

Electronic Supplementary Information

The reactivity game:
Theoretical predictions for heavy atom tunneling on adamantyl and related carbenes

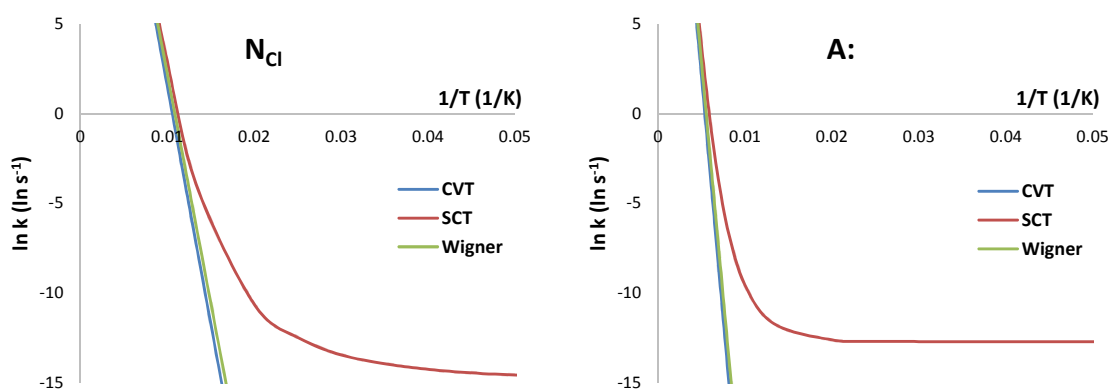
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Comparison of Wigner and SCT corrections:

A first-order tunneling correction for reactions at high temperatures or small imaginary frequencies is the Wigner correction:^{1,2}

$$Q_t = 1 + \frac{1}{24} \left(\frac{h\nu^\ddagger}{k_B T} \right)$$

where $\nu^\ddagger$ is the imaginary frequency of the reaction coordinate. Applying this method to the **N_{Cl}** ring opening and the **A:** H-shift we can see that its accuracy is severely compromised compared to SCT (see figure). In these two cases, below ~150 K Wigner cannot estimate the tunneling effect even in a qualitative manner.



1. E. Wigner, *Z. Phys. Chem. B*, 1932, **19**, 203.
2. R. P. Bell, *The tunnel effect in chemistry*, Chapman and Hall, London; New York, 1980.

Rates of reaction (Polyrate output):

A _H				A _H (¹³ C _α)				A _H (D)			
T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT
6	1.54E-216	1.52E-216	6.82E-04	6	9.11E-217	9.01E-217	5.16E-04	6	2.75E-209	2.75E-209	1.22E-03
8	1.09E-159	1.08E-159	6.82E-04	8	7.38E-160	7.31E-160	5.16E-04	8	3.00E-154	3.00E-154	1.22E-03
10	1.48E-125	1.47E-125	6.82E-04	10	1.08E-125	1.08E-125	5.16E-04	10	3.33E-121	3.32E-121	1.22E-03
20	3.50E-57	3.49E-57	6.82E-04	20	2.99E-57	2.98E-57	5.16E-04	20	5.23E-55	5.23E-55	1.22E-03
30	2.57E-34	2.57E-34	6.84E-04	30	2.32E-34	2.31E-34	5.18E-04	30	7.25E-33	7.25E-33	1.23E-03
40	7.60E-23	7.58E-23	7.15E-04	40	7.03E-23	7.01E-23	5.42E-04	40	9.28E-22	9.28E-22	1.30E-03
50	6.09E-16	6.08E-16	8.66E-04	50	5.72E-16	5.71E-16	6.60E-04	50	4.50E-15	4.50E-15	1.64E-03
75	1.08E-06	1.08E-06	6.15E-03	75	1.03E-06	1.03E-06	4.95E-03	75	4.08E-06	4.08E-06	1.40E-02
100	4.86E-02	4.86E-02	7.74E-01	100	4.71E-02	4.71E-02	6.99E-01	100	1.31E-01	1.31E-01	1.86E+00
125	3.12E+01	3.11E+01	1.19E+02	125	3.04E+01	3.04E+01	1.12E+02	125	6.85E+01	6.85E+01	2.50E+02
150	2.36E+03	2.36E+03	5.24E+03	150	2.31E+03	2.31E+03	4.99E+03	150	4.51E+03	4.51E+03	9.70E+03
175	5.25E+04	5.25E+04	8.81E+04	175	5.16E+04	5.15E+04	8.46E+04	175	9.05E+04	9.05E+04	1.48E+05
200	5.41E+05	5.41E+05	7.71E+05	200	5.33E+05	5.33E+05	7.45E+05	200	8.62E+05	8.62E+05	1.21E+06
225	3.33E+06	3.33E+06	4.29E+06	225	3.29E+06	3.29E+06	4.16E+06	225	4.99E+06	4.99E+06	6.32E+06
250	1.43E+07	1.43E+07	1.72E+07	250	1.41E+07	1.41E+07	1.67E+07	250	2.04E+07	2.04E+07	2.41E+07
275	4.73E+07	4.73E+07	5.41E+07	275	4.67E+07	4.67E+07	5.28E+07	275	6.44E+07	6.44E+07	7.29E+07
300	1.28E+08	1.28E+08	1.42E+08	300	1.27E+08	1.27E+08	1.39E+08	300	1.68E+08	1.68E+08	1.84E+08
325	2.98E+08	2.98E+08	3.21E+08	325	2.95E+08	2.95E+08	3.15E+08	325	3.80E+08	3.80E+08	4.06E+08
350	6.14E+08	6.13E+08	6.50E+08	350	6.08E+08	6.08E+08	6.37E+08	350	7.64E+08	7.63E+08	8.02E+08
375	1.15E+09	1.15E+09	1.20E+09	375	1.14E+09	1.14E+09	1.18E+09	375	1.40E+09	1.40E+09	1.45E+09
400	1.99E+09	1.99E+09	2.05E+09	400	1.97E+09	1.97E+09	2.02E+09	400	2.38E+09	2.38E+09	2.44E+09

A _H (¹³ C _γ)				A _H (¹³ C _β)				A _H (1,3-H-shift) 6-31G(d,p)			
T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT
6	3.26E-216	3.25E-216	3.46E-04	6	3.22E-217	3.16E-217	4.66E-04	6	0.00E+00	0.00E+00	NaN
8	1.92E-159	1.91E-159	3.46E-04	8	3.39E-160	3.34E-160	4.66E-04	8	0.00E+00	0.00E+00	NaN
10	2.33E-125	2.32E-125	3.46E-04	10	5.81E-126	5.75E-126	4.66E-04	10	0.00E+00	0.00E+00	NaN
20	4.38E-57	4.37E-57	3.46E-04	20	2.19E-57	2.18E-57	4.66E-04	20	1.35E-184	1.30E-184	7.77E-13
30	2.99E-34	2.98E-34	3.47E-04	30	1.88E-34	1.88E-34	4.68E-04	30	2.92E-119	2.85E-119	7.78E-13
40	8.49E-23	8.48E-23	3.66E-04	40	6.02E-23	6.00E-23	4.90E-04	40	1.48E-86	1.45E-86	7.97E-13
50	6.64E-16	6.64E-16	4.58E-04	50	5.05E-16	5.04E-16	5.99E-04	50	6.51E-67	6.41E-67	8.87E-13
75	1.14E-06	1.14E-06	4.10E-03	75	9.52E-07	9.51E-07	4.61E-03	75	1.12E-40	1.10E-40	2.47E-12
100	5.06E-02	5.06E-02	6.71E-01	100	4.43E-02	4.42E-02	6.57E-01	100	1.55E-27	1.54E-27	2.46E-11
125	3.21E+01	3.21E+01	1.06E+02	125	2.89E+01	2.89E+01	1.06E+02	125	1.22E-19	1.22E-19	6.13E-10
150	2.41E+03	2.41E+03	4.64E+03	150	2.22E+03	2.22E+03	4.76E+03	150	2.28E-14	2.26E-14	2.18E-08
175	5.33E+04	5.33E+04	7.83E+04	175	4.98E+04	4.98E+04	8.10E+04	175	1.33E-10	1.32E-10	7.87E-07
200	5.47E+05	5.47E+05	6.91E+05	200	5.17E+05	5.17E+05	7.17E+05	200	8.86E-08	8.82E-08	2.54E-05
225	3.36E+06	3.36E+06	3.88E+06	225	3.20E+06	3.20E+06	4.02E+06	225	1.40E-05	1.39E-05	6.67E-04
250	1.44E+07	1.44E+07	1.57E+07	250	1.38E+07	1.38E+07	1.62E+07	250	7.99E-04	7.95E-04	1.30E-02
275	4.74E+07	4.74E+07	4.98E+07	275	4.58E+07	4.58E+07	5.14E+07	275	2.19E-02	2.18E-02	1.80E-01
300	1.28E+08	1.28E+08	1.31E+08	300	1.24E+08	1.24E+08	1.35E+08	300	3.46E-01	3.44E-01	1.80E+00
325	2.97E+08	2.97E+08	2.99E+08	325	2.90E+08	2.90E+08	3.07E+08	325	3.57E+00	3.55E+00	1.35E+01
350	6.12E+08	6.12E+08	6.07E+08	350	5.98E+08	5.98E+08	6.24E+08	350	2.64E+01	2.63E+01	7.87E+01
375	1.14E+09	1.14E+09	1.13E+09	375	1.12E+09	1.12E+09	1.16E+09	375	1.50E+02	1.49E+02	3.72E+02
400	1.98E+09	1.98E+09	1.93E+09	400	1.95E+09	1.95E+09	1.98E+09	400	6.82E+02	6.78E+02	1.47E+03

A _{Cl}				N _H				N _{Cl} (¹³ C:)			
T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN	6	1.66E-03	1.35E-03	2.77E+11	6	1.35E-178	1.22E-178	2.21E-07
8	0.00E+00	0.00E+00	NaN	8	6.50E+00	5.58E+00	2.77E+11	8	3.07E-131	2.84E-131	2.21E-07
10	6.31E-307	5.81E-307	2.7E-31*	10	9.80E+02	8.7E+02	2.77E+11	10	8.35E-103	7.86E-103	2.22E-07
20	6.62E-148	6.35E-148	7.79E-31	20	2.85E+07	2.68E+07	2.77E+11	20	7.80E-46	7.57E-46	2.76E-07
30	7.32E-95	7.12E-95	4.71E-30	30	1.04E+09	1.00E+09	2.78E+11	30	8.66E-27	8.49E-27	5.87E-07
40	2.49E-68	2.44E-68	4.00E-29	40	6.86E+09	6.66E+09	2.82E+11	40	3.00E-17	2.96E-17	2.25E-06
50	2.10E-52	2.06E-52	5.36E-28	50	2.24E+10	2.18E+10	2.92E+11	50	1.61E-11	1.59E-11	1.53E-05
75	3.72E-31	3.68E-31	4.43E-24	75	1.20E+11	1.18E+11	3.62E+11	75	7.25E-04	7.20E-04	1.64E-02
100	1.63E-20	1.61E-20	9.67E-19	100	3.04E+11	3.01E+11	5.04E+11	100	4.98E+00	4.95E+00	1.82E+01
125	4.05E-14	4.02E-14	2.30E-13	125	5.60E+11	5.55E+11	7.13E+11	125	1.02E+03	1.01E+03	2.17E+03
150	7.61E-10	7.57E-10	2.17E-09	150	8.73E+11	8.65E+11	9.79E+11	150	3.57E+04	3.56E+04	5.97E+04
175	8.74E-07	8.69E-07	1.79E-06	175	1.23E+12	1.22E+12	1.29E+12	175	4.61E+05	4.59E+05	6.70E+05
200	1.75E-04	1.74E-04	2.96E-04	200	1.62E+12	1.61E+12	1.64E+12	200	3.17E+06	3.16E+06	4.23E+06
225	1.09E-02	1.08E-02	1.63E-02	225	2.04E+12	2.03E+12	2.02E+12	225	1.43E+07	1.43E+07	1.80E+07
250	2.99E-01	2.97E-01	4.13E-01	250	2.49E+12	2.47E+12	2.43E+12	250	4.83E+07	4.81E+07	5.82E+07
275	4.52E+00	4.50E+00	5.89E+00	275	2.95E+12	2.93E+12	2.86E+12	275	1.31E+08	1.31E+08	1.53E+08
300	4.38E+01	4.36E+01	5.45E+01	300	3.43E+12	3.41E+12	3.31E+12	300	3.03E+08	3.02E+08	3.45E+08
325	3.00E+02	2.99E+02	3.61E+02	325	3.92E+12	3.90E+12	3.77E+12	325	6.16E+08	6.15E+08	6.91E+08
350	1.57E+03	1.56E+03	1.84E+03	350	4.42E+12	4.40E+12	4.25E+12	350	1.14E+09	1.13E+09	1.26E+09
375	6.61E+03	6.58E+03	7.57E+03	375	4.93E+12	4.90E+12	4.73E+12	375	1.94E+09	1.93E+09	2.12E+09
400	2.33E+04	2.32E+04	2.62E+04	400	5.44E+12	5.42E+12	5.23E+12	400	3.10E+09	3.09E+09	3.35E+09

A _F				N _{Cl}				N _{Cl} (¹³ C _α)			
T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT	T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN	6	1.32E-178	1.21E-178	3.72E-07	6	8.93E-179	8.17E-179	2.44E-07
8	0.00E+00	0.00E+00	NaN	8	3.00E-131	2.82E-131	3.73E-07	8	2.25E-131	2.10E-131	2.44E-07
10		2.0E-390*	3.6E-35*	10	8.22E-103	7.80E-103	3.74E-07	10	6.52E-103	6.18E-103	2.45E-07
20	7.81E-190	7.56E-190	3.77E-35	20	7.74E-46	7.54E-46	4.66E-07	20	6.90E-46	6.72E-46	3.04E-07
30	8.60E-123	8.41E-123	6.67E-35	30	8.62E-27	8.48E-27	9.97E-07	30	7.99E-27	7.85E-27	6.51E-07
40	2.94E-89	2.90E-89	1.80E-34	40	2.99E-17	2.96E-17	3.79E-06	40	2.83E-17	2.79E-17	2.53E-06
50	3.94E-69	3.89E-69	8.56E-34	50	1.61E-11	1.60E-11	2.46E-05	50	1.54E-11	1.52E-11	1.73E-05
75	2.75E-42	2.73E-42	1.13E-30	75	7.26E-04	7.21E-04	1.99E-02	75	7.04E-04	6.99E-04	1.71E-02
100	7.42E-29	7.37E-29	9.89E-26	100	4.99E+00	4.96E+00	1.96E+01	100	4.87E+00	4.85E+00	1.82E+01
125	8.60E-21	8.55E-21	1.01E-19	125	1.02E+03	1.02E+03	2.30E+03	125	1.00E+03	9.96E+02	2.17E+03
150	2.07E-15	2.06E-15	8.09E-15	150	3.59E+04	3.58E+04	6.26E+04	150	3.53E+04	3.52E+04	5.96E+04
175	1.45E-11	1.45E-11	3.59E-11	175	4.64E+05	4.62E+05	6.99E+05	175	4.57E+05	4.56E+05	6.69E+05
200	1.13E-08	1.12E-08	2.16E-08	200	3.19E+06	3.18E+06	4.39E+06	200	3.15E+06	3.15E+06	4.23E+06
225	2.00E-06	1.99E-06	3.28E-06	225	1.44E+07	1.44E+07	1.87E+07	225	1.43E+07	1.43E+07	1.80E+07
250	1.27E-04	1.26E-04	1.87E-04	250	4.87E+07	4.86E+07	6.02E+07	250	4.82E+07	4.81E+07	5.83E+07
275	3.80E-03	3.79E-03	5.21E-03	275	1.32E+08	1.32E+08	1.58E+08	275	1.31E+08	1.31E+08	1.54E+08
300	6.50E-02	6.48E-02	8.43E-02	300	3.05E+08	3.05E+08	3.57E+08	300	3.03E+08	3.02E+08	3.47E+08
325	7.20E-01	7.18E-01	8.96E-01	325	6.23E+08	6.21E+08	7.12E+08	325	6.18E+08	6.16E+08	6.94E+08
350	5.68E+00	5.66E+00	6.83E+00	350	1.15E+09	1.15E+09	1.29E+09	350	1.14E+09	1.14E+09	1.26E+09
375	3.41E+01	3.40E+01	4.00E+01	375	1.96E+09	1.96E+09	2.18E+09	375	1.94E+09	1.94E+09	2.13E+09
400	1.64E+02	1.63E+02	1.88E+02	400	3.13E+09	3.13E+09	3.44E+09	400	3.11E+09	3.10E+09	3.36E+09

* Extrapolated values.

N_{Cl} (¹³C_β)

T(K)	TST	CVT	CVT/SCT
6	2.40E-179	2.24E-179	2.73E-07
8	8.39E-132	7.96E-132	2.73E-07
10	2.96E-103	2.84E-103	2.74E-07
20	4.64E-46	4.54E-46	3.43E-07
30	6.13E-27	6.04E-27	7.35E-07
40	2.32E-17	2.29E-17	2.83E-06
50	1.31E-11	1.30E-11	1.88E-05
75	6.33E-04	6.29E-04	1.65E-02
100	4.50E+00	4.48E+00	1.72E+01
125	9.39E+02	9.36E+02	2.06E+03
150	3.36E+04	3.35E+04	5.69E+04
175	4.38E+05	4.37E+05	6.43E+05
200	3.04E+06	3.03E+06	4.08E+06
225	1.38E+07	1.38E+07	1.75E+07
250	4.69E+07	4.68E+07	5.67E+07
275	1.28E+08	1.28E+08	1.50E+08
300	2.97E+08	2.96E+08	3.39E+08
325	6.06E+08	6.05E+08	6.81E+08
350	1.12E+09	1.12E+09	1.24E+09
375	1.92E+09	1.91E+09	2.09E+09
400	3.07E+09	3.06E+09	3.32E+09

N_{Cl} (³⁷Cl)

T(K)	TST	CVT	CVT/SCT
6	1.46E-178	1.33E-178	3.16E-07
8	3.24E-131	3.04E-131	3.16E-07
10	8.73E-103	8.28E-103	3.17E-07
20	7.97E-46	7.76E-46	3.96E-07
30	8.78E-27	8.62E-27	8.59E-07
40	3.03E-17	2.99E-17	3.38E-06
50	1.62E-11	1.61E-11	2.28E-05
75	7.28E-04	7.23E-04	1.95E-02
100	4.99E+00	4.97E+00	1.90E+01
125	1.02E+03	1.01E+03	2.20E+03
150	3.59E+04	3.58E+04	5.97E+04
175	4.63E+05	4.62E+05	6.66E+05
200	3.19E+06	3.18E+06	4.19E+06
225	1.44E+07	1.44E+07	1.79E+07
250	4.86E+07	4.85E+07	5.78E+07
275	1.32E+08	1.32E+08	1.52E+08
300	3.05E+08	3.05E+08	3.44E+08
325	6.22E+08	6.21E+08	6.88E+08
350	1.15E+09	1.15E+09	1.25E+09
375	1.96E+09	1.95E+09	2.11E+09
400	3.13E+09	3.12E+09	3.34E+09

N_F

T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN
8	7.11E-241	6.83E-241	7.27E-16
10	1.65E-190	1.59E-190	7.28E-16
20	1.12E-89	1.10E-89	8.02E-16
30	5.32E-56	5.27E-56	1.32E-15
40	3.86E-39	3.83E-39	3.64E-15
50	5.15E-29	5.12E-29	1.78E-14
75	1.67E-15	1.67E-15	1.07E-11
100	9.67E-09	9.64E-09	1.21E-07
125	1.11E-04	1.11E-04	3.82E-04
150	5.72E-02	5.71E-02	1.21E-01
175	4.98E+00	4.97E+00	8.21E+00
200	1.43E+02	1.43E+02	2.04E+02
225	1.96E+03	1.95E+03	2.54E+03
250	1.59E+04	1.59E+04	1.95E+04
275	8.91E+04	8.90E+04	1.04E+05
300	3.75E+05	3.75E+05	4.25E+05
325	1.27E+06	1.27E+06	1.40E+06
350	3.61E+06	3.61E+06	3.92E+06
375	8.97E+06	8.97E+06	9.60E+06
400	1.99E+07	1.99E+07	2.11E+07

B_{Cl}

T(K)	TST	CVT	CVT/SCT
6	3.24E-55	1.06E-55	5.57E+02
8	1.06E-38	4.60E-39	5.57E+02
10	9.07E-29	4.65E-29	5.60E+02
20	8.33E-09	5.96E-09	7.74E+02
30	4.28E-02	3.42E-02	2.12E+03
40	1.01E+02	8.54E+01	1.12E+04
50	1.08E+04	9.49E+03	1.05E+05
75	5.75E+06	5.26E+06	1.26E+07
100	1.37E+08	1.28E+08	2.10E+08
125	9.40E+08	8.91E+08	1.25E+09
150	3.47E+09	3.31E+09	4.24E+09
175	8.94E+09	8.59E+09	1.04E+10
200	1.84E+10	1.78E+10	2.08E+10
225	3.27E+10	3.17E+10	3.60E+10
250	5.23E+10	5.06E+10	5.65E+10
275	7.72E+10	7.49E+10	8.24E+10
300	1.08E+11	1.04E+11	1.14E+11
325	1.43E+11	1.39E+11	1.50E+11
350	1.84E+11	1.79E+11	1.91E+11
375	2.30E+11	2.23E+11	2.37E+11
400	2.80E+11	2.72E+11	2.87E+11

B_F

T(K)	TST	CVT	CVT/SCT
6	3.29E-173	1.82E-173	4.81E-07
8	3.39E-127	2.17E-127	4.81E-07
10	1.44E-99	1.01E-99	4.83E-07
20	3.27E-44	2.73E-44	5.71E-07
30	1.04E-25	9.21E-26	9.53E-07
40	1.91E-16	1.75E-16	2.44E-06
50	7.00E-11	6.52E-11	1.11E-05
75	1.87E-03	1.79E-03	1.75E-02
100	9.86E+00	9.53E+00	2.56E+01
125	1.71E+03	1.66E+03	3.00E+03
150	5.38E+04	5.26E+04	7.82E+04
175	6.39E+05	6.27E+05	8.36E+05
200	4.12E+06	4.05E+06	5.05E+06
225	1.77E+07	1.74E+07	2.07E+07
250	5.70E+07	5.63E+07	6.48E+07
275	1.49E+08	1.48E+08	1.66E+08
300	3.34E+08	3.31E+08	3.65E+08
325	6.63E+08	6.56E+08	7.14E+08
350	1.19E+09	1.18E+09	1.27E+09
375	1.99E+09	1.98E+09	2.11E+09
400	3.13E+09	3.10E+09	3.28E+09

B_F (¹³C:)

T(K)	TST	CVT	CVT/SCT
6	3.30E-173	1.79E-173	2.55E-07
8	3.40E-127	2.15E-127	2.55E-07
10	1.45E-99	1.00E-99	2.56E-07
20	3.27E-44	2.72E-44	3.04E-07
30	1.04E-25	9.17E-26	5.16E-07
40	1.91E-16	1.74E-16	1.37E-06
50	6.99E-11	6.50E-11	6.81E-06
75	1.87E-03	1.78E-03	1.55E-02
100	9.81E+00	9.47E+00	2.43E+01
125	1.70E+03	1.65E+03	2.87E+03
150	5.34E+04	5.22E+04	7.54E+04
175	6.33E+05	6.21E+05	8.08E+05
200	4.08E+06	4.01E+06	4.89E+06
225	1.75E+07	1.72E+07	2.01E+07
250	5.64E+07	5.57E+07	6.30E+07
275	1.48E+08	1.46E+08	1.61E+08
300	3.30E+08	3.27E+08	3.56E+08
325	6.55E+08	6.48E+08	6.96E+08
350	1.18E+09	1.17E+09	1.24E+09
375	1.97E+09	1.95E+09	2.06E+09
400	3.09E+09	3.06E+09	3.21E+09

B_F (¹³C_α)

T(K)	TST	CVT	CVT/SCT
6	2.49E-173	1.37E-173	2.95E-07
8	2.75E-127	1.76E-127	2.95E-07
10	1.22E-99	8.55E-100	2.96E-07
20	3.01E-44	2.51E-44	3.51E-07
30	9.81E-26	8.71E-26	5.92E-07
40	1.83E-16	1.68E-16	1.56E-06
50	6.77E-11	6.31E-11	7.48E-06
75	1.83E-03	1.75E-03	1.56E-02
100	9.69E+00	9.36E+00	2.41E+01
125	1.68E+03	1.64E+03	2.85E+03
150	5.31E+04	5.20E+04	7.50E+04
175	6.32E+05	6.20E+05	8.05E+05
200	4.08E+06	4.01E+06	4.88E+06
225	1.75E+07	1.73E+07	2.01E+07
250	5.66E+07	5.58E+07	6.30E+07
275	1.48E+08	1.46E+08	1.62E+08
300	3.32E+08	3.28E+08	3.56E+08
325	6.58E+08	6.51E+08	6.98E+08
350	1.19E+09	1.17E+09	1.25E+09
375	1.98E+09	1.96E+09	2.06E+09
400	3.10E+09	3.08E+09	3.22E+09

B_F (¹⁸F)

T(K)	TST	CVT	CVT/SCT
6	2.67E-173	1.49E-173	5.63E-07
8	2.90E-127	1.87E-127	5.64E-07
10	1.27E-99	8.99E-100	5.66E-07
20	3.07E-44	2.58E-44	6.63E-07
30	9.99E-26	8.89E-26	1.08E-06
40	1.86E-16	1.71E-16	2.71E-06
50	6.88E-11	6.42E-11	1.20E-05
75	1.86E-03	1.78E-03	1.73E-02
100	9.83E+00	9.50E+00	2.39E+01
125	1.71E+03	1.66E+03	2.75E+03
150	5.38E+04	5.27E+04	7.20E+04
175	6.39E+05	6.28E+05	7.73E+05
200	4.13E+06	4.06E+06	4.70E+06
225	1.77E+07	1.75E+07	1.94E+07
250	5.72E+07	5.64E+07	6.10E+07
275	1.50E+08	1.48E+08	1.57E+08
300	3.35E+08	3.31E+08	3.46E+08
325	6.64E+08	6.58E+08	6.80E+08
350	1.20E+09	1.19E+09	1.22E+09
375	2.00E+09	1.98E+09	2.02E+09
400	3.14E+09	3.11E+09	3.16E+09

A: (D_p)

T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN
8	6.52E-288	1.71E-288	5.10E-10
10	3.90E-228	1.34E-228	5.10E-10
20	1.78E-108	1.04E-108	5.10E-10
30	1.63E-68	1.15E-68	5.11E-10
40	1.70E-48	1.30E-48	5.29E-10
50	1.84E-36	1.48E-36	6.18E-10
75	2.24E-20	1.94E-20	3.12E-09
100	2.62E-12	2.36E-12	1.23E-07
125	1.86E-07	1.71E-07	1.88E-05
150	3.21E-04	2.99E-04	3.46E-03
175	6.58E-02	6.20E-02	2.93E-01
200	3.56E+00	3.38E+00	1.02E+01
225	7.92E+01	7.57E+01	1.74E+02
250	9.45E+02	9.08E+02	1.75E+03
275	7.17E+03	6.92E+03	1.18E+04
300	3.88E+04	3.75E+04	5.86E+04
325	1.61E+05	1.57E+05	2.29E+05
350	5.48E+05	5.34E+05	7.37E+05
375	1.58E+06	1.54E+06	2.04E+06
400	3.99E+06	3.90E+06	4.99E+06

B_F (¹³C_β)

T(K)	TST	CVT	CVT/SCT
6	1.19E-173	6.84E-174	3.88E-07
8	1.58E-127	1.04E-127	3.88E-07
10	7.86E-100	5.63E-100	3.89E-07
20	2.41E-44	2.04E-44	4.64E-07
30	8.46E-26	7.57E-26	7.85E-07
40	1.64E-16	1.51E-16	2.04E-06
50	6.19E-11	5.80E-11	9.37E-06
75	1.73E-03	1.65E-03	1.58E-02
100	9.28E+00	8.98E+00	2.36E+01
125	1.63E+03	1.59E+03	2.78E+03
150	5.17E+04	5.07E+04	7.33E+04
175	6.18E+05	6.07E+05	7.90E+05
200	4.01E+06	3.95E+06	4.80E+06
225	1.73E+07	1.70E+07	1.98E+07
250	5.58E+07	5.52E+07	6.22E+07
275	1.47E+08	1.45E+08	1.60E+08
300	3.29E+08	3.25E+08	3.53E+08
325	6.53E+08	6.46E+08	6.92E+08
350	1.18E+09	1.17E+09	1.24E+09
375	1.97E+09	1.95E+09	2.05E+09
400	3.09E+09	3.07E+09	3.20E+09

A: (H-Shift) 6-31G(d,p)

T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN
8	2.32E-276	2.07E-278	2.99E-06
10	6.80E-219	1.56E-220	2.99E-06
20	7.47E-104	1.13E-104	2.99E-06
30	1.98E-65	5.61E-66	2.99E-06
40	3.50E-46	1.36E-46	3.04E-06
50	1.30E-34	6.12E-35	3.30E-06
75	3.85E-19	2.33E-19	8.15E-06
100	2.23E-11	1.53E-11	7.19E-05
125	1.04E-06	7.69E-07	1.70E-03
150	1.36E-03	1.06E-03	6.43E-02
175	2.28E-01	1.84E-01	2.23E+00
200	1.07E+01	8.86E+00	4.88E+01
225	2.12E+02	1.80E+02	6.37E+02
250	2.31E+03	2.00E+03	5.36E+03
275	1.63E+04	1.43E+04	3.18E+04
300	8.31E+04	7.38E+04	1.43E+05
325	3.29E+05	2.95E+05	5.18E+05
350	1.07E+06	9.69E+05	1.57E+06
375	2.98E+06	2.71E+06	4.13E+06
400	7.28E+06	6.68E+06	9.67E+06

A: (D_d)

T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN
8	5.28E-278	1.58E-280	4.57E-08
10	3.30E-220	3.15E-222	4.57E-08
20	1.65E-104	1.61E-105	4.57E-08
30	7.22E-66	1.53E-66	4.58E-08
40	1.65E-46	5.15E-47	4.70E-08
50	7.12E-35	2.81E-35	5.30E-08
75	2.57E-19	1.38E-19	1.94E-07
100	1.64E-11	1.03E-11	4.00E-06
125	8.11E-07	5.60E-07	2.51E-04
150	1.10E-03	8.06E-04	2.03E-02
175	1.89E-01	1.46E-01	1.03E+00
200	9.01E+00	7.17E+00	2.63E+01
225	1.81E+02	1.48E+02	3.71E+02
250	2.00E+03	1.67E+03	3.27E+03
275	1.42E+04	1.21E+04	2.01E+04
300	7.31E+04	6.30E+04	9.31E+04
325	2.91E+05	2.54E+05	3.45E+05
350	9.52E+05	8.40E+05	1.07E+06
375	2.66E+06	2.37E+06	2.87E+06
400	6.52E+06	5.85E+06	6.83E+06

A: (¹³C:)

T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN
8	3.09E-276	2.54E-278	2.47E-06
10	8.55E-219	1.83E-220	2.47E-06
20	8.37E-104	1.23E-104	2.47E-06
30	2.13E-65	5.93E-66	2.47E-06
40	3.71E-46	1.42E-46	2.51E-06
50	1.36E-34	6.32E-35	2.73E-06
75	3.96E-19	2.38E-19	6.86E-06
100	2.28E-11	1.55E-11	6.26E-05
125	1.05E-06	7.77E-07	1.54E-03
150	1.37E-03	1.06E-03	6.06E-02
175	2.30E-01	1.85E-01	2.16E+00
200	1.07E+01	8.88E+00	4.77E+01
225	2.12E+02	1.80E+02	6.26E+02
250	2.31E+03	2.00E+03	5.28E+03
275	1.63E+04	1.43E+04	3.14E+04
300	8.31E+04	7.36E+04	1.41E+05
325	3.29E+05	2.94E+05	5.11E+05
350	1.07E+06	9.66E+05	1.55E+06
375	2.97E+06	2.70E+06	4.08E+06
400	7.26E+06	6.65E+06	9.56E+06

A: (¹³C_β)

T(K)	TST	CVT	CVT/SCT
6	0.00E+00	0.00E+00	NaN
8	1.88E-276	1.58E-278	2.18E-06
10	5.74E-219	1.25E-220	2.18E-06
20	6.86E-104	1.01E-104	2.18E-06
30	1.87E-65	5.22E-66	2.18E-06
40	3.35E-46	1.29E-46	2.22E-06
50	1.26E-34	5.86E-35	2.43E-06
75	3.76E-19	2.26E-19	6.25E-06
100	2.19E-11	1.49E-11	5.86E-05
125	1.02E-06	7.54E-07	1.50E-03
150	1.34E-03	1.04E-03	5.94E-02
175	2.25E-01	1.82E-01	2.11E+00
200	1.05E+01	8.73E+00	4.64E+01
225	2.09E+02	1.77E+02	6.07E+02
250	2.29E+03	1.97E+03	5.11E+03
275	1.62E+04	1.41E+04	3.03E+04
300	8.23E+04	7.29E+04	1.36E+05
325	3.26E+05	2.92E+05	4.94E+05
350	1.06E+06	9.59E+05	1.50E+06
375	2.95E+06	2.69E+06	3.95E+06
400	7.22E+06	6.61E+06	9.25E+06

XYZ Geometries

A _H			
H	-3.114496	-0.898527	0.036566
C	-2.738140	0.146519	-0.080274
C	-1.298211	0.027816	-0.277870
C	-1.018665	0.032586	1.309486
C	-0.614275	1.277352	-0.878648
C	-0.670288	-1.257776	-0.869692
C	0.519355	-0.006514	1.513189
C	0.906937	1.240373	-0.638636
C	0.853156	-1.284140	-0.630858
C	1.174002	1.235696	0.879507
C	1.117389	-1.281148	0.887755
C	1.500243	-0.037010	-1.269922
H	1.326291	-0.036758	-2.354821
H	2.197147	-1.315692	1.086805
H	0.695973	-0.007469	2.597397
H	2.588724	-0.061265	-1.121849
H	-1.065994	2.176455	-0.442916
H	0.775428	2.150781	1.338008
H	2.254485	1.222746	1.077750
H	-1.144790	-2.140981	-0.420485
H	-1.435686	0.930988	1.772569
H	0.678617	-2.175388	1.351575
H	-1.474593	-0.842326	1.787010
H	1.370932	2.126391	-1.091267
H	1.278134	-2.192753	-1.077413
H	-0.825951	1.307259	-1.956082
H	-0.883650	-1.292430	-1.946739

A _H to H _H ^{ene} TS			
H	-2.894861	-1.011797	0.335587
C	-2.550566	0.032938	0.203603
C	-1.320199	-0.008301	-0.456401
C	-1.142920	0.162441	1.411568
C	-0.627624	1.265775	-0.939153
C	-0.658957	-1.261647	-1.031659
C	0.412343	-0.005746	1.487154
C	0.890714	1.235353	-0.653469
C	0.837693	-1.286158	-0.672472
C	1.115920	1.218216	0.868206
C	0.973692	-1.299773	0.862749
C	1.519989	-0.034585	-1.262965
H	1.408962	-0.030707	-2.356121
H	2.031873	-1.392033	1.142749
H	0.622789	-0.022105	2.566119
H	2.597943	-0.054585	-1.052539
H	-1.112559	2.138831	-0.488665
H	0.734099	2.141454	1.324195
H	2.191042	1.174111	1.089165
H	-1.167508	-2.157302	-0.656880
H	-1.378009	1.152854	1.794413
H	0.459526	-2.178429	1.276407
H	-1.603068	-0.608518	2.031104
H	1.359374	2.127883	-1.087179
H	1.297906	-2.192642	-1.085941
H	-0.799585	1.331241	-2.023350
H	-0.784160	-1.246055	-2.124606

H _H ^{ene}			
H	-2.215119	-1.306873	0.696638
C	-1.816103	-0.307038	0.519887
C	-1.287736	-0.057711	-0.691269
C	-1.197314	0.359038	1.725705
C	-0.608298	1.258689	-1.024134
C	-0.681177	-1.246085	-1.385059
C	0.349883	0.082835	1.599189
C	0.894108	1.227843	-0.637049
C	0.740936	-1.275041	-0.707084
C	1.077332	1.251528	0.893977
C	0.708183	-1.267078	0.864754
C	1.536745	-0.052382	-1.201905
H	1.545338	-0.030032	-2.300439
H	1.721812	-1.541679	1.188741
H	0.755205	0.007346	2.618256
H	2.584642	-0.117157	-0.877200
H	-1.109106	2.094354	-0.521160
H	0.724618	2.207047	1.306111
H	2.153455	1.198610	1.114766
H	-1.225259	-2.172455	-1.166495
H	-1.373871	1.440315	1.795620
H	0.050168	-2.069984	1.222173
H	-1.588748	-0.082742	2.649196
H	1.390369	2.110612	-1.062876
H	1.252056	-2.196657	-1.019660
H	-0.694659	1.440806	-2.105258
H	-0.567488	-1.155214	-2.474619

A _H 6-31G(d,p)			
H	3.137456	0.873891	0.028594
C	2.755524	-0.166428	-0.107857
C	1.315480	-0.035128	-0.293288
C	1.047829	-0.073466	1.297056
C	0.619407	-1.267060	-0.915865
C	0.690177	1.266725	-0.851427
C	-0.487949	-0.029785	1.512800
C	-0.899418	-1.226482	-0.662474
C	-0.830994	1.296646	-0.599858
C	-1.154123	-1.254320	0.857412
C	-1.082850	1.261990	0.920379
C	-1.490758	0.067752	-1.260393
H	-1.326488	0.090316	-2.345617
H	-2.159664	1.299518	1.129279
H	-0.656032	-0.051671	2.597446
H	-2.576806	0.094871	-1.102423
H	1.068945	-2.177296	-0.503873
H	-0.755967	-2.180329	1.291410
H	-2.231873	-1.240992	1.064865
H	1.173095	2.136006	-0.386540
H	1.463249	-0.984133	1.735119
H	-0.634066	2.142009	1.399310
H	1.512896	0.787388	1.789012
H	-1.372143	-2.098900	-1.130471
H	-1.253915	2.216715	-1.022461
H	0.822085	-1.273883	-1.994427
H	0.895276	1.323833	-1.928143

A _H 1,3-H-Shift TS			
H	3.204593	0.525219	0.244711
C	2.606077	-0.309889	-0.159383
C	1.212859	0.149006	-0.492959
C	1.194409	-0.086301	1.008586
C	0.463744	-0.931447	-1.303278
C	0.563494	1.517364	-0.701336
C	-0.206569	-0.481782	1.496037
C	-0.987890	-1.058222	-0.833816
C	-0.899680	1.368518	-0.149178
C	-0.944693	-1.522214	0.636966
C	-0.935078	0.896268	1.332355
C	-1.672297	0.316970	-0.975955
H	-1.699774	0.606845	-2.034349
H	-1.981522	0.793882	1.648786
H	-0.201327	-0.784083	2.549914
H	-2.713813	0.268151	-0.632153
H	0.990257	-1.884838	-1.197161
H	-0.451993	-2.500169	0.703044
H	-1.958709	-1.648942	1.036912
H	1.103275	2.303641	-0.158843
H	2.189887	-0.954953	0.922871
H	-0.477495	1.643109	1.992097
H	1.514900	0.794824	1.558898
H	-1.520915	-1.804036	-1.436596
H	-1.406674	2.338554	-0.222211
H	0.516538	-0.658822	-2.365658
H	0.526513	1.812001	-1.758496

A _H Cyclopropane			
H	3.284295	0.500675	0.186323
C	2.464825	-0.189548	-0.001743
C	1.138093	0.273530	-0.582597
C	1.268151	0.031910	0.907023
C	0.443311	-0.851815	-1.370689
C	0.389470	1.589864	-0.757428
C	-0.040250	-0.498284	1.496884
C	-0.948170	-1.115561	-0.787031
C	-1.007751	1.306296	-0.079727
C	-0.745404	-1.590121	0.669325
C	-0.903682	0.808968	1.397451
C	-1.752673	0.199183	-0.858579
H	-1.887255	0.490187	-1.908876
H	-1.919099	0.616851	1.768355
H	0.045956	-0.813505	2.545118
H	-2.756513	0.060913	-0.435971
H	1.032902	-1.774699	-1.344434
H	-0.163275	-2.520791	0.675341
H	-1.711755	-1.819151	1.136590
H	0.899116	2.420447	-0.255576
H	2.796571	-1.169772	-0.332933
H	-0.476604	1.586960	2.041644
H	1.475352	0.975059	1.416271
H	-1.462766	-1.898259	-1.359211
H	-1.601771	2.228892	-0.098432
H	0.377444	-0.552986	-2.425715
H	0.231875	1.882630	-1.805840

A_{Cl}

Cl	3.289755	0.214359	0.001577
C	1.995804	-0.980142	-0.045638
C	0.646119	-0.352831	-0.116864
C	0.135594	-0.578649	1.363762
C	-0.213399	-1.254403	-1.057369
C	0.438330	1.131584	-0.491329
C	-1.357633	-0.190245	1.446174
C	-1.701537	-0.867851	-0.952480
C	-1.056730	1.502469	-0.394453
C	-2.183285	-1.080228	0.496490
C	-1.538703	1.289719	1.055145
C	-1.880973	0.612186	-1.346534
H	-1.557888	0.768556	-2.384952
H	-2.595937	1.572897	1.148398
H	-1.688114	-0.345384	2.481990
H	-2.942883	0.889547	-1.297546
H	-0.060128	-2.306689	-0.791850
H	-2.079007	-2.136473	0.779567
H	-3.249144	-0.829283	0.582073
H	1.026197	1.774698	0.173470
H	0.280117	-1.624679	1.655323
H	-0.973204	1.935368	1.740966
H	0.728074	0.040299	2.048470
H	-2.281007	-1.506651	-1.631852
H	-1.182379	2.556963	-0.672714
H	0.138115	-1.129465	-2.089768
H	0.809817	1.306539	-1.509800

A_{Cl} to H_C^{ene} TS

Cl	3.128815	0.172636	0.120632
C	1.721778	-0.623423	-0.786735
C	0.557785	0.149628	-0.750853
C	0.555933	-1.391602	0.465494
C	-0.562776	-0.256158	-1.703452
C	0.303062	1.478340	-0.066704
C	-0.840562	-1.094626	1.093190
C	-1.940727	-0.237728	-1.006760
C	-1.050617	1.415704	0.670200
C	-1.971916	-1.331288	0.074336
C	-0.994542	0.301370	1.734589
C	-2.178209	1.133605	-0.342965
H	-2.207778	1.927655	-1.101522
H	-1.921179	0.311343	2.323933
H	-0.922787	-1.849740	1.888603
H	-3.153555	1.139160	0.162017
H	-0.338243	-1.234131	-2.142996
H	-1.868737	-2.325372	-0.380675
H	-2.939973	-1.316134	0.592449
H	1.118876	1.720498	0.618211
H	0.513553	-2.366139	-0.016138
H	-0.170965	0.492057	2.435181
H	1.318179	-1.375644	1.241681
H	-2.719638	-0.432877	-1.754308
H	-1.225374	2.378375	1.166090
H	-0.547902	0.471821	-2.527102
H	0.280413	2.261386	-0.838212

H_C^{ene}

Cl	-2.834940	-0.167878	0.068989
C	-1.268793	0.293361	-0.661199
C	-0.355497	-0.641101	-0.975706
C	-0.781650	1.669050	-0.263816
C	0.930456	-0.219700	-1.677912
C	-0.178985	-1.831865	-0.076301
C	0.399895	1.450370	0.754627
C	2.059862	0.126404	-0.673951
C	0.781738	-1.213758	1.010759
C	1.769912	1.460686	0.039285
C	0.281222	0.143531	1.628416
C	2.166024	-0.996564	0.373528
H	2.518428	-1.928493	-0.089149
H	0.899871	0.312605	2.520343
H	0.381029	2.300099	1.450686
H	2.904899	-0.722086	1.138999
H	0.749528	0.624704	-2.352007
H	1.808105	2.293573	-0.676379
H	2.566637	1.646021	0.773726
H	-1.115111	-2.164608	0.374934
H	-0.434529	2.260280	-1.120982
H	-0.745955	0.028747	1.991756
H	-1.595267	2.235627	0.195965
H	3.007075	0.216150	-1.222647
H	0.863076	-1.936580	1.834148
H	1.254953	-1.060095	-2.308044
H	0.306119	-2.694488	-0.550531

A_F

F	3.181329	0.349124	0.007025
C	2.410788	-0.744083	-0.045482
C	0.981397	-0.291539	-0.120983
C	0.523776	-0.408240	1.381694
C	0.170347	-1.315773	-0.955495
C	0.696092	1.143635	-0.619349
C	-0.986182	-0.097586	1.471835
C	-1.335851	-1.005989	-0.851150
C	-0.814478	1.440954	-0.518537
C	-1.777805	-1.112420	0.622646
C	-1.256810	1.330277	0.955488
C	-1.604218	0.423192	-1.368403
H	-1.309484	0.503576	-2.423883
H	-2.326269	1.563550	1.048146
H	-1.291056	-0.176154	2.524000
H	-2.678984	0.646031	-1.319854
H	0.389079	-2.331298	-0.602964
H	-1.609298	-2.131890	0.995753
H	-2.854493	-0.913393	0.710826
H	1.266710	1.868971	-0.028173
H	0.734957	-1.414729	1.762029
H	-0.715629	2.063670	1.569093
H	1.096143	0.299952	1.994262
H	-1.895423	-1.730301	-1.457382
H	-1.008543	2.457591	-0.885118
H	0.493368	-1.267594	-2.004118
H	1.034622	1.245336	-1.659421

A_F to H_F^{ene} TS

F	2.966060	0.278550	0.223614
C	2.110974	-0.352117	-0.683948
C	0.879700	0.314617	-0.687510
C	0.944798	-1.367957	0.357976
C	-0.163357	-0.038582	-1.726974
C	0.539786	1.526069	0.153916
C	-0.490633	-1.234465	0.947385
C	-1.561696	-0.185079	-1.085345
C	-0.832066	1.297708	0.821184
C	-1.563772	-1.403805	-0.146503
C	-0.753017	0.063524	1.742842
C	-1.901591	1.079963	-0.269469
H	-1.950093	1.958576	-0.927406
H	-1.701431	-0.046658	2.285961
H	-0.568256	-2.082976	1.643344
H	-2.893815	0.970811	0.189040
H	0.137363	-0.944329	-2.266107
H	-1.380647	-2.325745	-0.714637
H	-2.551352	-1.509323	0.322469
H	1.328034	1.696926	0.891184
H	0.995016	-2.284581	-0.266419
H	0.029406	0.210101	2.499524
H	1.674879	-1.388750	1.166079
H	-2.305913	-0.328739	-1.878614
H	-1.086702	2.179212	1.422791
H	-0.176099	0.778785	-2.462761
H	0.500323	2.410480	-0.498297

H_F^{ene}

F	-2.599772	-0.433527	0.100663
C	-1.548193	0.072414	-0.625946
C	-0.561356	-0.758367	-0.982891
C	-1.276967	1.505566	-0.268769
C	0.661810	-0.217381	-1.700530
C	-0.276753	-1.881478	-0.016798
C	-0.066371	1.453243	0.735590
C	1.727460	0.287366	-0.691278
C	0.613842	-1.142802	1.046086
C	1.282124	1.595978	-0.007407
C	-0.037051	0.161181	1.638887
C	1.960306	-0.786117	0.388737
H	2.412409	-1.686097	-0.050186
H	0.550860	0.417400	2.530416
H	-0.169564	2.314637	1.409917
H	2.668830	-0.408201	1.139049
H	0.389452	0.585779	-2.395525
H	1.214189	2.408857	-0.743748
H	2.061013	1.892931	0.709557
H	-1.187367	-2.272378	0.440744
H	-1.027464	2.135687	-1.129781
H	-1.049050	-0.062622	1.994841
H	-2.167506	1.934364	0.200923
H	2.665059	0.478230	-1.231284
H	0.786589	-1.830553	1.885863
H	1.097470	-1.021666	-2.310195
H	0.279934	-2.722241	-0.450654

N_H

C	-2.363440	-0.317353	0.032462
H	-2.796637	0.690129	-0.165927
C	-1.053269	-0.098691	0.560195
C	-0.601644	-0.064090	-1.123941
C	0.162312	1.270783	-1.186354
C	0.385419	-1.238105	-1.184751
H	1.743372	-2.035596	0.368448
H	2.622375	0.233744	-0.265392
H	2.177635	0.192694	1.438471
H	1.354188	2.305356	0.363298
C	-0.438404	1.216187	1.089538
H	0.882575	1.251595	-2.013883
H	-0.514654	2.116089	-1.355886
H	-1.410335	-0.146283	-1.854626
C	1.046633	-1.204801	0.204193
H	-0.139474	-2.186275	-1.341375
H	1.090670	-1.098578	-2.013749
C	-0.211426	-1.274563	1.091133
H	-0.745627	-2.219181	0.948888
C	0.815191	1.363442	0.201942
H	0.004913	-1.156215	2.159024
H	-1.117281	2.065436	0.946910
H	-0.206457	1.142560	2.157907
C	1.767750	0.154612	0.420233

N_H to A_H^{ene} TS

C	2.215033	-0.484980	-0.088970
H	2.754917	0.459827	0.136562
C	1.011219	-0.145340	-0.732551
C	0.678183	-0.187498	1.143811
C	0.050186	1.210423	1.238924
C	-0.396932	-1.270854	1.149137
H	-1.912930	-1.862442	-0.341055
H	-2.543664	0.435753	0.469130
H	-2.237870	0.442816	-1.265338
H	-1.148264	2.416799	-0.165809
C	0.467891	1.234360	-1.112274
H	-0.622565	1.248286	2.106232
H	0.819195	1.977367	1.387361
H	1.465746	-0.355855	1.876189
C	-1.138364	-1.100875	-0.188578
H	0.056856	-2.264580	1.217569
H	-1.053877	-1.135826	2.018808
C	0.030386	-1.227150	-1.188705
H	0.500618	-2.212451	-1.124774
C	-0.684060	1.425197	-0.092368
H	-0.284732	-1.054364	-2.224404
H	1.226682	2.015688	-0.992937
H	0.110068	1.255095	-2.148369
C	-1.755237	0.319031	-0.286621

A_H^{ene}

C	-0.435219	0.916836	-1.392820
H	-1.362545	1.491872	-1.492542
C	-0.595485	-0.429907	-1.245727
C	0.458283	1.499214	-0.303841
C	-0.590853	1.343774	0.884350
C	1.691543	0.652815	0.054778
H	2.173441	-1.420677	0.522023
H	0.642217	-0.617878	2.353655
H	-0.031060	-2.021328	1.525868
H	-1.761486	-0.209596	1.867976
C	-1.719252	-0.717772	-0.282208
H	-0.127569	1.682634	1.821840
H	-1.457413	1.991630	0.705608
H	0.732064	2.554094	-0.433376
C	1.285853	-0.822241	0.275198
H	2.443471	0.715391	-0.742045
H	2.155890	1.061672	0.962444
C	0.630822	-1.300110	-1.035235
H	1.324680	-1.200883	-1.877035
C	-1.033025	-0.138326	1.048820
H	0.347469	-2.358708	-0.968882
H	-2.630897	-0.147212	-0.493534
H	-1.981552	-1.776630	-0.145463
C	0.229549	-0.961679	1.395596

N_{Cl}

C	2.487321	-0.427885	0.792052
Cl	3.796702	0.392125	-0.070886
C	1.175942	-0.032662	0.251236
C	0.011458	-0.118749	1.353576
C	-0.800651	1.173245	1.111237
C	-0.859652	-1.314998	0.911450
H	-1.165285	-2.076909	-1.148249
H	-2.378894	0.124570	-0.990287
H	-1.117229	0.195869	-2.218759
H	-1.077282	2.269278	-0.797350
C	0.878695	1.270639	-0.536986
H	-1.838313	1.073757	1.450033
H	-0.363201	2.035794	1.628893
H	0.405827	-0.215941	2.367404
C	-0.714293	-1.230100	-0.616644
H	-0.462267	-2.267499	1.281783
H	-1.893792	-1.224872	1.263387
C	0.820936	-1.230891	-0.734948
H	1.234694	-2.183406	-0.387425
C	-0.653862	1.333592	-0.414315
H	1.214294	-1.026792	-1.734763
H	1.343271	2.140019	-0.056686
H	1.246058	1.227381	-1.566478
C	-1.290674	0.114638	-1.137173

N_{Cl} to A_{Cl}^{ene} TS

C	1.663747	-0.954842	-0.259086
Cl	3.087706	0.194084	0.016296
C	0.571878	-0.298127	-0.851450
C	0.325806	-0.394206	1.145726
C	0.028964	1.101954	1.265264
C	-0.945775	-1.228467	1.133172
H	-2.602937	-1.431321	-0.301458
H	-2.708421	0.910460	0.632914
H	-2.504087	0.932422	-1.116053
H	-0.964101	2.586047	-0.020758
C	0.303204	1.164086	-1.134267
H	-0.573739	1.265204	2.169287
H	0.954732	1.673698	1.380377
H	1.083908	-0.742804	1.842452
C	-1.686592	-0.846404	-0.158985
H	-0.711523	-2.297583	1.147864
H	-1.533490	-1.000415	2.032841
C	-0.621657	-1.165232	-1.231913
H	-0.349278	-2.223846	-1.212349
C	-0.717185	1.517626	-0.012112
H	-0.957278	-0.910346	-2.243632
H	1.205317	1.773812	-1.052725
H	-0.129303	1.302814	-2.131323
C	-2.004096	0.669688	-0.174384

A_{Cl}^{ene}

C	1.663747	-0.954842	-0.259086
Cl	3.087706	0.194084	0.016296
C	0.571878	-0.298127	-0.851450
C	0.325806	-0.394206	1.145726
C	0.028964	1.101954	1.265264
C	-0.945775	-1.228467	1.133172
H	-2.602937	-1.431321	-0.301458
H	-2.708421	0.910460	0.632914
H	-2.504087	0.932422	-1.116053
H	-0.964101	2.586047	-0.020758
C	0.303204	1.164086	-1.134267
H	-0.573739	1.265204	2.169287
H	0.954732	1.673698	1.380377
H	1.083908	-0.742804	1.842452
C	-1.686592	-0.846404	-0.158985
H	-0.711523	-2.297583	1.147864
H	-1.533490	-1.000415	2.032841
C	-0.621657	-1.165232	-1.231913
H	-0.349278	-2.223846	-1.212349
C	-0.717185	1.517626	-0.012112
H	-0.957278	-0.910346	-2.243632
H	1.205317	1.773812	-1.052725
H	-0.129303	1.302814	-2.131323
C	-2.004096	0.669688	-0.174384

N_F

C 2.511732 -0.348774 0.769615
F 3.039011 0.852143 1.058922
C 1.227546 -0.113932 0.061496
C 0.125526 -0.149648 1.285890
C -0.646522 1.171334 1.083517
C -0.798486 -1.321945 0.899400
H -1.275171 -2.079738 -1.126711
H -2.402040 0.159227 -0.898040
H -1.224945 0.189590 -2.208798
H -1.033138 2.264966 -0.803723
C 0.912808 1.213648 -0.670342
H -1.657967 1.105410 1.501643
H -0.141697 2.017887 1.563951
H 0.570989 -0.253615 2.278911
C -0.754106 -1.249294 -0.636273
H -0.405949 -2.283021 1.251234
H -1.801646 -1.193954 1.323168
C 0.771593 -1.281210 -0.843747
H 1.196554 -2.232122 -0.502102
C -0.607427 1.319138 -0.447547
H 1.082202 -1.126466 -1.883146
H 1.434267 2.060880 -0.213913
H 1.203400 1.165575 -1.725609
C -1.326735 0.114120 -1.117696

N_F to A_F^{ene} TS

C 1.704755 -0.860335 -0.250794
F 2.636391 0.141682 -0.013943
C 0.575634 -0.289068 -0.870101
C 0.339643 -0.400246 1.153890
C 0.053999 1.098175 1.267564
C -0.933284 -1.229664 1.133129
H -2.582771 -1.432239 -0.312149
H -2.690484 0.901032 0.629283
H -2.477758 0.933193 -1.118186
H -0.953879 2.585390 -0.005200
C 0.315011 1.174238 -1.137297
H -0.534506 1.282385 2.177151
H 0.990501 1.656573 1.363244
H 1.085174 -0.748807 1.864268
C -1.664718 -0.850971 -0.164615
H -0.704702 -2.300249 1.154960
H -1.531499 -0.997808 2.025496
C -0.594092 -1.173905 -1.234305
H -0.307643 -2.229053 -1.190698
C -0.697782 1.518641 -0.005157
H -0.940222 -0.950459 -2.250397
H 1.228062 1.766146 -1.044339
H -0.118699 1.337754 -2.130435
C -1.981332 0.665896 -0.175671

A_F^{ene}

C 1.704755 -0.860335 -0.250794
F 2.636391 0.141682 -0.013943
C 0.575634 -0.289068 -0.870101
C 0.339643 -0.400246 1.153890
C 0.053999 1.098175 1.267564
C -0.933284 -1.229664 1.133129
H -2.582771 -1.432239 -0.312149
H -2.690484 0.901032 0.629283
H -2.477758 0.933193 -1.118186
H -0.953879 2.585390 -0.005200
C 0.315011 1.174238 -1.137297
H -0.534506 1.282385 2.177151
H 0.990501 1.656573 1.363244
H 1.085174 -0.748807 1.864268
C -1.664718 -0.850971 -0.164615
H -0.704702 -2.300249 1.154960
H -1.531499 -0.997808 2.025496
C -0.594092 -1.173905 -1.234305
H -0.307643 -2.229053 -1.190698
C -0.697782 1.518641 -0.005157
H -0.940222 -0.950459 -2.250397
H 1.228062 1.766146 -1.044339
H -0.118699 1.337754 -2.130435
C -1.981332 0.665896 -0.175671

B_{Cl}

C -1.477844 -0.970437 -0.410895
C -0.252607 -0.465060 0.195463
C 0.536573 0.272229 -1.138180
Cl -2.829467 0.137122 -0.112853
C 0.826271 -1.495432 0.630691
C -0.013321 0.572808 1.322231
C 2.008133 -0.533375 0.377157
C 1.420970 0.906206 0.849175
C 1.878993 -0.479540 -1.162411
C 1.025835 1.579604 -0.486398
H -0.047155 0.329114 -2.056381
H 0.864583 -2.395640 0.013406
H 0.676133 -1.795261 1.671938
H 2.979149 -0.808197 0.794271
H -0.675858 1.440236 1.308173
H -0.085561 0.100908 2.306521
H 2.056578 1.474095 1.531930
H 2.643603 0.112308 -1.676478
H 1.853688 -1.472850 -1.617604
H 1.853058 2.008798 -1.061544
H 0.264698 2.353384 -0.356732

B_{Cl} to N_{Cl}^{ene} TS

C -1.246289 -0.731314 -0.827219
C -0.190584 -0.844278 0.099496
C 0.283050 0.856419 -0.873650
Cl -2.678908 0.110221 -0.059973
C 1.101101 -1.586479 -0.223860
C 0.081159 -0.398799 1.531509
C 2.035821 -0.369193 -0.029316
C 1.315115 0.467468 1.159287
C 1.672635 0.422079 -1.305146
C 0.600243 1.613073 0.408832
H -0.409317 1.279150 -1.594306
H 1.136164 -2.005643 -1.230836
H 1.256844 -2.394709 0.498215
H 3.095216 -0.582087 0.130757
H -0.722067 0.170428 1.999771
H 0.319042 -1.260637 2.163332
H 1.971808 0.754790 1.983822
H 2.290764 1.314697 -1.466016
H 1.710437 -0.184926 -2.212167
H 1.249739 2.463336 0.163691
H -0.270700 1.997994 0.943679

N_{Cl}^{ene}

C -0.763942 0.074376 -0.723249
C -0.020081 -1.066490 -0.622587
C -0.042554 1.335866 -0.231274
Cl -2.482190 0.010711 -0.177803
C 1.423808 -0.998471 -1.102599
C 0.113269 -1.571819 0.807064
C 1.940802 -0.007090 -0.050876
C 1.013207 -0.318227 1.222463
C 1.456115 1.366981 -0.583712
C 0.127770 0.951156 1.298203
H -0.575428 2.273945 -0.406278
H 1.539891 -0.640537 -2.128396
H 1.880669 -1.993034 -1.037692
H 3.013318 -0.050692 0.160136
H -0.814767 -1.612112 1.377677
H 0.649084 -2.521808 0.911440
H 1.571110 -0.505357 2.145609
H 1.917349 2.208496 -0.054217
H 1.667692 1.494252 -1.649539
H 0.670210 1.767633 1.790744
H -0.812255 0.799423 1.832560

N_F

C	-1.869341	-0.729790	-0.494803
C	-0.581163	-0.379326	0.136331
C	0.390917	0.226407	-1.101209
F	-2.697881	0.307858	-0.288646
C	0.317418	-1.504352	0.705469
C	-0.359642	0.659520	1.265748
C	1.618260	-0.679805	0.561659
C	1.144443	0.828352	0.943713
C	1.649997	-0.655906	-0.984323
C	0.962854	1.497664	-0.439552
H	-0.089499	0.317452	-2.076111
H	0.328210	-2.424379	0.115707
H	0.030411	-1.756721	1.730748
H	2.506653	-1.043894	1.081820
H	-0.922962	1.589275	1.159897
H	-0.584408	0.230608	2.246829
H	1.763822	1.346540	1.679219
H	2.519106	-0.160656	-1.429273
H	1.567461	-1.655145	-1.420230
H	1.885735	1.815768	-0.935283
H	0.284837	2.354854	-0.402369

N_F to N_F^{ene} TS

C	-1.637034	-0.587597	-0.660900
C	-0.716453	-0.488513	0.407908
C	0.267191	0.236693	-1.250545
F	-2.381056	0.583367	-0.671700
C	0.323547	-1.526883	0.758971
C	-0.403286	0.626533	1.388352
C	1.550974	-0.629350	0.454773
C	1.035912	0.859246	0.848070
C	1.495882	-0.637795	-1.088171
C	0.706794	1.496741	-0.519914
H	-0.214381	0.324733	-2.218852
H	0.286595	-2.430071	0.146713
H	0.232121	-1.813681	1.812297
H	2.498300	-0.925068	0.911866
H	-1.046941	1.502473	1.302035
H	-0.430935	0.263207	2.421243
H	1.710705	1.419468	1.500349
H	2.354007	-0.141377	-1.560413
H	1.413391	-1.642731	-1.508387
H	1.579604	1.921272	-1.033410
H	-0.056771	2.275423	-0.454901

N_F^{ene}

C	-1.049387	-0.258405	-0.550709
C	-0.790345	-0.687698	0.713463
C	0.155156	0.148279	-1.389379
F	-2.048404	0.681976	-0.675252
C	0.403152	-1.605967	0.907263
C	-0.460831	0.509947	1.607335
C	1.496816	-0.628595	0.443589
C	0.900130	0.809854	0.841735
C	1.411654	-0.690797	-1.105308
C	0.574851	1.425929	-0.545932
H	-0.043594	0.352676	-2.445532
H	0.370748	-2.523562	0.313686
H	0.488048	-1.893752	1.961918
H	2.499960	-0.815092	0.838454
H	-1.161686	1.342402	1.535147
H	-0.306327	0.258817	2.662804
H	1.588517	1.426399	1.428993
H	2.267575	-0.207192	-1.590106
H	1.364881	-1.720056	-1.474315
H	1.476272	1.849556	-1.004528
H	-0.190462	2.204162	-0.511263

A: 6-31G(d,p)

C	1.590316	-0.852335	0.000000
C	0.781829	-0.593176	1.227469
C	0.781829	0.987045	1.243637
C	0.036704	1.498306	0.000000
C	0.781829	0.987045	-1.243637
C	0.781829	-0.593176	-1.227469
C	-0.686083	-1.088675	1.243434
C	-1.423221	-0.565261	0.000000
C	-0.686083	-1.088675	-1.243434
C	-1.415225	0.977310	0.000000
H	1.309305	-0.933536	2.127796
H	1.808554	1.366752	1.261270
H	0.295551	1.307135	2.173066
H	0.036676	2.596101	0.000000
H	1.808554	1.366752	-1.261270
H	0.295551	1.307135	-2.173066
H	1.309305	-0.933536	-2.127796
H	-0.705783	-2.185564	1.261318
H	-1.179363	-0.751538	2.165461
H	-2.459390	-0.926736	0.000000
H	-0.705783	-2.185564	-1.261318
H	-1.179363	-0.751538	-2.165461
H	-1.948076	1.356840	-0.881596
H	-1.948076	1.356840	0.881596

A: to DHA TS

C	-0.390795	1.199208	-1.222606
C	0.720199	1.437996	-0.233259
C	-0.506734	1.397038	0.702161
C	-0.944192	-0.005890	1.165040
C	-1.747237	-0.540791	-0.038045
C	-0.800730	-0.295734	-1.242026
C	1.811647	0.404347	0.024172
C	1.176433	-0.980702	0.186063
C	0.386860	-1.280655	-1.105304
C	0.248781	-0.950333	1.420651
H	1.134341	2.449551	-0.296721
H	-1.303210	1.733112	-0.119067
H	-0.573611	2.240059	1.391942
H	-1.568647	0.076189	2.061655
H	-2.679606	0.022263	-0.159240
H	-2.006909	-1.602611	0.057191
H	-1.339233	-0.486964	-2.178150
H	2.516600	0.406306	-0.817059
H	2.387786	0.679593	0.917532
H	1.957495	-1.736765	0.332268
H	1.058658	-1.197146	-1.969062
H	0.003789	-2.309899	-1.105452
H	-0.132851	-1.954861	1.643141
H	0.820007	-0.625737	2.299933

DHA

C	0.359177	1.323008	0.761525
C	-0.948503	1.387426	0.000000
C	0.359177	1.323008	-0.761525
C	0.907741	-0.059081	-1.189285
C	1.833046	-0.409522	0.000000
C	0.907741	-0.059081	1.189285
C	-1.892792	0.202945	0.000000
C	-1.075940	-1.099503	0.000000
C	-0.200923	-1.131016	1.274870
C	-0.200923	-1.131016	-1.274870
H	-1.432492	2.363151	0.000000
H	0.680142	2.197884	1.320163
H	0.680142	2.197884	-1.320163
H	1.445366	0.006477	-2.140813
H	2.718720	0.236317	0.000000
H	2.172438	-1.453451	0.000000
H	1.445366	0.006477	2.140813
H	-2.545564	0.241709	0.882427
H	-2.545564	0.241709	-0.882427
H	-1.758756	-1.957773	0.000000
H	-0.834628	-0.962983	2.154964
H	0.261331	-2.118720	1.398827
H	0.261331	-2.118719	-1.398827
H	-0.834628	-0.962983	-2.154964