.5012	0.5014
20.06	41.340	0.000	41.340	41.173	-0.167	41.340	3.639E-04	-0.5017	0.5021
21.47	41.348	0.000	41.348	41.170	-0.178	41.348	1.814E-04	-0.5023	0.5025
22.97	41.359	0.000	41.359	41.168	-0.191	41.359	1.049E-04	-0.5028	0.5029
24.58	41.377	0.000	41.377	41.172	-0.204	41.377	2.927E-04	-0.5034	0.5037
26.30	41.397	0.000	41.397	41.178	-0.218	41.397	5.286E-04	-0.5040	0.5045
28.14	41.404	0.000	41.404	41.171	-0.234	41.404	2.413E-04	-0.5045	0.5048
30.11	41.424	0.000	41.424	41.174	-0.250	41.424	3.718E-04	-0.5051	0.5055
32.21	41.430	0.006	41.424	41.162	-0.262	41.424	-2.050E-05	-0.5055	0.5055
34.47	41.467	0.006	41.461	41.180	-0.280	41.461	5.203E-04	-0.5060	0.5065
36.88	41.479	0.013	41.466	41.173	-0.294	41.466	3.115E-04	-0.5064	0.5067
39.47	41.507	0.054	41.453	41.179	-0.274	41.453	4.830E-04	-0.5059	0.5064
42.23	41.517	0.122	41.395	41.166	-0.229	41.395	1.502E-04	-0.5048	0.5049
45.18	41.547	0.279	41.268	41.171	-0.096	41.268	2.815E-04	-0.5017	0.5020
48.35	41.571	0.612	40.959	41.170	0.211	40.959	2.420E-04	-0.4952	0.4954
51.73	41.600	1.232	40.368	41.170	0.802	40.368	2.525E-04	-0.4833	0.4836
55.35	41.640	2.208	39.433	41.181	1.748	39.433	4.500E-04	-0.4657	0.4661
59.22	41.659	3.689	37.969	41.167	3.197	37.969	2.038E-04	-0.4403	0.4405
63.37	41.695	5.799	35.896	41.169	5.273	35.896	2.409E-04	-0.4064	0.4067
67.80	41.740	8.516	33.224	41.176	7.953	33.224	3.564E-04	-0.3655	0.3659
72.55	41.780	11.024	30.756	41.177	10.421	30.756	3.675E-04	-0.3303	0.3307
76.50	41.770	15.023	26.747	41.135	14.387	26.747	-2.014E-04	-0.2774	0.2772
79.56	41.862	17.962	23.900	41.201	17.301	23.900	6.516E-04	-0.2401	0.2407
82.74	41.842	21.143	20.699	41.154	20.455	20.699	7.129E-05	-0.2012	0.2012
86.05	41.893	24.493	17.400	41.178	23.778	17.400	3.562E-04	-0.1618	0.1621
89.50	41.900	27.683	14.217	41.156	26.939	14.217	1.102E-04	-0.1257	0.1259
93.08	41.943	30.517	11.426	41.169	29.743	11.426	2.487E-04	-0.0950	0.0953
96.80	41.974	32.706	9.268	41.170	31.901	9.268	2.549E-04	-0.0723	0.0725
100.67	42.033	34.411	7.622	41.196	33.574	7.622	5.204E-04	-0.0553	0.0559
104.70	41.961	35.869	6.091	41.090	34.999	6.091	-5.075E-04	-0.0414	0.0409
108.89	42.177	36.608	5.569	41.272	35.703	5.569	1.196E-03	-0.0349	0.0360
113.24	42.008	37.531	4.478	41.067	36.589	4.478	-6.525E-04	-0.0269	0.0262
117.77	42.158	38.004	4.154	41.179	37.025	4.154	3.192E-04	-0.0231	0.0234
122.48	42.130	38.591	3.539	41.112	37.573	3.539	-2.417E-04	-0.0185	0.0183
127.38	42.244	39.016	3.228	41.186	37.957	3.228	3.493E-04	-0.0155	0.0158
132.48	42.194	39.235	2.958	41.092	38.134	2.958	-3.690E-04	-0.0141	0.0137
137.77	42.260	39.535	2.724	41.114	38.390	2.724	-2.059E-04	-0.0122	0.0120
143.28	42.345	39.845	2.500	41.154	38.654	2.500	7.612E-05	-0.0103	0.0104
149.02	42.348	40.093	2.255	41.109	38.854	2.255	-2.290E-04	-0.0089	0.0087
154.98	42.396	40.212	2.185	41.108	38.923	2.185	-2.368E-04	-0.0085	0.0083
161.17	42.389	40.442	1.947	41.050	39.102	1.947	-6.076E-04	-0.0074	0.0068
167.62	42.465	40.572	1.893	41.072	39.179	1.893	-4.722E-04	-0.0069	0.0064
174.33	42.550	40.776	1.774	41.101	39.327	1.774	-3.047E-04	-0.0060	0.0057
181.30	42.467	40.873	1.594	40.960	39.366	1.594	-1.096E-03	-0.0058	0.0047
188.55	42.513	40.993	1.520	40.946	39.425	1.520	-1.174E-03	-0.0055	0.0043
196.10	42.631	41.072	1.559	41.001	39.442	1.559	-8.837E-04	-0.0054	0.0045
203.94	42.574	41.318	1.256	40.879	39.623	1.256	-1.497E-03	-0.0045	0.0030
212.10	42.723	41.257	1.466	40.960	39.494	1.466	-1.108E-03	-0.0051	0.0040
220.58	42.835	41.554	1.281	41.001	39.720	1.281	-9.147E-04	-0.0041	0.0032
229.40	42.642	41.419	1.222	40.735	39.512	1.222	-2.100E-03	-0.0050	0.0029
238.58	42.726	41.628	1.097	40.742	39.645	1.097	-2.067E-03	-0.0044	0.0024
248.12	42.725	41.717	1.007	40.662	39.655	1.007	-2.397E-03	-0.0044	0.0020
258.05	42.878	41.738	1.140	40.733	39.593	1.140	-2.117E-03	-0.0046	0.0025
268.37	42.810	41.906	0.904	40.579	39.675	0.904	-2.703E-03	-0.0043	0.0016
279.10	42.678	41.993	0.685	40.358	39.673	0.685	-3.509E-03	-0.0043	0.0008
290.27	43.018	41.943	1.075	40.605	39.530	1.075	-2.642E-03	-0.0048	0.0022
301.88	43.003	41.958	1.045	40.494	39.449	1.045	-3.019E-03	-0.0051	0.0021
313.95	42.790	42.082	0.708	40.180	39.472	0.708	-4.037E-03	-0.0050	0.0010
326.51	42.945	42.244	0.701	40.231	39.530	0.701	-3.878E-03	-0.0048	0.0010

SBV					$\Delta G^{\ddagger}$	
T	CVT	CVT+SCT	kappa	Class.	QMT	Corr.
10.54	7.10E-118	1.99E-04	2.80E+113	25.928	3.035	22.892
11.28	2.04E-109	1.99E-04	9.75E+104	25.928	3.255	22.673
12.07	1.58E-101	1.99E-04	1.26E+97	25.927	3.490	22.438
12.91	3.37E-94	1.99E-04	5.91E+89	25.927	3.740	22.188
13.82	2.92E-87	1.99E-04	6.82E+82	25.927	4.011	21.916
14.79	8.35E-81	1.99E-04	2.38E+76	25.927	4.301	21.626
15.82	8.19E-75	1.99E-04	2.43E+70	25.927	4.609	21.318
16.93	3.59E-69	1.99E-04	5.54E+64	25.927	4.942	20.985
18.11	6.26E-64	1.99E-04	3.18E+59	25.927	5.297	20.630
19.38	5.33E-59	1.99E-04	3.73E+54	25.927	5.679	20.248
20.74	2.18E-54	1.99E-04	9.13E+49	25.927	6.090	19.837
22.19	4.32E-50	1.99E-04	4.61E+45	25.927	6.528	19.399
23.74	4.46E-46	1.99E-04	4.46E+41	25.927	6.997	18.930
25.41	2.68E-42	1.99E-04	7.43E+37	25.927	7.504	18.423
27.18	8.48E-39	1.99E-04	2.35E+34	25.926	8.042	17.885
29.09	1.70E-35	1.99E-04	1.17E+31	25.926	8.623	17.303
31.12	1.98E-32	1.99E-04	1.01E+28	25.926	9.242	16.683
33.30	1.49E-29	1.99E-04	1.34E+25	25.927	9.909	16.018
35.63	7.30E-27	2.00E-04	2.74E+22	25.926	10.620	15.305
38.13	2.43E-24	2.00E-04	8.23E+19	25.925	11.387	14.538
40.80	5.48E-22	2.01E-04	3.67E+17	25.925	12.206	13.720
43.65	8.61E-20	2.04E-04	2.37E+15	25.926	13.078	12.848
46.71	9.94E-18	2.08E-04	2.09E+13	25.925	14.013	11.912
49.98	8.39E-16	2.15E-04	2.56E+11	25.925	15.008	10.916
53.47	5.27E-14	2.29E-04	4.35E+09	25.925	16.058	9.866
57.22	2.58E-12	2.54E-04	9.84E+07	25.924	17.168	8.756
61.22	9.71E-11	3.00E-04	3.09E+06	25.924	18.317	7.606
65.51	2.92E-09	3.94E-04	1.35E+05	25.923	19.489	6.434
70.09	7.01E-08	6.04E-04	8.62E+03	25.923	20.642	5.281
75.00	1.38E-06	1.05E-03	7.61E+02	25.923	21.786	4.137
78.00	7.11E-06	1.82E-03	2.56E+02	25.922	22.326	3.596
81.12	3.44E-05	3.50E-03	1.02E+02	25.922	22.804	3.118
84.36	1.57E-04	7.47E-03	4.76E+01	25.920	23.211	2.709
87.74	6.78E-04	1.75E-02	2.58E+01	25.920	23.549	2.372
91.25	2.77E-03	4.39E-02	1.58E+01	25.919	23.823	2.096
94.90	1.07E-02	1.16E-01	1.08E+01	25.920	24.040	1.881
98.69	3.94E-02	3.11E-01	7.89E+00	25.918	24.223	1.695
102.64	1.38E-01	8.48E-01	6.14E+00	25.919	24.370	1.549
106.75	4.64E-01	2.31E+00	4.98E+00	25.916	24.491	1.425
111.02	1.48E+00	6.19E+00	4.18E+00	25.918	24.597	1.321
115.46	4.55E+00	1.63E+01	3.58E+00	25.914	24.689	1.225
120.08	1.34E+01	4.22E+01	3.15E+00	25.911	24.766	1.145
124.88	3.78E+01	1.06E+02	2.80E+00	25.911	24.840	1.071
129.88	1.03E+02	2.62E+02	2.54E+00	25.908	24.900	1.008
135.07	2.69E+02	6.30E+02	2.34E+00	25.910	24.954	0.956
140.47	6.81E+02	1.47E+03	2.16E+00	25.906	25.008	0.899
146.09	1.67E+03	3.36E+03	2.01E+00	25.901	25.052	0.849
151.94	3.94E+03	7.48E+03	1.90E+00	25.903	25.094	0.810
158.01	9.02E+03	1.62E+04	1.80E+00	25.902	25.132	0.769
164.33	2.01E+04	3.43E+04	1.71E+00	25.896	25.166	0.730
170.91	4.33E+04	7.07E+04	1.63E+00	25.898	25.202	0.697
177.74	9.09E+04	1.42E+05	1.56E+00	25.895	25.236	0.659
184.85	1.86E+05	2.80E+05	1.51E+00	25.891	25.262	0.629
192.25	3.70E+05	5.39E+05	1.46E+00	25.891	25.290	0.601
199.94	7.17E+05	1.01E+06	1.41E+00	25.892	25.322	0.570
207.94	1.36E+06	1.87E+06	1.38E+00	25.889	25.339	0.551
216.25	2.51E+06	3.37E+06	1.34E+00	25.892	25.363	0.530
224.90	4.55E+06	5.95E+06	1.31E+00	25.889	25.387	0.502
233.90	8.05E+06	1.03E+07	1.28E+00	25.892	25.413	0.479
243.25	1.40E+07	1.76E+07	1.26E+00	25.887	25.424	0.463
252.99	2.38E+07	2.93E+07	1.23E+00	25.890	25.453	0.437
263.10	3.96E+07	4.81E+07	1.21E+00	25.896	25.471	0.425
273.63	6.49E+07	7.76E+07	1.20E+00	25.898	25.492	0.407
284.57	1.04E+08	1.23E+08	1.18E+00	25.911	25.514	0.397
295.96	1.65E+08	1.92E+08	1.16E+00	25.909	25.536	0.373
307.79	2.56E+08	2.95E+08	1.15E+00	25.920	25.558	0.363
320.11	3.92E+08	4.46E+08	1.14E+00	25.928	25.585	0.343
332.91	5.91E+08	6.66E+08	1.13E+00	25.937	25.607	0.331

		E_a			$\Delta H^{\ddagger}$			$\Delta S^{\ddagger}$	
$\bar{T}$	Class.	QMT	Corr.	Class.	QMT	Corr.	Class.	QMT	Corr.
10.91	26.017	0.000	26.017	25.926	-0.091	26.017	-1.261E-04	-0.2966	0.2965
11.68	26.029	0.000	26.029	25.932	-0.097	26.029	4.151E-04	-0.2972	0.2976
12.49	26.028	0.000	26.028	25.925	-0.104	26.028	-2.223E-04	-0.2977	0.2975
13.37	26.041	0.000	26.041	25.930	-0.111	26.041	2.102E-04	-0.2983	0.2985
14.31	26.046	0.000	26.046	25.927	-0.119	26.046	-2.207E-05	-0.2988	0.2988
15.31	26.057	0.000	26.057	25.930	-0.127	26.057	1.933E-04	-0.2994	0.2996
16.38	26.062	0.000	26.062	25.926	-0.136	26.062	-6.927E-05	-0.3000	0.2999
17.52	26.073	0.000	26.073	25.928	-0.146	26.073	3.659E-05	-0.3005	0.3006
18.75	26.084	0.000	26.084	25.929	-0.156	26.084	7.671E-05	-0.3011	0.3012
20.06	26.094	0.000	26.094	25.927	-0.167	26.094	4.395E-06	-0.3017	0.3017
21.47	26.111	0.000	26.111	25.932	-0.178	26.111	2.493E-04	-0.3022	0.3025
22.97	26.117	0.000	26.117	25.926	-0.191	26.117	-3.753E-05	-0.3028	0.3027
24.58	26.132	0.000	26.132	25.928	-0.204	26.132	4.583E-05	-0.3033	0.3034
26.30	26.148	0.000	26.148	25.929	-0.218	26.148	9.560E-05	-0.3039	0.3040
28.14	26.169	0.000	26.169	25.936	-0.234	26.169	3.367E-04	-0.3045	0.3048
30.11	26.178	0.000	26.178	25.928	-0.250	26.178	7.691E-05	-0.3050	0.3051
32.21	26.178	0.000	26.178	25.911	-0.268	26.178	-4.756E-04	-0.3056	0.3051
34.47	26.226	0.021	26.205	25.939	-0.265	26.205	3.814E-04	-0.3055	0.3059
36.88	26.241	0.000	26.241	25.935	-0.306	26.241	2.558E-04	-0.3067	0.3069
39.47	26.249	0.024	26.225	25.922	-0.304	26.225	-9.623E-05	-0.3066	0.3065
42.23	26.274	0.077	26.197	25.923	-0.274	26.197	-5.639E-05	-0.3059	0.3058
45.18	26.308	0.108	26.201	25.933	-0.268	26.201	1.664E-04	-0.3057	0.3059
48.35	26.330	0.196	26.133	25.928	-0.205	26.133	6.697E-05	-0.3044	0.3045
51.73	26.359	0.402	25.958	25.929	-0.028	25.958	9.144E-05	-0.3009	0.3009
55.35	26.395	0.703	25.692	25.935	0.243	25.692	1.901E-04	-0.2958	0.2960
59.22	26.417	1.212	25.205	25.925	0.720	25.205	1.270E-05	-0.2874	0.2875
63.37	26.456	2.119	24.337	25.929	1.592	24.337	8.568E-05	-0.2732	0.2733
67.80	26.493	3.561	22.932	25.930	2.998	22.932	9.696E-05	-0.2517	0.2518
72.55	26.526	4.922	21.604	25.923	4.320	21.604	6.057E-06	-0.2329	0.2329
76.50	26.580	8.918	17.662	25.944	8.282	17.662	2.848E-04	-0.1800	0.1803
79.56	26.583	11.026	15.557	25.922	10.365	15.557	-1.713E-07	-0.1533	0.1533
82.74	26.661	13.314	13.348	25.973	12.626	13.348	6.326E-04	-0.1255	0.1261
86.05	26.636	15.500	11.136	25.921	14.785	11.136	6.142E-06	-0.0999	0.0999
89.50	26.693	17.443	9.250	25.949	16.699	9.250	3.273E-04	-0.0781	0.0784
93.08	26.658	19.167	7.490	25.884	18.394	7.490	-3.818E-04	-0.0595	0.0591
96.80	26.783	20.263	6.520	25.978	19.458	6.520	6.082E-04	-0.0483	0.0489
100.67	26.727	21.388	5.339	25.890	20.551	5.339	-2.832E-04	-0.0372	0.0369
104.70	26.879	22.213	4.666	26.008	21.342	4.666	8.687E-04	-0.0295	0.0304
108.89	26.767	22.747	4.021	25.862	21.841	4.021	-5.017E-04	-0.0248	0.0243
113.24	26.959	23.241	3.717	26.017	22.300	3.717	8.971E-04	-0.0207	0.0216
117.77	26.951	23.735	3.216	25.972	22.756	3.216	5.026E-04	-0.0167	0.0172
122.48	26.938	23.924	3.014	25.919	22.905	3.014	6.728E-05	-0.0155	0.0156
127.38	27.036	24.406	2.630	25.978	23.348	2.630	5.328E-04	-0.0120	0.0125
132.48	26.979	24.658	2.322	25.878	23.557	2.322	-2.327E-04	-0.0103	0.0101
137.77	27.135	24.752	2.382	25.990	23.607	2.382	5.935E-04	-0.0100	0.0106
143.28	27.233	25.098	2.135	26.042	23.907	2.135	9.686E-04	-0.0078	0.0088
149.02	27.079	25.248	1.832	25.841	24.009	1.832	-4.122E-04	-0.0071	0.0067
154.98	27.238	25.413	1.825	25.950	24.125	1.825	3.038E-04	-0.0064	0.0067
161.17	27.372	25.625	1.747	26.032	24.285	1.747	8.253E-04	-0.0054	0.0062
167.62	27.235	25.669	1.566	25.842	24.276	1.566	-3.302E-04	-0.0054	0.0051
174.33	27.425	25.789	1.635	25.976	24.340	1.635	4.510E-04	-0.0050	0.0055
181.30	27.509	26.086	1.423	26.002	24.579	1.423	5.997E-04	-0.0037	0.0043
188.55	27.461	26.151	1.311	25.894	24.583	1.311	1.621E-05	-0.0037	0.0037
196.10	27.495	26.099	1.396	25.865	24.469	1.396	-1.360E-04	-0.0043	0.0041
203.94	27.661	26.617	1.045	25.966	24.921	1.045	3.705E-04	-0.0020	0.0024
212.10	27.571	26.499	1.072	25.807	24.736	1.072	-3.924E-04	-0.0029	0.0025
220.58	27.808	26.575	1.233	25.974	24.742	1.233	3.791E-04	-0.0029	0.0033
229.40	27.727	26.668	1.059	25.820	24.761	1.059	-3.069E-04	-0.0028	0.0025
238.58	27.998	27.106	0.892	26.015	25.123	0.892	5.278E-04	-0.0012	0.0018
248.12	27.875	26.775	1.100	25.813	24.713	1.100	-3.038E-04	-0.0029	0.0026
258.05	27.871	27.134	0.736	25.726	24.990	0.736	-6.488E-04	-0.0018	0.0012
268.37	28.082	27.188	0.894	25.852	24.957	0.894	-1.703E-04	-0.0020	0.0018
279.10	27.906	27.259	0.647	25.586	24.939	0.647	-1.142E-03	-0.0020	0.0009
290.27	28.376	27.378	0.999	25.964	24.965	0.999	1.856E-04	-0.0019	0.0021
301.88	28.121	27.497	0.624	25.612	24.987	0.624	-1.003E-03	-0.0019	0.0008
313.95	28.332	27.485	0.847	25.722	24.875	0.847	-6.446E-04	-0.0022	0.0016
326.51	28.420	27.756	0.663	25.706	25.042	0.663	-6.956E-04	-0.0017	0.0010

BBL					$\Delta G^{\ddagger}$	
T	CVT	CVT+SCT	kappa	Class.	QMT	Corr.
10.54	1.14E-161	5.00E-10	4.39E+151	34.765	4.165	30.599
11.28	2.45E-150	5.00E-10	2.04E+140	34.765	4.464	30.300
12.07	9.01E-140	5.00E-10	5.55E+129	34.765	4.784	29.981
12.91	5.93E-130	5.00E-10	8.43E+119	34.765	5.124	29.641
13.82	1.16E-120	5.00E-10	4.31E+110	34.765	5.493	29.272
14.79	5.14E-112	5.00E-10	9.73E+101	34.765	5.887	28.878
15.82	5.42E-104	5.00E-10	9.23E+93	34.765	6.305	28.459
16.93	1.94E-96	5.00E-10	2.58E+86	34.765	6.757	28.008
18.11	2.03E-89	5.00E-10	2.46E+79	34.765	7.239	27.526
19.38	8.07E-83	5.00E-10	6.20E+72	34.765	7.757	27.008
20.74	1.20E-76	5.00E-10	4.17E+66	34.765	8.313	26.452
22.19	6.77E-71	5.00E-10	7.39E+60	34.765	8.907	25.858
23.74	1.60E-65	5.00E-10	3.13E+55	34.765	9.542	25.222
25.41	1.82E-60	5.00E-10	2.75E+50	34.765	10.228	24.537
27.18	8.76E-56	5.00E-10	5.71E+45	34.765	10.956	23.810
29.09	2.28E-51	5.01E-10	2.20E+41	34.766	11.741	23.024
31.12	2.88E-47	5.01E-10	1.74E+37	34.766	12.578	22.187
33.30	2.04E-43	5.02E-10	2.46E+33	34.765	13.478	21.287
35.63	8.02E-40	5.03E-10	6.27E+29	34.766	14.440	20.326
38.13	1.88E-36	5.06E-10	2.69E+26	34.766	15.473	19.294
40.80	2.64E-33	5.12E-10	1.94E+23	34.765	16.575	18.190
43.65	2.27E-30	5.22E-10	2.30E+20	34.766	17.751	17.016
46.71	1.29E-27	5.42E-10	4.20E+17	34.766	19.007	15.760
49.98	4.82E-25	5.77E-10	1.20E+15	34.767	20.339	14.428
53.47	1.21E-22	6.38E-10	5.27E+12	34.768	21.745	13.023
57.22	2.18E-20	7.52E-10	3.45E+10	34.768	23.224	11.544
61.22	2.77E-18	9.71E-10	3.51E+08	34.767	24.752	10.015
65.51	2.59E-16	1.44E-09	5.56E+06	34.768	26.309	8.459
70.09	1.79E-14	2.60E-09	1.45E+05	34.770	27.843	6.927
75.00	9.52E-13	5.79E-09	6.08E+03	34.770	29.336	5.433
78.00	8.45E-12	1.15E-08	1.36E+03	34.770	30.090	4.680
81.12	6.90E-11	2.63E-08	3.81E+02	34.771	30.762	4.009
84.36	5.19E-10	6.92E-08	1.33E+02	34.772	31.340	3.432
87.74	3.64E-09	2.09E-07	5.74E+01	34.773	31.818	2.955
91.25	2.36E-08	7.01E-07	2.97E+01	34.775	32.202	2.573
94.90	1.43E-07	2.53E-06	1.77E+01	34.776	32.509	2.267
98.69	8.07E-07	9.52E-06	1.18E+01	34.777	32.752	2.025
102.64	4.28E-06	3.65E-05	8.53E+00	34.778	32.949	1.829
106.75	2.13E-05	1.40E-04	6.57E+00	34.781	33.110	1.671
111.02	9.98E-05	5.27E-04	5.28E+00	34.783	33.247	1.536
115.46	4.41E-04	1.94E-03	4.40E+00	34.786	33.363	1.422
120.08	1.84E-03	6.94E-03	3.77E+00	34.790	33.465	1.325
124.88	7.29E-03	2.40E-02	3.29E+00	34.792	33.555	1.237
129.88	2.74E-02	8.04E-02	2.93E+00	34.798	33.635	1.162
135.07	9.80E-02	2.59E-01	2.64E+00	34.801	33.710	1.091
140.47	3.34E-01	8.08E-01	2.42E+00	34.806	33.774	1.032
146.09	1.09E+00	2.43E+00	2.23E+00	34.810	33.836	0.974
151.94	3.39E+00	7.05E+00	2.08E+00	34.820	33.895	0.925
158.01	1.01E+01	1.97E+01	1.95E+00	34.828	33.950	0.878
164.33	2.90E+01	5.34E+01	1.84E+00	34.834	33.999	0.834
170.91	8.00E+01	1.40E+02	1.75E+00	34.842	34.047	0.795
177.74	2.12E+02	3.54E+02	1.67E+00	34.852	34.095	0.758
184.85	5.43E+02	8.67E+02	1.60E+00	34.861	34.142	0.719
192.25	1.34E+03	2.06E+03	1.54E+00	34.876	34.188	0.687
199.94	3.20E+03	4.75E+03	1.48E+00	34.889	34.232	0.657
207.94	7.41E+03	1.06E+04	1.43E+00	34.901	34.282	0.619
216.25	1.66E+04	2.32E+04	1.40E+00	34.916	34.314	0.602
224.90	3.61E+04	4.90E+04	1.36E+00	34.933	34.362	0.571
233.90	7.63E+04	1.01E+05	1.32E+00	34.952	34.407	0.545
243.25	1.57E+05	2.03E+05	1.29E+00	34.969	34.449	0.520
252.99	3.14E+05	3.99E+05	1.27E+00	34.994	34.490	0.504
263.10	6.12E+05	7.63E+05	1.25E+00	35.018	34.536	0.482
273.63	1.16E+06	1.43E+06	1.23E+00	35.054	34.578	0.476
284.57	2.16E+06	2.61E+06	1.21E+00	35.077	34.630	0.448
295.96	3.93E+06	4.67E+06	1.19E+00	35.105	34.681	0.425
307.79	6.97E+06	8.18E+06	1.17E+00	35.142	34.733	0.410
320.11	1.21E+07	1.40E+07	1.16E+00	35.185	34.797	0.388
332.91	2.07E+07	2.36E+07	1.14E+00	35.215	34.852	0.363

		E_a			$\Delta H^{\ddagger}$			$\Delta S^{\ddagger}$	
$\bar{T}$	Class.	QMT	Corr.	Class.	QMT	Corr.	Class.	QMT	Corr.
10.91	34.857	0.000	34.857	34.766	-0.091	34.857	1.236E-04	-0.4038	0.4039
11.68	34.860	0.000	34.860	34.763	-0.097	34.860	-1.042E-04	-0.4044	0.4043
12.49	34.869	0.000	34.869	34.765	-0.104	34.869	6.706E-05	-0.4049	0.4050
13.37	34.876	0.000	34.876	34.765	-0.111	34.876	1.635E-05	-0.4055	0.4055
14.31	34.881	0.000	34.881	34.763	-0.119	34.881	-1.369E-04	-0.4061	0.4059
15.31	34.892	0.000	34.892	34.765	-0.127	34.892	1.329E-05	-0.4066	0.4066
16.38	34.894	0.000	34.894	34.758	-0.136	34.894	-3.967E-04	-0.4072	0.4068
17.52	34.919	0.000	34.919	34.773	-0.146	34.919	4.918E-04	-0.4077	0.4082
18.75	34.916	0.000	34.916	34.760	-0.156	34.916	-2.482E-04	-0.4083	0.4081
20.06	34.924	0.000	34.924	34.757	-0.167	34.924	-3.983E-04	-0.4089	0.4085
21.47	34.948	0.000	34.948	34.770	-0.178	34.948	2.063E-04	-0.4094	0.4096
22.97	34.964	0.000	34.964	34.773	-0.191	34.964	3.481E-04	-0.4100	0.4103
24.58	34.964	0.000	34.964	34.760	-0.204	34.964	-1.959E-04	-0.4106	0.4104
26.30	34.979	0.000	34.979	34.760	-0.218	34.979	-1.861E-04	-0.4111	0.4109
28.14	34.993	0.007	34.986	34.759	-0.227	34.986	-2.135E-04	-0.4114	0.4112
30.11	35.017	0.000	35.017	34.767	-0.250	35.017	3.455E-05	-0.4122	0.4123
32.21	35.040	0.008	35.032	34.772	-0.260	35.032	2.226E-04	-0.4125	0.4128
34.47	35.043	0.008	35.034	34.756	-0.278	35.034	-2.598E-04	-0.4131	0.4128
36.88	35.061	0.027	35.034	34.754	-0.280	35.034	-3.191E-04	-0.4131	0.4128
39.47	35.109	0.057	35.052	34.782	-0.271	35.052	3.965E-04	-0.4129	0.4133
42.23	35.105	0.100	35.005	34.754	-0.250	35.005	-2.683E-04	-0.4124	0.4121
45.18	35.138	0.208	34.930	34.763	-0.167	34.930	-8.331E-05	-0.4105	0.4104
48.35	35.161	0.371	34.789	34.759	-0.030	34.789	-1.594E-04	-0.4076	0.4074
51.73	35.180	0.640	34.540	34.750	0.210	34.540	-3.351E-04	-0.4027	0.4024
55.35	35.233	1.115	34.118	34.773	0.655	34.118	9.960E-05	-0.3944	0.3945
59.22	35.276	1.861	33.415	34.784	1.369	33.415	2.877E-04	-0.3819	0.3822
63.37	35.273	3.063	32.210	34.746	2.537	32.210	-3.294E-04	-0.3629	0.3625
67.80	35.307	4.925	30.382	34.744	4.362	30.382	-3.710E-04	-0.3350	0.3346
72.55	35.373	7.127	28.246	34.770	6.524	28.246	8.968E-06	-0.3042	0.3042
76.50	35.399	11.126	24.273	34.763	10.490	24.273	-8.432E-05	-0.2513	0.2512
79.56	35.409	13.948	21.460	34.747	13.287	21.460	-2.897E-04	-0.2154	0.2151
82.74	35.435	16.989	18.446	34.747	16.301	18.446	-2.916E-04	-0.1783	0.1780
86.05	35.465	20.125	15.340	34.750	19.410	15.340	-2.571E-04	-0.1414	0.1412
89.50	35.451	22.951	12.500	34.707	22.207	12.500	-7.472E-04	-0.1095	0.1088
93.08	35.538	25.318	10.221	34.765	24.544	10.221	-1.147E-04	-0.0839	0.0838
96.80	35.555	27.227	8.328	34.750	26.423	8.328	-2.659E-04	-0.0641	0.0639
100.67	35.573	28.655	6.918	34.736	27.818	6.918	-4.074E-04	-0.0500	0.0496
104.70	35.570	29.798	5.772	34.700	28.927	5.772	-7.638E-04	-0.0392	0.0384
108.89	35.641	30.590	5.052	34.736	29.685	5.052	-4.242E-04	-0.0321	0.0317
113.24	35.667	31.283	4.384	34.726	30.342	4.384	-5.178E-04	-0.0262	0.0257
117.77	35.642	31.803	3.839	34.663	30.824	3.839	-1.057E-03	-0.0220	0.0209
122.48	35.761	32.229	3.532	34.743	31.211	3.532	-3.967E-04	-0.0188	0.0184
127.38	35.711	32.607	3.104	34.652	31.548	3.104	-1.123E-03	-0.0161	0.0149
132.48	35.816	32.876	2.940	34.715	31.775	2.940	-6.366E-04	-0.0143	0.0137
137.77	35.821	33.237	2.584	34.676	32.092	2.584	-9.302E-04	-0.0120	0.0110
143.28	35.910	33.429	2.481	34.719	32.238	2.481	-6.240E-04	-0.0109	0.0103
149.02	35.796	33.603	2.193	34.557	32.364	2.193	-1.728E-03	-0.0101	0.0083
154.98	35.901	33.793	2.108	34.613	32.504	2.108	-1.362E-03	-0.0092	0.0078
161.17	36.031	34.064	1.967	34.691	32.724	1.967	-8.680E-04	-0.0078	0.0069
167.62	36.012	34.205	1.806	34.618	32.812	1.806	-1.310E-03	-0.0072	0.0059
174.33	36.039	34.305	1.735	34.590	32.856	1.735	-1.475E-03	-0.0070	0.0055
181.30	36.136	34.415	1.721	34.629	32.908	1.721	-1.257E-03	-0.0067	0.0054
188.55	36.068	34.555	1.513	34.501	32.988	1.513	-1.948E-03	-0.0062	0.0043
196.10	36.177	34.721	1.456	34.547	33.091	1.456	-1.709E-03	-0.0057	0.0040
203.94	36.282	34.685	1.597	34.587	32.990	1.597	-1.509E-03	-0.0062	0.0047
212.10	36.289	35.242	1.047	34.526	33.479	1.047	-1.805E-03	-0.0039	0.0021
220.58	36.318	34.952	1.366	34.485	33.119	1.366	-1.994E-03	-0.0055	0.0035
229.40	36.369	35.150	1.219	34.462	33.244	1.219	-2.093E-03	-0.0050	0.0029
238.58	36.508	35.319	1.188	34.525	33.336	1.188	-1.827E-03	-0.0046	0.0027
248.12	36.413	35.499	0.914	34.351	33.437	0.914	-2.542E-03	-0.0042	0.0016
258.05	36.530	35.488	1.042	34.385	33.343	1.042	-2.405E-03	-0.0045	0.0021
268.37	36.349	35.708	0.641	34.118	33.478	0.641	-3.420E-03	-0.0040	0.0006
279.10	36.791	35.607	1.184	34.471	33.287	1.184	-2.131E-03	-0.0047	0.0026
290.27	36.798	35.770	1.028	34.385	33.357	1.028	-2.434E-03	-0.0045	0.0020
301.88	36.684	35.887	0.797	34.174	33.378	0.797	-3.145E-03	-0.0044	0.0013
313.95	36.677	35.731	0.946	34.067	33.121	0.946	-3.493E-03	-0.0052	0.0017
326.51	37.168	36.148	1.020	34.454	33.433	1.020	-2.286E-03	-0.0043	0.0020

BL					$\Delta G^{\ddagger}$	
T	CVT	CVT+SCT	kappa	Class.	QMT	Corr.
10.54	5.61E-283	1.32E-26	2.35E+256	59.243	7.511	51.732
11.28	1.09E-263	1.32E-26	1.21E+237	59.243	8.044	51.199
12.07	1.06E-245	1.32E-26	1.25E+219	59.242	8.615	50.628
12.91	5.42E-229	1.32E-26	2.44E+202	59.243	9.221	50.022
13.82	3.52E-213	1.32E-26	3.75E+186	59.243	9.879	49.364
14.79	1.83E-198	1.32E-26	7.21E+171	59.243	10.581	48.662
15.82	8.18E-185	1.32E-26	1.61E+158	59.243	11.327	47.916
16.93	5.85E-172	1.32E-26	2.26E+145	59.243	12.131	47.112
18.11	5.08E-160	1.32E-26	2.60E+133	59.243	12.986	46.256
19.38	8.56E-149	1.32E-26	1.54E+122	59.243	13.908	45.335
20.74	2.71E-138	1.32E-26	4.87E+111	59.243	14.896	44.347
22.19	1.63E-128	1.32E-26	8.10E+101	59.243	15.950	43.293
23.74	2.22E-119	1.33E-26	5.99E+92	59.243	17.076	42.167
25.41	8.75E-111	1.33E-26	1.52E+84	59.243	18.291	40.952
27.18	7.97E-103	1.34E-26	1.68E+76	59.243	19.579	39.664
29.09	2.55E-95	1.36E-26	5.33E+68	59.243	20.968	38.276
31.12	2.37E-88	1.41E-26	5.95E+61	59.243	22.439	36.804
33.30	8.20E-82	1.49E-26	1.82E+55	59.243	24.014	35.229
35.63	1.05E-75	1.65E-26	1.57E+49	59.242	25.684	33.558
38.13	5.54E-70	1.94E-26	3.50E+43	59.243	27.457	31.787
40.80	1.21E-64	2.47E-26	2.04E+38	59.244	29.320	29.924
43.65	1.16E-59	3.46E-26	2.98E+33	59.244	31.270	27.974
46.71	5.48E-55	5.38E-26	9.82E+28	59.244	33.318	25.926
49.98	1.27E-50	9.31E-26	7.33E+24	59.243	35.450	23.792
53.47	1.49E-46	1.80E-25	1.21E+21	59.244	37.663	21.581
57.22	9.88E-43	3.91E-25	3.96E+17	59.244	39.967	19.277
61.22	3.61E-39	9.69E-25	2.68E+14	59.245	42.333	16.911
65.51	7.87E-36	2.81E-24	3.57E+11	59.246	44.757	14.489
70.09	1.03E-32	9.87E-24	9.58E+08	59.245	47.193	12.052
75.00	8.51E-30	3.74E-23	4.39E+06	59.249	49.711	9.538
78.00	3.41E-28	1.06E-22	3.11E+05	59.251	51.049	8.202
81.12	1.19E-26	3.51E-22	2.95E+04	59.252	52.310	6.942
84.36	3.60E-25	1.39E-21	3.86E+03	59.254	53.461	5.793
87.74	9.68E-24	6.87E-21	7.10E+02	59.255	54.466	4.789
91.25	2.28E-22	4.22E-20	1.85E+02	59.259	55.298	3.961
94.90	4.77E-21	3.16E-19	6.62E+01	59.261	55.952	3.309
98.69	8.85E-20	2.73E-18	3.08E+01	59.263	56.449	2.814
102.64	1.48E-18	2.58E-17	1.74E+01	59.265	56.825	2.439
106.75	2.22E-17	2.52E-16	1.14E+01	59.269	57.113	2.156
111.02	2.99E-16	2.44E-15	8.16E+00	59.276	57.338	1.938
115.46	3.66E-15	2.29E-14	6.26E+00	59.279	57.519	1.760
120.08	4.07E-14	2.05E-13	5.04E+00	59.286	57.672	1.614
124.88	4.13E-13	1.74E-12	4.21E+00	59.290	57.797	1.493
129.88	3.84E-12	1.39E-11	3.62E+00	59.299	57.909	1.389
135.07	3.28E-11	1.04E-10	3.17E+00	59.303	58.007	1.296
140.47	2.58E-10	7.30E-10	2.83E+00	59.311	58.096	1.215
146.09	1.88E-09	4.82E-09	2.56E+00	59.319	58.176	1.144
151.94	1.27E-08	2.99E-08	2.35E+00	59.331	58.249	1.082
158.01	7.96E-08	1.73E-07	2.17E+00	59.341	58.322	1.020
164.33	4.66E-07	9.47E-07	2.03E+00	59.354	58.385	0.969
170.91	2.56E-06	4.88E-06	1.91E+00	59.366	58.449	0.917
177.74	1.31E-05	2.37E-05	1.81E+00	59.383	58.507	0.876
184.85	6.34E-05	1.09E-04	1.72E+00	59.395	58.563	0.833
192.25	2.89E-04	4.74E-04	1.64E+00	59.411	58.620	0.791
199.94	1.24E-03	1.96E-03	1.58E+00	59.432	58.671	0.761
207.94	5.06E-03	7.67E-03	1.52E+00	59.446	58.727	0.719
216.25	1.95E-02	2.86E-02	1.47E+00	59.467	58.778	0.689
224.90	7.15E-02	1.02E-01	1.43E+00	59.489	58.825	0.664
233.90	2.50E-01	3.45E-01	1.38E+00	59.512	58.885	0.626
243.25	8.33E-01	1.12E+00	1.34E+00	59.536	58.937	0.599
252.99	2.66E+00	3.49E+00	1.31E+00	59.560	58.989	0.571
263.10	8.09E+00	1.04E+01	1.29E+00	59.593	59.043	0.549
273.63	2.37E+01	2.98E+01	1.26E+00	59.622	59.100	0.521
284.57	6.65E+01	8.22E+01	1.24E+00	59.657	59.155	0.501
295.96	1.80E+02	2.19E+02	1.22E+00	59.691	59.208	0.483
307.79	4.67E+02	5.60E+02	1.20E+00	59.737	59.273	0.465
320.11	1.17E+03	1.39E+03	1.19E+00	59.789	59.330	0.459
332.91	2.85E+03	3.32E+03	1.16E+00	59.823	59.401	0.423

		E_a			$\Delta H^{\ddagger}$			$\Delta S^{\ddagger}$	
$\bar{T}$	Class.	QMT	Corr.	Class.	QMT	Corr.	Class.	QMT	Corr.
10.91	59.329	0.000	59.329	59.238	-0.091	59.329	-4.433E-04	-0.7212	0.7207
11.68	59.350	0.000	59.350	59.253	-0.097	59.350	8.539E-04	-0.7218	0.7226
12.49	59.340	0.000	59.340	59.236	-0.104	59.340	-5.282E-04	-0.7223	0.7218
13.37	59.353	0.000	59.353	59.242	-0.111	59.353	-5.485E-05	-0.7229	0.7228
14.31	59.366	0.000	59.366	59.248	-0.119	59.366	3.387E-04	-0.7234	0.7238
15.31	59.365	0.000	59.365	59.238	-0.127	59.365	-3.328E-04	-0.7240	0.7237
16.38	59.380	0.000	59.380	59.244	-0.136	59.380	7.896E-05	-0.7246	0.7246
17.52	59.388	0.000	59.388	59.243	-0.146	59.388	-1.158E-05	-0.7251	0.7251
18.75	59.397	0.000	59.397	59.242	-0.156	59.397	-7.196E-05	-0.7257	0.7256
20.06	59.413	0.000	59.413	59.247	-0.167	59.413	1.850E-04	-0.7263	0.7264
21.47	59.423	0.000	59.423	59.244	-0.178	59.423	7.584E-05	-0.7268	0.7269
22.97	59.433	0.021	59.411	59.242	-0.169	59.411	-3.566E-05	-0.7264	0.7264
24.58	59.443	0.000	59.443	59.238	-0.204	59.443	-1.799E-04	-0.7279	0.7277
26.30	59.458	0.024	59.434	59.240	-0.194	59.434	-1.173E-04	-0.7275	0.7274
28.14	59.479	0.051	59.428	59.245	-0.183	59.428	8.272E-05	-0.7271	0.7271
30.11	59.492	0.134	59.358	59.242	-0.116	59.358	-4.141E-05	-0.7248	0.7247
32.21	59.510	0.218	59.292	59.243	-0.049	59.292	-1.064E-05	-0.7226	0.7226
34.47	59.540	0.432	59.108	59.254	0.146	59.108	3.147E-04	-0.7168	0.7171
36.88	59.534	0.732	58.802	59.228	0.425	58.802	-4.175E-04	-0.7089	0.7085
39.47	59.559	1.170	58.389	59.231	0.842	58.389	-3.218E-04	-0.6980	0.6977
42.23	59.597	1.751	57.846	59.246	1.400	57.846	4.644E-05	-0.6843	0.6844
45.18	59.627	2.445	57.181	59.251	2.070	57.181	1.653E-04	-0.6690	0.6691
48.35	59.662	3.255	56.406	59.260	2.854	56.406	3.478E-04	-0.6522	0.6525
51.73	59.657	4.197	55.459	59.227	3.768	55.459	-3.114E-04	-0.6339	0.6336
55.35	59.692	5.262	54.430	59.233	4.803	54.430	-2.079E-04	-0.6145	0.6143
59.22	59.733	6.608	53.125	59.241	6.116	53.125	-5.471E-05	-0.5916	0.5915
63.37	59.750	8.276	51.475	59.224	7.749	51.475	-3.381E-04	-0.5649	0.5646
67.80	59.823	10.472	49.351	59.259	9.909	49.351	2.028E-04	-0.5320	0.5322
72.55	59.791	11.859	47.933	59.188	11.256	47.933	-8.112E-04	-0.5127	0.5119
76.50	59.837	16.890	42.947	59.201	16.255	42.947	-6.391E-04	-0.4461	0.4454
79.56	59.900	20.189	39.710	59.238	19.528	39.710	-1.613E-04	-0.4041	0.4040
82.74	59.876	24.169	35.707	59.188	23.481	35.707	-7.806E-04	-0.3554	0.3546
86.05	59.934	29.093	30.841	59.219	28.378	30.841	-4.185E-04	-0.2973	0.2969
89.50	59.916	34.427	25.490	59.173	33.683	25.490	-9.454E-04	-0.2369	0.2359
93.08	59.982	39.715	20.267	59.208	38.941	20.267	-5.518E-04	-0.1792	0.1787
96.80	60.009	44.304	15.704	59.204	43.500	15.704	-5.969E-04	-0.1312	0.1306
100.67	60.060	47.891	12.169	59.223	47.054	12.169	-4.084E-04	-0.0952	0.0948
104.70	60.025	50.516	9.509	59.155	49.646	9.509	-1.069E-03	-0.0699	0.0689
108.89	60.008	52.392	7.616	59.103	51.487	7.616	-1.559E-03	-0.0527	0.0511
113.24	60.125	53.748	6.376	59.183	52.807	6.376	-8.321E-04	-0.0408	0.0400
117.77	60.102	54.690	5.412	59.123	53.711	5.412	-1.355E-03	-0.0330	0.0316
122.48	60.190	55.551	4.639	59.172	54.533	4.639	-9.485E-04	-0.0261	0.0252
127.38	60.140	56.046	4.094	59.081	54.987	4.094	-1.677E-03	-0.0225	0.0208
132.48	60.282	56.559	3.722	59.181	55.458	3.722	-9.085E-04	-0.0189	0.0180
137.77	60.254	56.927	3.327	59.108	55.782	3.327	-1.443E-03	-0.0165	0.0150
143.28	60.297	57.304	2.993	59.106	56.113	2.993	-1.460E-03	-0.0141	0.0127
149.02	60.267	57.578	2.689	59.028	56.339	2.689	-1.992E-03	-0.0126	0.0106
154.98	60.358	57.728	2.630	59.070	56.440	2.630	-1.718E-03	-0.0119	0.0102
161.17	60.367	58.072	2.294	59.027	56.733	2.294	-1.990E-03	-0.0101	0.0081
167.62	60.458	58.188	2.270	59.065	56.794	2.270	-1.760E-03	-0.0097	0.0079
174.33	60.374	58.440	1.933	58.925	56.991	1.933	-2.581E-03	-0.0085	0.0059
181.30	60.584	58.626	1.959	59.077	57.119	1.959	-1.721E-03	-0.0078	0.0061
188.55	60.571	58.690	1.881	59.003	57.123	1.881	-2.121E-03	-0.0078	0.0057
196.10	60.529	58.994	1.536	58.899	57.364	1.536	-2.662E-03	-0.0065	0.0039
203.94	60.764	58.954	1.810	59.069	57.259	1.810	-1.815E-03	-0.0071	0.0052
212.10	60.695	59.212	1.483	58.932	57.449	1.483	-2.471E-03	-0.0061	0.0037
220.58	60.739	59.443	1.296	58.905	57.610	1.296	-2.595E-03	-0.0054	0.0028
229.40	60.832	59.219	1.613	58.925	57.312	1.613	-2.507E-03	-0.0067	0.0042
238.58	60.894	59.577	1.317	58.911	57.594	1.317	-2.567E-03	-0.0055	0.0030
248.12	60.993	59.707	1.286	58.931	57.645	1.286	-2.487E-03	-0.0053	0.0028
258.05	60.888	59.771	1.117	58.743	57.626	1.117	-3.230E-03	-0.0054	0.0022
268.37	61.099	59.841	1.259	58.869	57.610	1.259	-2.752E-03	-0.0054	0.0027
279.10	61.057	60.046	1.011	58.737	57.726	1.011	-3.233E-03	-0.0050	0.0018
290.27	61.219	60.245	0.974	58.806	57.832	0.974	-2.990E-03	-0.0046	0.0017
301.88	61.038	60.109	0.929	58.529	57.600	0.929	-3.927E-03	-0.0054	0.0015
313.95	61.069	60.450	0.619	58.460	57.841	0.619	-4.151E-03	-0.0047	0.0005
326.51	61.630	60.270	1.361	58.916	57.556	1.361	-2.725E-03	-0.0055	0.0028

Polyrate input files examples

.dat

```
*GENERAL

TITLE
  BBL
END

DL ISPE

ATOMS
1 C
2 C
3 H
4 H
5 C
6 C
7 H
8 C
9 C
10 C
11 H
12 C
13 H
14 H
15 H
16 H
17 C
18 H
19 H
END

NOSUPERMOL

*SECOND

HESSCAL hhook

FPRINT

*OPTIMIZATION

PRINT

OPTMIN ohook
OPTTS ohook

*REACT1
INITGEO hooks
GEOM
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
END
SPECIES nonlinrp

*PROD1
INITGEO hooks
GEOM
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
END
SPECIES nonlinrp

*START
INITGEO hooks
GEOM
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
END
SPECIES nonlints
PROJECT

*PATH
SYMMETRY
INTMU 3
SSTEP 0.001
RPM pagem
SRANGE
  SLP 20.
  SLM -20.
END
SPECSTOP
  CURVE VMEP
  PERCENTDOWN 99.9
END
PRPATH
  coord 1 2
  xmol
  freq 51
END

*TUNNEL
ZCT
SCT
#QRST
#  harmonic
#  mode 51
#  states all
#END

*RATE
FORWARDK
SIGMAF 1
TST
CVT
PRDELG
PRPART rtp
TEMP
75.00
78.00
81.12
84.36
87.74
91.25
94.90
98.69
102.64
106.75
111.02
115.46
120.08
124.88
129.88
135.07
140.47
146.09
151.94
158.01
164.33
170.91
177.74
184.85
192.25
199.94
207.94
216.25
224.90
233.90
243.25
252.99
263.10
273.63
284.57
295.96
307.79
320.11
332.91
END

ANALYSIS
75.00
78.00
81.12
84.36
87.74
91.25
94.90
98.69
102.64
106.75
111.02
115.46
120.08
124.88
129.88
135.07
140.47
146.09
151.94
158.01
164.33
170.91
177.74
184.85
192.25
199.94
207.94
216.25
224.90
233.90
243.25
252.99
263.10
273.63
284.57
295.96
```

```
307.79
320.11
332.91
END

EACT
75 78
87.74 91.25
102.64 106.75
120.08 124.88
140.47 146.09
164.33 170.91
192.25 199.94
224.9 233.9
263.1 273.63
307.79 320.11
END

GTLOG
```

.51

```
*ISPEGEN
ENERXN -0.
ENESAD 9.25
MEPTYPER one
MEPTYPEP one
RCINFO
 SRC -3.5376
END
PCINFO
 SPC 3.5376
END


*GRGENERAL
GRRESTART

*GRSTART
CHARGE 0
MULTIPLICITY 1

*GRCOMMON

GRENER
%mem=100gb
%nproc=16
#n pbe1pbe/def2tzvp  units(au) fchk
nosymm int(ultrafine)
END

GRFIRST
%mem=100gb
%nproc=16
#n pbe1pbe/def2tzvp  units(au) fchk
nosymm force int(ultrafine)
END

GRSEC
%mem=100gb
%nproc=16
#n pbe1pbe/def2tzvp  units(au) fchk
nosymm freq int(ultrafine)
END
```

.71

```
%mem=100gb
%nproc=16
#n pbe1pbe/def2tzvp  fchk  nosymm
int(ultrafine)


0 1
C 0.055507 1.399815 0.000000
C -0.751898 0.954382 1.189224
H 0.190697 2.482866 0.000000
H -1.383774 1.668800 1.705733
C -0.751898 -0.339715 1.522632
C 0.061982 -1.303139 0.785085
H -1.383147 -0.707121 2.325027
C 1.229824 -0.791239 -0.000000
C -0.751898 0.954382 -1.189224
C -0.751898 -0.339715 -1.522632
H -1.383774 1.668800 -1.705733
C 0.061982 -1.303139 -0.785085
H 0.149295 -2.294481 -1.212974
H 2.126117 -1.401503 -0.000000
H -1.383147 -0.707121 -2.325027
H 0.149295 -2.294481 1.212974
C 1.422168 0.697579 0.000000
H 1.987604 1.004488 -0.885300
H 1.987604 1.004488 0.885300
```

.73

```
%mem=100gb
%nproc=16
#n pbe1pbe/def2tzvp  fchk  nosymm
int(ultrafine)


0 1
C 0.055507 1.399815 0.000000
C -0.751898 0.954382 1.189224
H 0.190697 2.482866 0.000000
H -1.383774 1.668800 1.705733
C -0.751898 -0.339715 1.522632
C 0.061982 -1.303139 0.785085
H -1.383147 -0.707121 2.325027
C 1.229824 -0.791239 -0.000000
C -0.751898 0.954382 -1.189224
C -0.751898 -0.339715 -1.522632
H -1.383774 1.668800 -1.705733
C 0.061982 -1.303139 -0.785085
H 0.149295 -2.294481 -1.212974
H 2.126117 -1.401503 -0.000000
H -1.383147 -0.707121 -2.325027
H 0.149295 -2.294481 1.212974
C 1.422168 0.697579 0.000000
H 1.987604 1.004488 -0.885300
H 1.987604 1.004488 0.885300
```

.75

```
%mem=100gb
%nproc=16
#n pbe1pbe/def2tzvp  fchk  nosymm
int(ultrafine)


0 1
C 1.237556 -0.000000 0.725302
C 1.203902 1.006153 -0.367979
H 2.164025 -0.000000 1.297751
H 2.142956 1.352030 -0.781671
C 0.000000 1.499715 -0.838732
C -1.203902 1.006153 -0.367979
H 0.000000 2.182992 -1.680887
C -1.237556 0.000000 0.725302
C 1.203902 -1.006153 -0.367979
C -0.000000 -1.499715 -0.838732
H 2.142956 -1.352030 -0.781671
C -1.203902 -1.006153 -0.367979
H -2.142956 -1.352030 -0.781671
H -2.164025 0.000000 1.297751
H -0.000000 -2.182992 -1.680887
H -2.142956 1.352030 -0.781671
C 0.000000 0.000000 1.600240
H 0.000000 -0.885417 2.242085
H 0.000000 0.885417 2.24208
```