Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Kinetics of α Hydrogen Abstractions in Thiols, Sulfides and Thiocarbonyl Compounds

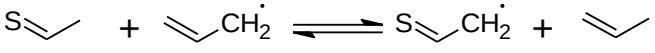
Aäron G. Vandeputte, Maarten K. Sabbe, Marie-Françoise Reyniers, Guy B. Marin

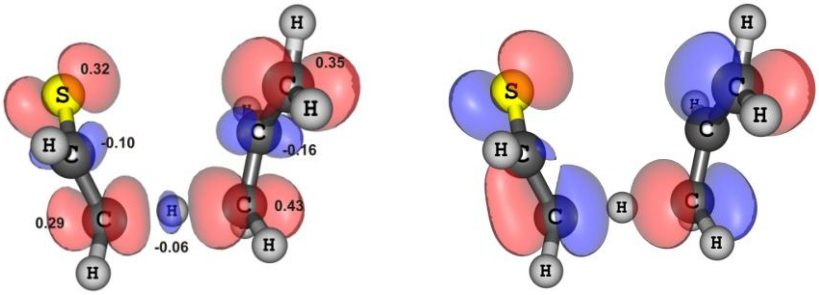
Laboratorium voor Chemische Technologie, Ghent University, Krijgslaan 281 S5, B-9000 Gent, Belgium

Resonance corrections

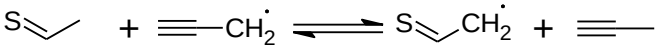
Left figure: Spin density plot (B3LYP/cbsb7, contour value = 0.005) and Mulliken atomic spin densities (|atomic spin densities| > 0.02 are displayed).
Right figure: SUMO of the transition state (B3LYP/cbsb7, contour value = 0.05)

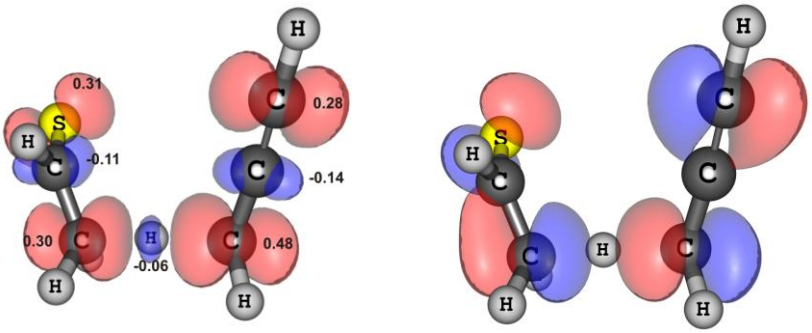
a) 

Figure S1: 



b) 

Figure S2: 



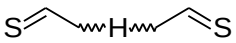
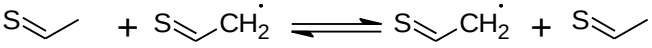
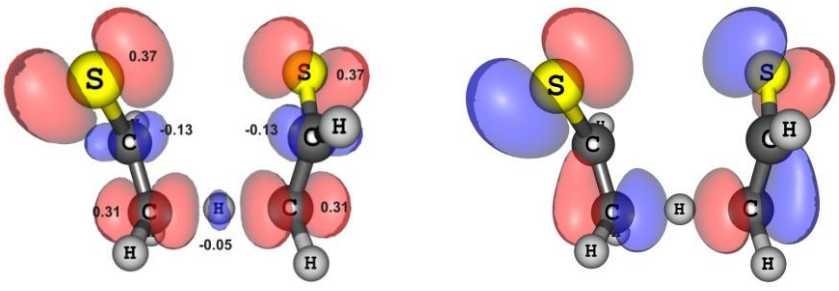
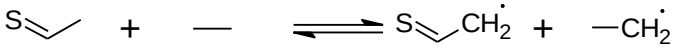
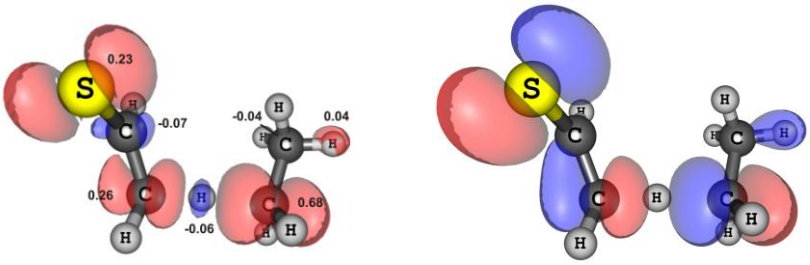
c) 

Figure S3: 



d) 

Figure S4: 



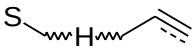
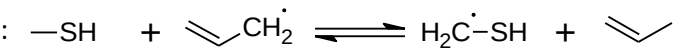
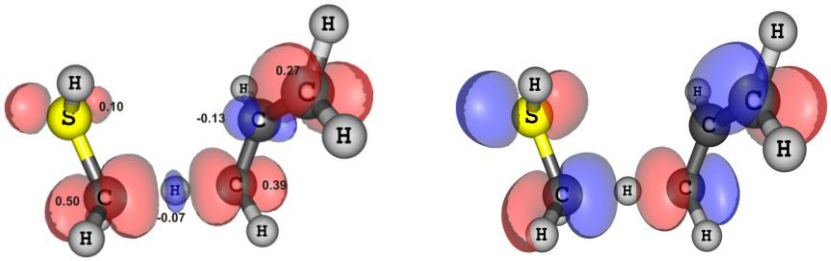
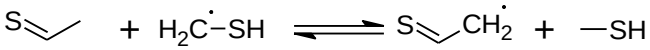
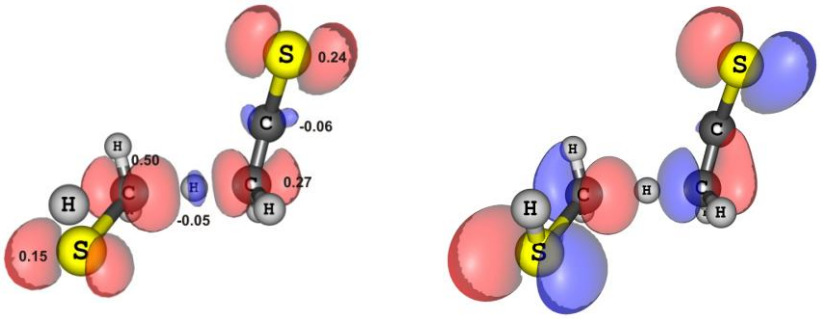
e) 

Figure S5: 



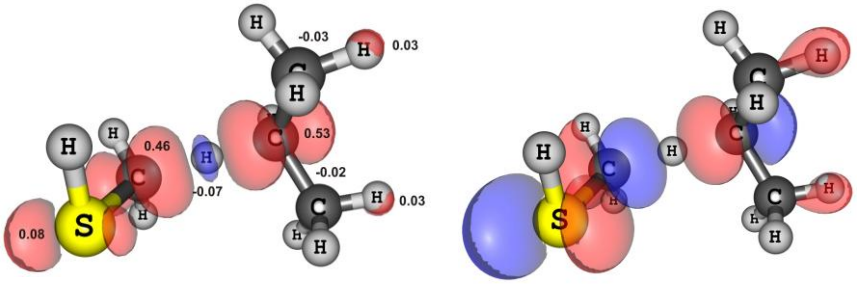
f) 

Figure S6: 



g) 

Figure S7: —SH +  ⇌ $H_2C^{\cdot}$–SH + 



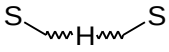
h) 

Figure S8: —SH + $H_2C^{\cdot}$–SH ⇌ $H_2C^{\cdot}$–SH + —SH

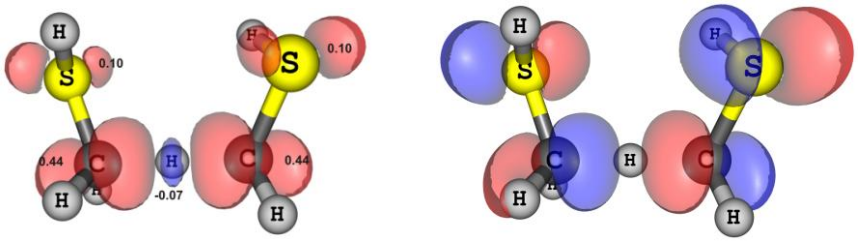


Table S1: Intrinsic Arrhenius parameters for the reference reaction, i.e. the hydrogen abstraction from methane by methyl, in the temperature range 300 – 1500K.

T K	log*A* $m^3\ mol^{-1}\ s^{-1}$	E_a $kJ\ mol^{-1}$
300	5.267	69.7
400	5.453	70.9
500	5.662	72.6
600	5.863	74.7
700	6.050	77.0
800	6.219	79.5
900	6.371	81.9
1000	6.509	84.4
1100	6.633	86.9
1200	6.746	89.4
1300	6.849	91.9
1400	6.944	94.3
1500	7.032	96.7

Rate coefficients in the temperature range 300 – 1500 K

Table S2: Rate coefficients ($m^3\ mol^{-1}\ s^{-1}$) for in the temperature range 300 – 1500 K for the reactions presented in Table 1 of the manuscript

	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K
1 →	5.2E-05	7.5E-03	2.7E-01	3.7E+00	2.7E+01	1.3E+02	4.5E+02	1.3E+03	3.2E+03	6.8E+03	1.3E+04	2.4E+04	4.1E+04
2 →	5.3E-02	1.4E+00	1.6E+01	9.7E+01	4.0E+02	1.2E+03	3.1E+03	6.7E+03	1.3E+04	2.4E+04	3.9E+04	6.2E+04	9.4E+04
3 →	3.2E-01	5.4E+00	4.3E+01	2.0E+02	6.9E+02	1.8E+03	4.1E+03	8.2E+03	1.5E+04	2.5E+04	3.9E+04	5.9E+04	8.6E+04
4 →	3.9E+00	4.0E+01	2.2E+02	8.1E+02	2.2E+03	5.1E+03	1.0E+04	1.9E+04	3.1E+04	4.9E+04	7.4E+04	1.1E+05	1.5E+05
5 →	3.8E+00	5.6E+01	3.5E+02	1.3E+03	3.8E+03	8.7E+03	1.7E+04	3.1E+04	5.2E+04	8.2E+04	1.2E+05	1.8E+05	2.4E+05
6 →	4.0E+01	3.9E+02	1.8E+03	5.6E+03	1.3E+04	2.7E+04	5.0E+04	8.3E+04	1.3E+05	1.9E+05	2.8E+05	3.8E+05	5.1E+05
7 →	2.2E+02	1.3E+03	4.5E+03	1.1E+04	2.3E+04	4.1E+04	6.8E+04	1.0E+05	1.5E+05	2.2E+05	3.0E+05	3.9E+05	5.1E+05
8 →	1.7E-02	7.1E-01	1.0E+01	7.5E+01	3.4E+02	1.1E+03	3.0E+03	6.9E+03	1.4E+04	2.6E+04	4.5E+04	7.3E+04	1.1E+05
9 →	2.9E-04	3.0E-02	8.6E-01	9.9E+00	6.3E+01	2.7E+02	9.0E+02	2.4E+03	5.6E+03	1.2E+04	2.2E+04	3.8E+04	6.4E+04
10 →	2.4E+00	3.2E+01	2.0E+02	7.9E+02	2.3E+03	5.5E+03	1.1E+04	2.1E+04	3.6E+04	5.8E+04	8.8E+04	1.3E+05	1.8E+05
11 →	1.3E+01	1.1E+02	5.1E+02	1.6E+03	4.0E+03	8.4E+03	1.6E+04	2.7E+04	4.3E+04	6.5E+04	9.4E+04	1.3E+05	1.8E+05
12 →	1.9E+01	2.1E+02	1.0E+03	3.3E+03	8.3E+03	1.8E+04	3.3E+04	5.6E+04	8.8E+04	1.3E+05	1.9E+05	2.7E+05	3.6E+05
13 →	8.2E+01	6.1E+02	2.4E+03	6.6E+03	1.5E+04	2.8E+04	4.9E+04	7.8E+04	1.2E+05	1.7E+05	2.4E+05	3.2E+05	4.2E+05
14 →	7.6E+00	7.0E+01	3.5E+02	1.2E+03	3.1E+03	6.9E+03	1.3E+04	2.3E+04	3.8E+04	5.9E+04	8.7E+04	1.2E+05	1.7E+05
15 →	6.0E+01	3.8E+02	1.4E+03	4.0E+03	9.1E+03	1.8E+04	3.1E+04	5.1E+04	7.9E+04	1.2E+05	1.6E+05	2.2E+05	3.0E+05
16 →	6.6E-01	1.1E+01	7.7E+01	3.3E+02	1.0E+03	2.6E+03	5.6E+03	1.1E+04	1.9E+04	3.1E+04	4.7E+04	7.0E+04	9.9E+04
17 →	2.4E+00	2.6E+01	1.4E+02	5.1E+02	1.4E+03	3.1E+03	6.1E+03	1.1E+04	1.8E+04	2.8E+04	4.1E+04	5.9E+04	8.1E+04
18 →	3.1E+00	4.3E+01	3.1E+02	1.4E+03	4.4E+03	1.1E+04	2.5E+04	4.8E+04	8.5E+04	1.4E+05	2.2E+05	3.3E+05	4.7E+05
19 →	3.8E+00	4.4E+01	2.7E+02	1.1E+03	3.1E+03	7.3E+03	1.5E+04	2.8E+04	4.7E+04	7.6E+04	1.1E+05	1.7E+05	2.3E+05
20 →	1.5E+01	1.4E+02	7.1E+02	2.3E+03	6.0E+03	1.3E+04	2.5E+04	4.3E+04	6.9E+04	1.1E+05	1.5E+05	2.2E+05	3.0E+05
21 →	2.3E+00	2.7E+01	1.8E+02	7.2E+02	2.2E+03	5.3E+03	1.1E+04	2.1E+04	3.7E+04	5.9E+04	9.1E+04	1.3E+05	1.9E+05
22 →	8.4E+00	8.9E+01	4.9E+02	1.7E+03	4.7E+03	1.1E+04	2.1E+04	3.7E+04	6.1E+04	9.5E+04	1.4E+05	2.0E+05	2.8E+05
23 →	4.7E-07	4.9E-04	3.9E-02	8.0E-01	7.5E+00	4.2E+01	1.7E+02	5.4E+02	1.4E+03	3.3E+03	6.7E+03	1.3E+04	2.2E+04
24 →	2.0E-06	1.2E-03	7.1E-02	1.2E+00	1.1E+01	5.6E+01	2.1E+02	6.4E+02	1.6E+03	3.7E+03	7.4E+03	1.4E+04	2.4E+04
1 ←	5.2E-05	7.5E-03	2.7E-01	3.7E+00	2.7E+01	1.3E+02	4.5E+02	1.3E+03	3.2E+03	6.8E+03	1.3E+04	2.4E+04	4.1E+04
2 ←	4.0E-09	6.4E-06	8.6E-04	2.8E-02	3.7E-01	2.8E+00	1.4E+01	5.4E+01	1.7E+02	4.4E+02	1.0E+03	2.1E+03	4.1E+03
3 ←	2.1E-09	3.8E-06	5.1E-04	1.6E-02	2.1E-01	1.6E+00	8.1E+00	3.1E+01	9.4E+01	2.5E+02	5.7E+02	1.2E+03	2.3E+03

4 ←	4.0E-09	7.3E-06	9.3E-04	2.8E-02	3.6E-01	2.6E+00	1.3E+01	4.8E+01	1.5E+02	3.8E+02	8.7E+02	1.8E+03	3.4E+03
5 ←	2.3E-16	5.8E-11	1.3E-07	2.5E-05	1.2E-03	2.4E-02	2.5E-01	1.7E+00	8.6E+00	3.4E+01	1.1E+02	3.0E+02	7.5E+02
6 ←	1.0E-18	9.5E-13	4.5E-09	1.4E-06	9.6E-05	2.4E-03	3.1E-02	2.5E-01	1.4E+00	6.2E+00	2.2E+01	6.6E+01	1.7E+02
7 ←	9.7E-21	2.6E-14	2.3E-10	1.1E-07	9.7E-06	3.0E-04	4.5E-03	4.2E-02	2.6E-01	1.2E+00	4.8E+00	1.5E+01	4.2E+01
8 ←	4.0E-03	2.3E-01	4.4E+00	3.8E+01	2.0E+02	7.7E+02	2.3E+03	5.7E+03	1.3E+04	2.5E+04	4.5E+04	7.6E+04	1.2E+05
9 ←	1.7E-12	2.2E-08	1.2E-05	9.5E-04	2.5E-02	3.1E-01	2.4E+00	1.2E+01	5.0E+01	1.6E+02	4.6E+02	1.1E+03	2.5E+03
10 ←	1.4E-16	3.1E-11	7.1E-08	1.4E-05	7.1E-04	1.4E-02	1.5E-01	1.1E+00	5.4E+00	2.1E+01	7.0E+01	2.0E+02	4.9E+02
11 ←	2.0E-17	5.1E-12	1.2E-08	2.3E-06	1.1E-04	2.2E-03	2.4E-02	1.7E-01	8.4E-01	3.3E+00	1.1E+01	3.0E+01	7.5E+01
12 ←	1.1E-22	1.6E-15	4.1E-11	4.1E-08	6.1E-06	2.8E-04	5.9E-03	6.9E-02	5.4E-01	3.0E+00	1.3E+01	4.9E+01	1.5E+02
13 ←	3.7E-24	1.0E-16	3.5E-12	4.4E-09	7.7E-07	4.0E-05	9.1E-04	1.1E-02	9.4E-02	5.6E-01	2.6E+00	9.6E+00	3.1E+01
14 ←	1.9E-15	1.9E-10	2.6E-07	3.8E-05	1.5E-03	2.5E-02	2.3E-01	1.5E+00	6.7E+00	2.5E+01	7.6E+01	2.0E+02	4.8E+02
15 ←	2.4E-16	3.4E-11	5.5E-08	9.0E-06	3.8E-04	6.9E-03	6.9E-02	4.6E-01	2.2E+00	8.6E+00	2.7E+01	7.6E+01	1.9E+02
16 ←	3.1E-15	2.7E-10	3.4E-07	4.7E-05	1.8E-03	2.9E-02	2.6E-01	1.6E+00	7.4E+00	2.7E+01	8.2E+01	2.2E+02	5.1E+02
17 ←	5.7E-15	3.6E-10	3.7E-07	4.3E-05	1.5E-03	2.2E-02	1.9E-01	1.1E+00	4.8E+00	1.7E+01	5.0E+01	1.3E+02	3.0E+02
18 ←	1.5E-09	5.1E-06	1.0E-03	4.3E-02	6.9E-01	6.0E+00	3.4E+01	1.4E+02	4.8E+02	1.4E+03	3.3E+03	7.3E+03	1.5E+04
19 ←	8.4E-10	2.8E-06	5.3E-04	2.1E-02	3.3E-01	2.8E+00	1.5E+01	6.4E+01	2.1E+02	5.8E+02	1.4E+03	3.1E+03	6.1E+03
20 ←	1.5E-11	1.7E-07	6.4E-05	3.9E-03	8.1E-02	8.5E-01	5.6E+00	2.6E+01	9.7E+01	3.0E+02	7.7E+02	1.8E+03	3.8E+03
21 ←	3.7E-12	4.1E-08	1.6E-05	1.0E-03	2.3E-02	2.5E-01	1.7E+00	8.1E+00	3.0E+01	9.4E+01	2.5E+02	5.8E+02	1.2E+03
22 ←	2.0E-14	1.2E-09	1.2E-06	1.5E-04	4.9E-03	7.2E-02	6.2E-01	3.6E+00	1.6E+01	5.5E+01	1.6E+02	4.2E+02	9.7E+02
23 ←	9.0E+02	4.2E+03	1.3E+04	3.3E+04	7.1E+04	1.3E+05	2.3E+05	3.6E+05	5.5E+05	8.1E+05	1.1E+06	1.5E+06	2.0E+06
24 ←	7.1E+01	5.1E+02	2.3E+03	7.3E+03	1.9E+04	4.1E+04	7.8E+04	1.4E+05	2.3E+05	3.5E+05	5.2E+05	7.4E+05	1.0E+06

Table S3: Rate coefficients ($m^3\ mol^{-1}\ s^{-1}$) for in the temperature range 300 – 1500 K for the reactions presented in Table 2 of the manuscript

	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K
3 →	3.2E-01	5.4E+00	4.3E+01	2.0E+02	6.9E+02	1.8E+03	4.1E+03	8.2E+03	1.5E+04	2.5E+04	3.9E+04	5.9E+04	8.6E+04
25 →	3.1E-01	4.6E+00	3.5E+01	1.6E+02	5.2E+02	1.4E+03	3.0E+03	5.9E+03	1.1E+04	1.8E+04	2.8E+04	4.2E+04	6.0E+04
26 →	5.0E-01	7.2E+00	5.2E+01	2.3E+02	7.5E+02	1.9E+03	4.3E+03	8.3E+03	1.5E+04	2.5E+04	3.9E+04	5.8E+04	8.3E+04
27 →	2.5E-01	3.7E+00	2.8E+01	1.3E+02	4.3E+02	1.1E+03	2.5E+03	4.9E+03	8.9E+03	1.5E+04	2.3E+04	3.5E+04	5.1E+04
28 →	2.8E-01	3.9E+00	2.9E+01	1.3E+02	4.2E+02	1.1E+03	2.4E+03	4.8E+03	8.6E+03	1.4E+04	2.2E+04	3.4E+04	4.9E+04
8 →	1.7E-02	7.1E-01	1.0E+01	7.5E+01	3.4E+02	1.1E+03	3.0E+03	6.9E+03	1.4E+04	2.6E+04	4.5E+04	7.3E+04	1.1E+05
29 →	4.9E-03	2.0E-01	2.8E+00	2.0E+01	8.8E+01	2.9E+02	7.7E+02	1.7E+03	3.5E+03	6.4E+03	1.1E+04	1.8E+04	2.7E+04
30 →	1.1E-02	2.9E-01	3.2E+00	1.9E+01	7.7E+01	2.3E+02	5.7E+02	1.2E+03	2.4E+03	4.2E+03	7.0E+03	1.1E+04	1.6E+04
2 →	5.3E-02	1.4E+00	1.6E+01	9.7E+01	4.0E+02	1.2E+03	3.1E+03	6.7E+03	1.3E+04	2.4E+04	3.9E+04	6.2E+04	9.4E+04
31 →	2.3E-01	5.1E+00	5.1E+01	2.9E+02	1.1E+03	3.2E+03	7.8E+03	1.6E+04	3.1E+04	5.5E+04	9.0E+04	1.4E+05	2.1E+05
32 →	4.1E-02	1.5E+00	2.0E+01	1.4E+02	6.5E+02	2.2E+03	5.8E+03	1.3E+04	2.7E+04	5.0E+04	8.6E+04	1.4E+05	2.2E+05
33 →	4.1E-02	9.5E-01	1.0E+01	5.9E+01	2.3E+02	7.0E+02	1.7E+03	3.7E+03	7.2E+03	1.3E+04	2.1E+04	3.3E+04	5.0E+04
3 →	3.2E-01	5.4E+00	4.3E+01	2.0E+02	6.9E+02	1.8E+03	4.1E+03	8.2E+03	1.5E+04	2.5E+04	3.9E+04	5.9E+04	8.6E+04
34 →	1.5E+00	2.1E+01	1.4E+02	6.3E+02	2.0E+03	5.0E+03	1.1E+04	2.1E+04	3.6E+04	6.0E+04	9.3E+04	1.4E+05	2.0E+05
35 →	4.7E-01	7.0E+00	5.3E+01	2.4E+02	7.9E+02	2.1E+03	4.6E+03	9.0E+03	1.6E+04	2.7E+04	4.3E+04	6.4E+04	9.2E+04
36 →	2.8E-01	4.5E+00	3.5E+01	1.6E+02	5.4E+02	1.4E+03	3.2E+03	6.3E+03	1.1E+04	1.9E+04	3.0E+04	4.5E+04	6.6E+04
37 →	5.2E-01	8.1E+00	6.3E+01	2.9E+02	9.7E+02	2.6E+03	5.8E+03	1.1E+04	2.1E+04	3.4E+04	5.4E+04	8.2E+04	1.2E+05
38 →	5.0E-01	1.1E+01	1.0E+02	5.4E+02	2.0E+03	5.6E+03	1.3E+04	2.7E+04	5.1E+04	8.8E+04	1.4E+05	2.2E+05	3.2E+05
10 →	2.4E+00	3.2E+01	2.0E+02	7.9E+02	2.3E+03	5.5E+03	1.1E+04	2.1E+04	3.6E+04	5.8E+04	8.8E+04	1.3E+05	1.8E+05
39 →	5.8E+00	7.6E+01	4.8E+02	1.9E+03	5.4E+03	1.3E+04	2.6E+04	4.9E+04	8.3E+04	1.3E+05	2.0E+05	2.9E+05	4.1E+05
40 →	2.7E-02	4.5E-01	3.8E+00	1.9E+01	6.7E+01	1.9E+02	4.4E+02	9.0E+02	1.7E+03	2.9E+03	4.6E+03	7.1E+03	1.0E+04
41 →	1.2E-01	1.6E+00	1.2E+01	5.2E+01	1.7E+02	4.5E+02	1.0E+03	2.0E+03	3.5E+03	5.9E+03	9.4E+03	1.4E+04	2.0E+04
3 ←	2.1E-09	3.8E-06	5.1E-04	1.6E-02	2.1E-01	1.6E+00	8.1E+00	3.1E+01	9.4E+01	2.5E+02	5.7E+02	1.2E+03	2.3E+03
25 ←	3.5E-09	5.1E-06	6.2E-04	1.8E-02	2.3E-01	1.6E+00	8.0E+00	3.0E+01	9.0E+01	2.3E+02	5.3E+02	1.1E+03	2.1E+03
26 ←	3.4E-09	5.3E-06	6.7E-04	2.0E-02	2.6E-01	1.9E+00	9.2E+00	3.4E+01	1.0E+02	2.7E+02	6.2E+02	1.3E+03	2.4E+03
27 ←	3.4E-09	4.9E-06	5.8E-04	1.7E-02	2.1E-01	1.5E+00	7.5E+00	2.8E+01	8.3E+01	2.1E+02	4.9E+02	1.0E+03	1.9E+03
28 ←	9.5E-09	9.1E-06	8.6E-04	2.2E-02	2.4E-01	1.6E+00	7.3E+00	2.6E+01	7.5E+01	1.9E+02	4.1E+02	8.3E+02	1.5E+03
8 ←	4.0E-03	2.3E-01	4.4E+00	3.8E+01	2.0E+02	7.7E+02	2.3E+03	5.7E+03	1.3E+04	2.5E+04	4.5E+04	7.6E+04	1.2E+05
29 ←	4.5E-03	2.5E-01	4.5E+00	3.9E+01	2.0E+02	7.5E+02	2.2E+03	5.5E+03	1.2E+04	2.3E+04	4.2E+04	7.2E+04	1.2E+05

30 ←	2.6E-03	1.5E-01	2.7E+00	2.4E+01	1.2E+02	4.7E+02	1.4E+03	3.5E+03	7.6E+03	1.5E+04	2.7E+04	4.6E+04	7.5E+04
2 ←	4.0E-09	6.4E-06	8.6E-04	2.8E-02	3.7E-01	2.8E+00	1.4E+01	5.4E+01	1.7E+02	4.4E+02	1.0E+03	2.1E+03	4.1E+03
31 ←	1.4E-09	3.2E-06	5.4E-04	2.0E-02	2.9E-01	2.3E+00	1.2E+01	4.9E+01	1.6E+02	4.2E+02	1.0E+03	2.1E+03	4.2E+03
32 ←	1.6E-09	3.8E-06	6.7E-04	2.6E-02	4.0E-01	3.3E+00	1.8E+01	7.5E+01	2.4E+02	6.7E+02	1.6E+03	3.5E+03	6.9E+03
33 ←	2.9E-08	2.7E-05	2.6E-03	6.6E-02	7.6E-01	5.1E+00	2.4E+01	8.4E+01	2.4E+02	6.1E+02	1.4E+03	2.7E+03	5.1E+03
3 ←	2.1E-09	3.8E-06	5.1E-04	1.6E-02	2.1E-01	1.6E+00	8.1E+00	3.1E+01	9.4E+01	2.5E+02	5.7E+02	1.2E+03	2.3E+03
34 ←	5.0E-10	1.3E-06	2.1E-04	7.5E-03	1.1E-01	8.5E-01	4.5E+00	1.8E+01	5.6E+01	1.5E+02	3.6E+02	7.6E+02	1.5E+03
35 ←	4.4E-09	5.4E-06	5.8E-04	1.6E-02	1.9E-01	1.3E+00	6.2E+00	2.3E+01	6.7E+01	1.7E+02	3.8E+02	7.7E+02	1.5E+03
36 ←	1.1E-08	1.7E-05	2.3E-03	7.6E-02	1.0E+00	8.2E+00	4.4E+01	1.8E+02	5.7E+02	1.6E+03	3.8E+03	8.4E+03	1.7E+04
37 ←	2.3E-09	3.1E-06	3.6E-04	1.0E-02	1.3E-01	9.0E-01	4.3E+00	1.6E+01	4.8E+01	1.2E+02	2.8E+02	5.7E+02	1.1E+03
38 ←	8.3E-10	2.2E-06	3.7E-04	1.4E-02	2.1E-01	1.7E+00	9.2E+00	3.7E+01	1.2E+02	3.2E+02	7.7E+02	1.7E+03	3.3E+03
10 ←	1.4E-16	3.1E-11	7.1E-08	1.4E-05	7.1E-04	1.4E-02	1.5E-01	1.1E+00	5.4E+00	2.1E+01	7.0E+01	2.0E+02	4.9E+02
39 ←	5.2E-17	1.5E-11	4.0E-08	9.0E-06	4.7E-04	9.9E-03	1.1E-01	8.0E-01	4.2E+00	1.7E+01	5.6E+01	1.6E+02	4.0E+02
40 ←	1.0E-06	3.8E-04	2.2E-02	3.9E-01	3.5E+00	1.9E+01	7.7E+01	2.4E+02	6.5E+02	1.5E+03	3.1E+03	6.0E+03	1.1E+04
41 ←	2.3E-07	1.2E-04	8.0E-03	1.6E-01	1.5E+00	9.0E+00	3.8E+01	1.2E+02	3.4E+02	8.0E+02	1.7E+03	3.3E+03	5.9E+03

Table S4: Rate coefficients ($m^3\ mol^{-1}\ s^{-1}$) for in the temperature range 300 – 1500 K for the reactions presented in Table 3 of the manuscript

	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K
42 →	6.1E-09	7.5E-06	9.4E-04	2.9E-02	3.8E-01	2.8E+00	1.4E+01	5.4E+01	1.7E+02	4.3E+02	1.0E+03	2.1E+03	4.0E+03
43 →	1.7E-10	4.7E-07	8.3E-05	3.2E-03	4.8E-02	4.0E-01	2.2E+00	8.7E+00	2.8E+01	7.7E+01	1.8E+02	4.0E+02	7.8E+02
44 →	1.2E-07	5.8E-05	4.0E-03	8.2E-02	8.1E-01	4.8E+00	2.0E+01	6.8E+01	1.9E+02	4.4E+02	9.4E+02	1.8E+03	3.3E+03
45 →	1.2E-08	1.2E-05	1.2E-03	3.0E-02	3.3E-01	2.2E+00	1.0E+01	3.6E+01	1.0E+02	2.5E+02	5.6E+02	1.1E+03	2.1E+03
46 →	3.6E-07	1.5E-04	1.0E-02	2.1E-01	2.1E+00	1.3E+01	5.3E+01	1.8E+02	4.9E+02	1.2E+03	2.5E+03	4.8E+03	8.7E+03
47 →	7.8E-06	1.3E-03	4.6E-02	6.2E-01	4.5E+00	2.1E+01	7.5E+01	2.1E+02	5.2E+02	1.1E+03	2.2E+03	3.9E+03	6.7E+03
48 →	2.0E-04	1.4E-02	2.9E-01	2.7E+00	1.5E+01	5.6E+01	1.7E+02	4.2E+02	9.2E+02	1.8E+03	3.2E+03	5.4E+03	8.6E+03
49 →	1.5E-06	4.0E-04	2.1E-02	3.7E-01	3.2E+00	1.8E+01	7.0E+01	2.2E+02	5.8E+02	1.3E+03	2.7E+03	5.2E+03	9.2E+03
50 →	4.7E-08	2.3E-05	1.5E-03	3.0E-02	2.9E-01	1.7E+00	7.2E+00	2.4E+01	6.5E+01	1.5E+02	3.2E+02	6.3E+02	1.1E+03
51 →	3.4E-05	4.0E-03	1.2E-01	1.4E+00	9.4E+00	4.2E+01	1.4E+02	3.8E+02	9.1E+02	1.9E+03	3.6E+03	6.5E+03	1.1E+04
52 →	1.1E-06	2.2E-04	7.9E-03	1.1E-01	7.7E-01	3.6E+00	1.3E+01	3.7E+01	8.9E+01	1.9E+02	3.7E+02	6.7E+02	1.1E+03
53 →	1.3E-03	5.4E-02	8.8E-01	7.0E+00	3.5E+01	1.3E+02	3.6E+02	8.8E+02	1.9E+03	3.6E+03	6.4E+03	1.1E+04	1.7E+04
54 →	5.4E-05	3.8E-03	8.9E-02	8.9E-01	5.3E+00	2.1E+01	6.8E+01	1.8E+02	4.0E+02	8.1E+02	1.5E+03	2.6E+03	4.3E+03
55 →	7.4E-05	4.5E-03	8.9E-02	8.1E-01	4.4E+00	1.7E+01	5.1E+01	1.3E+02	2.9E+02	5.7E+02	1.0E+03	1.8E+03	2.9E+03
56 →	1.7E-04	9.2E-03	1.6E-01	1.3E+00	6.8E+00	2.5E+01	7.2E+01	1.8E+02	3.8E+02	7.4E+02	1.3E+03	2.2E+03	3.5E+03
57 →	1.6E-03	4.3E-02	4.9E-01	3.1E+00	1.3E+01	4.0E+01	1.0E+02	2.3E+02	4.6E+02	8.3E+02	1.4E+03	2.3E+03	3.4E+03
58 →	2.4E-03	6.7E-02	8.1E-01	5.3E+00	2.3E+01	7.3E+01	1.9E+02	4.3E+02	8.6E+02	1.6E+03	2.7E+03	4.3E+03	6.6E+03
59 →	4.9E-03	1.2E-01	1.3E+00	8.1E+00	3.3E+01	1.0E+02	2.6E+02	5.8E+02	1.1E+03	2.1E+03	3.5E+03	5.6E+03	8.4E+03
60 →	9.1E-05	8.7E-03	2.4E-01	2.6E+00	1.6E+01	7.0E+01	2.3E+02	6.1E+02	1.4E+03	2.9E+03	5.5E+03	9.6E+03	1.6E+04
61 →	2.6E-05	3.1E-03	9.0E-02	1.0E+00	6.5E+00	2.8E+01	9.0E+01	2.4E+02	5.6E+02	1.1E+03	2.1E+03	3.7E+03	6.1E+03
62 →	8.2E-06	8.9E-04	2.3E-02	2.4E-01	1.4E+00	5.9E+00	1.8E+01	4.8E+01	1.1E+02	2.2E+02	4.0E+02	6.8E+02	1.1E+03
63 →	1.6E-03	8.1E-02	1.4E+00	1.2E+01	6.0E+01	2.2E+02	6.2E+02	1.5E+03	3.2E+03	6.2E+03	1.1E+04	1.8E+04	2.9E+04
64 →	1.5E-04	8.4E-03	1.5E-01	1.3E+00	6.4E+00	2.3E+01	6.8E+01	1.6E+02	3.5E+02	6.7E+02	1.2E+03	2.0E+03	3.1E+03
65 →	4.5E-04	2.0E-02	3.0E-01	2.2E+00	1.0E+01	3.6E+01	9.7E+01	2.2E+02	4.6E+02	8.6E+02	1.5E+03	2.4E+03	3.7E+03
66 →	1.5E-06	3.2E-04	1.4E-02	2.2E-01	1.7E+00	8.8E+00	3.3E+01	1.0E+02	2.5E+02	5.7E+02	1.1E+03	2.1E+03	3.7E+03
67 →	2.0E-04	1.7E-02	3.9E-01	3.9E+00	2.3E+01	9.4E+01	2.9E+02	7.6E+02	1.7E+03	3.5E+03	6.4E+03	1.1E+04	1.8E+04
68 →	1.5E-05	2.0E-03	6.1E-02	7.4E-01	4.9E+00	2.2E+01	7.4E+01	2.0E+02	4.8E+02	1.0E+03	1.9E+03	3.4E+03	5.7E+03
69 →	8.2E-03	2.5E-01	3.0E+00	1.9E+01	8.1E+01	2.5E+02	6.6E+02	1.5E+03	2.9E+03	5.2E+03	8.8E+03	1.4E+04	2.1E+04
70 →	2.3E-02	5.1E-01	4.5E+00	2.2E+01	7.6E+01	2.1E+02	4.7E+02	9.3E+02	1.7E+03	2.9E+03	4.5E+03	6.8E+03	9.9E+03
71 →	1.8E+00	1.8E+01	9.5E+01	3.3E+02	8.6E+02	1.9E+03	3.7E+03	6.4E+03	1.1E+04	1.6E+04	2.4E+04	3.4E+04	4.6E+04

72 →	8.8E-01	9.7E+00	5.1E+01	1.7E+02	4.5E+02	9.9E+02	1.9E+03	3.3E+03	5.4E+03	8.2E+03	1.2E+04	1.7E+04	2.3E+04
73 →	2.3E+01	9.5E+01	2.7E+02	6.2E+02	1.2E+03	2.1E+03	3.5E+03	5.3E+03	7.8E+03	1.1E+04	1.5E+04	2.0E+04	2.5E+04
42 ←	1.2E-03	4.4E-02	6.5E-01	4.8E+00	2.3E+01	7.8E+01	2.2E+02	5.1E+02	1.1E+03	2.0E+03	3.5E+03	5.7E+03	8.9E+03
43 ←	1.1E-02	2.2E-01	2.2E+00	1.2E+01	4.4E+01	1.3E+02	3.1E+02	6.5E+02	1.2E+03	2.2E+03	3.6E+03	5.5E+03	8.3E+03
44 ←	2.1E-03	5.2E-02	6.0E-01	3.8E+00	1.6E+01	5.1E+01	1.3E+02	2.9E+02	5.9E+02	1.1E+03	1.8E+03	2.9E+03	4.5E+03
45 ←	6.3E-02	9.0E-01	6.7E+00	3.1E+01	1.0E+02	2.7E+02	6.2E+02	1.2E+03	2.3E+03	3.8E+03	6.1E+03	9.2E+03	1.3E+04
46 ←	1.9E-04	1.1E-02	2.3E-01	2.2E+00	1.2E+01	5.0E+01	1.6E+02	4.1E+02	9.2E+02	1.9E+03	3.5E+03	6.2E+03	1.0E+04
47 ←	3.5E-04	1.4E-02	2.2E-01	1.8E+00	8.9E+00	3.2E+01	9.4E+01	2.3E+02	5.0E+02	9.7E+02	1.7E+03	3.0E+03	4.7E+03
48 ←	1.4E-03	4.1E-02	5.0E-01	3.4E+00	1.5E+01	5.0E+01	1.3E+02	3.1E+02	6.4E+02	1.2E+03	2.1E+03	3.5E+03	5.4E+03
49 ←	1.3E-03	6.1E-02	1.1E+00	9.7E+00	5.1E+01	1.9E+02	5.7E+02	1.4E+03	3.1E+03	6.1E+03	1.1E+04	1.8E+04	3.0E+04
50 ←	1.5E-02	3.5E-01	3.8E+00	2.3E+01	9.3E+01	2.8E+02	7.2E+02	1.6E+03	3.0E+03	5.5E+03	9.2E+03	1.5E+04	2.2E+04
51 ←	2.6E-03	9.5E-02	1.4E+00	1.1E+01	5.0E+01	1.7E+02	4.9E+02	1.2E+03	2.4E+03	4.6E+03	8.1E+03	1.3E+04	2.1E+04
52 ←	3.1E-02	5.2E-01	4.4E+00	2.3E+01	8.1E+01	2.3E+02	5.4E+02	1.1E+03	2.1E+03	3.7E+03	5.9E+03	9.2E+03	1.4E+04
53 ←	9.0E-10	1.8E-06	3.1E-04	1.2E-02	1.8E-01	1.6E+00	8.7E+00	3.6E+01	1.2E+02	3.3E+02	7.9E+02	1.7E+03	3.4E+03
54 ←	5.4E-05	3.8E-03	8.9E-02	8.9E-01	5.3E+00	2.1E+01	6.8E+01	1.8E+02	4.0E+02	8.1E+02	1.5E+03	2.6E+03	4.3E+03
55 ←	8.6E-04	2.9E-02	4.1E-01	2.9E+00	1.3E+01	4.5E+01	1.2E+02	2.8E+02	5.7E+02	1.1E+03	1.9E+03	3.0E+03	4.7E+03
56 ←	1.2E-02	2.3E-01	2.1E+00	1.1E+01	3.9E+01	1.1E+02	2.6E+02	5.5E+02	1.0E+03	1.8E+03	2.9E+03	4.5E+03	6.7E+03
57 ←	1.6E-03	4.3E-02	4.9E-01	3.1E+00	1.3E+01	4.0E+01	1.0E+02	2.3E+02	4.6E+02	8.3E+02	1.4E+03	2.3E+03	3.4E+03
58 ←	6.9E-05	7.6E-03	2.1E-01	2.4E+00	1.6E+01	6.8E+01	2.2E+02	6.1E+02	1.4E+03	3.0E+03	5.6E+03	9.9E+03	1.6E+04
59 ←	1.8E-03	8.6E-02	1.4E+00	1.1E+01	5.2E+01	1.8E+02	5.1E+02	1.2E+03	2.5E+03	4.8E+03	8.5E+03	1.4E+04	2.2E+04
60 ←	1.5E-08	1.1E-05	1.1E-03	2.9E-02	3.4E-01	2.3E+00	1.1E+01	3.9E+01	1.2E+02	2.9E+02	6.6E+02	1.3E+03	2.5E+03
61 ←	1.3E-06	3.4E-04	1.6E-02	2.5E-01	2.1E+00	1.1E+01	4.0E+01	1.2E+02	3.1E+02	7.0E+02	1.4E+03	2.6E+03	4.6E+03
62 ←	4.7E-05	5.7E-03	1.6E-01	1.8E+00	1.1E+01	4.9E+01	1.6E+02	4.3E+02	9.9E+02	2.0E+03	3.8E+03	6.7E+03	1.1E+04
63 ←	1.2E-09	2.8E-06	5.1E-04	2.1E-02	3.3E-01	2.8E+00	1.6E+01	6.6E+01	2.2E+02	6.2E+02	1.5E+03	3.3E+03	6.6E+03
64 ←	4.0E-08	2.9E-05	2.6E-03	6.3E-02	7.0E-01	4.6E+00	2.1E+01	7.4E+01	2.1E+02	5.3E+02	1.2E+03	2.3E+03	4.3E+03
65 ←	6.9E-06	1.6E-03	6.8E-02	1.0E+00	7.6E+00	3.8E+01	1.4E+02	4.1E+02	1.0E+03	2.2E+03	4.4E+03	8.1E+03	1.4E+04
66 ←	1.5E-06	3.2E-04	1.4E-02	2.2E-01	1.7E+00	8.8E+00	3.3E+01	1.0E+02	2.5E+02	5.7E+02	1.1E+03	2.1E+03	3.7E+03
67 ←	8.1E-08	3.9E-05	2.6E-03	5.3E-02	5.1E-01	3.0E+00	1.3E+01	4.2E+01	1.1E+02	2.7E+02	5.7E+02	1.1E+03	2.0E+03
68 ←	1.5E-05	2.0E-03	6.1E-02	7.4E-01	4.9E+00	2.2E+01	7.4E+01	2.0E+02	4.8E+02	1.0E+03	1.9E+03	3.4E+03	5.6E+03
69 ←	5.8E-09	4.8E-06	4.2E-04	1.0E-02	1.1E-01	6.8E-01	3.1E+00	1.1E+01	3.0E+01	7.3E+01	1.6E+02	3.1E+02	5.8E+02
70 ←	1.9E-11	1.1E-07	3.0E-05	1.5E-03	2.6E-02	2.4E-01	1.5E+00	6.3E+00	2.2E+01	6.2E+01	1.6E+02	3.5E+02	7.0E+02
71 ←	6.1E-13	9.7E-09	4.3E-06	2.9E-04	6.6E-03	7.3E-02	5.0E-01	2.4E+00	9.0E+00	2.8E+01	7.3E+01	1.7E+02	3.6E+02

72 ←	3.1E-13	1.2E-08	9.0E-06	8.5E-04	2.4E-02	3.1E-01	2.4E+00	1.3E+01	5.4E+01	1.8E+02	5.0E+02	1.2E+03	2.7E+03
73 ←	7.2E-09	1.5E-05	1.9E-03	5.5E-02	6.5E-01	4.5E+00	2.1E+01	7.6E+01	2.2E+02	5.6E+02	1.2E+03	2.5E+03	4.7E+03

Table S5: Rate coefficients ($m^3\ mol^{-1}\ s^{-1}$) for in the temperature range 300 – 1500 K for the reactions presented in Table 8 of the manuscript

	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K
74 →	2.0E-03	1.0E-01	1.8E+00	1.5E+01	7.5E+01	2.7E+02	7.8E+02	1.9E+03	4.0E+03	7.7E+03	1.4E+04	2.3E+04	3.6E+04
75 →	3.1E-01	5.8E+00	4.7E+01	2.2E+02	7.5E+02	2.0E+03	4.5E+03	8.9E+03	1.6E+04	2.7E+04	4.2E+04	6.4E+04	9.2E+04
76 →	1.4E-05	3.4E-03	1.3E-01	1.8E+00	1.3E+01	6.1E+01	2.1E+02	6.0E+02	1.5E+03	3.1E+03	6.0E+03	1.1E+04	1.8E+04
40 →	2.7E-02	4.5E-01	3.8E+00	1.9E+01	6.7E+01	1.9E+02	4.4E+02	9.0E+02	1.7E+03	2.9E+03	4.6E+03	7.1E+03	1.0E+04
77 →	1.2E-01	1.6E+00	1.2E+01	5.2E+01	1.7E+02	4.5E+02	1.0E+03	2.0E+03	3.5E+03	5.9E+03	9.4E+03	1.4E+04	2.0E+04
78 →	8.4E-04	5.2E-02	9.1E-01	7.3E+00	3.6E+01	1.3E+02	3.5E+02	8.4E+02	1.7E+03	3.3E+03	5.8E+03	9.6E+03	1.5E+04
79 →	4.2E-01	4.1E+00	2.3E+01	8.3E+01	2.3E+02	5.3E+02	1.1E+03	1.9E+03	3.3E+03	5.2E+03	7.8E+03	1.1E+04	1.6E+04
80 →	2.7E-01	3.0E+00	1.7E+01	6.6E+01	1.9E+02	4.4E+02	9.1E+02	1.7E+03	2.8E+03	4.5E+03	6.9E+03	1.0E+04	1.4E+04
81 →	7.5E-02	1.8E+00	1.9E+01	1.1E+02	4.2E+02	1.3E+03	3.1E+03	6.7E+03	1.3E+04	2.3E+04	3.8E+04	6.0E+04	9.0E+04
82 →	5.6E-03	1.4E-01	1.6E+00	9.8E+00	4.0E+01	1.3E+02	3.2E+02	7.0E+02	1.4E+03	2.5E+03	4.2E+03	6.7E+03	1.0E+04
83 →	3.7E-03	1.0E-01	1.2E+00	7.6E+00	3.2E+01	1.0E+02	2.6E+02	5.8E+02	1.1E+03	2.1E+03	3.5E+03	5.6E+03	8.5E+03
84 →	9.1E-03	1.8E-01	1.7E+00	9.1E+00	3.3E+01	9.6E+01	2.3E+02	4.8E+02	9.1E+02	1.6E+03	2.6E+03	4.0E+03	5.9E+03
85 →	6.6E-01	4.6E+00	2.1E+01	6.8E+01	1.8E+02	3.8E+02	7.5E+02	1.3E+03	2.2E+03	3.4E+03	5.0E+03	7.1E+03	9.8E+03
86 →	1.9E-03	6.9E-02	1.1E+00	8.2E+00	4.0E+01	1.4E+02	4.1E+02	9.7E+02	2.1E+03	3.9E+03	7.0E+03	1.2E+04	1.8E+04
87 →	1.9E-08	3.3E-05	3.9E-03	1.1E-01	1.3E+00	8.7E+00	4.1E+01	1.5E+02	4.2E+02	1.1E+03	2.3E+03	4.7E+03	8.8E+03
88 →	5.6E-06	1.2E-03	4.9E-02	7.0E-01	5.3E+00	2.6E+01	9.4E+01	2.8E+02	6.8E+02	1.5E+03	3.0E+03	5.4E+03	9.3E+03
89 →	2.8E-05	2.3E-03	6.5E-02	7.8E-01	5.3E+00	2.4E+01	8.2E+01	2.3E+02	5.5E+02	1.2E+03	2.3E+03	4.1E+03	6.9E+03
90 →	5.1E-05	3.9E-03	1.0E-01	1.2E+00	7.8E+00	3.4E+01	1.2E+02	3.2E+02	7.5E+02	1.6E+03	3.0E+03	5.4E+03	9.0E+03
91 →	8.4E-11	7.1E-07	2.1E-04	1.0E-02	1.9E-01	1.7E+00	1.0E+01	4.5E+01	1.5E+02	4.3E+02	1.1E+03	2.4E+03	4.8E+03
92 →	7.0E+01	4.1E+02	1.5E+03	4.4E+03	1.0E+04	2.0E+04	3.6E+04	6.0E+04	9.5E+04	1.4E+05	2.0E+05	2.8E+05	3.7E+05
93 →	2.6E+01	1.6E+02	6.6E+02	2.0E+03	4.8E+03	1.0E+04	1.9E+04	3.3E+04	5.2E+04	8.0E+04	1.2E+05	1.6E+05	2.2E+05
94 →	9.4E+00	6.7E+01	3.0E+02	9.9E+02	2.5E+03	5.6E+03	1.1E+04	1.9E+04	3.2E+04	4.9E+04	7.3E+04	1.0E+05	1.5E+05
95 →	2.8E-04	2.2E-02	4.9E-01	4.7E+00	2.6E+01	1.0E+02	3.1E+02	7.9E+02	1.8E+03	3.5E+03	6.4E+03	1.1E+04	1.8E+04
96 →	6.0E-02	9.8E-01	8.0E+00	3.9E+01	1.4E+02	3.7E+02	8.5E+02	1.7E+03	3.2E+03	5.4E+03	8.7E+03	1.3E+04	1.9E+04
97 →	2.3E-11	1.1E-07	2.7E-05	1.3E-03	2.4E-02	2.2E-01	1.3E+00	5.9E+00	2.0E+01	5.9E+01	1.5E+02	3.3E+02	6.7E+02
98 →	1.4E-08	9.6E-06	7.8E-04	1.8E-02	1.9E-01	1.2E+00	5.4E+00	1.8E+01	5.2E+01	1.3E+02	2.7E+02	5.4E+02	9.9E+02
99 →	8.5E-09	6.1E-06	5.0E-04	1.2E-02	1.2E-01	7.7E-01	3.4E+00	1.2E+01	3.3E+01	8.0E+01	1.7E+02	3.4E+02	6.3E+02
100 →	3.1E-11	1.0E-07	1.9E-05	7.4E-04	1.1E-02	9.4E-02	5.1E-01	2.1E+00	6.7E+00	1.8E+01	4.4E+01	9.5E+01	1.9E+02
101 →	1.1E-14	4.6E-10	3.4E-07	3.2E-05	8.9E-04	1.2E-02	9.0E-02	4.8E-01	2.0E+00	6.5E+00	1.8E+01	4.5E+01	9.9E+01

102 →	9.8E-09	7.3E-06	5.7E-04	1.3E-02	1.3E-01	8.0E-01	3.5E+00	1.2E+01	3.3E+01	7.9E+01	1.7E+02	3.3E+02	6.0E+02
74 ←	2.2E-06	6.3E-04	3.2E-02	5.3E-01	4.5E+00	2.4E+01	9.2E+01	2.8E+02	7.3E+02	1.7E+03	3.4E+03	6.3E+03	1.1E+04
75 ←	4.2E-16	5.3E-11	9.1E-08	1.5E-05	6.7E-04	1.2E-02	1.2E-01	8.2E-01	4.0E+00	1.5E+01	4.8E+01	1.3E+02	3.2E+02
76 ←	4.5E-01	8.6E+00	7.5E+01	3.9E+02	1.4E+03	3.9E+03	9.2E+03	1.9E+04	3.6E+04	6.2E+04	1.0E+05	1.5E+05	2.3E+05
40 ←	1.0E-06	3.8E-04	2.2E-02	3.9E-01	3.5E+00	1.9E+01	7.7E+01	2.4E+02	6.5E+02	1.5E+03	3.1E+03	6.0E+03	1.1E+04
77 ←	2.3E-07	1.2E-04	8.0E-03	1.6E-01	1.5E+00	9.0E+00	3.8E+01	1.2E+02	3.4E+02	8.0E+02	1.7E+03	3.3E+03	5.9E+03
78 ←	1.1E+00	2.1E+01	1.9E+02	9.6E+02	3.5E+03	1.0E+04	2.4E+04	5.0E+04	9.5E+04	1.7E+05	2.7E+05	4.2E+05	6.3E+05
79 ←	1.4E-13	5.0E-09	3.9E-06	3.9E-04	1.2E-02	1.6E-01	1.3E+00	7.1E+00	3.0E+01	1.0E+02	2.9E+02	7.3E+02	1.7E+03
80 ←	5.8E-14	2.8E-09	2.5E-06	2.8E-04	9.2E-03	1.3E-01	1.1E+00	6.5E+00	2.8E+01	9.8E+01	2.9E+02	7.4E+02	1.7E+03
81 ←	1.2E-08	1.4E-05	1.6E-03	4.4E-02	5.4E-01	3.8E+00	1.8E+01	6.6E+01	2.0E+02	5.1E+02	1.1E+03	2.3E+03	4.4E+03
82 ←	5.4E-06	1.4E-03	6.4E-02	1.0E+00	8.4E+00	4.4E+01	1.7E+02	5.0E+02	1.3E+03	2.9E+03	5.9E+03	1.1E+04	1.9E+04
83 ←	2.3E-04	2.1E-02	4.9E-01	5.0E+00	3.0E+01	1.2E+02	3.8E+02	9.9E+02	2.2E+03	4.5E+03	8.4E+03	1.4E+04	2.4E+04
84 ←	7.5E-03	2.3E-01	2.8E+00	1.7E+01	7.1E+01	2.2E+02	5.6E+02	1.2E+03	2.4E+03	4.4E+03	7.3E+03	1.2E+04	1.7E+04
85 ←	3.7E-08	2.5E-05	1.8E-03	3.5E-02	3.3E-01	1.9E+00	8.0E+00	2.6E+01	6.9E+01	1.6E+02	3.4E+02	6.4E+02	1.1E+03
86 ←	5.5E-09	6.3E-06	7.7E-04	2.4E-02	3.2E-01	2.5E+00	1.3E+01	4.9E+01	1.5E+02	4.0E+02	9.4E+02	2.0E+03	3.8E+03
87 ←	5.1E+01	3.6E+02	1.6E+03	5.1E+03	1.3E+04	2.8E+04	5.5E+04	9.6E+04	1.6E+05	2.5E+05	3.6E+05	5.2E+05	7.2E+05
88 ←	1.5E-02	2.8E-01	2.6E+00	1.4E+01	5.4E+01	1.6E+02	3.9E+02	8.3E+02	1.6E+03	2.8E+03	4.7E+03	7.3E+03	1.1E+04
89 ←	4.3E-09	2.9E-06	2.9E-04	8.2E-03	1.0E-01	7.4E-01	3.6E+00	1.4E+01	4.1E+01	1.1E+02	2.4E+02	5.1E+02	9.7E+02
90 ←	3.4E-08	1.4E-05	9.9E-04	2.2E-02	2.3E-01	1.5E+00	6.7E+00	2.3E+01	6.6E+01	1.6E+02	3.6E+02	7.1E+02	1.3E+03
91 ←	5.3E+01	3.0E+02	1.1E+03	3.1E+03	7.1E+03	1.4E+04	2.6E+04	4.3E+04	6.8E+04	1.0E+05	1.4E+05	2.0E+05	2.7E+05
92 ←	1.7E-09	5.4E-06	8.8E-04	3.0E-02	4.1E-01	3.1E+00	1.6E+01	6.1E+01	1.9E+02	4.9E+02	1.1E+03	2.4E+03	4.5E+03
93 ←	4.6E-08	4.3E-05	3.4E-03	7.4E-02	7.3E-01	4.4E+00	1.9E+01	6.1E+01	1.7E+02	4.0E+02	8.4E+02	1.6E+03	2.9E+03
94 ←	3.0E-06	9.3E-04	3.9E-02	5.5E-01	4.0E+00	1.9E+01	6.6E+01	1.9E+02	4.5E+02	9.7E+02	1.9E+03	3.4E+03	5.7E+03
95 ←	1.8E-07	1.0E-04	7.8E-03	1.7E-01	1.7E+00	1.0E+01	4.3E+01	1.4E+02	3.9E+02	9.3E+02	2.0E+03	3.8E+03	6.9E+03
96 ←	1.8E-05	2.5E-03	7.6E-02	8.8E-01	5.7E+00	2.5E+01	8.1E+01	2.2E+02	5.1E+02	1.1E+03	2.0E+03	3.5E+03	5.8E+03
97 ←	3.0E-02	5.0E-01	4.2E+00	2.1E+01	7.3E+01	2.0E+02	4.6E+02	9.4E+02	1.7E+03	3.0E+03	4.8E+03	7.3E+03	1.1E+04
98 ←	1.0E-03	3.6E-02	4.9E-01	3.4E+00	1.5E+01	5.0E+01	1.3E+02	3.1E+02	6.2E+02	1.1E+03	2.0E+03	3.2E+03	4.9E+03
99 ←	7.3E-03	2.0E-01	2.4E+00	1.5E+01	5.9E+01	1.8E+02	4.6E+02	1.0E+03	2.0E+03	3.6E+03	6.0E+03	9.5E+03	1.4E+04
100 ←	2.2E-01	2.9E+00	2.0E+01	8.5E+01	2.6E+02	6.6E+02	1.4E+03	2.8E+03	4.9E+03	8.0E+03	1.2E+04	1.8E+04	2.6E+04
101 ←	1.9E+01	1.1E+02	3.6E+02	9.2E+02	2.0E+03	3.6E+03	6.2E+03	9.8E+03	1.5E+04	2.1E+04	2.9E+04	3.9E+04	5.1E+04
102 ←	1.8E-01	2.6E+00	1.9E+01	8.5E+01	2.8E+02	7.1E+02	1.6E+03	3.1E+03	5.6E+03	9.3E+03	1.5E+04	2.2E+04	3.2E+04

Symmetry numbers

Table S6: Applied symmetry numbers and corresponding reaction path degeneracy for all reactions of Table 1, Table 2, Table 3 and Table 8. $n_{e,app}$ is the apparent reaction path degeneracy. Besides the number of equivalent reaction paths, $n_{e,app}$ includes mixing effects of swiftly interconverting, energetically equivalent conformers that are not accounted for within the calculated partition function.

Rx	Reactant 1				Reactant 2				Transition state				Rx path degeneracy	
	σ_{ext}	σ_{int}	n_{opt}	n_{conf}	σ_{ext}	σ_{int}	n_{opt}	n_{conf}	σ_{ext}	σ_{int}	n_{opt}	n_{conf}	n_e	$n_{e,app}$
Table 1														
1 →	6	1	1	1	12	1	1	1	3	3	1	1	8	8
1 ←	12	1	1	1	6	1	1	1	3	3	1	1	8	8
2 →	6	1	1	1	1	3	1	1	1	3	1	2	6	12
2 ←	12	1	1	1	1	2	1	1	1	3	1	2	8	16
3 →	6	1	1	1	1	3	1	2	1	9	2	1	4	2
3 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
4 →	6	1	1	1	1	9	1	2	1	27	1	2	2	2
4 ←	12	1	1	1	1	18	1	1	1	27	1	2	8	16
5 →	6	1	1	1	1	3	1	1	1	3	2	1	12	12
5 ←	12	1	1	1	1	1	1	1	1	3	2	1	8	8
6 →	6	1	1	1	1	3	1	1	1	9	2	1	4	4
6 ←	12	1	1	1	1	3	1	1	1	9	2	1	8	8
7 →	6	1	1	1	1	9	1	1	1	27	2	1	4	4
7 ←	12	1	1	1	1	9	1	1	1	27	2	1	8	8
8 →	6	1	1	1	1	1	1	1	1	3	1	2	2	4
8 ←	12	1	1	1	1	1	1	2	1	3	1	2	4	4
9 →	6	1	1	1	1	1	1	1	1	3	1	1	2	2
9 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
10 →	6	1	1	1	1	1	1	2	1	3	2	1	4	2
10 ←	12	1	1	1	1	1	1	1	1	3	2	1	8	8
11 →	6	1	1	1	1	3	2	1	1	9	2	1	2	2
11 ←	12	1	1	1	1	3	1	1	1	9	2	1	8	8
12 →	6	1	1	1	1	1	1	2	1	3	2	1	4	2
12 ←	12	1	1	1	1	1	1	1	1	3	2	1	8	8
13 →	6	1	1	1	1	3	2	1	1	9	2	1	2	2

13 ←	12	1	1	1	1	3	1	1	1	9	2	1	8	8
14 →	6	1	1	1	1	1	1	2	1	3	2	1	4	2
14 ←	12	1	1	1	1	1	1	1	1	3	2	1	8	8
15 →	6	1	1	1	1	3	2	1	1	9	2	1	2	2
15 ←	12	1	1	1	1	3	1	1	1	9	2	1	8	8
16 →	6	1	1	1	1	2	1	2	1	3	2	1	8	4
16 ←	12	1	1	1	1	1	1	1	1	3	2	1	8	8
17 →	6	1	1	1	1	6	2	1	1	9	2	1	4	4
17 ←	12	1	1	1	1	3	1	1	1	9	2	1	8	8
18 →	6	1	1	1	2	1	1	1	1	3	1	1	4	4
18 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
19 →	6	1	1	1	1	3	1	1	1	9	1	1	2	2
19 ←	12	1	1	1	1	3	1	1	1	9	1	1	4	4
20 →	6	1	1	1	1	1	1	1	1	3	1	1	2	2
20 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
21 →	6	1	1	1	1	1	1	1	1	3	1	1	2	2
21 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
22 →	6	1	1	1	1	1	1	1	1	3	1	1	2	2
22 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
23 →	6	1	1	1	2	1	1	1	1	3	1	1	4	4
23 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
24 →	6	1	1	1	2	1	1	1	1	3	1	1	4	4
24 ←	12	1	1	1	1	1	1	1	1	3	1	1	4	4
Table 2														
3 →	6	1	1	1	1	3	1	2	1	9	2	1	4	2
3 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
25 →	6	1	1	1	1	3	1	2	1	9	2	1	4	2
25 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
26 →	6	1	1	1	1	3	1	2	1	9	2	1	4	2
26 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
27 →	6	1	1	1	1	9	1	2	1	27	2	1	4	2
27 ←	12	1	1	1	1	9	1	2	1	27	2	1	8	4
28 →	6	1	1	1	1	81	1	2	1	243	2	1	4	2
28 ←	12	1	1	1	1	81	1	2	1	243	2	1	8	4
8 →	6	1	1	1	1	1	1	1	1	3	1	2	2	4

8 ←	12	1	1	1	1	1	1	2	1	3	1	2	4	4
29 →	6	1	1	1	1	3	1	2	1	9	1	2	2	2
29 ←	12	1	1	1	1	3	1	2	1	9	1	2	4	4
30 →	6	1	1	1	1	9	1	2	1	27	1	2	2	2
30 ←	12	1	1	1	1	9	1	2	1	27	1	2	4	4
2 →	6	1	1	1	1	3	1	1	1	3	1	2	6	12
2 ←	12	1	1	1	1	2	1	1	1	3	1	2	8	16
31 →	6	1	1	1	2	9	1	1	1	9	1	2	12	24
31 ←	12	1	1	1	1	6	1	1	1	9	1	2	8	16
32 →	6	1	1	1	1	3	1	1	1	3	1	2	6	12
32 ←	12	1	1	1	1	2	1	2	1	3	1	2	8	8
33 →	6	1	1	1	1	3	1	2	1	3	1	2	6	6
33 ←	12	1	1	1	1	2	1	2	1	3	1	2	8	8
3 →	6	1	1	1	1	3	1	2	1	9	2	1	4	2
3 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
34 →	6	1	1	1	1	9	1	1	1	27	2	1	4	4
34 ←	12	1	1	1	1	9	1	2	1	27	2	1	8	4
35 →	6	1	1	1	1	3	1	2	1	9	2	1	4	2
35 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
36 →	6	1	1	1	1	9	1	2	1	27	2	1	4	2
36 ←	12	1	1	1	1	9	1	2	1	27	2	1	8	4
37 →	6	1	1	1	2	9	1	2	1	27	2	1	8	4
37 ←	12	1	1	1	1	9	1	2	1	27	2	1	8	4
38 →	6	1	1	1	1	3	1	1	1	9	2	1	4	4
38 ←	12	1	1	1	1	3	1	2	1	9	2	1	8	4
10 →	6	1	1	1	1	1	1	2	1	3	2	1	4	2
10 ←	12	1	1	1	1	1	1	1	1	3	2	1	8	8
39 →	6	1	1	1	1	1	1	2	1	3	2	1	4	2
39 ←	12	1	1	1	1	1	1	2	1	3	2	1	8	4
40 →	1	6	1	1	1	3	1	2	1	9	2	1	4	2
40 ←	6	3	1	1	1	3	1	2	1	9	2	1	12	6
41 →	1	6	1	1	1	9	1	1	1	27	2	1	4	4
41 ←	6	3	1	1	1	9	1	2	1	27	2	1	12	6
Table 3														
42 →	1	3	1	1	2	1	1	1	1	1	2	1	12	12

42 ←	1	2	1	1	1	3	1	1	1	1	2	1	12	12
43 →	1	3	1	1	1	3	1	1	1	3	2	1	6	6
43 ←	1	2	1	1	1	3	1	2	1	3	2	1	4	2
44 →	1	3	1	2	2	1	1	1	1	3	2	1	4	2
44 ←	1	3	1	2	1	3	1	1	1	3	2	1	6	3
45 →	1	3	1	2	1	3	1	1	1	9	2	1	2	1
45 ←	1	3	1	2	1	3	1	2	1	9	2	1	2	0.5
46 →	1	3	1	1	2^2	1	1	1	1	1	1	2	6	12
46 ←	1	2	1	1	1	6	1	1	1	1	1	2	12	24
47 →	1	3	1	2	2^2	1	1	1	1	3	2	1	4	2
47 ←	1	3	1	2	1	6	1	1	1	3	2	1	12	6
48 →	1	9	1	2	2^2	1	1	1	1	9	1	2	2	2
48 ←	1	18	1	1	1	6	1	1	1	9	1	2	12	24
49 →	1	3	1	1	2	1	1	1	1	1	1	2	6	12
49 ←	1	2	1	1	3	1	1	1	1	1	1	2	6	12
50 →	1	3	1	1	1	3	1	1	1	3	2	1	6	6
50 ←	1	2	1	1	1	3	1	1	1	3	2	1	4	4
51 →	1	3	1	2	2	1	1	1	1	3	2	1	4	2
51 ←	1	3	1	2	3	1	1	1	1	3	2	1	6	3
52 →	1	3	1	2	1	3	1	1	1	9	2	1	2	1
52 ←	1	3	1	2	1	3	1	1	1	9	2	1	2	1
53 →	1	1	1	2	2	1	1	1	1	1	2	1	4	2
53 ←	1	1	1	1	3	1	1	1	1	1	2	1	6	6
54 →	1	3	1	1	1	2	1	1	1	1	1	2	6	12
54 ←	1	2	1	1	1	3	1	1	1	1	1	2	6	12
55 →	1	3	1	1	1	3	1	2	1	3	2	1	6	3
55 ←	1	2	1	1	1	3	1	2	1	3	2	1	4	2
56 →	1	3	1	1	1	18	1	1	1	9	1	2	6	12
56 ←	1	2	1	1	1	9	1	2	1	9	1	2	2	2
57 →	1	3	1	2	1	3	1	2	1	9	2	1	2	0.5
57 ←	1	3	1	2	1	3	1	2	1	9	2	1	2	0.5
58 →	1	3	1	1	1	9	1	1	1	9	1	2	3	6
58 ←	1	2	1	1	2	9	1	1	1	9	1	2	4	8
59 →	1	3	1	1	3	27	1	1	1	81	1	2	3	6
59 ←	1	2	1	1	3	27	1	1	1	81	1	2	2	4

60 →	1	3	1	1	2	1	1	1	1	1	2	1	12	12
60 ←	1	1	1	1	1	3	1	1	1	1	2	1	6	6
61 →	1	3	1	1	1	3	1	1	1	3	2	1	6	6
61 ←	1	1	1	1	1	3	1	2	1	3	2	1	2	1
62 →	1	3	1	1	1	9	1	1	1	9	2	1	6	6
62 ←	1	1	1	1	1	9	1	1	1	9	2	1	2	2
63 →	1	3	1	1	2	1	1	1	1	1	2	1	12	12
63 ←	1	1	1	1	3	1	1	1	1	1	2	1	6	6
64 →	1	3	1	1	1	3	1	1	1	3	2	1	6	6
64 ←	1	1	1	1	1	3	1	1	1	3	2	1	2	2
65 →	1	3	1	1	2	9	1	1	1	9	2	1	12	12
65 ←	1	1	1	1	1	9	1	1	1	9	2	1	2	2
66 →	1	3	1	1	1	1	1	1	1	1	2	1	6	6
66 ←	1	1	1	1	1	3	1	1	1	1	2	1	6	6
67 →	1	3	1	1	1	1	1	1	1	3	2	1	2	2
67 ←	1	3	1	1	1	3	1	1	1	3	2	1	6	6
68 →	1	3	1	1	1	3	1	1	1	9	2	1	2	2
68 ←	1	3	1	1	1	3	1	1	1	9	2	1	2	2
69 →	1	9	1	1	1	1	1	1	1	9	2	1	2	2
69 ←	1	9	1	1	1	3	1	1	1	9	2	1	6	6
70 →	1	3	1	1	1	2	1	1	1	1	2	1	12	12
70 ←	1	1	1	1	1	3	1	1	1	1	2	1	6	6
71 →	1	3	1	1	1	2	1	1	1	3	2	1	4	4
71 ←	1	3	1	1	1	3	1	1	1	3	2	1	6	6
72 →	1	3	1	1	1	6	1	1	1	3	2	1	12	12
72 ←	1	1	1	1	6	3	1	1	1	3	2	1	12	12
73 →	1	3	1	1	3	27	1	1	1	81	2	1	6	6
73 ←	1	1	1	1	3	27	1	1	1	81	2	1	2	2
Table 8														
74 →	1	3	1	2	6	1	1	1	1	3	1	2	6	6
74 ←	1	2	1	2	12	1	1	1	1	3	1	2	8	8
75 →	1	3	1	1	6	1	1	1	1	3	1	1	6	6
75 ←	1	2	1	1	12	1	1	1	1	3	1	1	8	8
76 →	1	1	1	1	6	1	1	1	1	3	1	1	2	2
76 ←	1	1	1	1	12	1	1	1	1	3	1	1	4	4

40 →	1	3	1	2	1	6	1	1	1	9	2	1	4	2
40 ←	1	3	1	2	6	3	1	1	1	9	2	1	12	6
77 →	1	9	1	1	1	6	1	1	1	27	2	1	4	4
77 ←	1	9	1	2	6	3	1	1	1	27	2	1	12	6
78 →	1	1	1	1	1	6	1	1	1	3	1	2	2	4
78 ←	1	1	1	2	6	3	1	1	1	3	1	2	6	6
79 →	1	1	1	2	1	6	1	1	1	3	2	1	4	2
79 ←	1	1	1	1	6	3	1	1	1	3	2	1	12	12
80 →	1	3	1	2	1	6	1	1	1	9	2	1	4	2
80 ←	1	3	1	1	6	3	1	1	1	9	2	1	12	12
81 →	2	9	1	2	6	1	1	1	1	9	1	2	12	12
81 ←	1	6	1	2	12	1	1	1	1	9	1	2	8	8
82 →	2	9	1	2	1	6	1	1	1	9	1	2	12	12
82 ←	1	6	1	2	6	3	1	1	1	9	1	2	12	12
83 →	2	9	1	2	1	9	1	1	1	27	1	2	6	6
83 ←	1	6	1	2	2	9	1	1	1	27	1	2	4	4
84 →	2	9	1	2	3	27	1	1	1	243	1	2	6	6
84 ←	1	6	1	2	3	27	1	1	1	243	1	2	2	2
85 →	1	1	1	2	1	18	1	1	1	9	2	1	4	2
85 ←	1	1	1	1	1	9	1	2	1	9	2	1	2	1
86 →	1	1	1	2	2	1	1	1	1	1	2	1	4	2
86 ←	1	1	1	1	3	1	1	1	1	1	2	1	6	6
87 →	1	1	1	1	2	1	1	1	1	1	1	2	2	4
87 ←	1	1	1	2	3	1	1	1	1	1	1	2	3	3
88 →	1	9	1	2	2	1	1	1	1	9	2	1	4	2
88 ←	1	18	1	1	1	3	1	1	1	9	2	1	12	12
89 →	1	1	1	2	2	1	1	1	1	1	2	1	4	2
89 ←	1	1	1	1	1	3	1	1	1	1	2	1	6	6
90 →	1	1	1	2	2	1	1	1	1	1	2	1	4	2
90 ←	1	1	1	1	1	3	1	1	1	1	2	1	6	6
91 →	1	1	1	1	2	1	1	1	1	1	2	1	4	4
91 ←	1	1	1	2	1	3	1	1	1	1	2	1	6	3
92 →	1	3	1	1	1	1	1	1	1	1	1	2	3	6
92 ←	1	2	1	1	4	1	1	1	1	1	1	2	8	16
93 →	1	3	1	1	1	3	1	1	1	3	1	2	3	6

93 ←	1	2	1	1	1	3	1	1	1	3	1	2	2	4
94 →	1	3	1	1	1	1	1	2	1	1	1	2	3	3
94 ←	1	2	1	1	1	1	1	1	1	1	1	2	2	4
95 →	1	3	1	1	1	1	1	1	1	1	2	1	6	6
95 ←	1	2	1	1	2	1	1	1	1	1	2	1	8	8
96 →	1	3	1	1	2 [2]	1	1	1	1	1	1	2	6	12
96 ←	1	2	1	1	1	1	1	1	1	1	1	2	2	4
97 →	1	3	1	1	1	1	1	1	1	1	2	1	6	6
97 ←	1	2	1	1	1	1	1	2	1	1	2	1	4	2
98 →	1	3	1	1	1	3	1	1	1	3	2	1	6	6
98 ←	1	2	1	1	1	6	1	1	1	3	2	1	8	8
99 →	1	3	1	1	2 [2]	9	1	1	1	9	1	2	6	12
99 ←	1	2	1	1	1	18	1	1	1	9	1	2	4	8
100 →	1	3	1	1	1	9	1	1	1	9	2	1	6	6
100 ←	1	2	1	1	1	9	1	1	1	9	2	1	4	4
101 →	1	3	1	1	1	9	1	1	1	9	2	1	6	6
101 ←	1	2	1	1	1	9	1	1	1	9	2	1	4	4
102 →	1	3	1	1	2	9	1	1	1	9	1	2	6	3
102 ←	1	2	1	1	1	9	1	1	1	9	1	2	2	1

[1] As $n_{e,app}$ accounts for mixing effects, this value is rather difficult to interpret and retrieve without the geometry of the reactants and transition state. Users of the GA method presented in this work are therefore advised to use the easily retrievable n_e value.

[2] External symmetry number calculated by Gaussian was 1.

Tunneling coefficients

Table S7: Eckart tunneling coefficients for all reactions of Table 1, Table 2, Table 3 and Table 8.

Rx	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500
Table 2													
1	49.1	6.1	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
2	28.5	5.1	2.7	2.0	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1
3	17.6	4.3	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
4	11.7	3.7	2.3	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
5	4.0	2.1	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
6	2.6	1.7	1.4	1.3	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0
7	1.8	1.4	1.2	1.2	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0	1.0
8	26.6	5.1	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
9	30.3	4.9	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
10	8.3	3.0	2.0	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
11	5.5	2.5	1.8	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1
12	2.7	1.7	1.4	1.3	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.0	1.0
13	2.0	1.4	1.3	1.2	1.1	1.1	1.1	1.1	1.1	1.0	1.0	1.0	1.0
14	8.6	3.1	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1
15	5.5	2.5	1.8	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1
16	9.0	3.1	2.0	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
17	6.7	2.7	1.9	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1
18	18.7	4.4	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
19	12.9	3.8	2.3	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
20	7.1	2.8	1.9	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
21	17.7	4.4	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
22	7.7	2.9	2.0	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
23	4.6	2.4	1.8	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1
24	9.1	3.3	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
Table 3													
3	17.6	4.3	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
25	19.2	4.5	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
26	18.4	4.4	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1

27	20.0	4.6	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
28	22.0	4.8	2.6	1.9	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1
8	26.6	5.1	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
29	25.4	5.0	2.7	2.0	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
30	27.9	5.4	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
2	28.5	5.1	2.7	2.0	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1
31	23.3	4.8	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
32	28.5	5.1	2.7	1.9	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1
33	29.1	5.3	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
3	17.6	4.3	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
34	14.9	4.0	2.4	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
35	19.4	4.5	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
36	19.1	4.5	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
37	19.4	4.5	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
38	18.4	4.3	2.5	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
10	8.3	3.0	2.0	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
39	7.8	2.9	2.0	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1	1.1
40	29.4	5.6	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
41	25.1	5.3	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
Table 4													
42	38.1	5.8	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
43	21.9	4.7	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
44	35.6	5.9	3.0	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1
45	20.7	4.9	2.7	2.0	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
46	44.4	6.2	3.0	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
47	36.2	5.9	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1
48	30.0	5.7	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
49	51.5	6.6	3.1	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
50	32.3	5.7	2.9	2.1	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1
51	39.4	6.1	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
52	26.7	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
53	44.7	6.3	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
54	49.0	6.6	3.1	2.2	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
55	38.3	6.2	3.1	2.2	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
56	26.3	5.5	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1

57	29.5	5.9	3.0	2.1	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
58	39.0	6.1	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
59	30.5	5.7	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
60	33.1	5.3	2.7	2.0	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1
61	20.8	4.4	2.4	1.8	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
62	16.7	4.0	2.4	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
63	31.4	5.2	2.7	2.0	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1
64	24.6	4.8	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
65	18.0	4.2	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
66	29.4	5.0	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
67	20.4	4.4	2.4	1.8	1.6	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
68	19.6	4.3	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
69	15.8	4.0	2.4	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
70	10.1	3.3	2.1	1.7	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1
71	6.3	2.7	1.9	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1
72	4.3	2.2	1.6	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
73	3.9	2.2	1.7	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1
Table 9													
74	33.3	5.4	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
75	12.2	3.6	2.2	1.7	1.5	1.4	1.3	1.2	1.2	1.1	1.1	1.1	1.1
76	18.0	4.4	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
40	29.4	5.6	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
77	25.1	5.3	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
78	20.5	4.8	2.7	2.0	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
79	12.1	3.8	2.3	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
80	11.4	3.6	2.2	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
81	28.4	5.2	2.7	2.0	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
82	36.2	5.9	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
83	30.9	5.6	2.9	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.1	1.1
84	22.4	5.1	2.8	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1
85	15.2	4.6	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.2	1.1
86	51.6	6.8	3.2	2.2	1.8	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
87	10.2	3.6	2.3	1.8	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1	1.1
88	31.3	5.8	3.0	2.1	1.7	1.5	1.4	1.3	1.3	1.2	1.2	1.2	1.1
89	87.4	8.1	3.4	2.3	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1

90	76.5	7.7	3.4	2.3	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1
91	6.5	2.9	2.0	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1
92	7.8	3.1	2.1	1.7	1.5	1.3	1.3	1.2	1.2	1.1	1.1	1.1	1.1
93	11.9	3.9	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
94	11.8	3.9	2.4	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
95	22.0	4.5	2.5	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
96	23.4	5.0	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
97	23.9	5.1	2.7	2.0	1.7	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
98	28.0	5.2	2.7	2.0	1.6	1.5	1.4	1.3	1.2	1.2	1.2	1.1	1.1
99	22.4	4.8	2.6	1.9	1.6	1.4	1.3	1.3	1.2	1.2	1.2	1.1	1.1
100	14.6	4.1	2.4	1.8	1.6	1.4	1.3	1.3	1.2	1.2	1.1	1.1	1.1
101	3.0	1.9	1.5	1.3	1.2	1.2	1.1	1.1	1.1	1.1	1.1	1.1	1.1
102	19.4	4.7	2.6	1.9	1.6	1.5	1.3	1.3	1.2	1.2	1.2	1.1	1.1

Determination of the number of single events

The number of single events for a bimolecular reaction A + B is calculated as:

$$n_e = \frac{n_{\mathrm{opt},\ddagger}}{n_{\mathrm{opt,A}}\, n_{\mathrm{opt,B}}} \frac{\sigma_{\mathrm{A}}\sigma_{\mathrm{B}}}{\sigma_{\ddagger}}$$

with σ the total symmetry number of the molecule and n_{opt} the number of chiral species. The total symmetry number σ is the product of the external symmetry number and internal rotational symmetry numbers:

$$\sigma = \sigma_{\mathrm{ext}} \prod_i \sigma_{\mathrm{int},i}$$

Symmetry numbers are introduced to avoid the overcounting of indistinguishable configurations in the phase space and the corresponding energy levels in the partition functions. The partition functions obtained within the HO approximation correspond with a single well on the potential energy surface. In some cases compounds exist of multiple distinguishable, swiftly interconverting and energetically equivalent conformations, of which only one is accounted for within the HO approximation. One can opt to explicitly account for these energetically equivalent conformations by multiplying the partition function with a factor n_{conf} (=number of equivalent conformations) or by dividing the symmetry number σ by n_{conf}. The ratio σ/n_{conf} is often referred to as the apparent symmetry number σ_{app}.

a) σ_{ext}

The external symmetry number is defined as the number of different but indistinguishable atomic rearrangements that can be obtained by rotating a given molecule as a whole. It is found by multiplying the order of the independent simple rotational axes of the point group to which the molecule belongs.

Table S8: The various points groups and their corresponding external symmetry number

Point group	σ_{ext}
C_1, C_i, C_s, $C_{\infty v}$	1
$D_{\infty h}$	2
C_n, C_{nv}, C_{nh}	n
D_n, D_{nh}, D_{nd}	$2n$
S_n (n even)	$n/2$
T_d	12
O_h	24
I_h	60

b) σ_{int}

The internal symmetry number is defined as the number of different but indistinguishable atomic rearrangements that can be obtained by internal rotations around a single bond. The internal rotational symmetry number is equal to the least common multiple (lcm) of the rotational symmetry numbers of the two rotating fragments. For example, in toluene, the methyl and phenyl fragment have a rotational symmetry number of 3 and 2, respectively. The internal symmetry number for rotation around the C−C bond hence amounts to lcm(3,2)=6.

Table S9: Various rotating fragments and the corresponding rotational symmetry number

Rotating fragment	σ_{rot}
$-CH_3$	3
$-C(CH_3)_3$	3
$-C_6H_5$ (phenyl)	2
$-C^{\bullet}H_2$	2
$-C^{\bullet}(CH_3)_2$	2

The use of the internal symmetry number is only valid in case rotation is fast compared to the time scale reaction takes place. Therefore for rotational barriers of the same order of magnitude or exceeding the reaction barrier no internal symmetry number is accounted for. In particular rotations around a bond between a radical site and a neighboring π system are hindered and not considered to be rotating. For example, the internal symmetry number for the benzyl radical is 1.

Table S10: Hindered rotations

Rotation	σ_{int}
$C^{\bullet} - C_B$	1
$C^{\bullet} - C_d$	1

c) n_{opt}

A chiral carbon atom contribute a factor 2 to n_{opt}. Contributions of diastereomers are excluded.

In analogy with previous work (Sabbe et al. *PCCP* (2010) 12, 1278 – 1298), a n_{opt} of 2 is also assigned to transition states having a C=C or C=S double bond in gauche position transition state bond C_1—H—C_2. Rotation around C^{TS}–C_d or C^{TS}–CS bonds is hampered due to resonance and will not occur in the time scale of reaction.

Reassessment of the rate coefficient for the reaction $C^{\bullet}_2H_5 + C_2H_5SC_2H_5 \rightarrow C_2H_6 + CH_3C^{\bullet}HSC_2H_5$ reported in Ekwenchi et al. Can. J. Chem 59 3226 (1981)

Table S11: Effect of temperature and diethylsulfide (DES) pressure on the quantum yields of the products (I_a = 1.06 10^{-2} μeinstein min^{-1}, V = 200 cm^3). This table corresponds with Table 2 in Ekwenchi et al. Can. J. Chem 59 3226 (1981).

Temp	P(DES)	$\varphi = R/I_a$					
(°C)	(Torr)	C2H6	C2H4	C4H10	MTH	C2H5SH	Σ
170	31.6	1.51	0.114	0.197	~0	2.01	2.02
170	**20.0**	**1.49**	**0.107**	**0.197**	**~0**	**2.01**	**1.99**
167	10.0	1.45	0.0982	0.236	~0	2.01	2.02
150	**20.0**	**1.19**	**0.11**	**0.291**	**0.136**	**2.01**	**2.02**
130	**20.0**	**0.984**	**0.107**	**0.321**	**0.272**	**2.01**	**2.01**
110	**20.0**	**0.652**	**0.104**	**0.363**	**0.527**	**2.01**	**2.01**
25	20.0	0.630	0.0982	0.407	~0	1.53	1.54

Hydrogen atoms were generated by the mercury-photosensitized decomposition of H_2. The hydrogen radicals will initiate the following radical reactions:

[1] $H^{\bullet} + C_2H_5SC_2H_5 \rightarrow C^{\bullet}_2H_5 + C_2H_5SH$

[2] $C^{\bullet}_2H_5 + C^{\bullet}_2H_5 \rightarrow C_2H_6 + CH_2{=}CH_2$

[3] $C^{\bullet}_2H_5 + C^{\bullet}_2H_5 \rightarrow C_4H_{10}$

[4] $C^{\bullet}_2H_5 + C_2H_5SC_2H_5 \rightarrow C_2H_6 + CH_3C^{\bullet}HSC_2H_5$

[5] $C^{\bullet}_2H_5 + CH_3C^{\bullet}HSC_2H_5 \rightarrow C_2H_6 + CH_2{=}CHSC_2H_5$

[6] $C^{\bullet}_2H_5 + CH_3C^{\bullet}HSC_2H_5 \rightarrow CH_2{=}CH_2 + C_2H_5SC_2H_5$

The total rates of ethane and ethene formation are then expressed as:

$R_{C2H6} = R_2 + R_4 + R_5$

$R_{CH2=CH2} = R_2 + R_6$

Assuming that $R_5 = R_6$

$R_{C2H6} = R_{CH2=CH2} + R_4 \rightarrow \varphi_{C2H6} = \varphi_{CH2=CH2} + R_4/I_a$

The *n*-butane rate is:

$R_{C4H10} = R_3 \rightarrow \varphi_{C4H10} = R_3/I_a$

The value of R_4 can hence be calculated directly from the quantum yields presented in Table S11. However in order to obtain the rate coefficient, the calculated rate is divided by the root of R_{C4H10}. The rate coefficient for reaction [3] can be retrieved from the NIST Chemical kinetics database as 1.0 10^7 m^3 mol^{-1} s^{-1}.

$R_4 = k_4 [C^{\bullet}_2H_5] [DES]$

$R_3 = k_3 [C^{\bullet}_2H_5]^2$ with k_3 = 1.0 10^7 m^3 mol^{-1} s^{-1}

Hence $(\varphi_{C2H6} - \varphi_{CH2=CH2})/\varphi_{C4H10}^{1/2} = R_4 / (I_a R_3)^{1/2} = k_4 [DES] / (I_a k_3)^{1/2}$. This leads to an expression for k_4:

$$k_{C_2H_5+C_2H_5SC_2H_5} = \frac{\sqrt{k_{C_2H_5+C_2H_5}}}{[C_2H_5SC_2H_5]} \frac{\varphi_{C_2H_6} - \varphi_{CH_2=CH_2}}{\sqrt{\varphi_{C_4H_{10}}}} \sqrt{I_a}$$

(k_4= $k_{C_2H_5+C_2H_5SC_2H_5}$ and k_3 = $k_{C_2H_5+C_2H_5}$)

Eckwenchi et al. do not report which formula has been used to obtain the rate coefficient from the reported quantum yields. However, from their derivation we suspect the discrepancies are mainly due to the fact that the authors did not multiply the right hand side of the aforementioned formula with $\sqrt{I_a}$.

Table S12: Rate coefficients $k_{C2H5+C2H5SC2H5}$ calculated in the temperature range 110 to 170°C for the bold data in Table S11 (I_a = 1.06 10^{-2} µeinstein min^{-1}, V = 200 cm^3) Rate coefficients reported by Ekwenchi et al. are presented in the last column.

Temp (°C)	P(DES) (Torr)	[DES] (mol m^{-3})	I_a (mol m^{-3} s^{-1})	$\frac{\varphi_{C_2H_6} - \varphi_{CH_2=CH_2}}{\sqrt{\varphi_{C_4H_{10}}}}$ (-)	k (m^3 mol^{-1} s^{-1})	$k_{Ekwenchi}$ (m^3 mol^{-1} s^{-1})
170	20.0	0.724	8.83E-07	3.12	12.8	3.1 10^4
150	20.0	0.758	8.83E-07	2.00	7.9	2.1 10^4
130	20.0	0.796	8.83E-07	1.55	5.8	1.4 10^4
110	20.0	0.837	8.83E-07	0.91	3.2	9.0 10^3

Fitting of Arrhenius parameters to the calculated rate coefficients results to the following expression:

$$k_{C_2H_5+C_2H_5SC_2H_5} = 6.2\,10^4 \exp(-31300/RT)$$

with R in J mol^{-1} K^{-1}.

Geometries of the reactants, products and transition states for all reactions considered in this work

Geometries (Å), HO frequencies (cm^{-1}) in the transition state, rotational barrier in (kJ mol^{-1}), fitted Fourrier coefficients for the 1D HR treatment (kJ mol^{-1}), substituted frequency (cm^{-1}) and reduced moment of inertia (amu $bohr^2$)

Notation for Fourier coefficients

cos = C_1, C_2, C_3, (C_4, C_5)
sin = D_1, D_2, D_3, (D_4, D_5)

Indicates that the potential energy profile for rotation can be approximated by the Fourrier expansion:

$$V(\phi) = \sum_{i=1}^{5} \frac{1}{2} C_i (1 - \cos(i\phi)) + \sum_{i=1}^{5} D_i \sin(i\phi)$$

Reaction01

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C 0.000000 0.000000 1.347599
C 0.000000 0.000000 -1.347599
H 0.000000 1.049672 1.632870
H 0.909043 -0.524836 1.632870
H -0.909043 -0.524836 1.632870
H 0.000000 0.000000 0.000000
H 0.000000 -1.049672 -1.632870
H -0.909043 0.524836 -1.632870
H 0.909043 0.524836 -1.632870

Frequencies = -1637.95, 39.3441, 331.935, 331.937, 505.902, 694.107, 694.108, 1148.59, 1178.95, 1357.36, 1357.36, 1439.94, 1439.94, 1457.05, 1457.05, 3054.23, 3055.68, 3183.37, 3183.37, 3184.38, 3184.38
cos = 0, 0, .10
sin = 0, 0, 0
barrier = 0.307
Substituted frequency = 39.34 (from HO analysis)
Reduced moment of inertia = 5.949

Reaction02

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

TRANSITION STATE

H -1.256196 -0.851797 1.121689
S -1.382204 -0.279868 -0.088506

C -0.020806 0.878466 0.058632
H 1.132195 0.282804 0.023470
C 2.411321 -0.316868 -0.023909
H -0.032659 1.455793 0.982056
H -0.024145 1.527051 -0.816491
H 2.536070 -0.763446 0.959527
H 2.315743 -1.039249 -0.830457
H 3.101162 0.497146 -0.232029

Frequencies = -1603.18, 35.2783, 117.566, 199.177, 348.117, 457.516, 559.751, 644.662, 735.595, 853.152, 1054.15, 1120.55, 1127.77, 1392.36, 1398.39, 1422.07, 1439.9, 1444.3, 2657.47, 3057.54, 3075.57, 3159.3, 3191.67, 3195.53
cos = .01, .01, .31, .01, .01
sin = 0, 0, .03, 0, 0
barrier = 0.327
Substituted frequency = 35.28 (from HO analysis)
Reduced moment of inertia = 10.669

Reaction03

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

TRANSITION STATE

C 0.029507 0.377383 -0.465626
S 1.353764 -0.749457 0.015164
H 0.038252 0.407240 -1.556942
C 0.039219 1.753732 0.168983
H -0.807797 2.344448 -0.193709
H -0.040838 1.688201 1.257972
H 0.960332 2.296020 -0.065486
H -1.104883 -0.166983 -0.197311
C -2.398784 -0.710499 0.087259
H -2.295097 -1.747204 -0.221269
H -2.516605 -0.573563 1.159309
H -3.092576 -0.129398 -0.514747
H 1.179345 -0.651140 1.345872

Frequencies = -1544.59, 43.9917, 106.334, 155.51, 218.413, 254.105, 314.88, 449.518, 532.563, 553.199, 673.158, 866.59, 896.935, 1017.54, 1083.65, 1124.34, 1139.18, 1300.61, 1385.63, 1406.5, 1410.46, 1438.38, 1444.07, 1486.98, 1492.1, 2650.54, 3016.44, 3059.07, 3074.89, 3079.56, 3094.77, 3193, 3198.81
cos = 0, 0, .37, 0, 0
sin = 0, 0, -.03, 0, 0
barrier = 0.369
Substituted frequency = 43.99 (from HO analysis)
Reduced moment of inertia = 11.616

Reaction04

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -0.416743 0.016648 0.401914
S 1.370091 -0.080624 -0.092069
C -1.092896 1.273450 -0.142201
C -1.091922 -1.265135 -0.089637
H -0.436704 0.030165 1.494167
H 1.749074 1.095395 0.437615
H -0.614345 -2.155502 0.325257
H -2.142662 -1.270770 0.214075
H -1.055862 -1.333473 -1.180727
H -2.143622 1.299170 0.167520
H -0.613112 2.182183 0.228997
H -1.054854 1.293045 -1.234244

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745

H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.085389 1.313238 0.036768
C 0.384580 0.008453 -0.166818
S -1.359504 -0.096411 0.035726
C 1.125045 -1.280188 0.007989
H -1.655216 1.176510 -0.281170
H 1.189097 1.567951 1.104198
H 2.094663 1.272829 -0.385000
H 0.556706 2.144567 -0.439850
H 2.079005 -1.245228 -0.528633
H 1.360984 -1.490121 1.064115
H 0.556743 -2.132957 -0.372915

TRANSITION STATE

H -1.121415 -1.459417 1.130067
S -1.321410 -0.925550 -0.087681
C -0.030624 0.355280 0.013699
H 1.090304 -0.250337 -0.003172
C 2.404701 -0.867454 -0.026803
C -0.052261 1.162756 1.299788
C -0.056047 1.197658 -1.251987
H 2.487682 -1.337284 0.949711
H 2.321231 -1.566567 -0.854174
H 3.102636 -0.051087 -0.192398
H 0.791141 1.889459 -1.253364
H 0.011987 0.578174 -2.149626
H -0.974463 1.791996 -1.317458
H 0.782801 1.871137 1.311486
H -0.983970 1.731002 1.392856
H 0.040006 0.522282 2.180777

Frequencies = -1471.43, 38.9781, 100.959, 118.073, 190.513, 231.172, 242.644, 303.23, 315.115, 342.028, 487.937, 528.19, 539.281, 644.753, 872.137, 916.815, 958.178, 995.787, 1102, 1133.59, 1179.73, 1190.07, 1380.66, 1394, 1404.06, 1418.09, 1435.21, 1439.84, 1481.93, 1483.45, 1496.07, 1501.92, 2656.65, 3010.94, 3015.53, 3060.77, 3071.17, 3074.82, 3087.42, 3096.03, 3196.05, 3201.05
cos = 0, 0, .35, 0, 0
sin = 0, 0, .02, 0, 0
barrier = 0.361
Substituted frequency = 38.98 (from HO analysis)
Reduced moment of inertia = 11.776

Reaction05

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

TRANSITION STATE

C -2.783925 -0.631028 0.054601
C -0.583440 1.002568 -0.303834
H -0.967325 1.971706 0.022033
C 0.559714 0.522189 0.463409
S 1.754890 -0.442075 -0.098985
H -1.531920 0.252769 -0.081381
H -0.455040 0.938961 -1.383299
H 0.576532 0.813064 1.516243
H -3.497100 -0.126218 -0.587653
H -2.389794 -1.573571 -0.308919
H -2.967690 -0.565880 1.121688

Frequencies = -1114.17, 34.4532, 66.283, 167.22, 358.099, 391.041, 494.221, 589.142, 686.568, 835.484, 882.168, 1035.48, 1092.07, 1106.45, 1193.5, 1361.04, 1388.3, 1420.01, 1420.58, 1437.52, 1467.79, 3062.82, 3074.59, 3076.33, 3150.71, 3231.09, 3234.48
cos = 0, 0, .36, 0, 0
sin = 0, 0, .02, 0, 0
barrier = 0.364
Substituted frequency = 34.45 (from HO analysis)
Reduced moment of inertia = 11.572

Reaction06

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -1.327332 0.192629 0.000000
C 0.000000 0.890905 0.000000
S 1.475337 0.219519 0.000000
H -0.077991 1.981482 0.000000
C -1.311691 -1.331367 0.000000
H -1.883617 0.577607 0.867672
H -1.883617 0.577607 -0.867672
H -2.333686 -1.718270 0.000000
H -0.796169 -1.721869 -0.879633
H -0.796169 -1.721869 0.879633

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -2.363629 0.049719 0.000009
C -0.939547 -0.390541 -0.000022
C 0.137524 0.455049 -0.000015
S 1.751584 -0.074704 0.000008
H -0.049834 1.528545 -0.000028
H -0.742501 -1.459462 -0.000028
H -2.889317 -0.347800 0.876519
H -2.460269 1.136849 -0.000232
H -2.889508 -0.348227 -0.876186

TRANSITION STATE

C -2.682688 -1.012618 -0.340837
C -0.544407 0.481309 0.644543
H -0.915226 0.706453 1.650411
C 0.638066 -0.385279 0.712640
S 1.900712 -0.419876 -0.324321
H -1.438467 -0.245377 0.238576
C -0.517739 1.696178 -0.266129
H 0.626493 -1.100096 1.538956
H -3.481233 -0.292185 -0.203995
H -2.344120 -1.175092 -1.357934
H -2.698018 -1.881303 0.308157
H -1.491009 2.192691 -0.268498
H 0.232703 2.416347 0.071982
H -0.261919 1.419038 -1.289832

Frequencies = -975.532, 23.8245, 67.3924, 116.379, 180.595, 230.613, 271.42, 462.821, 504.662, 568.869, 605.367, 792.448, 839.692, 905.349, 986.247, 1072.87, 1097.74, 1117.27, 1190.66, 1299.03, 1379.7, 1391.48, 1416.49, 1418.55, 1422.05, 1428.76, 1488.87, 1498.71, 3034.93, 3042.66, 3072.85, 3077.71, 3093.69, 3115.51, 3233.7, 3236.38
cos = 0, 0, .29, 0, 0
sin = 0, 0, .01, 0, 0
barrier = 0.285
Substituted frequency = 23.82 (from HO analysis)
Reduced moment of inertia = 11.939

Reaction07

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.132027 -0.835770 0.000000
C -0.358696 0.583412 0.000000
S 0.548402 1.925752 0.000000
H -1.449374 0.681652 0.000000
H 1.225030 -0.815693 0.000000
C -0.358696 -1.557557 1.271321
C -0.358696 -1.557557 -1.271321
H -0.004581 -2.591851 1.273036
H 0.013651 -1.067890 2.173865
H -1.451930 -1.576841 1.318633
H -0.004581 -2.591851 -1.273036
H -1.451930 -1.576841 -1.318633
H 0.013651 -1.067890 -2.173865

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.821897 -0.025137 0.000086
C -0.378047 -0.711838 -0.000009
S -1.929833 -0.032719 -0.000199
H -0.315203 -1.799063 0.000046
C 0.921964 1.466291 0.000032
C 2.115592 -0.784099 0.000254
H 1.483398 1.807508 -0.877872
H -0.059619 1.936413 -0.000109
H 1.483179 1.807583 0.878048
H 2.717700 -0.518090 -0.876885
H 2.717517 -0.518016 0.877498
H 1.961914 -1.864141 0.000284

TRANSITION STATE

C -2.207041 1.788808 -0.043986
C -0.490788 -0.435617 -0.002339
C -1.289710 -1.492124 -0.773391
C 0.748892 -0.035058 -0.696500
S 2.169477 0.420723 -0.033985

H -1.171759 0.563918 -0.081815
C -0.377025 -0.724589 1.488286
H 0.661037 -0.020241 -1.786451
H -3.024117 1.377022 0.537077
H -1.582407 2.526981 0.445715
H -2.384467 1.927083 -1.104591
H -1.368332 -0.882074 1.921078
H 0.216952 -1.627992 1.658878
H 0.114079 0.092236 2.018128
H -0.796513 -2.467617 -0.712558
H -2.293095 -1.598781 -0.353814
H -1.388983 -1.230622 -1.830308

Frequencies = -786.819, 47.6446, 61.7045, 110.244, 138.018, 194.371, 218.021, 245.318, 352.426, 395.052, 461.42, 492.323, 516.84, 617.647, 777.488, 877.632, 943.823, 954.007, 992.28, 1068.38, 1101.71, 1152.11, 1188.04, 1231.13, 1304.94, 1375.78, 1399.51, 1405.09, 1416.67, 1419, 1428.37, 1480.61, 1486.97, 1500.45, 1507.84, 3021.34, 3029.96, 3060.39, 3079.96, 3082.79, 3087.85, 3096.77, 3117.82, 3236.81, 3239.81
cos = 0, 0, .30, 0, 0
sin = 0, 0, -.01, 0, 0
barrier = 0.295
Substituted frequency = 47.64 (from HO analysis)
Reduced moment of inertia = 12.084

Reaction08

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.748228 0.124075 0.039321
C 0.565049 -0.440481 -0.067799
S -1.053621 0.123840 -0.050080
H 2.653636 -0.427995 -0.197380
H 1.877846 1.151585 0.382815
H -1.553214 -0.806591 0.786707

TRANSITION STATE

C -2.433049 -0.642262 -0.028863
C 0.019880 0.443686 0.062839
S 1.397989 -0.634956 -0.067098
C 0.045721 1.767720 0.021699
H -0.878795 2.334697 -0.023247
H 0.973023 2.334435 0.033457
H -1.171346 -0.130358 0.041277
H 0.973089 -1.555549 0.818181
H -3.077888 0.219556 -0.181597
H -2.398887 -1.321722 -0.876828
H -2.582330 -1.136628 0.928271

Frequencies = -1601.42, 22.737, 104.695, 161.526, 234.861, 303.59, 464.924, 512.904, 550.534, 653.173, 722.942, 907.725, 952.511, 1078.51, 1156.69, 1237.84, 1376.76, 1414.95, 1436.48, 1445.11, 1658.74, 2642.93, 3058.28, 3110.1, 3189.46, 3190.7, 3193.57
cos = 0, 0, .30, 0, 0
sin = 0, 0, -.03, 0, 0
barrier = 0.301
Substituted frequency = 22.74 (from HO analysis)
Reduced moment of inertia = 11.482

Reaction09

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 0.449465 0.000000
S -1.623646 0.295698 0.000000
H 0.443032 1.448356 0.000000
C 0.948150 -0.645188 0.000000
C 2.273801 -0.441563 0.000000
H 0.536627 -1.649548 0.000000
H 2.976058 -1.266614 0.000000
H 2.690923 0.560357 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 2.283924 -0.300143 0.000050
C 1.089013 0.201111 -0.000153
C -0.143437 0.709500 0.000051
S -1.545164 -0.275462 0.000051
H 2.802260 -0.524828 -0.928356
H 2.802745 -0.522713 0.928693
H -0.259384 1.792137 -0.000840

TRANSITION STATE

C 1.612149 1.921054 0.000011
H 2.697108 1.833987 0.000027
C 0.739418 -0.618025 0.000000
C -0.683166 -0.826786 0.000042
C 1.673822 -1.568370 -0.000022
H 2.733046 -1.331499 -0.000043
H 1.412702 -2.626854 -0.000029
H 1.164716 0.692990 -0.000008
H 1.210663 2.365171 0.907423
H 1.210688 2.365195 -0.907400
S -1.843450 0.320903 -0.000017
H -0.987059 -1.880683 0.000129

Frequencies = -1539.68, 38.6224, 46.1489, 90.49, 193.866, 244.394, 409.62, 486.992, 507.03, 560.667, 566.029, 880.711, 893.173, 961.546, 1080.85, 1187.93, 1216.07, 1281.82, 1320.24, 1361.91, 1437.09, 1438.88, 1455.86, 1646.56, 3019.19, 3057.83, 3086.27, 3182.95, 3184.44, 3192.94
cos = 0, 0, .22, 0, 0
sin = 0, 0, .01, 0, 0
barrier = 0.228
Substituted frequency = 38.62 (from HO analysis)
Reduced moment of inertia = 11.705

Reaction10

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935
C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000
H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

TRANSITION STATE

C -1.225825 2.340702 -0.086024
C 0.068192 -0.032876 0.392612
S -1.065385 -1.379636 -0.072050
C 1.316870 -0.060877 -0.393679
C 2.538325 0.104476 0.120983
H -2.166237 -0.870538 0.510057
H -0.527086 1.038265 0.145249
H 0.243079 -0.002953 1.469047
H 1.201590 -0.190278 -1.467765
H 3.419017 0.120175 -0.510243
H 2.696329 0.228126 1.187735
H -1.958117 2.393624 0.714148
H -0.412258 3.056238 -0.018145
H -1.635526 2.192969 -1.080638

Frequencies = -1374.01, 45.8209, 79.2285, 123.012, 157.621, 187.841, 258.837, 396.587, 463.65, 503.858, 550.753, 663.991, 766.503, 892.059, 936.01, 958.83, 1017.37, 1029.67, 1104.09, 1155.06, 1238.56, 1319.61, 1340.79, 1415.33, 1425.62, 1435.33, 1457.46, 1672.05, 2657.48, 3066.22, 3084.14, 3129.4, 3136.15, 3210.6, 3214.39, 3217.62
cos = 0, 0, .54, 0, 0
sin = 0, 0, -.02, 0, 0
barrier = 0.542
Substituted frequency = 45.82 (from HO analysis)
Reduced moment of inertia = 11.909

Reaction11

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -2.339486 -0.507714 -0.142716
C -1.212392 -0.086409 0.425239
C 0.006068 0.345939 -0.331324
S 1.442783 -0.778971 0.046708
H 0.824558 -1.928656 -0.272199
C 0.445122 1.770747 0.024498
H -0.179918 0.280671 -1.405151
H -1.130818 -0.039972 1.509213
H -3.197322 -0.804153 0.449787
H -2.444762 -0.571413 -1.221690
H 1.344781 2.055000 -0.526501
H -0.351392 2.474690 -0.228640
H 0.654475 1.861995 1.093666

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 2.369655 -0.455338 0.000000
C 1.034479 -0.769329 0.000000
C -0.020009 0.153602 0.000000
S -1.709963 -0.334849 0.000000
H 3.119525 -1.235537 0.000000
H 2.723690 0.568159 0.000000
H 0.770163 -1.824297 0.000000
C 0.196373 1.640624 0.000000
H -1.520278 -1.665490 0.000000
H -0.746400 2.190666 0.000000
H 0.764802 1.953383 0.883011
H 0.764923 1.953352 -0.882988

TRANSITION STATE

C -1.400603 2.267658 -0.348132
C 0.037187 -0.026548 0.167462
C 0.311476 0.044510 1.660526
C 1.214643 0.001525 -0.737863
C 2.486422 0.177128 -0.371241
S -1.047453 -1.421327 -0.324226
H -2.135194 -1.021845 0.360154
H -0.619275 0.993340 -0.105479
H 0.982774 -0.103700 -1.795344
H 3.276420 0.218841 -1.111870
H 2.786248 0.280950 0.664992
H -1.826188 2.064215 -1.325712
H -2.111331 2.299463 0.472072
H -0.625757 3.027330 -0.323086
H -0.622681 0.077744 2.224923
H 0.877948 -0.827390 1.999440
H 0.881530 0.946638 1.903011

Frequencies = -1275.97, 57.6602, 80.6207, 111.842, 127.281, 207.115, 238.568, 266.091, 313.089, 323.007, 427.752, 498.421, 510.254, 550.334, 622.325, 739.838, 856.458, 928.848, 935.842, 1002.84, 1031.88, 1065.57, 1106.75, 1124.07, 1205.54, 1325.02, 1334.61, 1391.57, 1407.22, 1425.1, 1427.64, 1447.98, 1490.72, 1494.66, 1672.93, 2648.58, 3023.86, 3068.21, 3087.11, 3100.02, 3133.38, 3145.31, 3213.13, 3217.3, 3224.41
cos = 0, 0, .56, 0, 0
sin = 0, 0, -.02, 0, 0
barrier = 0.560
Substituted frequency = 57.66 (from HO analysis)
Reduced moment of inertia = 11.967

Reaction12

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -0.510027 0.799014 -0.303335
C 0.659584 0.342385 0.503980
S 2.039526 -0.250290 -0.104797
H 0.520589 0.408009 1.584599
H -0.289907 0.816146 -1.368870
S -1.968938 -0.278332 0.042517
H -0.832436 1.793567 0.019804
H -1.425002 -1.408162 -0.442915

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -0.647835 0.957924 -0.000020
S -1.692207 -0.406648 0.000014
C 0.741522 0.926690 -0.000157
S 1.694221 -0.456905 0.000003
H 1.235336 1.895918 0.000733
H -1.165772 1.910923 -0.000072
H -0.663922 -1.297678 0.000114

TRANSITION STATE

C 1.181440 2.547712 0.063427
C 0.346121 -0.073296 -0.342229
S 1.777229 -1.164403 -0.069211
C -0.866598 -0.352448 0.441701
S -2.389284 -0.109103 -0.082532
H 1.946341 -0.891244 1.237145

H 0.692088 1.066522 -0.094306
H 0.150627 -0.044605 -1.413992
H -0.698942 -0.697714 1.463939
H 2.086708 2.519291 -0.532375
H 0.339175 3.091499 -0.349128
H 1.311096 2.600539 1.139203

Frequencies = -988.431, 44.5957, 54.174, 110.924, 160.386, 198.984, 259.478, 348.606, 469.03, 500.865, 592.415, 714.252, 832.619, 889.885, 952.7, 1043.67, 1092.88, 1189.81, 1225.47, 1291.1, 1385.12, 1417.32, 1417.55, 1439.8, 2661.81, 3076.79, 3081.39, 3116.47, 3231.44, 3238.86
cos = 0, 0, .49, 0, 0
sin = 0, 0, -.05, 0, 0
barrier = 0.488
Substituted frequency = 44.60 (from HO analysis)
Reduced moment of inertia = 12.112

Reaction13

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -0.455238 0.405530 -0.342395
S -1.656197 -0.958224 0.049612
C 0.768662 0.163563 0.483239
S 2.236115 -0.212804 -0.095289
H 0.608693 0.252347 1.560226
H -0.212111 0.350775 -1.402616
C -1.129089 1.741256 -0.009084
H -0.898545 -1.961896 -0.425911
H -2.034965 1.869348 -0.604920
H -1.399931 1.798853 1.048348
H -0.447830 2.564921 -0.234848

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.663770 0.400460 -0.000103
C -0.640322 0.897897 -0.000114
S -2.060952 0.002792 0.000047
H -0.722315 1.983548 -0.000229
S 1.016214 -1.296668 -0.000016
C 1.851618 1.318797 0.000068
H -0.301716 -1.644776 0.000114
H 2.478056 1.150206 0.881769
H 2.479947 1.148299 -0.879892
H 1.531436 2.361806 -0.001355

TRANSITION STATE

C -1.427631 2.448786 -0.372003
C -0.324678 -0.068931 0.199262
C 0.880582 -0.201251 -0.646501
S 2.427553 -0.005210 -0.175449
S -1.582469 -1.284855 -0.372347
H -2.631482 -0.702236 0.235040
H -0.779152 1.003941 -0.122181
C -0.131754 -0.024376 1.705943
H 0.668464 -0.410006 -1.697105
H -2.164888 2.507745 0.420648
H -0.548761 3.074799 -0.268759
H -1.801293 2.286636 -1.376652
H -1.082949 0.165674 2.207237
H 0.265866 -0.974472 2.069149
H 0.573747 0.763587 1.977157

Frequencies = -822.845, 44.2788, 60.0395, 103.982, 121.651, 168.251, 206.829, 241.669, 295.107, 346.495, 439.329, 482.295, 490.303, 617.107, 668.199, 836.096, 878.618, 932.665, 1046.9, 1057.91, 1080.8, 1141.26, 1210.98, 1264.79, 1367.57, 1401.95, 1415.52, 1416.22, 1417.81, 1482.77, 1486.78, 2657.63, 3039.89, 3079.09, 3081.86, 3109.81, 3112.94, 3237.43, 3240.25
cos = 0, 0, .55, 0, 0
sin = 0, 0, .03, 0, 0
barrier = 0.549
Substituted frequency = 44.28 (from HO analysis)
Reduced moment of inertia = 12.164

Reaction14

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 1.275072 0.157942 -0.000791
C -0.003799 0.840478 0.061607
C 2.332294 -0.411226 -0.034669
H 3.266389 -0.915805 -0.072492
H -0.090502 1.423579 0.979934
H -0.113254 1.531514 -0.777702
S -1.469790 -0.282226 -0.079388
H -1.167393 -1.046849 0.983591

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745

H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 2.361273 -0.341462 0.000000
C 1.253535 0.166078 0.000000
C 0.000000 0.724962 0.000000
S -1.495795 -0.181980 0.000000
H 3.330556 -0.775632 0.000000
H -0.140578 1.798264 0.000000
H -0.946110 -1.408414 0.000000

TRANSITION STATE

C -1.635759 2.047436 -0.162851
C 0.027313 -0.006123 0.561378
C 1.364442 0.321557 0.166973
C 2.460696 0.645574 -0.212921
S -0.642080 -1.572460 -0.086981
H -0.294945 -1.363721 -1.368616
H -0.731081 0.929626 0.210032
H -0.102149 -0.038962 1.644597
H 3.438260 0.913804 -0.530483
H -2.616540 1.620443 0.022349
H -1.337655 2.848790 0.506217
H -1.382765 2.198713 -1.207869

Frequencies = -1404.08, 40.8925, 86.9922, 135.506, 170.579, 217.159, 360.467, 440.191, 472.478, 525.151, 586.01, 639.75, 674.445, 705.01, 879.79, 997.21, 1031.1, 1108.69, 1256, 1352.39, 1407.87, 1425.27, 1430.8, 2192, 2669.85, 3067.23, 3089.22, 3213.45, 3215.8, 3475.99
cos = 0, 0, .32, 0, 0
sin = 0, 0, .02, 0, 0
barrier = 0.320
Substituted frequency = 40.89 (from HO analysis)
Reduced moment of inertia = 11.909

Reaction15

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 1.288198 -0.221995 -0.137998
C -0.004220 0.380144 -0.432363
C 2.361948 -0.692048 0.127014
H 3.307341 -1.120088 0.354129
C -0.160521 1.771404 0.198805
H -0.114788 0.462685 -1.518138
S -1.403228 -0.763362 0.016023
H -1.065056 -0.897974 1.310283
H -1.128131 2.199023 -0.067109
H -0.093569 1.710220 1.286808
H 0.633429 2.434902 -0.155086

PRODUCT 1

C 2.446234 -0.538497 0.000390
C 1.298527 -0.127532 -0.000501
C 0.003230 0.335306 -0.002978
C -0.351686 1.795185 0.000805
S -1.364916 -0.781363 0.000000
H 3.447787 -0.891498 0.001764
H -0.652416 -1.919597 0.005617
H -0.975353 2.056596 -0.861894
H -0.912242 2.067626 0.902923
H 0.553052 2.401923 -0.034841

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C -1.644401 1.994362 -0.567643
C 0.036518 -0.004491 0.286052
C -0.213652 -0.070114 1.792468
S -0.536868 -1.563446 -0.499642
C 1.372863 0.368592 -0.086918
C 2.470270 0.733096 -0.424983
H -0.080743 -1.290763 -1.733638
H -0.716705 0.894656 -0.133781
H 3.446404 1.037233 -0.713317
H -2.620161 1.540383 -0.426547
H -1.402643 2.812646 0.103422
H -1.339170 2.134320 -1.599948
H -1.265033 -0.287008 1.995992
H 0.400685 -0.844266 2.259058
H 0.037670 0.889279 2.249175

Frequencies = -1308.32, 44.9671, 87.1651, 107.857, 161.893, 201.002, 223.017, 244.117, 289.787, 426.844, 475.699, 502.313, 521.487, 566.746, 643.624, 675.21, 694.979, 867.688, 900.678, 1060.58, 1094.14, 1114.37, 1177.23, 1343.73, 1385.99, 1408.85, 1423.89, 1426.26, 1488.54, 1495.12, 2188.99, 2677.39, 3033.23, 3068.7, 3101.47, 3110.24, 3215.44, 3217.38, 3475.5
cos = 0, 0, .35, 0, 0
sin = 0, 0, .01, 0, 0
barrier = 0.345
Substituted frequency = 44.97 (from HO analysis)
Reduced moment of inertia = 11.973

Reaction16

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 2.672635 -0.162290 -0.337779
H 3.709633 -0.278885 -0.631540
C 2.110084 1.107145 -0.243221
C 0.776923 1.253253 0.137375
C -0.010951 0.135658 0.426391
C 0.564695 -1.136214 0.325319
C 1.895004 -1.284540 -0.050812
H 2.707448 1.985240 -0.461956
H 0.345764 2.246423 0.216256
C -1.449410 0.307354 0.835285
H -0.038632 -2.012931 0.536087
H 2.327557 -2.276406 -0.120511
H -1.702496 -0.349011 1.670523
H -1.647868 1.332460 1.147844
S -2.678922 -0.162925 -0.467546
H -2.192532 0.637708 -1.431317

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.677225 -1.390843 0.000064
C 2.689255 -0.426663 -0.000026
C 2.344109 0.929241 -0.000081
C 1.015862 1.315712 -0.000044
C -0.030614 0.352696 0.000053
C 0.343315 -1.017761 0.000100
C -1.376136 0.790673 0.000154
S -2.737843 -0.306392 -0.000170
H 3.730505 -0.726568 -0.000022
H 3.121701 1.685214 -0.000155
H 0.758763 2.369779 -0.000114
H -0.423702 -1.784347 0.000197
H 1.936105 -2.444037 0.000078
H -1.603596 1.847533 0.000293
H -3.692369 0.636373 0.001117

TRANSITION STATE

C 2.255565 2.280725 0.703229
H 1.685519 1.093467 0.004375
C 1.203697 0.119674 -0.619177
S 2.166200 -1.351148 -0.146102
H 1.367699 0.370536 -1.667188
H 1.495900 3.039709 0.543312
H 3.199753 2.457250 0.196219
H 2.339469 1.916760 1.722771
H 3.381282 -0.807219 -0.339521
C -0.244065 0.016258 -0.289426
C -1.203250 0.424705 -1.227629
C -2.560528 0.390413 -0.923084
C -2.986724 -0.055173 0.326438
C -2.043566 -0.463548 1.268736
C -0.686621 -0.427068 0.966648
H -0.879591 0.766115 -2.205428
H -3.286014 0.706084 -1.664605
H -4.044054 -0.085584 0.563670
H -2.366558 -0.810968 2.243836
H 0.040336 -0.743703 1.705792

Frequencies = -1377.53, 38.9176, 48.2625, 68.6346, 111.078, 146.352, 185.879, 244.127, 334.992, 414.93, 430.74, 476.804, 522.82, 571.837, 598.007, 634.714, 710.293, 729.707, 778.353, 827.301, 854.212, 924.814, 948.295, 981.046, 999.384, 1006.26, 1015.26, 1050.88, 1104.67, 1106.33, 1182.19, 1201.01, 1207.26, 1253.61, 1332.24, 1351.72, 1363.47, 1418.15, 1426.18, 1443.02, 1482.87, 1524.07, 1617.45, 1639.85, 2650.35, 3065.52, 3091.89, 3157.93, 3164.81, 3174.17, 3182.21, 3190.71, 3208.71, 3212.8
cos = 0, 0, .44, 0, 0
sin = 0, 0, .02, 0, 0
barrier = 0.440
Substituted frequency = 48.26 (from HO analysis)
Reduced moment of inertia = 12.030

Reaction17

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -2.023932 -1.292915 0.311212
C -2.917192 -0.303049 -0.100272
C -2.437938 0.963002 -0.421110
C -1.073825 1.237224 -0.327330
C -0.170511 0.254903 0.087850
C -0.664075 -1.017693 0.401323
C 1.300062 0.592779 0.209556
S 2.373681 -0.450415 -0.899810
H -3.976804 -0.520634 -0.172463
H -3.122280 1.739058 -0.745509
H -0.707042 2.227920 -0.577395
H 0.024247 -1.800098 0.700318
H -2.389085 -2.283783 0.557788
H 1.445573 1.626871 -0.106683
C 1.844359 0.439929 1.635738
H 1.675048 -0.248671 -2.029936
H 2.896983 0.729103 1.685189

H 1.278071 1.081602 2.315229
H 1.754702 -0.589808 1.988614

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -2.068685 -1.349604 -0.088564
C -2.944928 -0.267238 0.027172
C -2.419605 1.024368 0.105714
C -1.050736 1.236823 0.071018
C -0.136912 0.153002 -0.047117
C -0.699026 -1.151044 -0.124976
C 1.274202 0.381493 -0.080105
S 2.353254 -0.996047 0.140296
H -4.016246 -0.427560 0.055067
H -3.086654 1.874402 0.200669
H -0.677426 2.249369 0.153696
H -0.044277 -2.006227 -0.240098
H -2.461292 -2.358252 -0.157702
C 1.883818 1.751794 -0.115267
H 3.455822 -0.424062 -0.371576
H 1.992454 2.175421 0.892731
H 2.881059 1.733150 -0.561867
H 1.275722 2.442951 -0.702912

TRANSITION STATE

C 1.631533 1.745381 0.392370
C 1.119765 0.355135 0.049438
C 2.041701 -1.177784 2.137253
S 1.872495 -0.322801 -1.480074
H 1.358039 2.476441 -0.373758
H 1.230154 2.077736 1.354602
H 2.720794 1.740765 0.471101
H 1.531218 -0.376910 0.973302
H 2.047180 -2.182466 1.726063
H 1.294545 -0.994269 2.903144
H 3.022061 -0.754705 2.335877
H 3.152702 -0.223099 -1.076452
C -0.370769 0.166927 0.004843
C -0.911427 -1.112637 -0.208652
C -2.285582 -1.318084 -0.216214
C -3.157538 -0.249265 -0.010279
C -2.637879 1.023478 0.204328
C -1.259784 1.230301 0.213062
H -0.242415 -1.950020 -0.369778
H -2.677784 -2.315377 -0.381826
H -4.229788 -0.408765 -0.017225
H -3.305173 1.863514 0.362691
H -0.881570 2.231261 0.376546

Frequencies = -1317.08, 31.1659, 42.6295, 71.7952, 104.254, 133.33, 210.175, 234.475, 268.749, 288.982, 317.705, 382.583, 414.242, 438.516, 486.679, 519.004, 531.785, 606.606, 635.028, 674.489, 712.012, 779.194, 797.127, 853.913, 918.44, 934.194, 981.914, 1002.72, 1015.02, 1043.45, 1057.08, 1068.74, 1084.82, 1110.43, 1126.07, 1183.41, 1210.1, 1248.69, 1320.6, 1342.65, 1358.34, 1400.63, 1408.78, 1425.88, 1430.19, 1478.28, 1492.51, 1494.44, 1525.86, 1617.04, 1641.07, 2652.01, 3022.17, 3066.67, 3086.2, 3096.52, 3161.54, 3169.74, 3181.41, 3189.27, 3198.04, 3209.1, 3214.03
cos = 0, 0, .38, 0, 0
sin = 0, 0, -.02, 0, 0
barrier = 0.381
Substituted frequency = 31.17 (from HO analysis)
Reduced moment of inertia = 12.048

Reaction18

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

S 0.000000 0.000000 0.585090
C 0.000000 0.000000 -1.025528
H 0.000000 0.923638 -1.604133
H 0.000000 -0.923638 -1.604133

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.035528 1.056377 0.000000
S 0.035528 -0.507317 0.000000
H -0.781621 1.778818 0.000000

TRANSITION STATE

C 0.141352 0.708905 0.000000
S 1.409589 -0.254953 0.000000
C -2.423643 -0.218188 0.000000
H -1.063195 0.263710 0.000000
H 0.191266 1.800743 0.000000
H -2.849787 0.174719 0.919448
H -2.856084 0.191302 -0.909233
H -2.281873 -1.295525 -0.010225

Frequencies = -1568.91, 28.9235, 134.144, 200.194, 456.239, 531.501, 561.124, 1048.02,

1099.4, 1154.99, 1242.53, 1418.04, 1428.14, 1458.6, 3058.59, 3073.23, 3197.1, 3201.15
cos = 0, 0, .22, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.216
Substituted frequency = 28.92 (from HO analysis)
Reduced moment of inertia = 9.723

Reaction19

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.697236 0.123111 -0.000046
C 0.336006 -0.439010 -0.000051
S -1.150039 0.073332 0.000002
H 2.240478 -0.247620 0.876072
H 2.242086 -0.250258 -0.873981
H 1.718599 1.219956 -0.001550

TRANSITION STATE

C -2.460891 -0.582796 -0.000002
C 0.142707 0.266817 0.000001
S 1.332646 -0.805188 -0.000001
H -1.064145 -0.150309 0.000013
C 0.200455 1.754104 -0.000006
H -2.880529 -0.172344 0.914746
H -2.880797 -0.171515 -0.914253
H -2.344062 -1.662919 -0.000502
H 1.223703 2.133013 -0.000234
H -0.335286 2.139194 -0.875912
H -0.334845 2.139148 0.876194

Frequencies = -1499.3, 28.0088, 107.331, 126.894, 179.388, 311.448, 485.059, 498.513, 529.552, 833.353, 949.016, 1074.56, 1128.18, 1222.17, 1237.81, 1382.04, 1411.15, 1429.04, 1445.14, 1464.29, 1479.12, 3008.78, 3058, 3059.14, 3110.41, 3196.29, 3202.45
cos = 0, 0, .22, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.220
Substituted frequency = 28.01 (from HO analysis)
Reduced moment of inertia = 11.581

Reaction20

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 0.607073 0.000000
S 1.539936 0.089100 0.000000
H -0.239706 1.671448 0.000000
S -1.469763 -0.325069 0.000000
H -0.883060 -1.538389 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -0.092187 0.490785 -0.000091
S -1.568218 -0.080596 0.000022
S 1.468518 -0.165952 -0.000005
H 2.148326 1.000056 0.000283

TRANSITION STATE

C -2.583248 -0.688769 -0.000005
C 0.098819 -0.106341 0.000006
S 0.369553 1.603466 -0.000007
S 1.218354 -1.263107 0.000001
H -1.123108 -0.376000 0.000005
H -2.956758 -0.244538 0.918174
H -2.956867 -0.244045 -0.917900
H -2.531959 -1.773290 -0.000295
H -0.931242 1.962784 0.000097

Frequencies = -1358.37, 44.0337, 95.0525, 178.152, 258.409, 403.111, 446.64, 503.475, 513.466, 745.739, 949.485, 1103.77, 1168.96, 1178.45, 1395.69, 1426.71, 1430.51, 2615.11, 3064.07, 3207.21, 3212.19
cos = 0, 0, .51, 0, 0

sin = 0, 0, .01, 0, 0
barrier = 0.510
Substituted frequency = 44.03 (from HO analysis)
Reduced moment of inertia = 11.820

Reaction21

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 0.449465 0.000000
S -1.623646 0.295698 0.000000
H 0.443032 1.448356 0.000000
C 0.948150 -0.645188 0.000000
C 2.273801 -0.441563 0.000000
H 0.536627 -1.649548 0.000000
H 2.976058 -1.266614 0.000000
H 2.690923 0.560357 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -2.242465 -0.401880 -0.000098
C -1.186816 0.495149 0.000125
C 0.135291 0.202444 -0.000003
S 1.656401 -0.114385 -0.000011
H -1.401391 1.564074 -0.000160
H -3.259573 -0.037592 -0.000058
H -2.077517 -1.470599 0.000256

TRANSITION STATE

C -1.133855 2.232225 0.000031
H -0.295903 2.924101 -0.000293
C 0.243184 -0.131667 -0.000041
C -0.586018 -1.317141 0.000054
S 1.852324 -0.044503 -0.000008
H -0.428461 0.966794 -0.000067
H -1.720366 2.237445 0.915333
H -1.720905 2.237285 -0.914928
C -1.926246 -1.264867 -0.000037
H -0.073064 -2.276448 0.000193
H -2.524268 -2.168580 0.000019
H -2.456615 -0.319855 -0.000170

Frequencies = -1566.48, 61.2297, 97.3348, 109.898, 174.34, 243.783, 418.896, 484.524, 496.504, 536.331, 655.483, 899.944, 989.082, 1020.35, 1093.35, 1141.11, 1214.34, 1227.47, 1317.74, 1391.42, 1431.87, 1432.25, 1468.53, 1648.42, 3056.95, 3131.93, 3148.81, 3194.02, 3199.09, 3236.54
cos = 0, 0, .91, 0, 0
sin = 0, 0, .02, 0, 0
barrier = 0.904
Substituted frequency = 61.23 (from HO analysis)
Reduced moment of inertia = 11.769

Reaction22

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

S -1.498234 0.010007 0.000000
C 0.000000 0.656162 0.000000
C 1.202204 -0.081586 0.000000
C 2.246728 -0.685637 0.000000
H 3.157243 -1.234676 0.000000
H 0.120912 1.740921 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.000000 0.050530 0.000000
S -0.166266 1.601227 0.000000
C 0.108145 -1.255540 0.000000
C 0.316309 -2.477500 0.000000
H 0.113535 -3.524578 0.000000

TRANSITION STATE

C -1.862706 1.885108 0.000000
H -2.776260 1.298720 0.000000
C 0.017937 -0.119340 0.000000
C 1.325154 0.372594 0.000000
S -0.492073 -1.651977 0.000000
H -0.835042 0.796244 0.000000
H -1.649431 2.424138 -0.917977
H -1.649432 2.424138 0.917977
C 2.417886 0.890905 0.000000
H 3.393710 1.312786 0.000000

Frequencies = -1363.2, 26.6123, 86.2989, 146.011, 188.086, 330.846, 429.336, 507.145, 523.799,

547.255, 620.603, 721.95, 903.713, 1106.71, 1152.56, 1214.74, 1407.39, 1421.82, 1431.03, 2152.85, 3066.63, 3213.99, 3216.96, 3469.19
cos = 0, 0, .23, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.233
Substituted frequency = 26.61 (from HO analysis)
Reduced moment of inertia = 11.906

Reaction23

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 1.239640 -0.008781
S 0.000000 0.000000 1.193707
C 0.000000 -1.239640 -0.008781
C 0.000000 -0.712734 -1.269488
C 0.000000 0.712734 -1.269488
H 0.000000 -2.277239 0.286893
H 0.000000 -1.317289 -2.166933
H 0.000000 1.317289 -2.166933
H 0.000000 2.277239 0.286893

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.000000 1.186068 0.000000
S -1.214242 -0.065876 0.000000
C 0.018210 -1.249863 0.000000
C 1.285292 -0.775347 0.000000
C 1.261202 0.662188 0.000000
H -0.300993 2.222620 0.000000
H 2.157226 1.270041 0.000000
H 2.183420 -1.376926 0.000000

TRANSITION STATE

H 2.342623 1.906249 0.000000
C 1.597579 1.120527 0.000000
C 0.186819 1.365070 0.000000
H -0.257667 2.351839 0.000000
C -0.523709 0.203497 0.000000
H -1.947284 0.099633 0.000710
C -3.204378 0.061569 0.000136
H -3.530228 1.095453 -0.096232
H -3.480942 -0.549665 -0.856666
H -3.487758 -0.384403 0.951372
S 0.479806 -1.193443 0.000000
C 1.910186 -0.209317 0.000000
H 2.885379 -0.672100 0.000000

Frequencies = -1269.77, 17.6232, 77.6727, 80.4791, 392.197, 415.203, 466.898, 501.421, 552.558, 632.863, 692.625, 730.272, 812.334, 840.146, 905.592, 938.148, 1050.02, 1100.71, 1220.9, 1228.68, 1247.45, 1324.76, 1368.73, 1425.59, 1448.53, 1458.62, 1551.15, 3055.36, 3178.13, 3179.98, 3189.26, 3204.23, 3239.89
cos = .01, .01, .06, .01, .01
sin = 0, 0, 0, 0, 0
barrier = 0.074
Substituted frequency = 17.62 (from HO analysis)
Reduced moment of inertia = 11.442

Reaction24

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.000000 1.239640 -0.008781
S 0.000000 0.000000 1.193707
C 0.000000 -1.239640 -0.008781
C 0.000000 -0.712734 -1.269488
C 0.000000 0.712734 -1.269488
H 0.000000 -2.277239 0.286893
H 0.000000 -1.317289 -2.166933
H 0.000000 1.317289 -2.166933
H 0.000000 2.277239 0.286893

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -1.205550 -0.099406 0.000000
S 0.000000 1.141693 0.000000
C 1.300928 -0.029786 0.000000
C 0.752639 -1.259017 0.000000
C -0.656806 -1.355107 0.000000
H -2.250229 0.173699 0.000000
H -1.226316 -2.273435 0.000000
H 2.329277 0.292543 0.000000

TRANSITION STATE

C 1.177647 -1.264368 0.000000
S -0.469946 -1.785984 0.000000
C -1.047563 -0.143067 0.000000
C 0.000000 0.717738 0.000000
C 1.279211 0.100465 0.000000
H 1.971279 -1.996435 0.000000
H 2.220778 0.633446 0.000000
H -0.164728 2.105046 0.000000
H -2.108035 0.055366 0.000000
C -0.305912 3.382273 0.000000
H -1.380436 3.554679 0.000000
H 0.179992 3.732700 0.908293
H 0.179992 3.732700 -0.908293

Frequencies = -1452.71, 17.8061, 84.1683, 89.1217, 373.448, 440.38, 474.548, 519.678, 582.175, 617.455, 668.866, 757.028, 762.465, 822.666, 884.22, 884.767, 1078.85, 1101.97, 1200.51, 1203.64, 1256.68, 1333.92, 1377.21, 1433.86, 1447.06, 1456.21, 1526.18, 3054.66, 3178.71, 3180.75, 3201.42, 3237.32, 3242.9
cos = 0, 0, .09, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.090
Substituted frequency = 17.81 (from HO analysis)
Reduced moment of inertia = 11.333

Reaction03

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

TRANSITION STATE

C 0.029507 0.377383 -0.465626
S 1.353764 -0.749457 0.015164
H 0.038252 0.407240 -1.556942
C 0.039219 1.753732 0.168983
H -0.807797 2.344448 -0.193709
H -0.040838 1.688201 1.257972
H 0.960332 2.296020 -0.065486
H -1.104883 -0.166983 -0.197311
C -2.398784 -0.710499 0.087259
H -2.295097 -1.747204 -0.221269
H -2.516605 -0.573563 1.159309
H -3.092576 -0.129398 -0.514747
H 1.179345 -0.651140 1.345872

Frequencies = -1544.59, 43.9917, 106.334, 155.51, 218.413, 254.105, 314.88, 449.518, 532.563, 553.199, 673.158, 866.59, 896.935, 1017.54, 1083.65, 1124.34, 1139.18, 1300.61, 1385.63, 1406.5, 1410.46, 1438.38, 1444.07, 1486.98, 1492.1, 2650.54, 3016.44, 3059.07, 3074.89, 3079.56, 3094.77, 3193, 3198.81
cos = 0, 0, .37, 0, 0
sin = 0, 0, -.03, 0, 0
barrier = 0.37
Substituted frequency = 43.99 (from HO analysis)
Reduced moment of inertia = 11.616

Reaction25

REACTANT 1

H 1.773519 -0.850168 1.001666
S 1.791079 -0.046598 -0.076287
C 0.064735 0.568549 0.079912
C -1.010901 -0.507453 -0.065592
H -0.023859 1.310467 -0.718438
H -0.034256 1.102500 1.027480
H -0.865511 -1.031154 -1.014998
H -0.879508 -1.256840 0.722740
C -2.427915 0.073165 0.006912
H -2.602005 0.797179 -0.794875
H -2.602429 0.583217 0.959179
H -3.178736 -0.715203 -0.089553

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.128285 0.532035 0.407768
C -0.179115 0.748219 -0.284638
S -1.584944 -0.246464 -0.024218
H -0.222684 1.299719 -1.216806
H -1.330088 -0.591558 1.252618
H 0.954057 0.316908 1.469462
C 1.990514 -0.597783 -0.196806
H 1.696328 1.468858 0.373977
H 2.932559 -0.700821 0.349990
H 1.464245 -1.554486 -0.155977
H 2.226584 -0.390020 -1.243714

TRANSITION STATE

C 0.469694 2.455877 0.094029
C -0.139610 -0.149204 -0.404539
C 0.856152 -1.015717 0.349874
S -1.886880 -0.413650 -0.041757
H -0.037980 -0.229633 -1.489607
C 2.303462 -0.791819 -0.102821
H 0.768125 -0.812694 1.423891
H 0.585026 -2.069867 0.217101
H 0.146027 1.087666 -0.168928
H -0.488810 2.948709 -0.045146
H 0.831187 2.464038 1.119477
H 1.221376 2.722557 -0.644330
H -1.802263 -0.273079 1.293918
H 2.987590 -1.437090 0.454099
H 2.423688 -1.020054 -1.166119
H 2.617933 0.243029 0.054500

Frequencies = -1561.46, 61.0468, 93.0292, 111.64, 154.628, 215.848, 239.785, 262.439, 362.373, 450.183, 532.191, 550.994, 728.684, 788.03, 883.459, 916.04, 951.261, 1046.88, 1106.93, 1125.57, 1150.84, 1269.51, 1300.07, 1354.53, 1386.29, 1407.54, 1417.23, 1437.96, 1443.39, 1487.23, 1501.71, 1507.96, 2649.44, 3008.54, 3027.84, 3034.01, 3058.22, 3077.54, 3090.03, 3097.04, 3192, 3197.52
cos = 0, 0, .57, 0, 0
sin = 0, 0, -.08, 0, 0
barrier = 0.59
Substituted frequency = 61.05 (from HO analysis)
Reduced moment of inertia = 11.810

Reaction26

REACTANT 1

C 3.018848 -0.407916 -0.031024
C 1.794207 0.509738 0.030755
C 0.467556 -0.261066 -0.016142
C -0.750786 0.658456 0.055859
S -2.370638 -0.202143 -0.084224
H -2.260561 -0.935999 1.036994
H 3.030508 -1.108435 0.809538
H 3.948271 0.166608 0.002335
H 3.024716 -0.997338 -0.952863
H 1.828303 1.221207 -0.802967
H 1.833833 1.111117 0.946884
H 0.432336 -0.974898 0.815496
H 0.414148 -0.855670 -0.934041
H -0.753005 1.359996 -0.782708
H -0.747288 1.252422 0.972220

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.440059 -0.207481 -0.475525
C 0.498326 0.655928 0.397990
C -0.879977 0.828570 -0.151781
S -2.132150 -0.374322 -0.015550
H -1.072070 1.545706 -0.941396
H -1.725380 -0.931375 1.141413
H 0.447807 0.212360 1.401486
H 0.950201 1.647781 0.523931
C 2.842173 -0.342568 0.123732
H 0.991690 -1.197457 -0.607574
H 1.502886 0.237594 -1.474404
H 3.486944 -0.955992 -0.511252
H 3.321251 0.634880 0.237719
H 2.807584 -0.811043 1.112384

TRANSITION STATE

C -0.934955 2.533071 0.163810
C -0.644257 -0.101769 -0.450926
S -2.150872 -0.972264 0.026638
C 0.655206 -0.593788 0.165000
C 1.895733 0.129657 -0.377829
H -0.625871 -0.102590 -1.543471
H 0.608242 -0.471747 1.254739
H 0.753029 -1.672058 -0.015254
H -0.782968 1.147395 -0.157019
H -2.008452 2.673379 0.069428

H -0.560949 2.624530 1.180705
H -0.346562 3.069314 -0.576157
H -1.985898 -0.870337 1.358194
C 3.198510 -0.383949 0.242208
H 1.935337 0.005515 -1.466491
H 1.801757 1.205270 -0.194634
H 4.065954 0.142037 -0.164996
H 3.203454 -0.241765 1.327285
H 3.335462 -1.452051 0.047889

Frequencies = -1562.21, 49.5454, 69.5661, 79.8546, 114.413, 151.153, 177.83, 242.456, 245.001, 330.792, 370.646, 464.895, 533.544, 552.332, 735.845, 751.245, 849.074, 876.698, 914.002, 979.78, 1024.28, 1062.46, 1114.84, 1125.61, 1155.93, 1249.82, 1276.5, 1324.92, 1331.4, 1377.49, 1391.38, 1407.83, 1415.68, 1437.85, 1442.91, 1481.92, 1496.17, 1501.96, 1510.88, 2650.97, 2996.9, 3014.86, 3021.77, 3023.4, 3050.65, 3058.19, 3079.33, 3085.05, 3089.47, 3191.86, 3197.34
cos = 0, 0, .56, 0, 0
sin = 0, 0, -.09, 0, 0
barrier = 0.58
Substituted frequency = 49.55 (from HO analysis)
Reduced moment of inertia = 11.891

Reaction27

REACTANT 1

S -1.972545 0.016415 -0.013545
H -2.005394 -0.342637 -1.308776
C -0.310675 -0.681291 0.362724
H -0.224114 -0.592856 1.450039
H -0.330950 -1.747146 0.128488
C 0.881598 0.004915 -0.323218
C 2.162033 -0.800134 -0.049511
H 0.696616 -0.013241 -1.404923
C 1.045463 1.465348 0.111194
H 1.877659 1.936816 -0.418518
H 0.141960 2.043975 -0.089279
H 1.255995 1.528363 1.184739
H 3.018546 -0.354195 -0.562375
H 2.390915 -0.819608 1.021426
H 2.068968 -1.835148 -0.391223

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.852902 -0.008213 -0.297767
C -0.376808 -0.496323 0.411367
S -1.998581 -0.036958 -0.023919
H -0.302681 -0.869458 1.427599
H -1.788113 0.148516 -1.341374
H 0.634885 0.020574 -1.374555
C 1.242903 1.425073 0.130581
C 2.021516 -0.983242 -0.077277
H 2.114194 1.773683 -0.433118
H 0.421654 2.124768 -0.040005
H 1.494263 1.453448 1.195164
H 2.913639 -0.648503 -0.613943
H 2.277348 -1.047426 0.985324
H 1.769026 -1.988044 -0.423804

TRANSITION STATE

C -1.925985 2.055021 0.087210
C -0.279246 -0.054395 -0.412180
S -1.227729 -1.545172 -0.039696
C 1.048217 0.153550 0.315935
C 1.637910 1.529158 -0.035713
H -0.168797 -0.027218 -1.499944
H 0.840756 0.138387 1.394296
C 2.063497 -0.961020 0.012024
H -1.044294 0.958459 -0.167260
H -2.898153 1.610429 -0.108270
H -1.756344 2.314738 1.129442
H -1.639144 2.831867 -0.616677
H -1.316780 -1.354509 1.289767
H 2.578765 1.691302 0.497218
H 1.849046 1.599154 -1.108090
H 0.957820 2.342129 0.227039
H 2.987806 -0.800226 0.574710
H 1.668726 -1.944318 0.272378
H 2.317901 -0.971330 -1.053132

Frequencies = -1578.9, 54.9316, 69.3529, 109.563, 154.919, 214.957, 224.21, 229.028, 258.917, 338.411, 355.666, 426.409, 460.118, 537.131, 596.957, 724.539, 839.049, 889.362, 935.841, 943.228, 962.468, 987.302, 1116.76, 1124.32, 1162.17, 1185.09, 1270.14, 1334.73, 1364.33, 1383.9, 1397.95, 1403.47, 1420.25, 1438.77, 1441.6, 1490.6, 1492.24, 1504.12, 1513.53, 2649.25, 2995.08, 3019.21, 3024.52, 3057.86, 3070.38, 3077.11, 3085.22, 3102.6, 3109.46, 3191.33, 3197.53
cos = 0, 0, 1.07, 0, 0
sin = 0, 0, -.04, 0, 0
barrier = 1.08
Substituted frequency = 64.01 (from rotational profile)
Reduced moment of inertia = 11.817

Reaction28

REACTANT 1

S -2.100262 -0.077640 0.017187
H -2.147473 1.228142 -0.293714
C -0.464566 -0.448993 -0.744658
H -0.464717 -1.538454 -0.836145
H -0.468813 -0.044572 -1.759017
C 0.806384 0.006474 0.011371
C 2.013076 -0.447204 -0.836040
C 0.838159 1.537013 0.157730
C 0.881029 -0.653317 1.398188
H 1.792416 -0.346924 1.919718
H 0.024858 -0.372947 2.015424
H 0.894598 -1.744846 1.314964
H 2.951937 -0.161405 -0.353011
H 2.021747 -1.534003 -0.964488
H 1.996502 0.009613 -1.830445
H 1.777176 1.857426 0.618012
H 0.759550 2.031912 -0.816046
H 0.021928 1.894465 0.790211

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 0.783767 -0.006860 -0.009977
C -0.522498 -0.679041 -0.375179
S -2.123178 -0.088377 -0.019130
H -0.524047 -1.753974 -0.524519
H -1.890457 1.230461 -0.142068
C 0.821842 1.465097 -0.469295
C 1.009722 -0.068152 1.522203
C 1.915798 -0.779718 -0.719439
H 1.969102 0.389004 1.786188
H 0.218255 0.463262 2.056208
H 1.016843 -1.103048 1.874351
H 2.889431 -0.346020 -0.474160
H 1.927745 -1.828726 -0.409206
H 1.790709 -0.748590 -1.804961
H 1.800373 1.901475 -0.250189
H 0.644011 1.546694 -1.544792
H 0.077097 2.075538 0.049350

TRANSITION STATE

C -1.955392 2.129261 -0.000439
C -0.445031 -0.069585 -0.543350
S -1.436856 -1.506282 -0.077914
C 0.985361 0.091347 0.005430
C 1.553467 1.410371 -0.559121
H -0.454167 -0.056622 -1.636331
C 0.996334 0.150023 1.542618
C 1.870694 -1.079086 -0.472209
H -1.135379 0.988859 -0.246331
H -2.953360 1.715791 -0.120309
H -1.724362 2.443971 1.014271
H -1.678841 2.853657 -0.762104
H -1.525096 -1.252424 1.239528
H 2.589142 1.547883 -0.235528
H 1.543662 1.408029 -1.653409
H 0.977303 2.273805 -0.217681
H 2.896032 -0.949932 -0.111713
H 1.494671 -2.035085 -0.102589
H 1.902746 -1.128120 -1.564833
H 2.010573 0.335693 1.907082
H 0.354889 0.953080 1.916537
H 0.659281 -0.792052 1.982452

Frequencies = -1597.1, 42.7718, 61.4747, 107.574, 152.1, 206.203, 218.888, 248.924, 271.479, 295.292, 316.013, 326.248, 375.556, 408.857, 421.48, 490.455, 542.214, 598.124, 704.142, 778.428, 887.196, 913.857, 929.375, 941.426, 962.675, 983.753, 1044.19, 1068.66, 1123.25, 1209.47, 1224.56, 1259.11, 1314.14, 1379.07, 1396.46, 1400.04, 1405.32, 1430.03, 1439.58, 1443.42, 1481.68, 1490.74, 1491.98, 1505.31, 1510.82, 1523.01, 2664.02, 3019.33, 3022.62, 3029.07, 3058.19, 3072.99, 3079.28, 3085.36, 3089.6, 3092.72, 3098.04, 3103.75, 3191.87, 3196.08
cos = 0, 0, .63, 0, 0
sin = 0, 0, -.03, 0, 0
barrier = 0.63
Substituted frequency = 42.77 (from HO analysis)
Reduced moment of inertia = 11.821

Reaction08

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.748228 0.124075 0.039321
C 0.565049 -0.440481 -0.067799
S -1.053621 0.123840 -0.050080
H 2.653636 -0.427995 -0.197380
H 1.877846 1.151585 0.382815
H -1.553214 -0.806591 0.786707

TRANSITION STATE

C -2.433049 -0.642262 -0.028863
C 0.019880 0.443686 0.062839
S 1.397989 -0.634956 -0.067098
C 0.045721 1.767720 0.021699
H -0.878795 2.334697 -0.023247
H 0.973023 2.334435 0.033457
H -1.171346 -0.130358 0.041277
H 0.973089 -1.555549 0.818181
H -3.077888 0.219556 -0.181597
H -2.398887 -1.321722 -0.876828
H -2.582330 -1.136628 0.928271

Frequencies = -1601.42, 22.737, 104.695, 161.526, 234.861, 303.59, 464.924, 512.904, 550.534, 653.173, 722.942, 907.725, 952.511, 1078.51, 1156.69, 1237.84, 1376.76, 1414.95, 1436.48, 1445.11, 1658.74, 2642.93, 3058.28, 3110.1, 3189.46, 3190.7, 3193.57
cos = 0, 0, .30, 0, 0
sin = 0, 0, -.03, 0, 0
barrier = 0.30
Substituted frequency = 22.74 (from HO analysis)
Reduced moment of inertia = 11.482

Reaction29

REACTANT 1

C -1.841625 -0.679452 -0.029926
C -1.169855 0.659543 0.008974
C 0.142333 0.897732 0.005206
S 1.390455 -0.372721 0.041517
H -1.821195 1.529084 0.056084
H 0.522044 1.911381 0.048240
H 2.352095 0.344319 -0.562214
H -2.663917 -0.678867 -0.752117
H -1.146132 -1.475672 -0.304044
H -2.275298 -0.933645 0.944263

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 1.042505 0.388531 0.106672
C -0.062162 -0.327698 0.031404
S -1.730144 0.045715 -0.090798
H 0.966338 1.459667 0.318688
H -2.167265 -0.720783 0.928470
C 2.434167 -0.160183 -0.055594
H 3.030594 0.026441 0.844079
H 2.417333 -1.233826 -0.245932
H 2.948243 0.333161 -0.887424

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C 2.720536 -0.917077 -0.028083
C 0.158286 -0.123973 0.062371
S -0.156148 1.600148 -0.071931
C -0.723591 -1.116997 0.018417
H -0.317266 -2.127699 -0.010714
C -2.222970 -1.009230 0.006043
H 1.430336 -0.475734 0.042513
H 0.691163 1.998372 0.895176
H 2.647529 -1.997174 -0.129444
H 3.125671 -0.419906 -0.905928
H 3.172022 -0.595748 0.907783
H -2.556019 0.012581 0.193625
H -2.628250 -1.328905 -0.960818
H -2.660385 -1.664488 0.766219

Frequencies = -1601.81, 25.648, 94.9106, 114.755, 138.21, 193.676, 222.335, 364.315, 375.03, 500.269, 538.187, 570.042, 770.796, 813.874, 930.231, 983.581, 1055.66, 1108.5, 1153.85, 1227.35, 1306.43, 1393.11, 1407.04, 1435.65, 1448.3, 1484.49, 1486.28, 1683.8, 2645.3, 3015.37, 3057.35, 3061.22, 3101.56, 3117.99, 3187.83, 3192.09
cos = 0, 0, .34, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.34
Substituted frequency = 25.65 (from HO analysis)
Reduced moment of inertia = 11.667

Reaction30

REACTANT 1

C 2.182053 -0.786509 0.026848
C 0.874179 -0.035006 -0.016668
C 0.984874 1.466181 -0.028890
C -0.281815 -0.708092 -0.017357
S -1.952639 -0.102300 -0.014374
H -0.278247 -1.793126 -0.018483
H -1.718608 1.139000 0.438754
H 2.800464 -0.543664 -0.845238
H 2.764633 -0.508445 0.913458
H 2.031920 -1.867521 0.048938
H 1.834603 1.781192 -0.642190
H 0.091629 1.949368 -0.428780
H 1.160085 1.860556 0.979932

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.871735 -0.056722 0.023260
C -0.331656 -0.604789 0.080897
S -1.940679 -0.039454 -0.099645
H -2.439150 -0.512595 1.060542
C 2.107731 -0.926073 -0.036259
H 2.761717 -0.722650 0.819460
H 1.852155 -1.985569 -0.035554
H 2.686936 -0.707188 -0.940557
C 1.118290 1.437977 0.031545
H 0.192795 2.002475 0.143739
H 1.794813 1.706354 0.850360
H 1.604997 1.748081 -0.900334

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C 2.141571 -0.764640 0.020118
C 1.023031 0.251094 0.026170
C -0.271433 -0.070148 0.063657
S -0.982251 -1.672208 -0.083580
C 1.471976 1.692573 -0.017197
H -1.166648 0.910042 0.044897
H -1.826200 -1.583398 0.962164
H 2.887272 -0.509866 0.781035
H 1.778763 -1.774576 0.209015
H 2.659467 -0.759362 -0.946235
H 2.131053 1.912247 0.830382
H 2.053334 1.886035 -0.926176
H 0.634353 2.388493 0.006535
C -2.113956 1.894250 -0.015639
H -1.920104 2.433020 -0.940064
H -3.049550 1.339615 -0.027498
H -1.972861 2.494312 0.880567

Frequencies = -1635.72, 57.6065, 80.6827, 112.082, 137.662, 161.876, 209.655, 224.779, 240.075, 350.127, 381.996, 435.541, 488.179, 526.218, 545.222, 786.666, 871.595, 944.891, 963.346, 985.278, 1096.56, 1103.48, 1150.17, 1213.49, 1234.72, 1388.75, 1397.99, 1413.71, 1437.75, 1451.67, 1477.49, 1480.75, 1490.32, 1496.17, 1682.39, 2637.33, 3009.71, 3015, 3053.04, 3054.84, 3057.2, 3122.38, 3128.97, 3185.39, 3187.3
cos = .01, .01, .69, .01, .01
sin = 0, 0, -.05, 0, 0
barrier = 0.72
Substituted frequency = 57.61 (from HO analysis)
Reduced moment of inertia = 11.752

Reaction02

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

TRANSITION STATE

H -1.256196 -0.851797 1.121689
S -1.382204 -0.279868 -0.088506
C -0.020806 0.878466 0.058632
H 1.132195 0.282804 0.023470

C 2.411321 -0.316868 -0.023909
H -0.032659 1.455793 0.982056
H -0.024145 1.527051 -0.816491
H 2.536070 -0.763446 0.959527
H 2.315743 -1.039249 -0.830457
H 3.101162 0.497146 -0.232029

Frequencies = -1603.18, 35.2783, 117.566, 199.177, 348.117, 457.516, 559.751, 644.662, 735.595, 853.152, 1054.15, 1120.55, 1127.77, 1392.36, 1398.39, 1422.07, 1439.9, 1444.3, 2657.47, 3057.54, 3075.57, 3159.3, 3191.67, 3195.53
cos = .01, .01, .31, .01, .01
sin = 0, 0, .03, 0, 0
barrier = 0.33
Substituted frequency = 35.28 (from HO analysis)
Reduced moment of inertia = 10.669

Reaction31

REACTANT 1

S 0.000000 0.000000 0.659855
C 0.000000 1.391958 -0.513348
C 0.000000 -1.391958 -0.513348
H -0.894042 1.378637 -1.139879
H 0.000000 2.306474 0.081008
H 0.894042 1.378637 -1.139879
H 0.894042 -1.378637 -1.139879
H 0.000000 -2.306474 0.081008
H -0.894042 -1.378637 -1.139879

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 1.351111 0.579062 0.041325
H 1.158163 1.597234 -0.268138
H 2.364842 0.212777 0.116372
S 0.111021 -0.605863 -0.018286
C -1.387724 0.426812 0.019945
H -1.410991 1.094962 -0.842141
H -1.426565 1.002162 0.945140
H -2.242110 -0.248576 -0.026286

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C -2.632733 0.467548 -0.204507
C -0.412029 -0.911982 0.558986
S 1.047843 -0.496059 -0.372261
C 1.362055 1.189228 0.240929
H -1.442978 -0.229766 0.181640
H -0.313216 -0.726245 1.630263
H -0.677813 -1.949970 0.359320
H -2.594083 1.410523 0.335383
H -2.520258 0.564549 -1.281387
H -3.447488 -0.183609 0.102046
H 2.265843 1.544037 -0.255400
H 0.533907 1.854182 -0.008058
H 1.526831 1.184472 1.319920

Frequencies = -1575.36, 38.9483, 71.0142, 115.686, 179.398, 273.495, 348.257, 453.31, 556.49, 658.996, 689.382, 759.114, 939.798, 966.965, 1049.78, 1074.95, 1117.76, 1354.91, 1393.06, 1402.63, 1416.72, 1438.38, 1445.03, 1468.6, 1483.83, 3035.88, 3054.5, 3056.53, 3114.41, 3130.97, 3142.85, 3190.9, 3194.07
cos = 0, 0, .27, 0, 0
sin = 0, 0, .04, 0, 0
barrier = 0.27
Substituted frequency = 38.95 (from HO analysis)
Reduced moment of inertia = 11.511

Reaction32

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -1.283939 0.994588 0.000000
S -0.676956 -0.716065 0.000000
C 1.067705 -0.500304 0.000000
C 1.776367 0.629229 0.000000
H -0.953297 1.523887 -0.894920
H -2.372236 0.932347 -0.000423
H -0.953885 1.523958 0.894961
H 1.566351 -1.465205 -0.000190
H 2.858945 0.588106 0.000000
H 1.324620 1.612872 0.000188

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.786404 0.574854 -0.067317
C 1.021357 -0.509115 0.066061
S -0.734079 -0.615242 -0.034003
C -1.289561 0.996623 0.033779
H 2.861821 0.496353 0.037404
H 1.379159 1.551160 -0.297388
H 1.451258 -1.485413 0.265195
H -2.328537 1.152420 -0.216759
H -0.727637 1.755192 0.560460

TRANSITION STATE

C -2.678371 1.153042 -0.202066
C -1.093123 -0.948012 0.471552
S 0.481503 -0.935441 -0.367762
C 1.315673 0.374658 0.472359
H -1.830022 0.061647 0.134289
H -1.000825 -0.898038 1.557666
H -1.649632 -1.831820 0.160837
H -2.013460 2.011940 -0.161775
H -3.027776 0.909309 -1.202113
H -3.458086 1.154202 0.555551
C 2.269150 1.119613 -0.084245
H 1.039829 0.495931 1.516336
H 2.808064 1.852654 0.504398
H 2.547898 1.015433 -1.126591

Frequencies = -1586.56, 40.4882, 48.8563, 77.639, 125.35, 227.204, 340.398, 400.659, 457.713, 560.659, 602.587, 655.375, 702.016, 753.632, 914.268, 982.526, 1005.1, 1053.2, 1070.05, 1122.39, 1295.71, 1392.08, 1402.74, 1413.51, 1418.2, 1440.27, 1443.54, 1645.85, 3057.89, 3061.11, 3134.87, 3147.37, 3148.75, 3193.7, 3195.54, 3224.94
cos = .01, .01, .21, 0, .01
sin = 0, 0, -.06, 0, 0
barrier = 0.24
Substituted frequency = 40.49 (from HO analysis)
Reduced moment of inertia = 11.763

Reaction33

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

S -0.485847 -0.707246 0.014367
S 1.370399 0.244028 -0.087618
C -1.663975 0.690512 -0.004658
H 1.577787 0.434367 1.232037
H -2.657149 0.236046 -0.047719
H -1.578431 1.287677 0.902614
H -1.511186 1.310313 -0.886956

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

S 1.366695 0.189887 -0.061734
S -0.597305 -0.632772 -0.013053
H 1.446062 0.516028 1.243790
C -1.634314 0.719663 -0.005987
H -1.397118 1.610059 -0.571634
H -2.553298 0.642093 0.560352

TRANSITION STATE

C -2.694817 -0.859184 -0.192281
H -2.785973 -0.704327 -1.264347
C -0.898261 1.009848 0.582606
S 0.615095 0.949973 -0.365010
S 1.383170 -0.954187 0.058566
H 2.093390 -0.634294 1.159882
H -1.393323 1.956753 0.356699
H -0.757169 0.864856 1.653194
H -1.741023 0.095047 0.197037
H -3.588153 -0.607585 0.373846
H -2.241524 -1.807007 0.084836

Frequencies = -1611.3, 42.8546, 56.7402, 112.805, 243.327, 288.145, 349.285, 457.73, 478.73, 569.728, 669.502, 724.379, 873.162, 1004.68, 1053.96, 1133.22, 1377.25, 1394.23, 1406.17, 1436.74, 1443.52, 2615.12, 3057.93, 3059.49, 3145.32, 3194.68, 3199.75
cos = 0, 0, .46, 0, 0
sin = 0, 0, -.05, 0, 0
barrier = 0.46
Substituted frequency = 42.85 (from HO analysis)
Reduced moment of inertia = 11.738

Reaction03

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 0.000000 0.000000 0.000000

H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

TRANSITION STATE

C 0.029507 0.377383 -0.465626
S 1.353764 -0.749457 0.015164
H 0.038252 0.407240 -1.556942
C 0.039219 1.753732 0.168983
H -0.807797 2.344448 -0.193709
H -0.040838 1.688201 1.257972
H 0.960332 2.296020 -0.065486
H -1.104883 -0.166983 -0.197311
C -2.398784 -0.710499 0.087259
H -2.295097 -1.747204 -0.221269
H -2.516605 -0.573563 1.159309
H -3.092576 -0.129398 -0.514747
H 1.179345 -0.651140 1.345872

Frequencies = -1544.59, 43.9917, 106.334, 155.51, 218.413, 254.105, 314.88, 449.518, 532.563, 553.199, 673.158, 866.59, 896.935, 1017.54, 1083.65, 1124.34, 1139.18, 1300.61, 1385.63, 1406.5, 1410.46, 1438.38, 1444.07, 1486.98, 1492.1, 2650.54, 3016.44, 3059.07, 3074.89, 3079.56, 3094.77, 3193, 3198.81
cos = 0, 0, .37, 0, 0
sin = 0, 0, -.03, 0, 0
barrier = 0.37
Substituted frequency = 43.99 (from HO analysis)
Reduced moment of inertia = 11.616

Reaction34

REACTANT 1

C -0.231045 -1.003023 0.000000
S 0.000000 0.815120 0.000000
C 1.819011 0.898786 0.000000
H 0.258801 -1.416127 0.885912
C -1.718608 -1.346806 0.000000
H 0.258801 -1.416127 -0.885912
H 2.235252 0.430102 -0.893849
H 2.086858 1.956027 0.000000
H 2.235252 0.430102 0.893849
H -1.854919 -2.431670 0.000000
H -2.218096 -0.943987 0.884465
H -2.218096 -0.943987 -0.884465

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

S 0.491290 -0.615357 0.032517
C 1.954305 0.465737 -0.049597
H 1.940928 1.051893 -0.968648
H 1.992892 1.124962 0.818778
H 2.829839 -0.183737 -0.044297
C -0.793793 0.545786 0.007098
C -2.207643 0.067765 -0.042449
H -0.565615 1.545712 0.359930
H -2.601062 -0.209490 0.947814
H -2.861949 0.851010 -0.437189
H -2.312886 -0.810372 -0.686970

TRANSITION STATE

C -1.929197 1.768120 -0.197675
C -0.480203 -0.449508 0.463629
S 1.079872 -0.486540 -0.424416
C -1.377934 -1.621423 0.111937
H -2.343164 -1.518483 0.615316
H -0.313589 -0.347811 1.539491
H -1.564323 -1.668811 -0.964444
H -0.938708 -2.575675 0.419725
H -1.119080 0.615639 0.147314
H -1.548177 2.572605 0.426326
H -1.729756 1.891715 -1.258977
H -2.948810 1.472069 0.035056
C 1.931882 0.924921 0.348238
H 2.919687 0.987125 -0.109358
H 1.393518 1.854843 0.161127
H 2.047163 0.768769 1.422306

Frequencies = -1515.48, 22.8614, 63.1181, 101.635, 149.232, 167.705, 204.124, 223.557, 345.937, 453.711, 522.051, 555.275, 686.943,

720.855, 894.577, 969.488, 970.644, 1018.48, 1089.79, 1097.3, 1118.24, 1278.18, 1355.21, 1384.88, 1409.79, 1413.51, 1436.59, 1446.82, 1468.23, 1483.15, 1489.47, 1498.4, 3020.45, 3036.61, 3052.25, 3057.85, 3078.89, 3093, 3115.09, 3130.74, 3192.53, 3195.77
cos = 0, 0, .20, 0, 0
sin = 0, 0, .05, 0, 0
barrier = 0.21
Substituted frequency = 22.86 (from HO analysis)
Reduced moment of inertia = 11.771

Reaction35

REACTANT 1

C 1.985948 -0.872770 -0.235725
C 1.368231 0.305722 0.504153
S -0.181554 0.964366 -0.238774
S -1.589288 -0.529895 0.149761
H -1.428904 -1.270778 -0.965689
H 2.030074 1.178233 0.483516
H 1.166774 0.069747 1.550244
H 2.922816 -1.171323 0.245067
H 1.317681 -1.736845 -0.223246
H 2.199944 -0.618286 -1.276257

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -1.927548 -0.965269 0.120293
C -1.415836 0.376861 -0.274839
S 0.102161 1.019651 0.156664
H -1.985975 0.992402 -0.963681
S 1.561604 -0.551676 -0.149773
H -1.583608 -1.746165 -0.571729
H -1.585099 -1.249793 1.118748
H -3.020938 -0.978318 0.107102
H 1.615671 -0.975273 1.126595

TRANSITION STATE

C 1.131362 -1.492436 0.962614
C 0.951804 -0.742597 -0.339939
S -0.726945 -0.482579 -0.939379
S -1.616382 0.739920 0.515115
H -2.118383 -0.225463 1.311063
H 1.475424 -1.199895 -1.185182
H 1.532952 0.404380 -0.228880
H 2.194672 -1.575466 1.206800
H 0.640172 -0.969932 1.787157
H 0.715559 -2.503570 0.903721
C 2.241683 1.631163 -0.089932
H 2.076691 2.117898 -1.047446
H 1.754669 2.118497 0.750074
H 3.272381 1.339322 0.094458

Frequencies = -1564.73, 48.7321, 57.3176, 98.2795, 144.259, 182.72, 244.236, 307.952, 358.583, 448.653, 475.557, 537.306, 574.266, 659.529, 868.119, 875.949, 998.066, 1074.9, 1090.65, 1126.3, 1280.96, 1380.81, 1392.38, 1406.61, 1436.74, 1441, 1484.53, 1493.8, 2628.53, 3017.29, 3060.28, 3060.8, 3077.51, 3093.74, 3196.99, 3201.68
cos = 0, 0, .45, 0, 0
sin = 0, 0, -.04, 0, 0
barrier = 0.45
Substituted frequency = 48.73 (from HO analysis)
Reduced moment of inertia = 11.861

Reaction36

REACTANT 1

H -2.633731 0.644458 1.000327
C -2.240780 -0.353982 0.814496
S -1.153801 -0.349873 -0.658783
S 0.299969 1.055778 -0.171815
C 1.583601 0.082543 0.724715
C 2.341466 -0.916019 -0.140178
H -3.064465 -1.031175 0.574919
H -1.715034 -0.726770 1.692921
H 2.250777 0.859954 1.111723
H 1.113135 -0.399091 1.583898
H 3.099101 -1.435406 0.455513
H 1.664188 -1.666984 -0.552243
H 2.841616 -0.414711 -0.971689

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C -2.125886 1.096488 -0.256417
C -1.633978 -0.063121 0.540861
S -0.374353 -1.136637 0.076366
S 1.193002 0.074197 -0.704210
C 1.979499 0.715065 0.818316
H 2.380698 -0.100791 1.418154
H -2.076765 -0.284466 1.506935
H -3.221875 1.117688 -0.264563

H -1.796306 2.054434 0.168625
H -1.769090 1.057355 -1.286700
H 2.796422 1.360518 0.486641
H 1.270733 1.303704 1.399857

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C -2.793387 -1.244722 -0.642801
C -1.269959 0.735655 0.417604
S 0.163021 0.032600 1.257788
S 1.268132 -0.903501 -0.245537
C 2.507894 0.360965 -0.713357
C -1.035899 1.745885 -0.685308
H 2.041638 1.221449 -1.190597
H 3.079034 0.673441 0.159597
H 3.175873 -0.132701 -1.423723
H -1.969723 -0.229270 -0.074653
H -1.992611 2.082605 -1.095996
H -0.461390 1.303557 -1.502655
H -0.494732 2.624755 -0.319666
H -1.904641 1.110271 1.226700
H -2.202348 -1.622310 -1.472611
H -2.913222 -1.947865 0.177061
H -3.708226 -0.736209 -0.936296

Frequencies = -1563.44, 36.5835, 45.4746, 78.4968, 106.385, 127.934, 160.978, 209.378, 229.355, 257.894, 358.695, 449.379, 475.223, 535.753, 571.214, 658.266, 673.617, 873.047, 970.389, 973.277, 999.445, 1073.94, 1092.63, 1124.02, 1281.33, 1348.5, 1383.11, 1394.86, 1403.96, 1437.22, 1440.89, 1458.8, 1479.42, 1485.87, 1498.3, 3016.71, 3039.86, 3059.05, 3060.36, 3076.11, 3097, 3123.52, 3143.52, 3196.28, 3200.72
cos = 0, 0, .46, 0, -.01
sin = 0, 0, .07, 0, 0
barrier = 0.47
Substituted frequency = 36.58 (from HO analysis)
Reduced moment of inertia = 11.883

Reaction37

REACTANT 1

S -0.810617 0.652147 -0.588754
S 0.810617 -0.652147 -0.588754
C 0.375876 -1.901758 0.695612
C -0.375876 1.901758 0.695612
H -1.296877 2.487285 0.785856
H -0.226139 1.383068 1.644423
C 0.810617 2.788583 0.341431
H 0.992971 3.515519 1.139527
H 1.716960 2.192851 0.214861
H 0.628897 3.334623 -0.586855
H 1.296877 -2.487285 0.785856
H 0.226139 -1.383068 1.644423
C -0.810617 -2.788583 0.341431
H -0.992971 -3.515519 1.139527
H -1.716960 -2.192851 0.214861
H -0.628897 -3.334623 -0.586855

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C -2.708377 0.443647 0.682918
C -1.706675 -0.698497 0.572017
S -0.598366 -0.609603 -0.897405
S 0.669395 1.028240 -0.427045
C 1.849176 0.415163 0.670383
C 2.630298 -0.839328 0.477184
H -2.211982 -1.661385 0.445355
H -1.075652 -0.774740 1.459461
H -3.342234 0.306370 1.565019
H -2.196714 1.403205 0.782184
H -3.350963 0.489957 -0.198879
H 2.120057 1.117530 1.452021
H 2.954253 -1.251769 1.437144
H 2.044023 -1.597821 -0.046438
H 3.536216 -0.655433 -0.119677

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C -3.306159 -1.099290 -0.456503
C -1.589967 0.825818 0.390083
S -0.174535 0.073805 1.218713
S 0.770056 -1.060554 -0.259129
C 2.111936 0.038329 -0.886051
C 3.221019 0.318901 0.119880
C -1.337113 1.736387 -0.792217
H 2.493737 -0.518935 -1.748125
H 1.663369 0.958942 -1.261094
H 3.996495 0.942819 -0.336297
H 2.832174 0.849638 0.991436
H 3.683435 -0.608971 0.463418
H -2.381938 -0.114814 0.000299
H -2.285937 2.114330 -1.185068
H -0.718273 2.596134 -0.514558

H -0.835144 1.197539 -1.599186
H -2.155844 1.302969 1.196232
H -3.522500 -1.669491 0.442983
H -4.150595 -0.536045 -0.845543
H -2.745622 -1.647005 -1.208989

Frequencies = -1564.52, 43.3954, 52.3051, 55.987, 86.7507, 113.04, 141.728, 187.354, 209.004, 251.542, 273.315, 353.642, 360.424, 449.485, 475.397, 535.999, 572.242, 622.547, 657.484, 768.589, 873.929, 977.255, 999.814, 1049.23, 1069.43, 1075.38, 1092.21, 1124.21, 1273.02, 1280.1, 1295.95, 1382.28, 1394.34, 1403.62, 1412.82, 1437.58, 1441.2, 1464.16, 1486.25, 1491.27, 1497.8, 1503.93, 3015.15, 3026.75, 3037.72, 3058.68, 3060.33, 3074.73, 3088.18, 3094.19, 3096.7, 3116, 3196.03, 3200.89
cos = 0, 0, .49, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.50
Substituted frequency = 52.31 (from HO analysis)
Reduced moment of inertia = 11.894

Reaction38

REACTANT 1

C 2.132184 0.943494 0.000007
C 1.680176 -0.311472 0.000054
S 0.023968 -0.901113 -0.000002
C -0.958439 0.641241 -0.000013
C -2.449122 0.308246 -0.000003
H 2.375693 -1.145951 -0.000081
H 3.199070 1.132209 -0.000150
H 1.482755 1.809196 0.000046
H -0.688225 1.219770 0.886472
H -0.688083 1.219623 -0.886556
H -3.035596 1.230752 -0.000212
H -2.728917 -0.268635 -0.884621
H -2.728964 -0.268209 0.884870

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 2.079677 0.988653 -0.093390
H 3.135972 1.222689 -0.036069
C 1.668622 -0.274457 0.020954
H 1.395514 1.810652 -0.260792
S 0.015746 -0.888200 -0.011186
H 2.373852 -1.087971 0.158191
C -0.979301 0.505865 0.177063
C -2.444415 0.408755 -0.096171
H -0.583336 1.318369 0.775377
H -2.839531 1.383194 -0.401137
H -2.661579 -0.305029 -0.895157
H -3.020318 0.096397 0.787825

TRANSITION STATE

C -1.628784 2.241099 -0.195053
C -1.005333 -0.328663 0.452286
C -2.203681 -1.170946 0.057764
S 0.501557 -0.842514 -0.388505
C 1.722250 0.085976 0.486609
H -3.108536 -0.770465 0.522857
H -0.846259 -0.289910 1.532796
H -2.355001 -1.165947 -1.025125
H -2.092518 -2.211955 0.377354
H -1.267779 0.886647 0.133302
H -0.673837 2.759279 -0.177515
H -2.071604 2.157116 -1.184161
H -2.323009 2.550517 0.582133
C 2.865323 0.501179 -0.056565
H 1.506984 0.246147 1.539605
H 3.617329 0.990311 0.551522
H 3.090664 0.356623 -1.106933

Frequencies = -1532.65, 46.4068, 52.3602, 71.1132, 103.208, 157.901, 171.936, 221.16, 333.212, 388.146, 453.525, 531.203, 560.403, 607.195, 706.044, 716.264, 891.407, 914.843, 983.912, 1015.69, 1041.31, 1085.85, 1098.78, 1121.64, 1271.83, 1302.8, 1382.77, 1411.5, 1415.19, 1418.86, 1437.21, 1448.94, 1489.34, 1497.89, 1646.29, 3020.92, 3058.88, 3060.85, 3080.36, 3094.14, 3134.67, 3147.66, 3194.13, 3198.13, 3224.44
cos = .01, .01, .36, 0, .01
sin = 0, 0, -.05, 0, 0
barrier = 0.38
Substituted frequency = 52.36 (from HO analysis)
Reduced moment of inertia = 11.876

Reaction10

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935

C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000
H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

TRANSITION STATE

C -1.225825 2.340702 -0.086024
C 0.068192 -0.032876 0.392612
S -1.065385 -1.379636 -0.072050
C 1.316870 -0.060877 -0.393679
C 2.538325 0.104476 0.120983
H -2.166237 -0.870538 0.510057
H -0.527086 1.038265 0.145249
H 0.243079 -0.002953 1.469047
H 1.201590 -0.190278 -1.467765
H 3.419017 0.120175 -0.510243
H 2.696329 0.228126 1.187735
H -1.958117 2.393624 0.714148
H -0.412258 3.056238 -0.018145
H -1.635526 2.192969 -1.080638

Frequencies = -1374.01, 45.8209, 79.2285, 123.012, 157.621, 187.841, 258.837, 396.587, 463.65, 503.858, 550.753, 663.991, 766.503, 892.059, 936.01, 958.83, 1017.37, 1029.67, 1104.09, 1155.06, 1238.56, 1319.61, 1340.79, 1415.33, 1425.62, 1435.33, 1457.46, 1672.05, 2657.48, 3066.22, 3084.14, 3129.4, 3136.15, 3210.6, 3214.39, 3217.62
cos = 0, 0, .54, 0, 0
sin = 0, 0, -.02, 0, 0
barrier = 0.54
Substituted frequency = 45.82 (from HO analysis)
Reduced moment of inertia = 11.909

Reaction39

REACTANT 1

C -2.453050 1.126711 0.053773
C -1.882589 -0.009576 -0.340277
C -0.978382 -0.839160 0.514148
S 0.730881 -1.001416 -0.171795
C 1.292008 0.672015 -0.083708
H -1.324645 -1.875540 0.560096
H -0.917036 -0.455817 1.533920
H -2.051677 -0.379960 -1.348404
H -3.102921 1.692713 -0.603709
H -2.298059 1.525315 1.051882
C 2.566185 1.011495 0.101878
H 0.525558 1.420017 -0.263679
H 2.868593 2.051624 0.060127
H 3.341056 0.275397 0.283599

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 2.164166 1.329800 -0.172565
C 2.094214 0.013339 0.021993
S 0.655699 -1.010378 0.037039
C -0.656681 0.105770 0.242923
C -1.943994 -0.172714 -0.223615
C -3.050765 0.594914 0.036744
H 3.122400 1.833764 -0.131621
H 1.292786 1.935896 -0.386340
H 2.985801 -0.577776 0.205674
H -0.455639 0.984525 0.846794
H -2.069594 -1.060013 -0.840221
H -4.020422 0.333483 -0.366084
H -2.988149 1.489522 0.646303

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C 0.406530 2.657935 -0.203076
C 0.778043 -0.024913 0.292077
C 2.056468 -0.441925 -0.320543
C 3.184561 -0.661855 0.358455
S -0.637586 -0.932580 -0.385992
C -1.966323 -0.210907 0.526947
H 0.597243 1.184136 0.037710
H 0.793208 -0.076410 1.383354

H 2.063485 -0.525974 -1.405318
H 4.107404 -0.918183 -0.148462
H 3.222134 -0.592260 1.441047
H -0.658955 2.795064 -0.048382
H 1.052496 3.118438 0.538277
H 0.740822 2.752746 -1.231876
C -3.211677 -0.111317 0.064628
H -1.717502 0.088437 1.541294
H -4.007756 0.253317 0.703282
H -3.476805 -0.400143 -0.945983

Frequencies = -1350.91, 19.9049, 46.7414, 68.0974, 80.1725, 110.414, 158.594, 164.469, 294.443, 354.93, 424.067, 462.137, 503.797, 551.465, 606.715, 666.616, 713.178, 793.073, 915.806, 934.745, 955.212, 983.566, 990.469, 1026.22, 1046.4, 1098.95, 1144.92, 1230.31, 1298.7, 1322.67, 1343.73, 1416.47, 1418.61, 1425.38, 1438.77, 1457.01, 1645.34, 1675.96, 3066.93, 3067.1, 3128.66, 3134.33, 3135.02, 3147.3, 3211.28, 3216.18, 3217.34, 3223.99
cos = .01, .01, .39, .01, .01
sin = 0, 0, -.03, 0, 0
barrier = 0.41
Substituted frequency = 19.90 (from HO analysis)
Reduced moment of inertia = 12.029

Reaction40

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

PRODUCT 1

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

PRODUCT 2

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

TRANSITION STATE

C -1.898751 0.627707 0.418190
C 0.665101 0.409354 -0.454469
C 1.402626 1.650950 0.002654
S 1.347277 -1.178647 0.059355
H 0.541293 0.352871 -1.537599
H 0.898020 2.549463 -0.366427
H 1.436698 1.711927 1.094605
H 2.434488 1.664293 -0.362911
H -0.576132 0.504927 -0.019107
C -2.678580 -0.492720 -0.225908
H -1.787676 0.555361 1.500651
H -2.177808 1.634552 0.106351
H 1.400013 -0.917518 1.378607
H -3.725349 -0.499152 0.106089
H -2.688768 -0.401052 -1.316057
H -2.253590 -1.469081 0.023323

Frequencies = -1660.57, 26.5491, 77.3941, 127.251, 185.207, 192.646, 216.764, 253.574, 329.144, 462.265, 565.461, 673.083, 824.946, 871.327, 888.739, 909.698, 1014.82, 1041.33, 1084.37, 1137.03, 1158.31, 1225.09, 1302.02, 1403.45, 1406.36, 1412.74, 1436.22, 1464.04, 1486.43, 1491.56, 1492.52, 1493.75, 2650.85, 2993.99, 3013.14, 3051.04, 3066.21, 3071.07, 3076.54, 3082.49, 3093.85, 3139.54
cos = 1.07, -.20, .59, .12, .02
sin = .05, -.06, .07, .01, .03
barrier = 1.72
Substituted frequency = 24.45 (from rotational profile)
Reduced moment of inertia = 67.271

Reaction41

REACTANT 1

C -0.231045 -1.003023 0.000000
S 0.000000 0.815120 0.000000
C 1.819011 0.898786 0.000000
H 0.258801 -1.416127 0.885912
C -1.718608 -1.346806 0.000000
H 0.258801 -1.416127 -0.885912
H 2.235252 0.430102 -0.893849
H 2.086858 1.956027 0.000000

H 2.235252 0.430102 0.893849
H -1.854919 -2.431670 0.000000
H -2.218096 -0.943987 0.884465
H -2.218096 -0.943987 -0.884465

REACTANT 2

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

PRODUCT 1

S 0.491290 -0.615357 0.032517
C 1.954305 0.465737 -0.049597
H 1.940928 1.051893 -0.968648
H 1.992892 1.124962 0.818778
H 2.829839 -0.183737 -0.044297
C -0.793793 0.545786 0.007098
C -2.207643 0.067765 -0.042449
H -0.565615 1.545712 0.359930
H -2.601062 -0.209490 0.947814
H -2.861949 0.851010 -0.437189
H -2.312886 -0.810372 -0.686970

PRODUCT 2

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

TRANSITION STATE

C 2.062122 -0.544695 0.717865
C -0.298088 0.812432 0.535616
C 0.083373 2.195495 0.042628
S -1.430550 -0.027438 -0.574372
C -1.825522 -1.507698 0.409955
H 0.847171 2.628477 0.694774
H -0.684144 0.814701 1.558508
H 0.491073 2.158349 -0.971460
H -0.774250 2.876418 0.032874
H 0.816544 0.124175 0.626122
H 1.803774 -1.446700 1.273760
C 2.550046 -0.774111 -0.692216
H 2.664576 0.137386 1.318459
H -2.533666 -2.096258 -0.174122
H -0.932158 -2.105764 0.594289
H -2.290683 -1.230225 1.357543
H 3.489114 -1.344004 -0.709586
H 1.820475 -1.335908 -1.282748
H 2.739393 0.169827 -1.211541

Frequencies = -1653.23, 25.5575, 69.0358, 77.2793, 109.269, 163.422, 175.204, 188.175, 209.682, 286.601, 356.461, 454.704, 552.76, 686.94, 720.495, 836.463, 851.515, 928.894, 970.233, 972.189, 1017.47, 1040.46, 1091.56, 1104.93, 1154.09, 1223.52, 1278.02, 1357.88, 1405.23, 1407.78, 1417.32, 1442.1, 1464.38, 1470.38, 1484.21, 1487.7, 1491.88, 1492.19, 1498.78, 2989.23, 3016.39, 3036.8, 3049.5, 3052.25, 3065.32, 3073.41, 3080.58, 3090.2, 3114.6, 3130.59, 3137.49
cos = .13, .72, .23, .22, .05
sin = 0, -.12, .09, .10, -.04
barrier = 1.20
Substituted frequency = 23.99 (from rotational profile)
Reduced moment of inertia = 85.393

Reaction42

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000

H -1.620529 -0.881510 0.000000

TRANSITION STATE

C -2.485826 -0.903244 0.423872
C -1.829057 -0.154845 -0.478887
C -1.306985 1.187405 -0.242019
H -0.037800 1.071776 0.066065
C 1.323491 0.944101 0.445727
H -2.818101 -1.908564 0.193544
H -2.720993 -0.522701 1.413433
H -1.623059 -0.587571 -1.455699
H -1.261458 1.833247 -1.118851
H -1.721978 1.700688 0.626213
S 1.972914 -0.589496 -0.171397
H 1.282964 -1.410324 0.639527
H 1.818745 1.780084 -0.043610
H 1.305314 1.034792 1.529567

Frequencies = -1657.61, 33.4907, 62.9277, 112.317, 219.571, 249.106, 397.285, 424.821, 466.455, 634.595, 690.438, 757.764, 854.551, 899.842, 953.923, 985.258, 1009.08, 1034.99, 1095.9, 1124.39, 1207.15, 1318.35, 1388.58, 1415.45, 1419.54, 1436.88, 1480.99, 1637.13, 2665.6, 3068.12, 3085.12, 3123.17, 3128.12, 3146.51, 3179.22, 3214.38
cos = 1.92, 1.35, .27, .16, .05
sin = .22, -.18, -.07, -.04, 0
barrier = 2.93
Substituted frequency = 31.22 (from rotational profile)
Reduced moment of inertia = 69.202

Reaction43

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C 1.313608 1.343078 0.000000
C 0.000000 0.632143 0.000000
C -0.149896 -0.745657 0.000000
C -1.356259 -1.420691 0.000000
H 2.152068 0.642019 0.000000
H 1.418728 1.994231 0.877425
H 1.418728 1.994231 -0.877425
H -0.897812 1.246981 0.000000
H 0.761290 -1.343310 0.000000
H -1.398264 -2.502272 0.000000
H -2.299458 -0.885116 0.000000

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C -1.727687 -0.246806 -0.294228
C -0.539011 0.519974 0.308071
C 0.724146 -0.294054 0.340439
C 1.857831 0.017219 -0.280789
H -1.928687 -1.166347 0.263750
H -1.526830 -0.525021 -1.332111
H -2.636870 0.360122 -0.274235
H -0.365390 1.442057 -0.255997
H -0.796587 0.822146 1.331471
H 0.676814 -1.216634 0.918783
H 2.734122 -0.618652 -0.221704
H 1.951753 0.924338 -0.870918

TRANSITION STATE

C 1.275977 0.554264 0.348635
C 1.525139 1.845836 -0.413744
C -1.409432 0.580280 0.874233
S -2.279654 -0.324107 -0.382559
H -1.832129 -1.549427 -0.056963
H 0.001147 0.557049 0.591476
H -1.479177 0.163088 1.876284
H -1.679157 1.632971 0.828016
C 1.540536 -0.701016 -0.360867
H 1.690623 0.564505 1.360367
H 2.593388 1.995211 -0.607628
H 1.013383 1.836844 -1.380959
H 1.167417 2.713884 0.146843
C 1.963105 -1.843133 0.203329
H 1.333298 -0.696496 -1.430408
H 2.104182 -2.745941 -0.379288
H 2.189543 -1.903355 1.263692

Frequencies = -1598.46, 30.2769, 59.8153, 96.8898, 156.418, 193.523, 222.857, 282.512, 285.041, 448.921, 464.052, 538.267, 656.908, 752.904, 848.37, 869.414, 884.022, 908.712, 996.6, 1019.39, 1045.7, 1082.5, 1108.48, 1127.39, 1208.3, 1311.8, 1323.7, 1388.46, 1413.47, 1415.92, 1422.39, 1460.48, 1492.18, 1501.64, 1644.88, 2667.82, 3011.08, 3057.79, 3067.5, 3086.07, 3088.01, 3116.26, 3127.15, 3181.27, 3212.93
cos = 1.96, 1.54, .36, -.01, .02
sin = -.21, .23, 0, .03, .03
barrier = 3.04
Substituted frequency = 23.66 (from rotational profile)
Reduced moment of inertia = 105.987

Reaction44

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

PRODUCT 1

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000
H -1.620529 -0.881510 0.000000

TRANSITION STATE

C 1.430790 0.524853 1.089495
C -1.214390 0.536227 0.428065
C -1.336161 1.620568 -0.616973
S -1.666501 -1.129845 -0.034018
H -1.708056 0.760121 1.374277
H -1.011084 2.581827 -0.207326
H -0.714488 1.400038 -1.489738
H -2.369364 1.731848 -0.964491
H 0.141049 0.504105 0.794339
H 1.406010 0.292755 2.153899
C 2.095226 -0.462398 0.247030
H 1.706645 1.562292 0.897732
H -0.947297 -1.187769 -1.170202
C 2.716615 -0.201364 -0.916913
H 2.037118 -1.496952 0.579308
H 3.162119 -0.990031 -1.511523
H 2.808871 0.811977 -1.296219

Frequencies = -1681.97, 28.2704, 58.3, 96.8829, 169.433, 214.242, 223.896, 287.735, 326.729, 409.881, 464.78, 612.429, 635.205, 689.755, 853.378, 894.763, 898.02, 955.202, 992.059, 1018.95, 1033.1, 1066.3, 1102.86, 1137.47, 1209.11, 1307.86, 1318.07, 1391.3, 1408.78, 1422.85, 1437.7, 1480.8, 1485.62, 1490.25, 1633.76, 2650.41, 3009.12, 3066.06, 3069.88, 3080.82, 3105.67, 3123.38, 3128.29, 3148.3, 3214.92
cos = 2.09, 1.15, .43, .03, -.05
sin = .84, -.33, -.05, 0, -.01
barrier = 3.44
Substituted frequency = 19.08 (from rotational profile)
Reduced moment of inertia = 133.768

Reaction45

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 1.313608 1.343078 0.000000
C 0.000000 0.632143 0.000000
C -0.149896 -0.745657 0.000000
C -1.356259 -1.420691 0.000000
H 2.152068 0.642019 0.000000
H 1.418728 1.994231 0.877425
H 1.418728 1.994231 -0.877425
H -0.897812 1.246981 0.000000
H 0.761290 -1.343310 0.000000
H -1.398264 -2.502272 0.000000
H -2.299458 -0.885116 0.000000

PRODUCT 1

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945

H -1.627682 -1.165027 -0.565273

PRODUCT 2

C -1.727687 -0.246806 -0.294228
C -0.539011 0.519974 0.308071
C 0.724146 -0.294054 0.340439
C 1.857831 0.017219 -0.280789
H -1.928687 -1.166347 0.263750
H -1.526830 -0.525021 -1.332111
H -2.636870 0.360122 -0.274235
H -0.365390 1.442057 -0.255997
H -0.796587 0.822146 1.331471
H 0.676814 -1.216634 0.918783
H 2.734122 -0.618652 -0.221704
H 1.951753 0.924338 -0.870918

TRANSITION STATE

C -2.211994 -1.782459 -0.291785
C -1.828120 -0.519282 -0.538403
C -1.409381 0.458623 0.467856
C -1.704695 1.921191 0.178860
C 1.317855 0.334094 0.585396
C 1.622700 -0.763473 1.577077
S 1.924993 0.147970 -1.085446
H -0.101243 0.397820 0.503661
H -2.476094 -2.462262 -1.093300
H -2.283128 -2.167302 0.721178
H -1.783116 -0.184579 -1.574316
H -1.668734 0.157618 1.486536
H 1.466320 -1.100780 -1.290243
H 1.579987 1.337804 0.920847
H -1.230556 2.576037 0.915274
H -1.336456 2.208213 -0.810770
H -2.781600 2.123893 0.202235
H 2.701897 -0.892368 1.718789
H 1.178997 -0.531353 2.550184
H 1.215650 -1.722430 1.243055

Frequencies = -1640.38, 9.3346, 59.8555, 74.3349, 147.838, 182.476, 192.665, 212.65, 228.016, 285.236, 303.448, 335.588, 453.416, 503.344, 655.995, 689.91, 842.388, 866.996, 882.602, 897.492, 905.031, 996.446, 1019.14, 1030, 1080.85, 1088.16, 1115.76, 1136.28, 1209.39, 1308.13, 1310.74, 1322.85, 1396.11, 1405.43, 1411.48, 1428.97, 1459.59, 1484.91, 1490.05, 1492.81, 1499.54, 1640.31, 2651.58, 3006.79, 3009.76, 3056.92, 3063.82, 3066.22, 3080.6, 3087.44, 3107.51, 3114.49, 3126.96, 3212.99
cos = 3.01, 1.65, .66, -.08, -.10
sin = 1.04, -.58, 0, .08, .02
barrier = 4.83
Substituted frequency = 16.80 (from rotational profile)
Reduced moment of inertia = 209.947

Reaction46

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C 0.000000 0.993596 0.000000
C -1.216254 0.251259 0.000000
C -1.209617 -1.131393 0.000000
C 0.000000 -1.835757 0.000000
C 1.209615 -1.131314 0.000000
C 1.216317 0.251207 0.000000
H -2.157326 0.790828 0.000000
H -2.148915 -1.673415 0.000000
H 0.000000 -2.919393 0.000000
H 2.148773 -1.673586 0.000000
H 2.157286 0.790962 0.000000
C 0.000000 2.397411 0.000000
H -0.926886 2.957174 0.000000
H 0.926708 2.957383 0.000000

PRODUCT 1

C -0.012612 2.422864 0.000000
H 1.000842 2.828304 0.000000
H -0.530228 2.814544 0.880890
H -0.530228 2.814544 -0.880890
C 0.000000 0.911991 0.000000
C -1.199466 0.189711 0.000000
C -1.198091 -1.201720 0.000000
C 0.007954 -1.901531 0.000000
C 1.207772 -1.196479 0.000000
C 1.200802 0.197836 0.000000
H -2.143997 0.725304 0.000000
H -2.138732 -1.741767 0.000000
H 0.010467 -2.985728 0.000000
H 2.151993 -1.730155 0.000000
H 2.141729 0.738918 0.000000

PRODUCT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

TRANSITION STATE

S 2.974765 -0.932839 -0.273700
C 2.614057 0.802457 -0.429752
C 0.405276 1.483270 1.012388
H 0.335207 2.557155 0.841554
H 0.733107 1.248642 2.024632
H 3.412840 1.384525 0.025688

H 2.375669 1.130128 -1.439649
H 1.936387 -1.392747 -0.993136
H 1.473890 1.143249 0.310055
C -0.735538 0.696898 0.526972
C -1.010351 -0.581367 1.048861
C -2.062359 -1.345814 0.557544
C -2.867327 -0.857602 -0.471969
C -2.608058 0.405829 -1.003926
C -1.556727 1.171163 -0.513134
H -0.390752 -0.968520 1.851054
H -2.258698 -2.324875 0.980982
H -3.689251 -1.452946 -0.852838
H -3.231229 0.796388 -1.801151
H -1.367262 2.155423 -0.929896

Frequencies = -1666.03, 20.3589, 40.57, 59.9398, 122.451, 215.307, 246.873, 342.975, 414.795, 435.257, 450.228, 523.502, 553.977, 632.633, 647.569, 707.928, 752.597, 764.013, 819.494, 849.387, 854.008, 913.008, 975.707, 996.023, 1005.07, 1012.21, 1044.6, 1047.94, 1080.78, 1117.25, 1125.45, 1179.79, 1200.43, 1251.1, 1330.76, 1357.02, 1393.29, 1417.99, 1420.36, 1472.13, 1482.18, 1522.13, 1609.13, 1633.38, 2667.75, 3075.46, 3082.05, 3149.12, 3153.25, 3158.48, 3169.1, 3175.09, 3175.68, 3188.44
cos = 1.31, 1.48, .46, -.04, .01
sin = -.41, .19, .21, .04, -.01
barrier = 3.00
Substituted frequency = 19.41 (from rotational profile)
Reduced moment of inertia = 144.324

Reaction47

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 0.000000 0.993596 0.000000
C -1.216254 0.251259 0.000000
C -1.209617 -1.131393 0.000000
C 0.000000 -1.835757 0.000000
C 1.209615 -1.131314 0.000000
C 1.216317 0.251207 0.000000
H -2.157326 0.790828 0.000000
H -2.148915 -1.673415 0.000000
H 0.000000 -2.919393 0.000000
H 2.148773 -1.673586 0.000000
H 2.157286 0.790962 0.000000
C 0.000000 2.397411 0.000000
H -0.926886 2.957174 0.000000
H 0.926708 2.957383 0.000000

PRODUCT 1

C -0.012612 2.422864 0.000000
H 1.000842 2.828304 0.000000
H -0.530228 2.814544 0.880890
H -0.530228 2.814544 -0.880890
C 0.000000 0.911991 0.000000
C -1.199466 0.189711 0.000000
C -1.198091 -1.201720 0.000000
C 0.007954 -1.901531 0.000000
C 1.207772 -1.196479 0.000000
C 1.200802 0.197836 0.000000
H -2.143997 0.725304 0.000000
H -2.138732 -1.741767 0.000000
H 0.010467 -2.985728 0.000000
H 2.151993 -1.730155 0.000000
H 2.141729 0.738918 0.000000

PRODUCT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

TRANSITION STATE

C -1.693567 1.258314 0.126151
C -0.967021 0.284708 0.838429
C -1.349650 -1.061932 0.682962
C -2.409785 -1.415967 -0.143325
C -3.117641 -0.436697 -0.840984
C -2.753551 0.902662 -0.699559
C 0.183032 0.652640 1.671217
C 2.442280 0.506702 0.156542
S 2.700374 -1.202802 -0.309274
H 0.196571 1.686090 2.015739
H 0.425801 -0.051559 2.466029
H 3.218770 0.766355 0.877322
C 2.256452 1.517898 -0.951785
H 1.667725 -1.298688 -1.166814
H 1.290090 0.570246 0.927330
H -0.806602 -1.830229 1.223487
H -2.689367 -2.459400 -0.241085
H -3.946152 -0.713331 -1.482892
H -3.302316 1.672275 -1.231606
H -1.422171 2.303800 0.233468
H 3.131141 1.558180 -1.610342
H 1.386004 1.274320 -1.567614
H 2.101231 2.516802 -0.532515

Frequencies = -1674.73, 22.3314, 37.7876, 50.6648, 111.819, 155.039, 207.25, 243.111, 306.624, 329.081, 343.822, 415.169, 442.057, 511.699, 547.814, 606.327, 636.379, 686.231, 708.022, 758.62, 816.415, 849.741, 853.921, 899.057, 916.005, 976.554, 996.328, 1008.18, 1011.45, 1030.74, 1047.11, 1074.64, 1100.42, 1116.8, 1137.06, 1179.46, 1199.74, 1252.5, 1307.12, 1330.65, 1356.62, 1398.45, 1410.99, 1425.16, 1471.61, 1481.74, 1485.72, 1489.97, 1521.24, 1607.61, 1631.88, 2655.73, 3010.18, 3068.09, 3077.49, 3081.28, 3102.62, 3151.66, 3153.74, 3158.13, 3168.67, 3175.1, 3188.07
cos = 1.57, 1.50, .62, -.09, .12
sin = -.94, .29, .24, .07, .05
barrier = 3.80
Substituted frequency = 16.06 (from rotational profile)
Reduced moment of inertia = 284.529

Reaction48

REACTANT 1

C -0.416743 0.016648 0.401914
S 1.370091 -0.080624 -0.092069
C -1.092896 1.273450 -0.142201
C -1.091922 -1.265135 -0.089637
H -0.436704 0.030165 1.494167
H 1.749074 1.095395 0.437615
H -0.614345 -2.155502 0.325257
H -2.142662 -1.270770 0.214075
H -1.055862 -1.333473 -1.180727
H -2.143622 1.299170 0.167520
H -0.613112 2.182183 0.228997
H -1.054854 1.293045 -1.234244

REACTANT 2

C 0.000000 0.993596 0.000000
C -1.216254 0.251259 0.000000
C -1.209617 -1.131393 0.000000
C 0.000000 -1.835757 0.000000
C 1.209615 -1.131314 0.000000
C 1.216317 0.251207 0.000000
H -2.157326 0.790828 0.000000
H -2.148915 -1.673415 0.000000
H 0.000000 -2.919393 0.000000
H 2.148773 -1.673586 0.000000
H 2.157286 0.790962 0.000000
C 0.000000 2.397411 0.000000
H -0.926886 2.957174 0.000000
H 0.926708 2.957383 0.000000

PRODUCT 1

C -0.012612 2.422864 0.000000
H 1.000842 2.828304 0.000000
H -0.530228 2.814544 0.880890
H -0.530228 2.814544 -0.880890
C 0.000000 0.911991 0.000000
C -1.199466 0.189711 0.000000
C -1.198091 -1.201720 0.000000
C 0.007954 -1.901531 0.000000
C 1.207772 -1.196479 0.000000
C 1.200802 0.197836 0.000000
H -2.143997 0.725304 0.000000
H -2.138732 -1.741767 0.000000
H 0.010467 -2.985728 0.000000
H 2.151993 -1.730155 0.000000
H 2.141729 0.738918 0.000000

PRODUCT 2

C 1.085389 1.313238 0.036768
C 0.384580 0.008453 -0.166818
S -1.359504 -0.096411 0.035726
C 1.125045 -1.280188 0.007989
H -1.655216 1.176510 -0.281170
H 1.189097 1.567951 1.104198
H 2.094663 1.272829 -0.385000
H 0.556706 2.144567 -0.439850
H 2.079005 -1.245228 -0.528633
H 1.360984 -1.490121 1.064115
H 0.556743 -2.132957 -0.372915

TRANSITION STATE

C 1.917363 -1.313094 -0.033423
C 1.204221 -0.401808 0.770126
C 1.689206 0.918736 0.850019
C 2.833034 1.306078 0.162124
C 3.525778 0.388524 -0.628751
C 3.060769 -0.923808 -0.720805
C -0.027626 -0.797513 1.456880
C -2.167602 -0.275693 -0.144166
S -2.218612 1.516235 -0.375398
H -0.140803 -1.866359 1.634317
H -0.287520 -0.201753 2.330896
C -3.357991 -0.736308 0.674175
C -1.897652 -1.080160 -1.398753
H -1.118070 1.616964 -1.140956
H -1.076826 -0.516103 0.654277
H 1.158429 1.638856 1.463970
H 3.189831 2.326997 0.245511
H 4.419341 0.691005 -1.162640
H 3.595625 -1.646741 -1.327324
H 1.568629 -2.338429 -0.106522
H -4.293496 -0.646347 0.108172
H -3.237307 -1.788574 0.948133
H -3.465224 -0.156749 1.594648
H -2.708667 -0.961151 -2.127311
H -0.965076 -0.776837 -1.880660
H -1.818072 -2.144265 -1.152704

Frequencies = -1672.86, 22.1208, 42.888, 55.4725, 110.655, 132.695, 188.5, 203.394, 231.77, 248.145, 308.171, 321.762, 342.199, 345.124, 416.146, 481.559, 521.128, 545.221, 613.552, 636.915, 660.484, 707.901, 763.451, 821.329, 849.676,

879.566, 910.042, 922.565, 961.495, 976.45, 992.711, 995.743, 1010.91, 1015.75, 1046.96, 1071.74, 1116.25, 1124.65, 1179.28, 1184.24, 1199.76, 1210.37, 1253.27, 1330.51, 1357.09, 1397.63, 1403.98, 1418.42, 1431.29, 1470.4, 1480.05, 1481.73, 1482.89, 1493.91, 1500.24, 1521.07, 1606.48, 1630.92, 2664.92, 3002.21, 3006.19, 3061.62, 3064.92, 3077.77, 3090.98, 3093.13, 3151.57, 3153.61, 3158.39, 3168.9, 3175.3, 3188.09
cos = .75, 1.84, .93, -.02, -.03
sin = -1.08, .26, .34, 0, .05
barrier = 4.05
Substituted frequency = 14.52 (from rotational profile)
Reduced moment of inertia = 367.460

Reaction49

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C 0.000000 0.000000 1.337862
C 0.000000 0.000000 0.115777
C 0.000000 0.000000 -1.251352
H 0.000000 0.000000 2.400040
H 0.000000 0.929833 -1.806877
H 0.000000 -0.929833 -1.806877

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.000000 0.000000 -1.238052
H 0.000000 1.021022 -1.629805
H -0.884231 -0.510511 -1.629805
H 0.884231 -0.510511 -1.629805
C 0.000000 0.000000 0.219184
C 0.000000 0.000000 1.420084
H 0.000000 0.000000 2.482121

TRANSITION STATE

C -1.189092 0.868574 0.532706
S -1.940497 -0.552491 -0.222813
C 1.372057 1.170864 -0.332027
H 1.728270 2.031212 0.235071
C 2.055410 -0.046536 -0.062172
C 2.574843 -1.106350 0.196065
H 0.108820 1.026425 0.078279
H 1.248012 1.399271 -1.390866
H -1.705563 1.772319 0.215051
H -1.069839 0.805689 1.612501
H -1.202852 -1.488226 0.399992
H 3.061791 -2.026150 0.407560

Frequencies = -1689.17, 19.7549, 64.1861, 148.289, 236.371, 338.181, 378.587, 458.324, 493.068, 602.75, 628.464, 659.677, 755.264, 851.14, 997.275, 1028.83, 1070.07, 1092.2, 1126.21, 1393.56, 1412.55, 1420.41, 1449.04, 2162.75, 2667.89, 3069.39, 3082.42, 3135.64, 3175.43, 3475.31
cos = 1.52, .58, .08, .04, .04
sin = -.59, .35, .02, .02, .01
barrier = 2.45
Substituted frequency = 20.92 (from rotational profile)
Reduced moment of inertia = 70.378

Reaction50

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C -1.496297 0.827933 0.000000
C 0.000000 0.753661 0.000000
C 0.705702 -0.422428 0.000000
C 1.330359 -1.472517 0.000000
H -1.863079 1.372446 0.878966
H -1.946492 -0.165292 0.000000
H -1.863079 1.372446 -0.878966
H 0.559299 1.684823 0.000000
H 1.874768 -2.384319 0.000000

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C -1.526705 0.649900 0.000000
C 0.000000 0.844781 0.000000
C 0.740610 -0.414795 0.000000

C 1.331703 -1.461080 0.000000
H 1.859218 -2.382941 0.000000
H -2.033076 1.618332 0.000000
H -1.847178 0.093855 0.883415
H -1.847178 0.093855 -0.883415
H 0.297285 1.432031 0.876023
H 0.297285 1.432031 -0.876023

TRANSITION STATE

C 1.358256 -0.352402 0.987659
S 2.183214 0.309437 -0.439612
C -1.305465 -0.629966 0.476261
C -1.775163 0.683106 0.166002
C -2.112783 1.810912 -0.104198
H -1.687634 -0.994766 1.432965
H -0.019133 -0.494483 0.733367
C -1.382798 -1.665791 -0.638719
H 1.711956 -1.362382 1.184469
H 1.379155 0.286187 1.868275
H 1.639709 1.538499 -0.397833
H -2.438429 2.793736 -0.340880
H -0.919839 -2.604407 -0.323279
H -2.422105 -1.876583 -0.910983
H -0.867379 -1.311955 -1.534342

Frequencies = -1659.03, 25.9777, 61.6413, 98.6566, 188.214, 197.541, 221.345, 262.889, 416.672, 474.705, 517.782, 558.219, 608.268, 664.937, 751.636, 844.851, 857.115, 877.976, 1049.88, 1074.86, 1098.32, 1106.08, 1129.04, 1324.03, 1403.24, 1409.42, 1414.36, 1421.23, 1489.94, 1498.16, 2164.32, 2667.54, 3021.24, 3063.99, 3080.18, 3083.88, 3105.26, 3177.82, 3475.16
cos = 1.81, .91, .44, .20, .04
sin = -.60, .44, .07, -.01, 0
barrier = 3.12
Substituted frequency = 25.12 (from rotational profile)
Reduced moment of inertia = 107.704

Reaction51

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 0.000000 0.000000 1.337862
C 0.000000 0.000000 0.115777
C 0.000000 0.000000 -1.251352
H 0.000000 0.000000 2.400040
H 0.000000 0.929833 -1.806877
H 0.000000 -0.929833 -1.806877

PRODUCT 1

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

PRODUCT 2

C 0.000000 0.000000 -1.238052
H 0.000000 1.021022 -1.629805
H -0.884231 -0.510511 -1.629805
H 0.884231 -0.510511 -1.629805
C 0.000000 0.000000 0.219184
C 0.000000 0.000000 1.420084
H 0.000000 0.000000 2.482121

TRANSITION STATE

C 1.479442 0.070529 1.239434
C -1.073213 0.556281 0.439032
C -0.940226 1.670530 -0.573966
S -1.793463 -0.988615 -0.101995
H -1.576141 0.843605 1.363581
H -0.479140 2.549531 -0.113645
H -0.311511 1.365618 -1.415017
H -1.916435 1.966836 -0.972534
H 0.204033 0.295626 0.860485
H 1.358029 -0.785192 1.903556
C 2.246132 -0.184608 0.070791
H 1.752018 0.977921 1.778466
H -1.047091 -1.138966 -1.211732
C 2.840857 -0.392143 -0.960864
H 3.393693 -0.580669 -1.847805

Frequencies = -1685, 16.4193, 63.9833, 104.797, 189.335, 222.57, 272.69, 323.915, 340.531, 439.427, 470.762, 554.24, 595.663, 658.364, 686.805, 845.718, 899.772, 998.246, 1021.59, 1070.06, 1083.24, 1096.69, 1138.73, 1306.62, 1394.91, 1409.45, 1417.56, 1449.35, 1484.65, 1488.54, 2157.94, 2657.96, 3013.66, 3071.5, 3073.24, 3083.57, 3102.74, 3138.82, 3475.1
cos = 2.51, .20, .41, .13, -.03
sin = 1.20, -.37, -.11, .02, 0
barrier = 3.56
Substituted frequency = 17.54 (from rotational profile)
Reduced moment of inertia = 132.921

Reaction52

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C -1.496297 0.827933 0.000000
C 0.000000 0.753661 0.000000
C 0.705702 -0.422428 0.000000
C 1.330359 -1.472517 0.000000
H -1.863079 1.372446 0.878966
H -1.946492 -0.165292 0.000000
H -1.863079 1.372446 -0.878966
H 0.559299 1.684823 0.000000
H 1.874768 -2.384319 0.000000

PRODUCT 1

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

PRODUCT 2

C -1.526705 0.649900 0.000000
C 0.000000 0.844781 0.000000
C 0.740610 -0.414795 0.000000
C 1.331703 -1.461080 0.000000
H 1.859218 -2.382941 0.000000
H -2.033076 1.618332 0.000000
H -1.847178 0.093855 0.883415
H -1.847178 0.093855 -0.883415
H 0.297285 1.432031 0.876023
H 0.297285 1.432031 -0.876023

TRANSITION STATE

C 1.269691 -0.126476 0.675948
S 1.812797 -0.531839 -0.978721
C -1.450202 -0.299080 0.705720
C -1.769036 -1.739851 0.327388
C -1.894306 0.716448 -0.193817
C -2.214352 1.578180 -0.978304
H -1.678050 -0.063443 1.748149
H -0.119750 -0.228974 0.694896
H 1.584606 -0.938180 1.332964
C 1.568881 1.259197 1.200079
H 1.291733 0.547548 -1.590737
H -2.525106 2.331705 -1.659191
H -1.308824 -2.433461 1.035910
H -2.849078 -1.920445 0.331467
H -1.393763 -1.971154 -0.671788
H 2.646808 1.452452 1.231075
H 1.108960 2.026419 0.570897
H 1.173654 1.376446 2.213822

Frequencies = -1672.1, 23.9, 61.8374, 79.5097, 185.091, 188.725, 189.368, 216.853, 227.175, 280.302, 333.123, 446.759, 482.903, 537.618, 599.702, 664.422, 686.666, 833.442, 857.597, 892.414, 899.34, 1024.99, 1073.28, 1085.85, 1099.23, 1118.6, 1136.95, 1307.45, 1325.85, 1403.75, 1406.73, 1415, 1422.75, 1484.82, 1489.81, 1490.19, 1497.4, 2158.86, 2657.68, 3011.19, 3020.09, 3064.58, 3069.78, 3078.99, 3082.69, 3104.09, 3106.2, 3474.94
cos = 3.14, .79, .99, .27, .04
sin = -1.46, .60, .05, -.07, -.01
barrier = 5.09
Substituted frequency = 22.24 (from rotational profile)
Reduced moment of inertia = 206.111

Reaction53

REACTANT 1

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935
C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

REACTANT 2

C 0.000000 0.000000 1.337862
C 0.000000 0.000000 0.115777
C 0.000000 0.000000 -1.251352
H 0.000000 0.000000 2.400040
H 0.000000 0.929833 -1.806877
H 0.000000 -0.929833 -1.806877

PRODUCT 1

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000

H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

PRODUCT 2

C 0.000000 0.000000 -1.238052
H 0.000000 1.021022 -1.629805
H -0.884231 -0.510511 -1.629805
H 0.884231 -0.510511 -1.629805
C 0.000000 0.000000 0.219184
C 0.000000 0.000000 1.420084
H 0.000000 0.000000 2.482121

TRANSITION STATE

C -1.321893 -1.363612 0.533861
C 0.812115 0.092473 -0.339291
C 2.036621 -0.444904 0.260479
C 2.871403 -1.293257 -0.353885
S 0.454823 1.797420 0.133127
H -0.818248 1.812620 -0.302728
H -0.203489 -0.608003 0.115167
H 0.728799 -0.076820 -1.413499
H 2.234776 -0.155807 1.290522
H 3.736636 -1.700056 0.155590
H 2.715683 -1.602493 -1.382513
C -2.481921 -0.721968 0.047008
H -1.092552 -2.334176 0.096950
H -1.175885 -1.329396 1.612534
C -3.434530 -0.124915 -0.401909
H -4.293653 0.372508 -0.779626

Frequencies = -1694.23, 24.7952, 56.3649, 96.6879, 151.85, 176.444, 232.464, 257.791, 343.077, 370.695, 418.253, 492.74, 552.477, 588.645, 658.725, 675.463, 772.657, 908.231, 926.006, 963.994, 1000.15, 1014.9, 1022.23, 1061.9, 1078.71, 1170.17, 1241.69, 1320.23, 1358.5, 1417.76, 1448.67, 1455.89, 1651.39, 2139.62, 2655.17, 3082.13, 3088.95, 3130.77, 3136.13, 3155.17, 3221.32, 3473.6
cos = 3.44, 1.52, .21, .10, .08
sin = .08, -.47, -.02, -.01, -.01
barrier = 4.39
Substituted frequency = 22.29 (from rotational profile)
Reduced moment of inertia = 150.960

Reaction54

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

TRANSITION STATE

C -1.341246 1.059342 -0.220956
S -2.025411 -0.553065 0.127651
C 1.341161 1.059364 0.220964
S 2.025400 -0.553018 -0.127697
H 1.491178 -1.199609 0.922958
H -0.000071 1.058073 0.000022
H 1.746893 1.778939 -0.488623
H 1.467165 1.384336 1.252444
H -1.467312 1.384323 -1.252427
H -1.747010 1.778836 0.488689
H -1.490151 -1.199795 -0.922386

Frequencies = -1703.53, 45.0599, 71.7402, 187.415, 216.491, 273.077, 407.094, 451.437, 617.795, 733.282, 751.545, 844.884, 851.8, 1040.64, 1053.51, 1119.95, 1121.58, 1401.07, 1416.93, 1420.45, 1439.54, 2666.36, 2666.94, 3076.08, 3077.12, 3164.27, 3165.49
cos = 3.08, 2.43, .57, .18, .02
sin = .58, -.25, -.21, -.07, .01
barrier = 5.14
Substituted frequency = 46.31 (from rotational profile)
Reduced moment of inertia = 49.708

Reaction55

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000

H -0.430914 1.557520 -0.895039

REACTANT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

TRANSITION STATE

C 1.446501 0.757044 0.785932
S 2.311393 -0.275011 -0.387190
C -1.242642 0.528341 0.449474
S -1.617106 -1.192331 0.091323
C -1.632245 1.552805 -0.594489
H -1.643512 0.736889 1.443065
H -1.351886 2.557783 -0.263565
H -1.126730 1.360103 -1.545390
H -2.710964 1.546604 -0.783545
H 0.087142 0.627523 0.624679
H 1.634232 0.502616 1.827599
H 1.664743 1.801838 0.570676
H -1.081199 -1.223722 -1.142637
H 1.989904 -1.461311 0.157499

Frequencies = -1695.89, 32.9811, 71.3978, 111.82, 199.375, 214.62, 274.444, 295.45, 324.74, 451.31, 516.895, 676.85, 741.729, 847.936, 850.992, 897.922, 1019.24, 1053.82, 1085.2, 1117.15, 1137.49, 1304.13, 1400.69, 1411.48, 1418.4, 1443.19, 1485.45, 1491.56, 2657.45, 2668.84, 3011.48, 3069.29, 3076.67, 3077.71, 3095.37, 3166.64
cos = 3.22, 2.55, .69, .01, -.02
sin = .74, -.42, -.19, -.05, -.01

barrier = 5.53
Substituted frequency = 31.73 (from rotational profile)
Reduced moment of inertia = 95.386

Reaction56

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C 1.085389 1.313238 0.036768
C 0.384580 0.008453 -0.166818
S -1.359504 -0.096411 0.035726
C 1.125045 -1.280188 0.007989
H -1.655216 1.176510 -0.281170
H 1.189097 1.567951 1.104198
H 2.094663 1.272829 -0.385000
H 0.556706 2.144567 -0.439850
H 2.079005 -1.245228 -0.528633
H 1.360984 -1.490121 1.064115
H 0.556743 -2.132957 -0.372915

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C -0.416743 0.016648 0.401914
S 1.370091 -0.080624 -0.092069
C -1.092896 1.273450 -0.142201
C -1.091922 -1.265135 -0.089637
H -0.436704 0.030165 1.494167
H 1.749074 1.095395 0.437615
H -0.614345 -2.155502 0.325257
H -2.142662 -1.270770 0.214075
H -1.055862 -1.333473 -1.180727
H -2.143622 1.299170 0.167520
H -0.613112 2.182183 0.228997
H -1.054854 1.293045 -1.234244

TRANSITION STATE

C 1.486420 -1.007131 -0.508996
S 2.623180 0.203162 0.145959
C -1.088331 -0.337606 0.065856
C -1.289331 -0.774822 1.503796
S -1.231831 1.450204 -0.207895

H -0.507627 1.839892 0.855647
H 0.174270 -0.643194 -0.221884
C -1.931561 -1.086599 -0.950883
H 1.518849 -1.110655 -1.592073
H 1.640081 -1.955637 0.002902
H 2.322207 1.199979 -0.704453
H -2.305343 -0.550727 1.849142
H -1.132671 -1.855115 1.593203
H -0.587492 -0.277681 2.178419
H -3.003333 -0.939379 -0.771155
H -1.715182 -0.764704 -1.972938
H -1.728523 -2.159687 -0.884475

Frequencies = -1669.08, 36.3906, 69.0799, 113.802, 160.863, 199.316, 227.372, 236.98, 279.454, 307.275, 310.976, 347.141, 484.082, 527.791, 649.032, 743.344, 848.787, 876.165, 917.083, 960.131, 993.007, 1042.88, 1115.31, 1123.41, 1182.32, 1201.79, 1400.49, 1402.95, 1418.27, 1420.47, 1446.46, 1481.53, 1483.46, 1495.13, 1501.3, 2660.4, 2668, 3004.6, 3008.76, 3063.16, 3066.25, 3078.45, 3086.63, 3090.8, 3167.8
cos = 3.03, 2.41, 1.07, -.15, 0
sin = .86, -.67, -.16, -.09, .06
barrier = 5.59
Substituted frequency = 30.55 (from rotational profile)
Reduced moment of inertia = 106.862

Reaction57

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

PRODUCT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

PRODUCT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

TRANSITION STATE

C 1.358787 0.696162 -0.066394
S 1.886461 -0.875725 -0.759266
C -1.358909 0.696010 0.066560
S -1.886123 -0.876238 0.758948
H -1.573571 -1.636682 -0.306365
H 0.000000 0.684346 0.000000
H -1.569589 1.457909 0.819069
C -1.860639 1.044267 -1.317750
C 1.860127 1.043909 1.318192
H 1.569588 1.458424 -0.818504
H 1.573812 -1.636630 0.305689
H -2.954636 1.087737 -1.353006
H -1.472982 2.019700 -1.628419
H -1.532754 0.304271 -2.053786
H 2.954107 1.087509 1.353742
H 1.472257 2.019159 1.629166
H 1.532154 0.303567 2.053840

Frequencies = -1704.72, 23.8897, 75.7692, 78.0903, 184.125, 192.774, 210.393, 213.987, 287.938, 314.092, 328.959, 333.079, 461.286, 668.492, 687.351, 841.421, 854.722, 889.639, 898.836, 1011.36, 1032.71, 1080.18, 1091.68, 1132.2, 1137.91, 1303.23, 1304.41, 1403.62, 1405.92, 1415.03, 1448.29, 1484.83, 1485.21, 1491.09, 1491.86, 2647.67, 2648.74, 3009.49, 3009.74, 3066.9, 3067.45, 3075.91, 3076.69, 3095.61, 3096.04
cos = 3.95, 3.04, .92, -.14, -.07
sin = 1.01, -.68, -.15, .02, .01
barrier = 6.81
Substituted frequency = 23.36 (from rotational profile)
Reduced moment of inertia = 186.952

Reaction58

REACTANT 1

S 0.047809 -0.669761 0.000000

C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C 0.010170 0.535277 0.000000
H -0.207782 1.597871 0.000000
C 0.010170 -0.197547 1.297818
C 0.010170 -0.197547 -1.297818
H 0.757439 -1.001216 -1.307030
H -0.960273 -0.683110 -1.499120
H 0.215195 0.464839 -2.142558
H 0.757439 -1.001216 1.307030
H 0.215195 0.464839 2.142558
H -0.960273 -0.683110 1.499120

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.000000 1.276840 -0.259553
C 0.000000 0.000000 0.585554
C 0.000000 -1.276840 -0.259553
H 0.882751 1.322941 -0.905415
H 0.000000 2.173102 0.367188
H -0.882751 1.322941 -0.905415
H -0.875663 0.000000 1.244299
H 0.875663 0.000000 1.244299
H 0.000000 -2.173102 0.367188
H -0.882751 -1.322941 -0.905415
H 0.882751 -1.322941 -0.905415

TRANSITION STATE

C -1.735423 1.352875 -0.109835
C -1.564859 -0.043204 0.447432
C -1.898086 -1.181248 -0.491691
C 1.082125 -0.323292 0.993123
S 2.116856 0.030281 -0.426840
H 1.940302 1.362691 -0.446422
H -0.237668 -0.169869 0.718433
H 1.282891 0.311156 1.855073
H 1.179553 -1.379827 1.238749
H -2.005677 -0.163382 1.440745
H -2.786985 1.560366 -0.352071
H -1.410493 2.117367 0.602012
H -1.162171 1.482746 -1.033676
H -2.958779 -1.164673 -0.778332
H -1.312686 -1.116853 -1.414592
H -1.700537 -2.155009 -0.034654

Frequencies = -1693.76, 16.0413, 75.7544, 112.336, 188.515, 191.531, 229.976, 285.372, 368.905, 455.111, 515.368, 732.588, 828.712, 854.113, 885.837, 928.414, 952.964, 1060.12, 1106.75, 1127.79, 1172.29, 1189.69, 1347.48, 1396.86, 1412.52, 1419.49, 1424.83, 1437.76, 1481.39, 1488.26, 1497.19, 1499.37, 2666.56, 2986.43, 2990.21, 3044.5, 3047.86, 3057.57, 3075.3, 3079.95, 3087.38, 3161.82
cos = .04, .14, .68, .10, -.07
sin = .08, -.04, -.02, .02, -.01
barrier = 0.88
Substituted frequency = 16.04 (from HO analysis)
Reduced moment of inertia = 80.912

Reaction59

REACTANT 1

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

REACTANT 2

C 0.000000 1.486187 -0.014859
C 0.000000 0.000000 0.149312
C 1.287076 -0.743093 -0.014859
C -1.287076 -0.743093 -0.014859
H 0.000000 1.783483 -1.079233
H 0.886704 1.944418 0.434881
H -0.886704 1.944418 0.434881
H -1.240564 -1.740117 0.434881
H -2.127268 -0.204301 0.434881
H -1.544541 -0.891741 -1.079233
H 1.240564 -1.740117 0.434881
H 1.544541 -0.891741 -1.079233
H 2.127268 -0.204301 0.434881

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.000000 0.000000 0.371940
C 0.000000 1.461427 -0.095749
C -1.265633 -0.730714 -0.095749
C 1.265633 -0.730714 -0.095749
H 0.000000 0.000000 1.469892
H 0.884045 1.995279 0.265249
H 0.000000 1.519937 -1.189845

H -0.884045 1.995279 0.265249
H -1.285940 -1.763245 0.265249
H -2.169985 -0.232035 0.265249
H -1.316304 -0.759968 -1.189845
H 1.285940 -1.763245 0.265249
H 1.316304 -0.759968 -1.189845
H 2.169985 -0.232035 0.265249

TRANSITION STATE

C 1.218886 1.025671 -0.110475
S 2.516671 -0.191641 0.086633
C -1.278004 -0.050470 0.005929
C -1.386925 -0.572168 1.426225
C -1.286690 -1.137529 -1.052520
C -2.200177 1.115365 -0.299472
H -1.088896 -0.730887 -2.049365
H -0.538299 -1.907365 -0.842826
H -2.265403 -1.637187 -1.094286
H -0.039251 0.462310 -0.059499
H 1.237159 1.696967 0.746732
H 1.260316 1.569570 -1.052790
H 2.381125 -0.791239 -1.108849
H -3.253564 0.802024 -0.267327
H -2.080468 1.924105 0.427902
H -2.014696 1.525830 -1.296876
H -2.362217 -1.051211 1.594940
H -0.614440 -1.316681 1.638952
H -1.290641 0.234799 2.159032

Frequencies = -1668.67, 10.6169, 70.2406, 105.999, 162.668, 189.605, 218.611, 220.848, 224.225, 312.178, 365.493, 375.304, 502.95, 518.163, 736.683, 789.617, 843.893, 940.404, 943.44, 963.26, 997.635, 1006.24, 1047.48, 1115.38, 1184.05, 1245.83, 1247.58, 1394.4, 1396.89, 1415.82, 1422.6, 1428.12, 1434.45, 1474.72, 1482.06, 1483.55, 1499.29, 1500.64, 1508.31, 2658.89, 2980.15, 2981.33, 2988.75, 3046.26, 3048.44, 3052.72, 3076.04, 3078.69, 3082.07, 3086.16, 3163.28
cos = 0, 0, 1.01, 0, 0
sin = 0, 0, .08, 0, 0
barrier = 1.02
Substituted frequency = 10.62 (from HO analysis)
Reduced moment of inertia = 93.070

Reaction60

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000
H -1.620529 -0.881510 0.000000

TRANSITION STATE

S 2.068795 -0.784563 -0.287734
C 1.341643 0.350150 0.664918
C 0.740175 1.564420 0.195887
H -0.517383 1.253642 -0.072014
C -1.858528 1.012875 -0.408530
C -1.974537 -0.421584 -0.479565
C -2.342489 -1.209804 0.552949
H 1.253711 0.150138 1.734065
H 0.609473 2.358295 0.931343
H -1.907127 1.568667 -1.341339
H -2.346347 1.508352 0.428925
H -1.692120 -0.892466 -1.417535
H -2.378024 -2.287830 0.457040
H -2.623960 -0.790256 1.513692
H 1.063480 1.908123 -0.784378

Frequencies = -1579.31, 33.6988, 48.7929, 87.213, 190.698, 263.544, 387.223, 413.589, 450.039, 508.623, 622.303, 771.781, 839.129, 901.796, 914.019, 956.6, 997.716, 1000.18, 1029.13, 1093.54, 1139.95, 1196.68, 1250.61, 1313.97, 1332.93, 1353.09, 1388.34, 1438.8, 1473.98, 1490.36, 1610.24, 3077.72, 3087.53, 3094.77, 3133.75, 3145.33, 3169.22, 3182.52, 3227.54
cos = 1.59, 2.00, .71, .27, .12
sin = .31, .13, -.34, -.05, -.01
barrier = 3.87

Substituted frequency = 32.41 (from rotational profile)
Reduced moment of inertia = 110.612

Reaction61

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 1.313608 1.343078 0.000000
C 0.000000 0.632143 0.000000
C -0.149896 -0.745657 0.000000
C -1.356259 -1.420691 0.000000
H 2.152068 0.642019 0.000000
H 1.418728 1.994231 0.877425
H 1.418728 1.994231 -0.877425
H -0.897812 1.246981 0.000000
H 0.761290 -1.343310 0.000000
H -1.398264 -2.502272 0.000000
H -2.299458 -0.885116 0.000000

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C -1.727687 -0.246806 -0.294228
C -0.539011 0.519974 0.308071
C 0.724146 -0.294054 0.340439
C 1.857831 0.017219 -0.280789
H -1.928687 -1.166347 0.263750
H -1.526830 -0.525021 -1.332111
H -2.636870 0.360122 -0.274235
H -0.365390 1.442057 -0.255997
H -0.796587 0.822146 1.331471
H 0.676814 -1.216634 0.918783
H 2.734122 -0.618652 -0.221704
H 1.951753 0.924338 -0.870918

TRANSITION STATE

C -0.719905 -1.275108 0.860141
C -1.653444 -0.195949 0.758762
S -2.440949 0.257972 -0.622443
C 1.750994 -0.333725 0.226623
C 1.518192 0.981908 -0.334972
C 1.505188 2.126388 0.374974
H 0.471204 -0.750159 0.561742
H -1.805088 0.398776 1.660757
H -0.528021 -1.664646 1.859918
C 2.266429 -1.439553 -0.666745
H 2.175930 -0.325225 1.232066
H 1.285887 1.023153 -1.397144
H 1.284020 3.078731 -0.090812
H 1.721025 2.136744 1.438775
H -0.778575 -2.034219 0.082776
H 2.181374 -2.417220 -0.185684
H 1.717496 -1.474568 -1.611538
H 3.325204 -1.282675 -0.904463

Frequencies = -1524.03, 21.3657, 45.1724, 81.2819, 162.735, 175.719, 216.03, 269.41, 279.394, 398.594, 448.125, 485.037, 604.735, 697.606, 837.089, 863.712, 878.29, 917.663, 945.97, 1000.64, 1012.74, 1041.52, 1089.9, 1103.32, 1146.35, 1204.48, 1234.82, 1312.79, 1323.24, 1355.42, 1362.98, 1398.23, 1417.16, 1463.77, 1476.48, 1489.97, 1497.57, 1621.28, 3012.65, 3069.39, 3077.01, 3083.39, 3088.63, 3101.24, 3132.21, 3136.14, 3167.88, 3225.39
cos = 0, 3.03, .52, .35, .05
sin = .73, -.08, -.25, -.06, .02
barrier = 4.35
Substituted frequency = 25.07 (from rotational profile)
Reduced moment of inertia = 189.085

Reaction62

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 0.257358 -2.083274 0.000000
C 0.733479 -0.787214 0.000000
C 0.000000 0.398983 0.000000
C -1.499325 0.444678 0.000000
C 0.696711 1.727848 0.000000
H 0.943168 -2.920686 0.000000
H -0.799592 -2.318264 0.000000
H 1.816210 -0.670869 0.000000
H 1.783302 1.620820 0.000000
H -1.958204 -0.543545 0.000000
H -1.872158 0.987818 0.878018
H -1.872158 0.987818 -0.878018
H 0.415048 2.325393 0.877522
H 0.415048 2.325393 -0.877522

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C -0.039118 -2.155117 0.000000
C 0.468489 -0.926272 0.000000
C -0.328860 0.352844 0.000000
C -0.039118 1.176572 1.267632
C -0.039118 1.176572 -1.267632
H -1.111703 -2.326848 0.000000
H 0.594781 -3.034933 0.000000
H 1.552036 -0.801120 0.000000
H -1.392759 0.086675 0.000000
H -0.625702 2.100094 -1.275359
H -0.625702 2.100094 1.275359
H -0.281411 0.610329 -2.170251
H -0.281411 0.610329 2.170251
H 1.019109 1.453891 -1.319421
H 1.019109 1.453891 1.319421

TRANSITION STATE

C 0.814788 -1.297437 -0.320714
C 1.993471 -0.564993 -0.662969
S 3.059340 0.106835 0.411907
C -1.262760 0.435244 -0.097155
C -1.078351 0.853573 1.347691
C -2.435217 -0.372265 -0.442326
C -3.289886 -0.956842 0.412509
C -0.867942 1.488089 -1.116076
H -0.219627 -0.443221 -0.264315
H 2.173924 -0.416296 -1.729114
H 0.418457 -1.969283 -1.082337
H -2.600261 -0.516955 -1.508839
H -4.119765 -1.551490 0.049777
H -3.199826 -0.853999 1.487491
H 0.765665 -1.686538 0.694125
H 0.168217 1.807556 -0.974192
H -0.979634 1.121896 -2.140003
H -1.502415 2.376430 -1.009225
H -0.087017 1.284347 1.502318
H -1.822402 1.611773 1.620961
H -1.189360 0.014204 2.037081

Frequencies = -1492.58, 20.4075, 53.5829, 85.177, 129.116, 157.765, 187.226, 214.608, 231.859, 288.116, 317.896, 372.846, 396.419, 472.558, 542.677, 656.823, 699.488, 785.818, 838.834, 882.363, 925.5, 953.842, 962.014, 997.914, 1023.66, 1059.7, 1068.56, 1084.23, 1127.25, 1200.7, 1221.46, 1280.91, 1329.9, 1351.48, 1373.17, 1394.01, 1403.1, 1414.67, 1454.28, 1474.58, 1480.39, 1484.27, 1502.44, 1504.91, 1638.7, 3008.75, 3014.1, 3068.23, 3075.63, 3081.7, 3084.2, 3096.19, 3109.36, 3120.67, 3145.71, 3169.32, 3227.49
cos = .71, 1.95, .09, .41, .14
sin = -.17, .29, -.05, .06, -.04
barrier = 2.78
Substituted frequency = 21.14 (from rotational profile)
Reduced moment of inertia = 216.985

Reaction63

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 0.000000 0.000000 1.337862
C 0.000000 0.000000 0.115777
C 0.000000 0.000000 -1.251352
H 0.000000 0.000000 2.400040
H 0.000000 0.929833 -1.806877
H 0.000000 -0.929833 -1.806877

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C 0.000000 0.000000 -1.238052
H 0.000000 1.021022 -1.629805
H -0.884231 -0.510511 -1.629805
H 0.884231 -0.510511 -1.629805
C 0.000000 0.000000 0.219184
C 0.000000 0.000000 1.420084
H 0.000000 0.000000 2.482121

TRANSITION STATE

C 0.603177 1.458946 0.361631
C 1.230071 0.201081 0.678173
S 2.163410 -0.682384 -0.349479
C -1.927134 0.975257 -0.531810
C -2.291859 -0.313195 -0.099803
C -2.525936 -1.429082 0.304993
H 1.023460 -0.200414 1.671338
H 0.381928 2.107264 1.210391

H 1.003821 1.979822 -0.505776
H -0.601865 1.172397 -0.040805
H -1.752882 1.098562 -1.598604
H -2.443497 1.812474 -0.066799
H -2.755429 -2.410004 0.642815

Frequencies = -1595.96, 12.3849, 55.7784, 89.7113, 237.911, 335.066, 383.507, 405.854, 430.268, 478.826, 625.447, 662.698, 755.796, 833.572, 888.271, 992.815, 1018.23, 1069.07, 1096.42, 1138.66, 1212.12, 1350.73, 1351.47, 1386.35, 1451.35, 1471.56, 2142.67, 3073.91, 3090.77, 3092.71, 3165.64, 3169.34, 3471.76
cos = .51, 1.20, -.09, .02, -.02
sin = 1.00, -.34, -.08, -.09, -.04
barrier = 2.52
Substituted frequency = 14.14 (from rotational profile)
Reduced moment of inertia = 109.713

Reaction64

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C -1.496297 0.827933 0.000000
C 0.000000 0.753661 0.000000
C 0.705702 -0.422428 0.000000
C 1.330359 -1.472517 0.000000
H -1.863079 1.372446 0.878966
H -1.946492 -0.165292 0.000000
H -1.863079 1.372446 -0.878966
H 0.559299 1.684823 0.000000
H 1.874768 -2.384319 0.000000

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C -1.526705 0.649900 0.000000
C 0.000000 0.844781 0.000000
C 0.740610 -0.414795 0.000000
C 1.331703 -1.461080 0.000000
H 1.859218 -2.382941 0.000000
H -2.033076 1.618332 0.000000
H -1.847178 0.093855 0.883415
H -1.847178 0.093855 -0.883415
H 0.297285 1.432031 0.876023
H 0.297285 1.432031 -0.876023

TRANSITION STATE

C -0.570302 -1.159689 0.345028
C -1.716374 -0.357495 0.672513
S -2.916983 0.070959 -0.374057
C 1.434148 0.489044 -0.459601
C 1.212769 1.740385 0.365449
C 2.628754 -0.247167 -0.274036
C 3.622214 -0.908994 -0.082372
H -1.759162 0.022609 1.694929
H -0.076634 -1.661924 1.177684
H -0.655067 -1.764719 -0.555446
H 0.396145 -0.351109 -0.016018
H 1.113590 0.565498 -1.499348
H 4.505962 -1.478349 0.071825
H 0.171990 2.066667 0.298702
H 1.465111 1.572337 1.414296
H 1.842542 2.557141 -0.003590

Frequencies = -1559.62, 22.2147, 53.457, 99.165, 131.956, 179.323, 208.703, 276.924, 372.526, 405.208, 455.428, 541.187, 623.965, 668.9, 682.211, 836.932, 850.211, 882.841, 930.3, 1055.18, 1076.56, 1098.97, 1103.63, 1122.32, 1192.48, 1340.57, 1350.65, 1380.18, 1407.96, 1409.71, 1473, 1488.5, 1493.12, 2147.59, 3022.01, 3074.84, 3080.72, 3083.84, 3094.65, 3114.45, 3167.64, 3472.07
cos = 2.61, 1.41, .10, 0, .14
sin = -1.36, .65, -.10, .10, -.02
barrier = 4.76
Substituted frequency = 18.98 (from rotational profile)
Reduced moment of inertia = 176.864

Reaction65

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 0.000000 0.000000 1.043643
C 0.000000 0.000000 2.265132
C 0.000000 0.000000 -0.332748
H 0.000000 0.000000 3.326998
C 0.000000 1.288872 -1.104719

C 0.000000 -1.288872 -1.104719
H 0.000000 2.156753 -0.445259
H 0.879523 1.352850 -1.759006
H -0.879523 1.352850 -1.759006
H 0.000000 -2.156753 -0.445259
H -0.879523 -1.352850 -1.759006
H 0.879523 -1.352850 -1.759006

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

H -1.494578 0.497337 0.000000
C -0.402762 0.385740 0.000000
C -0.112137 -1.050895 0.000000
C 0.141538 -2.226011 0.000000
H 0.361479 -3.265166 0.000000
C 0.141538 1.060591 1.274591
C 0.141538 1.060591 -1.274591
H -0.121966 2.121770 1.281913
H -0.271032 0.595988 2.172321
H 1.230409 0.976104 1.318597
H -0.121966 2.121770 -1.281913
H 1.230409 0.976104 -1.318597
H -0.271032 0.595988 -2.172321

TRANSITION STATE

C -0.728605 -1.270792 -0.333460
C -1.859422 -0.813757 0.419059
S -3.049058 0.188145 -0.140436
C 1.344003 0.443965 0.038745
C 1.133255 1.396455 -1.128030
C 2.488858 -0.398815 -0.044159
C 3.430668 -1.151544 -0.121484
C 1.035137 1.012422 1.413798
H -1.905439 -1.139027 1.459983
H -0.253341 -2.189101 0.012586
H -0.808463 -1.184498 -1.415221
H 0.279052 -0.441997 -0.113951
H 4.270446 -1.799129 -0.187819
H 0.125854 1.818282 -1.102663
H 1.850014 2.224044 -1.070413
H 1.279900 0.893293 -2.085121
H 0.016349 1.407503 1.446022
H 1.145956 0.256839 2.193494
H 1.721243 1.835854 1.643277

Frequencies = -1520.27, 20.9931, 50.0835, 101.207, 114.997, 175.281, 178.186, 190.045, 221.221, 299.581, 341.085, 377.899, 411.417, 556.808, 585.143, 633.981, 670.197, 681.478, 774.218, 841.06, 882.441, 955.087, 977.108, 1002.14, 1068.35, 1085.15, 1128.36, 1191.87, 1199.42, 1266.26, 1350.49, 1376.94, 1397.28, 1400.12, 1417.17, 1474.29, 1478.56, 1480.1, 1498.02, 1498.79, 2153.62, 3014.64, 3018.39, 3075.49, 3078.92, 3083.13, 3084.11, 3112.58, 3116.72, 3168.24, 3471.63
cos = 3.26, .33, .78, .07, .23
sin = -.43, .61, -.14, .06, .02
barrier = 4.61
Substituted frequency = 21.12 (from rotational profile)
Reduced moment of inertia = 206.030

Reaction66

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

TRANSITION STATE

C 1.312195 1.562442 -0.355007
C 1.580862 0.203279 -0.698834
S 2.007254 -0.967997 0.386649
C -1.312536 1.562375 0.354948
C -1.581135 0.203209 0.698857

S -2.006929 -0.968281 -0.386623
H -1.719444 1.918242 -0.588712
H -1.301369 2.293019 1.162088
H -0.000123 1.527072 0.000001
H -1.431646 -0.078536 1.740978
H 1.300709 2.293008 -1.162209
H 1.719311 1.918437 0.588517
H 1.431048 -0.078626 -1.740865

Frequencies = -1578.53, 30.5337, 62.0729, 70.5668, 238.775, 266.865, 387.208, 396.883, 445.966, 547.653, 738.551, 837.978, 847.083, 890.98, 951.366, 986.896, 1082.31, 1090.75, 1130.25, 1175.98, 1258.37, 1297.13, 1333.14, 1362.08, 1405.1, 1476.5, 1478.26, 3089.66, 3090.32, 3107.76, 3107.8, 3182.63, 3184.11
cos = 2.11, 3.23, 1.35, .79, .41
sin = -2.05, -.16, .45, .05, .07
barrier = 7.62
Substituted frequency = 38.43 (from rotational profile)
Reduced moment of inertia = 169.106

Reaction67

REACTANT 1

C -1.327332 0.192629 0.000000
C 0.000000 0.890905 0.000000
S 1.475337 0.219519 0.000000
H -0.077991 1.981482 0.000000
C -1.311691 -1.331367 0.000000
H -1.883617 0.577607 0.867672
H -1.883617 0.577607 -0.867672
H -2.333686 -1.718270 0.000000
H -0.796169 -1.721869 -0.879633
H -0.796169 -1.721869 0.879633

REACTANT 2

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 1

C -2.363629 0.049719 0.000009
C -0.939547 -0.390541 -0.000022
C 0.137524 0.455049 -0.000015
S 1.751584 -0.074704 0.000008
H -0.049834 1.528545 -0.000028
H -0.742501 -1.459462 -0.000028
H -2.889317 -0.347800 0.876519
H -2.460269 1.136849 -0.000232
H -2.889508 -0.348227 -0.876186

PRODUCT 2

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

TRANSITION STATE

C 0.932449 -1.507891 0.847807
C 1.743046 -0.343297 0.748148
S 2.436212 0.196021 -0.657263
C -1.585846 -0.701910 0.208521
C -1.350946 0.539850 -0.475688
S -1.093215 1.987570 0.268743
H -1.933012 -0.581521 1.235360
C -2.170958 -1.878577 -0.545066
H -0.327177 -1.043188 0.505936
H -1.272682 0.485809 -1.562871
H 0.740676 -1.909141 1.841473
H 1.026765 -2.245968 0.054500
H 1.863348 0.252201 1.652516
H -2.021930 -2.812576 0.002039
H -3.249721 -1.748047 -0.679820
H -1.720693 -1.984073 -1.535152

Frequencies = -1532.53, 29.6032, 45.9816, 62.2354, 171.393, 173.795, 247.305, 264.962, 275.507, 397.732, 424.665, 466.767, 647.757, 838.147, 863.491, 873.683, 891.504, 959.496, 1005.4, 1043.92, 1082.08, 1094.95, 1127.42, 1182.91, 1232.99, 1285.22, 1314.52, 1347.37, 1390.51, 1415.05, 1435.61, 1478.64, 1488.44, 1499.81, 3024.76, 3081.39, 3089.18, 3090.26, 3097.22, 3110.56, 3112.18, 3182.73
cos = .16, 4.52, 1.23, .93, .30
sin = -2.75, .08, .44, .07, .06
barrier = 8.59
Substituted frequency = 31.99 (from rotational profile)
Reduced moment of inertia = 251.409

Reaction68

REACTANT 1

C -1.327332 0.192629 0.000000
C 0.000000 0.890905 0.000000
S 1.475337 0.219519 0.000000
H -0.077991 1.981482 0.000000
C -1.311691 -1.331367 0.000000
H -1.883617 0.577607 0.867672
H -1.883617 0.577607 -0.867672
H -2.333686 -1.718270 0.000000
H -0.796169 -1.721869 -0.879633
H -0.796169 -1.721869 0.879633

REACTANT 2

C -2.363629 0.049719 0.000009
C -0.939547 -0.390541 -0.000022
C 0.137524 0.455049 -0.000015
S 1.751584 -0.074704 0.000008
H -0.049834 1.528545 -0.000028
H -0.742501 -1.459462 -0.000028
H -2.889317 -0.347800 0.876519
H -2.460269 1.136849 -0.000232
H -2.889508 -0.348227 -0.876186

PRODUCT 1

C -2.363629 0.049719 0.000009
C -0.939547 -0.390541 -0.000022
C 0.137524 0.455049 -0.000015
S 1.751584 -0.074704 0.000008
H -0.049834 1.528545 -0.000028
H -0.742501 -1.459462 -0.000028
H -2.889317 -0.347800 0.876519
H -2.460269 1.136849 -0.000232
H -2.889508 -0.348227 -0.876186

PRODUCT 2

C -1.327332 0.192629 0.000000
C 0.000000 0.890905 0.000000
S 1.475337 0.219519 0.000000
H -0.077991 1.981482 0.000000
C -1.311691 -1.331367 0.000000
H -1.883617 0.577607 0.867672
H -1.883617 0.577607 -0.867672
H -2.333686 -1.718270 0.000000
H -0.796169 -1.721869 -0.879633
H -0.796169 -1.721869 0.879633

TRANSITION STATE

C -1.348055 1.007507 0.167169
C -1.668911 -0.376541 0.347509
S -1.827957 -1.471216 -0.879888
C 1.349040 1.006583 -0.167153
C 1.668888 -0.377700 -0.347509
S 1.826411 -1.472660 0.879822
H 1.559308 1.387562 0.833050
C 1.561525 1.986075 -1.302064
H 0.000463 0.924015 0.000000
H 1.748684 -0.727903 -1.377566
C -1.559682 1.987091 1.302159
H -1.558200 1.388698 -0.832980
H -1.748538 -0.726796 1.377560
H 1.002615 2.911088 -1.140420
H 2.619971 2.255964 -1.380861
H 1.252542 1.560555 -2.259810
H -1.000000 2.911646 1.140562
H -2.617901 2.257865 1.380995
H -1.251036 1.561224 2.259859

Frequencies = -1530.93, 28.8041, 46.8849, 58.3652, 149.536, 168.825, 180.407, 187.173, 239.232, 281.059, 284.166, 303.646, 422.998, 433.092, 511.019, 848.245, 861.962, 868.707, 889.684, 890.121, 961.143, 1002.22, 1033.58, 1069.14, 1085.9, 1099.88, 1124, 1190.66, 1221.75, 1277.9, 1297.14, 1317.95, 1383.32, 1412.64, 1413.93, 1428.06, 1442.6, 1488.12, 1489.85, 1497.49, 1501.79, 3023.66, 3023.79, 3079.44, 3080.28, 3093.03, 3093.35, 3096.94, 3097.11, 3111.36, 3111.68
cos = -1.54, 7.58, 1.18, .91, .06
sin = -4.62, -.09, .81, .39, .07
barrier = 13.20
Substituted frequency = 26.23 (from rotational profile)
Reduced moment of inertia = 402.012

Reaction69

REACTANT 1

C 0.132027 -0.835770 0.000000
C -0.358696 0.583412 0.000000
S 0.548402 1.925752 0.000000
H -1.449374 0.681652 0.000000
H 1.225030 -0.815693 0.000000
C -0.358696 -1.557557 1.271321
C -0.358696 -1.557557 -1.271321
H -0.004581 -2.591851 1.273036
H 0.013651 -1.067890 2.173865
H -1.451930 -1.576841 1.318633
H -0.004581 -2.591851 -1.273036
H -1.451930 -1.576841 -1.318633
H 0.013651 -1.067890 -2.173865

REACTANT 2

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 1

C 0.821897 -0.025137 0.000086
C -0.378047 -0.711838 -0.000009
S -1.929833 -0.032719 -0.000199
H -0.315203 -1.799063 0.000046
C 0.921964 1.466291 0.000032
C 2.115592 -0.784099 0.000254
H 1.483398 1.807508 -0.877872
H -0.059619 1.936413 -0.000109
H 1.483179 1.807583 0.878048
H 2.717700 -0.518090 -0.876885
H 2.717517 -0.518016 0.877498
H 1.961914 -1.864141 0.000284

PRODUCT 2

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

TRANSITION STATE

C -1.007480 -1.571794 0.628815
C -1.893141 -0.473934 0.796219
S -2.825810 0.171070 -0.413348
C 1.401718 -0.573210 -0.162533
C 1.017569 0.716827 -0.709000
S 0.874856 2.131800 0.114516
C 2.157520 -0.608791 1.153154
C 1.833839 -1.619037 -1.179957
H 0.189677 -0.975875 0.200394
H 0.736431 0.703570 -1.763347
H -1.160508 -2.203629 -0.242735
H -0.652256 -2.079972 1.523629
H 2.167609 -1.620345 1.566462
H 3.196687 -0.302401 0.992438
H 1.724546 0.076853 1.881769
H 2.873236 -1.446291 -1.480202
H 1.780522 -2.625550 -0.757156
H 1.214722 -1.588309 -2.079570
H -1.915560 -0.004341 1.779453

Frequencies = -1510.35, 29.3069, 39.0147, 62.4924, 133.921, 167.011, 191.552, 219.435, 238.256, 247.104, 345.183, 356.639, 401.316, 464.662, 540.176, 681.952, 782.533, 839.193, 874.722, 896.03, 955.713, 962.067, 1003.61, 1029.8, 1081.72, 1087.54, 1139.12, 1180.14, 1209.08, 1267.54, 1316.87, 1337.33, 1368.51, 1388.58, 1404.05, 1424.78, 1476.41, 1480.61, 1484.37, 1498.03, 1505.8, 3019.82, 3027.64, 3078.54, 3085.09, 3087.57, 3090.23, 3103.43, 3105.69, 3123.2, 3185.42
cos = -1.11, 3.01, .76, .72, .21
sin = 1.85, -.06, -.15, -.15, .04
barrier = 5.23
Substituted frequency = 25.89 (from rotational profile)
Reduced moment of inertia = 256.766

Reaction70

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

TRANSITION STATE

C -1.574535 0.432956 0.812885
S -2.720270 -0.397863 -0.228988
C 0.656565 1.151712 -0.606375
C 1.829870 0.724428 0.119590
S 2.521619 -0.765277 0.036525
H 0.542914 2.230596 -0.722039
H -0.367450 0.838885 0.088222
H 0.442852 0.590765 -1.515440
H 2.249135 1.450521 0.819442
H -1.968457 1.388168 1.149499
H -1.113196 -0.165178 1.594041
H -2.078778 -1.578086 -0.290931

Frequencies = -1389.35, 17.8612, 62.0032, 109.738, 202.866, 269.126, 394.921, 455.089, 525.549, 680.586, 779.132, 841.091, 865.394, 874.112, 1030.25, 1052, 1095.5, 1120.17, 1187.71, 1363.74, 1384.03, 1418.48, 1434.57, 1471.92, 2668.69, 3066.99, 3076.45, 3098.23, 3153.51, 3200.81
cos = .63, 1.19, -.17, -.03, -.03
sin = -.23, -.06, .17, .04, .02
barrier = 1.79
Substituted frequency = 11.42 (from rotational profile)
Reduced moment of inertia = 104.081

Reaction71

REACTANT 1

C -1.327332 0.192629 0.000000

C 0.000000 0.890905 0.000000
S 1.475337 0.219519 0.000000
H -0.077991 1.981482 0.000000
C -1.311691 -1.331367 0.000000
H -1.883617 0.577607 0.867672
H -1.883617 0.577607 -0.867672
H -2.333686 -1.718270 0.000000
H -0.796169 -1.721869 -0.879633
H -0.796169 -1.721869 0.879633

REACTANT 2

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 1

C -2.363629 0.049719 0.000009
C -0.939547 -0.390541 -0.000022
C 0.137524 0.455049 -0.000015
S 1.751584 -0.074704 0.000008
H -0.049834 1.528545 -0.000028
H -0.742501 -1.459462 -0.000028
H -2.889317 -0.347800 0.876519
H -2.460269 1.136849 -0.000232
H -2.889508 -0.348227 -0.876186

PRODUCT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

TRANSITION STATE

C -1.860985 0.259557 0.982828
S -2.521439 -0.586105 -0.408010
C 0.696216 1.166129 0.447421
C 1.601744 0.084656 0.801640
S 2.266696 -1.027523 -0.208174
H 0.749910 1.989919 1.165900
H -0.449813 0.707244 0.727020
C 0.591588 1.620022 -0.995819
H 1.809792 -0.003671 1.870672
H -2.377604 1.199572 1.155901
H -1.699331 -0.336661 1.876805
H -1.841962 -1.736569 -0.257124
H -0.195865 2.369359 -1.107764
H 1.535072 2.063683 -1.328251
H 0.374322 0.782997 -1.660630

Frequencies = -1302.64, 21.0716, 49.0919, 97.4601, 143.07, 170.593, 226.148, 274.648, 340.261, 464.701, 536.142, 578.339, 772.837, 783.638, 840.759, 870.864, 902.246, 972.29, 1060.53, 1083.04, 1100.28, 1123.48, 1184.62, 1317.77, 1374.91, 1381.17, 1409.12, 1420.21, 1426.06, 1482.49, 1495.6, 2670.26, 3030.91, 3050.31, 3072.68, 3088.67, 3097.91, 3117.19, 3200.46
cos = .25, .10, .41, .12, .07
sin = -.28, -.25, .17, .06, .01
barrier = 1.19
Substituted frequency = 18.47 (from rotational profile)
Reduced moment of inertia = 118.322

Reaction72

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

TRANSITION STATE

H -0.913675 0.099554 1.686895
C -1.026366 0.330062 0.625272
S -2.094794 -0.550562 -0.254909

C -0.153486 1.370853 0.110906
H 0.136469 2.125691 0.844439
H 0.936322 0.848044 -0.178557
C 2.267869 0.261900 -0.591570
H 2.032752 0.032580 -1.628065
H 2.914646 1.126910 -0.465127
C 2.463118 -0.895414 0.340636
H -0.471615 1.798559 -0.838692
H 3.370883 -1.457193 0.079502
H 2.575529 -0.569221 1.378018
H 1.628579 -1.600346 0.288671

Frequencies = -1158.39, 37.6382, 62.2745, 111.102, 149.674, 267.364, 388.117, 428.45, 537.265, 701.109, 817.758, 840.722, 868.95, 903.91, 1035.47, 1070.41, 1094.69, 1137.6, 1214.72, 1218.89, 1367.84, 1387.55, 1405.31, 1426.29, 1467.19, 1471.9, 1484.22, 1491.21, 2991.19, 3055.14, 3064.68, 3076.09, 3092.2, 3098.33, 3151.62, 3185.97
cos = .87, .55, .21, .04, .05
sin = .42, .13, -.10, .01, -.01
barrier = 1.62
Substituted frequency = 22.69 (from rotational profile)
Reduced moment of inertia = 66.750

Reaction73

REACTANT 1

C 0.000000 0.619438 0.000000
S 0.876535 -0.742834 0.000000
C -1.489657 0.715256 0.000000
H 0.521754 1.579998 0.000000
H -1.958447 -0.268040 0.000000
H -1.824962 1.282607 0.877050
H -1.824962 1.282607 -0.877050

REACTANT 2

C 0.000000 1.486187 -0.014859
C 0.000000 0.000000 0.149312
C 1.287076 -0.743093 -0.014859
C -1.287076 -0.743093 -0.014859
H 0.000000 1.783483 -1.079233
H 0.886704 1.944418 0.434881
H -0.886704 1.944418 0.434881
H -1.240564 -1.740117 0.434881
H -2.127268 -0.204301 0.434881
H -1.544541 -0.891741 -1.079233
H 1.240564 -1.740117 0.434881
H 1.544541 -0.891741 -1.079233
H 2.127268 -0.204301 0.434881

PRODUCT 1

C 1.346643 0.927884 0.000000
H 1.752961 1.934400 0.000000
H 2.041117 0.095867 0.000000
H -0.667474 1.571777 0.000000
C 0.000000 0.712273 0.000000
S -0.700404 -0.840186 0.000000

PRODUCT 2

C 0.000000 0.000000 0.371940
C 0.000000 1.461427 -0.095749
C -1.265633 -0.730714 -0.095749
C 1.265633 -0.730714 -0.095749
H 0.000000 0.000000 1.469892
H 0.884045 1.995279 0.265249
H 0.000000 1.519937 -1.189845
H -0.884045 1.995279 0.265249
H -1.285940 -1.763245 0.265249
H -2.169985 -0.232035 0.265249
H -1.316304 -0.759968 -1.189845
H 1.285940 -1.763245 0.265249
H 1.316304 -0.759968 -1.189845
H 2.169985 -0.232035 0.265249

TRANSITION STATE

H -1.820151 1.177613 1.345786
C -1.739864 0.743174 0.347103
S -2.794754 -0.452329 -0.069508
C -0.662433 1.245642 -0.471550
H -0.345694 2.265912 -0.247555
H 0.391717 0.591959 -0.193717
C 1.635152 -0.148647 0.027082
C 2.704604 0.891700 -0.198963
C 1.434087 -0.591194 1.454934
C 1.544018 -1.237771 -1.013450
H -0.765512 1.048110 -1.537504
H 2.406054 -1.916286 -0.930641
H 0.640455 -1.839304 -0.888571
H 1.549082 -0.830324 -2.027934
H 2.269854 -1.228153 1.778965
H 1.389171 0.259160 2.141120
H 0.517689 -1.176536 1.569214
H 3.702344 0.452872 -0.051196
H 2.675122 1.288019 -1.217733
H 2.612545 1.726790 0.500961

Frequencies = -1215.56, 27.8828, 55.7611, 106.319, 133.335, 172.069, 195.016, 206.716, 219.44, 303.487, 376.695, 379.288, 397.048, 580.78, 646.089, 797.177, 837.299, 874.075, 936.429, 939.986, 970.369, 1007.34, 1014.83, 1066.87, 1093.63, 1164.06, 1210.64, 1271.02, 1273.71, 1371.36, 1391.85, 1399.22, 1406.24, 1418.37, 1437.17, 1468.37, 1470.31, 1479.7, 1480.97, 1494.82, 1495.61, 1507.51, 2979.87, 2982.64, 2989.7, 3054.04, 3057.82, 3061.65, 3064.68, 3076.16, 3091.46, 3095.74, 3101, 3152.13
cos = .05, .06, .92, .05, .07
sin = 0, 0, -.11, .01, .02
barrier = 1.08
Substituted frequency = 18.06 (from rotational profile)

Reduced moment of inertia = 170.589

Reaction74

REACTANT 1

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C -1.666874 -0.359382 -0.061911
C -0.610249 0.646879 0.090364
S 1.117950 -0.106542 -0.076867
H -0.615395 1.386684 -0.712455
H -0.643518 1.167364 1.046411
H 1.008288 -0.948225 0.965098
H -1.917446 -0.743280 -1.042640
H -2.056393 -0.882848 0.802736

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C -0.659832 0.699894 -0.059184
C 0.259703 -0.480525 0.084225
S 2.058508 -0.051458 -0.077348
H 0.116910 -0.999536 1.032849
H 0.102134 -1.206865 -0.716425
H 2.121855 0.758354 0.993830
H -1.902072 0.260303 -0.024878
H -0.583420 1.210115 -1.019094
H -0.614834 1.408440 0.769080
C -3.221423 -0.184811 0.003953
H -3.331490 -0.782024 -0.898044
H -3.300964 -0.758892 0.924075
H -3.814944 0.726081 0.002216

Frequencies = -1616.85, 33.7382, 70.8354, 98.9467, 210.189, 274.366, 378.533, 472.466, 559.33, 664.611, 682.47, 758.672, 895.622, 1038.47, 1081.25, 1125.35, 1142.65, 1285.47, 1287.9, 1382.95, 1387.02, 1443.91, 1444.58, 1468.21, 1480.32, 2662.87, 3056.36, 3057.28, 3070.95, 3101.71, 3145.91, 3189.34, 3190.7
cos = .01, .01, .24, .01, .01
sin = 0, 0, .03, 0, 0
barrier = 0.26
Substituted frequency = 33.74 (from HO analysis)
Reduced moment of inertia = 10.431

Reaction75

REACTANT 1

C 2.437725 -0.058335 0.000000
C 1.006539 0.396140 0.000000
C -0.039200 -0.428417 0.000000
S -1.763051 -0.014461 0.000000
H 0.839581 1.471339 0.000000
H 0.098431 -1.505959 0.000000
H -1.617702 1.322039 0.000000
H 2.972334 0.317905 -0.879443
H 2.972192 0.317906 0.879572
H 2.513607 -1.148175 0.000000

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C -2.422802 0.046977 0.000244
C -1.114586 -0.372293 -0.000189
C -0.006881 0.472983 -0.000154
S 1.672537 -0.005660 0.000000
H -0.925672 -1.444303 -0.000290
H -0.129994 1.550287 -0.000177
H 1.478381 -1.336431 0.000240
H -3.237366 -0.665062 0.000414
H -2.680330 1.100065 0.000375

TRANSITION STATE

C 1.491843 1.063646 -0.037584
C 0.172943 0.591254 0.401519
C -0.824558 0.253820 -0.430752
S -2.419593 -0.381679 -0.016297
H 0.026380 0.471359 1.473107

H -0.714466 0.361576 -1.505809
H -2.246675 -0.425530 1.316347
H 1.942850 1.805807 0.623332
H 2.329027 0.124859 -0.000855
H 1.528035 1.393733 -1.076927
C 3.367196 -0.948573 -0.018041
H 3.444720 -1.226294 1.029164
H 2.913261 -1.698762 -0.658702
H 4.245808 -0.460765 -0.429767

Frequencies = -1435.69, 32.8165, 64.0476, 112.384, 224.653, 251.956, 253.516, 357.356, 399.43, 492.112, 560.52, 672.741, 760.649, 793.186, 950.092, 955.579, 1012.26, 1066.01, 1103.82, 1152.04, 1299.82, 1325.38, 1401.71, 1407.77, 1432.34, 1433, 1467.9, 1634.56, 2667.16, 3059.46, 3064.13, 3117.96, 3134.26, 3157.08, 3206.76, 3209.05
cos = 0, 0, .29, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.29
Substituted frequency = 32.82 (from HO analysis)
Reduced moment of inertia = 11.720

Reaction76

REACTANT 1

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

REACTANT 2

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

PRODUCT 1

C 1.232501 1.268150 0.000000
C 0.000000 0.849234 0.000000
S -0.588583 -0.856356 0.000000
H 2.248466 0.910357 0.000000
H -0.844615 1.534149 0.000000
H 0.618476 -1.447103 0.000000

PRODUCT 2

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

TRANSITION STATE

C 0.661915 -0.633669 0.000477
C -0.260507 0.307681 -0.000217
S -2.037728 0.118717 -0.000267
H 1.965672 -0.229229 0.000340
H 0.537743 -1.710206 0.001155
H 0.003190 1.362155 -0.000868
H -2.062258 -1.225059 0.000543
C 3.214693 0.176539 0.000185
H 3.162563 1.263324 -0.001189
H 3.649817 -0.230752 0.910120
H 3.650316 -0.233019 -0.908493

Frequencies = -1546.79, 19.6926, 98.2163, 99.8293, 256.856, 309.915, 465.361, 479.764, 596.287, 684.598, 697.556, 915.239, 919.298, 1085.88, 1186.13, 1232.96, 1286.21, 1376.06, 1441.61, 1454.85, 1625.09, 2672, 3055.62, 3142.11, 3182.08, 3184.78, 3186.37
cos = 0, 0, .17, 0, 0
sin = 0, 0, 0, 0, 0
barrier = 0.16
Substituted frequency = 19.69 (from HO analysis)
Reduced moment of inertia = 9.712

Reaction40

REACTANT 1

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

REACTANT 2

C 1.650140 -0.350957 -0.052298
C 0.503087 0.643515 0.090543
S -1.171828 -0.100377 -0.080954
H 0.551662 1.178189 1.040536
H 0.537320 1.392866 -0.703596
H -1.095818 -0.912980 0.987742
H 1.599963 -0.873197 -1.009835
H 2.612680 0.167673 0.009282
H 1.624076 -1.101871 0.741667

PRODUCT 1

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

PRODUCT 2

C -1.683734 -0.249204 0.034496
C -0.455990 0.583549 -0.114113
S 1.155602 -0.058278 0.038605
H -0.494973 1.657824 0.016409
H 0.893568 -1.312027 -0.377328
H -1.855256 -0.561790 1.076166
H -2.566939 0.307395 -0.289945
H -1.627682 -1.165027 -0.565273

TRANSITION STATE

C -1.898751 0.627707 0.418190
C 0.665101 0.409354 -0.454469
C 1.402626 1.650950 0.002654
S 1.347277 -1.178647 0.059355
H 0.541293 0.352871 -1.537599
H 0.898020 2.549463 -0.366427
H 1.436698 1.711927 1.094605
H 2.434488 1.664293 -0.362911
H -0.576132 0.504927 -0.019107
C -2.678580 -0.492720 -0.225908
H -1.787676 0.555361 1.500651
H -2.177808 1.634552 0.106351
H 1.400013 -0.917518 1.378607
H -3.725349 -0.499152 0.106089
H -2.688768 -0.401052 -1.316057
H -2.253590 -1.469081 0.023323

Frequencies = -1660.57, 26.5491, 77.3941, 127.251, 185.207, 192.646, 216.764, 253.574, 329.144, 462.265, 565.461, 673.083, 824.946, 871.327, 888.739, 909.698, 1014.82, 1041.33, 1084.37, 1137.03, 1158.31, 1225.09, 1302.02, 1403.45, 1406.36, 1412.74, 1436.22, 1464.04, 1486.43, 1491.56, 1492.52, 1493.75, 2650.85, 2993.99, 3013.14, 3051.04, 3066.21, 3071.07, 3076.54, 3082.49, 3093.85, 3139.54
cos = 1.07, -.20, .59, .12, .02
sin = .05, -.06, .07, .01, .03
barrier = 1.72
Substituted frequency = 24.45 (from rotational profile)
Reduced moment of inertia = 67.271

Reaction77

REACTANT 1

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

REACTANT 2

C -0.231045 -1.003023 0.000000
S 0.000000 0.815120 0.000000
C 1.819011 0.898786 0.000000
H 0.258801 -1.416127 0.885912
C -1.718608 -1.346806 0.000000
H 0.258801 -1.416127 -0.885912
H 2.235252 0.430102 -0.893849
H 2.086858 1.956027 0.000000
H 2.235252 0.430102 0.893849
H -1.854919 -2.431670 0.000000
H -2.218096 -0.943987 0.884465
H -2.218096 -0.943987 -0.884465

PRODUCT 1

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

PRODUCT 2

S 0.491290 -0.615357 0.032517
C 1.954305 0.465737 -0.049597
H 1.940928 1.051893 -0.968648
H 1.992892 1.124962 0.818778
H 2.829839 -0.183737 -0.044297
C -0.793793 0.545786 0.007098
C -2.207643 0.067765 -0.042449
H -0.565615 1.545712 0.359930
H -2.601062 -0.209490 0.947814
H -2.861949 0.851010 -0.437189
H -2.312886 -0.810372 -0.686970

TRANSITION STATE

C 2.062122 -0.544695 0.717865
C -0.298088 0.812432 0.535616
C 0.083373 2.195495 0.042628
S -1.430550 -0.027438 -0.574372
C -1.825522 -1.507698 0.409955
H 0.847171 2.628477 0.694774
H -0.684144 0.814701 1.558508
H 0.491073 2.158349 -0.971460
H -0.774250 2.876418 0.032874
H 0.816544 0.124175 0.626122
H 1.803774 -1.446700 1.273760
C 2.550046 -0.774111 -0.692216
H 2.664576 0.137386 1.318459
H -2.533666 -2.096258 -0.174122
H -0.932158 -2.105764 0.594289
H -2.290683 -1.230225 1.357543
H 3.489114 -1.344004 -0.709586
H 1.820475 -1.335908 -1.282748
H 2.739393 0.169827 -1.211541

Frequencies = -1653.23, 25.5575, 69.0358, 77.2793, 109.269, 163.422, 175.204, 188.175, 209.682, 286.601, 356.461, 454.704, 552.76, 686.94, 720.495, 836.463, 851.515, 928.894, 970.233, 972.189, 1017.47, 1040.46, 1091.56, 1104.93, 1154.09, 1223.52, 1278.02, 1357.88, 1405.23, 1407.78, 1417.32, 1442.1, 1464.38, 1470.38, 1484.21, 1487.7, 1491.88, 1492.19, 1498.78, 2989.23, 3016.39, 3036.8, 3049.5, 3052.25, 3065.32, 3073.41, 3080.58, 3090.2, 3114.6, 3130.59, 3137.49
cos = .13, .72, .23, .22, .05
sin = 0, -.12, .09, .10, -.04
barrier = 1.20
Substituted frequency = 23.99 (from rotational profile)
Reduced moment of inertia = 85.393

Reaction78

REACTANT 1

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

REACTANT 2

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

PRODUCT 1

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

PRODUCT 2

C 1.748228 0.124075 0.039321
C 0.565049 -0.440481 -0.067799
S -1.053621 0.123840 -0.050080
H 2.653636 -0.427995 -0.197380
H 1.877846 1.151585 0.382815
H -1.553214 -0.806591 0.786707

TRANSITION STATE

C -1.945222 0.163617 0.671619
C 0.661561 0.534080 0.121102
C 0.990978 1.778588 -0.192629
S 1.668119 -0.891878 -0.060299
H 0.245988 2.567995 -0.165002
H 1.999732 2.063272 -0.481729
H -0.641275 0.316576 0.443724
H 1.264383 -1.524107 1.057267
H -2.278958 1.179467 0.886180
C -2.562552 -0.470274 -0.553389
H -1.958938 -0.455778 1.569709
H -3.638186 -0.637777 -0.414884
H -2.442572 0.164295 -1.435448
H -2.108669 -1.439961 -0.775263

Frequencies = -1596.19, 30.0577, 81.2301, 105.142, 175.975, 202.196, 299.165, 309.033, 463.209, 557.751, 637.74, 721.726, 845.218, 886.782, 905.721, 957.506, 1026.28, 1078.94, 1162.22, 1225.18, 1304.02, 1401.05, 1408.99, 1421.1, 1465.28, 1491.35, 1494.89, 1655.23, 2646.47, 3003.67, 3057.83, 3067.84, 3088.3, 3104.8, 3136.54, 3184.39
cos = .25, .28, .33, .11, -.02
sin = .01, -.02, .07, -.01, .01
barrier = 0.72
Substituted frequency = 30.06 (from HO analysis)
Reduced moment of inertia = 67.680

Reaction79

REACTANT 1

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

REACTANT 2

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935
C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

PRODUCT 1

C 0.000000 0.000000 0.764767

H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

PRODUCT 2

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000
H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

TRANSITION STATE

C -2.099267 0.080151 0.748159
C 0.623664 -0.056462 0.497187
C 1.058739 1.048058 -0.373200
C 1.612759 2.185108 0.062861
S 1.018674 -1.688551 -0.200991
H 0.177387 -2.402134 0.569335
H -0.643606 -0.006488 0.604316
H 0.973290 0.043407 1.525756
H 0.867357 0.922408 -1.436811
H 1.866239 2.987077 -0.620271
H 1.830129 2.347711 1.113795
H -2.342345 -0.899098 1.158293
H -2.190893 0.880967 1.480372
C -2.619571 0.373750 -0.632451
H -3.714220 0.469424 -0.635788
H -2.216020 1.312921 -1.021896
H -2.364042 -0.423008 -1.336584

Frequencies = -1522.57, 32.6762, 75.864, 86.5413, 127.825, 165.518, 191.028, 251.766, 270.812, 403.467, 480.067, 553.029, 636.573, 764.456, 840.355, 870.587, 900.759, 924.441, 964.116, 1015.88, 1027.46, 1056.66, 1141.07, 1168.91, 1221.54, 1239.34, 1318.65, 1359.35, 1404.93, 1428.55, 1453.48, 1466.53, 1489.15, 1492, 1660.11, 2650.13, 2988.99, 3051.28, 3079.5, 3083.32, 3085.67, 3129.72, 3135.96, 3159.48, 3218.44
cos = .96, .09, .49, .16, -.07
sin = -.74, -.09, .20, -.02, .02
barrier = 1.77
Substituted frequency = 19.11 (from rotational profile)
Reduced moment of inertia = 86.602

Reaction80

REACTANT 1

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

REACTANT 2

C -2.345361 0.600972 0.033244
C -1.474846 -0.321599 -0.370034
C -0.379493 -0.882954 0.479971
S 1.303157 -0.499297 -0.164209
C 1.342675 1.306065 0.069784
H -0.409632 -1.976236 0.487056
H -0.455109 -0.537577 1.514084
H -1.520494 -0.699652 -1.388565
H -3.117915 0.979484 -0.626309
H -2.322204 1.003923 1.041460
H 2.292027 1.650864 -0.341819
H 0.524428 1.788485 -0.465877
H 1.300534 1.564568 1.129522

PRODUCT 1

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

PRODUCT 2

C -2.733643 0.208185 0.000151
C -1.364780 0.354653 -0.000279
C -0.457171 -0.702180 -0.000006
S 1.278912 -0.645313 -0.000082
H -0.817828 -1.725961 0.000374
C 1.660113 1.131154 0.000186
H -0.971604 1.367247 -0.000877
H -3.387710 1.070151 -0.000183
H -3.198280 -0.771361 0.000821
H 2.747805 1.202929 0.000393
H 1.269076 1.615725 -0.895157
H 1.268838 1.615416 0.895624

TRANSITION STATE

C 1.176029 1.824420 0.722247
C -0.005775 -0.638277 0.381472
C 1.003743 -1.472155 -0.298064
C 1.790907 -2.363774 0.311750
S -1.524072 -0.465801 -0.581669
C -2.479290 0.639497 0.505382
H 0.493407 0.521019 0.532933

H -0.212791 -0.965720 1.403635
H 1.126447 -1.299930 -1.365544
H 2.549623 -2.912828 -0.233408
H 1.700762 -2.573266 1.373027
H 0.391798 2.454324 1.139736
H 1.929933 1.548181 1.458008
C 1.682867 2.205586 -0.642293
H 2.228055 3.159566 -0.618857
H 2.372841 1.453996 -1.036905
H 0.864039 2.320295 -1.358417
H -3.448154 0.786429 0.026923
H -2.634725 0.182981 1.484520
H -1.986963 1.605993 0.618087

Frequencies = -1499.98, 20.2143, 57.407, 79.7271, 86.1708, 123.028, 161.825, 166.561, 193.331, 265.466, 316.604, 400.865, 473.063, 552.046, 639.925, 705.995, 785.182, 838.53, 875.132, 924.039, 956.932, 964.375, 982.211, 1003.43, 1026.33, 1053.64, 1134.08, 1159.34, 1220.39, 1234.22, 1321.18, 1353, 1368.96, 1404.05, 1435.73, 1454.04, 1465.04, 1469.55, 1483.42, 1488.89, 1491.59, 1667.06, 2985.84, 3036.99, 3048.97, 3058.78, 3078.82, 3083.08, 3115.56, 3126.81, 3130.4, 3133.15, 3157.76, 3216.04
cos = 1.13, .77, .11, .18, -.20
sin = -1.37, .19, .15, -.03, .09
barrier = 2.86
Substituted frequency = 12.67 (from rotational profile)
Reduced moment of inertia = 95.161

Reaction81

REACTANT 1

C 0.000000 0.000000 0.000000
H 0.000000 1.080238 0.000000
H 0.935514 -0.540119 0.000000
H -0.935514 -0.540119 0.000000

REACTANT 2

C 0.981892 1.640379 0.795309
S 0.981892 0.339913 -0.493232
S -0.981892 -0.339913 -0.493232
C -0.981892 -1.640379 0.795309
H 1.983742 2.076655 0.777378
H 0.247197 2.408969 0.560125
H 0.792582 1.219645 1.782359
H -1.983742 -2.076655 0.777378
H -0.247197 -2.408969 0.560125
H -0.792582 -1.219645 1.782359

PRODUCT 1

C 0.000000 0.000000 0.000000
H 0.629745 0.629745 0.629745
H -0.629745 -0.629745 0.629745
H -0.629745 0.629745 -0.629745
H 0.629745 -0.629745 -0.629745

PRODUCT 2

C 1.765498 0.867708 -0.340662
S 0.911065 -0.570438 0.400827
S -1.015322 -0.425306 -0.442601
C -1.776759 0.824125 0.446336
H 2.766565 0.877945 0.096825
H 1.840163 0.758016 -1.421657
H 1.249320 1.791260 -0.081846
H -2.542678 1.396984 -0.059851
H -1.577687 0.956715 1.500869

TRANSITION STATE

C 2.352407 -0.443749 0.796908
H 2.957220 0.438950 0.594771
H 2.984672 -1.334302 0.759836
H 1.889762 -0.373496 1.780721
S 1.095002 -0.674572 -0.513191
S 0.025724 1.113808 -0.452264
C -1.236597 0.819154 0.782020
H -1.835617 1.727439 0.875535
H -0.849110 0.487636 1.744815
H -2.075927 -0.097167 0.392156
C -3.018934 -1.064486 0.006307
H -3.492539 -0.627507 -0.869167
H -2.412599 -1.940833 -0.206243
H -3.678731 -1.174018 0.863453

Frequencies = -1613.33, 34.8899, 42.7205, 74.0104, 125.198, 153.963, 228.286, 262.495, 342.511, 458.27, 480.848, 567.142, 663.486, 675.131, 721.503, 970.24, 972.38, 1001.85, 1050.74, 1130.21, 1348.47, 1380.22, 1395.67, 1406.54, 1437.48, 1443.26, 1461.43, 1478.82, 3039.76, 3058.24, 3059.01, 3122.25, 3141.81, 3144.25, 3193.66, 3198.47
cos = .01, .01, .49, .01, .01
sin = 0, 0, .05, 0, 0
barrier = 0.51
Substituted frequency = 34.89 (from HO analysis)
Reduced moment of inertia = 11.807

Reaction82

REACTANT 1

C 0.010147 -0.693349 0.000000
C 0.010147 0.794179 0.000000
H -1.012817 -1.105011 0.000000
H 0.506076 -1.101141 0.886082
H 0.506076 -1.101141 -0.886082
H -0.060551 1.351156 -0.926074
H -0.060551 1.351156 0.926074

REACTANT 2

C 0.981892 1.640379 0.795309

S 0.981892 0.339913 -0.493232
S -0.981892 -0.339913 -0.493232
C -0.981892 -1.640379 0.795309
H 1.983742 2.076655 0.777378
H 0.247197 2.408969 0.560125
H 0.792582 1.219645 1.782359
H -1.983742 -2.076655 0.777378
H -0.247197 -2.408969 0.560125
H -0.792582 -1.219645 1.782359

PRODUCT 1

C 0.000000 0.000000 0.764767
H 0.000000 1.018335 1.163569
H 0.881904 -0.509167 1.163569
H -0.881904 -0.509167 1.163569
C 0.000000 0.000000 -0.764767
H 0.000000 -1.018335 -1.163569
H -0.881904 0.509167 -1.163569
H 0.881904 0.509167 -1.163569

PRODUCT 2

C 1.765498 0.867708 -0.340662
S 0.911065 -0.570438 0.400827
S -1.015322 -0.425306 -0.442601
C -1.776759 0.824125 0.446336
H 2.766565 0.877945 0.096825
H 1.840163 0.758016 -1.421657
H 1.249320 1.791260 -0.081846
H -2.542678 1.396984 -0.059851
H -1.577687 0.956715 1.500869

TRANSITION STATE

C -2.532885 -0.794074 0.654296
C -3.395786 -0.362843 -0.507213
C -0.581925 1.067610 0.906367
S 0.502866 1.092790 -0.514320
S 1.433103 -0.774332 -0.474029
C 2.869338 -0.490260 0.624361
H 3.490525 0.317012 0.239244
H 3.438213 -1.423265 0.615592
H 2.549894 -0.274769 1.643415
H -1.131990 2.010531 0.928942
H -0.078513 0.864579 1.850970
H -1.525347 0.132156 0.782727
H -3.016682 -0.770970 1.631386
H -1.970133 -1.714695 0.501318
H -4.203366 -1.082478 -0.694963
H -3.866838 0.607150 -0.322281
H -2.813730 -0.283165 -1.429633

Frequencies = -1668.75, 24.6344, 37.3154, 70.4967, 86.657, 154.707, 158.098, 186.339, 241.382, 262.3, 454.557, 475.889, 481.085, 611.798, 675.16, 719.711, 845.172, 898.128, 970.192, 970.568, 997.787, 1034.3, 1058.47, 1161.9, 1225.69, 1347.2, 1401.98, 1402.83, 1408.55, 1419.62, 1460.93, 1467.05, 1479.12, 1491.42, 1493.9, 2997.63, 3039.73, 3052.48, 3058.1, 3069.7, 3083.05, 3122.18, 3141.76, 3144.86, 3145.34
cos = .28, .79, -.01, .11, .09
sin = -.26, .13, .11, -.13, .05
barrier = 1.55
Substituted frequency = 20.19 (from rotational profile)
Reduced moment of inertia = 90.491

Reaction83

REACTANT 1

C 0.010170 0.535277 0.000000
H -0.207782 1.597871 0.000000
C 0.010170 -0.197547 1.297818
C 0.010170 -0.197547 -1.297818
H 0.757439 -1.001216 -1.307030
H -0.960273 -0.683110 -1.499120
H 0.215195 0.464839 -2.142558
H 0.757439 -1.001216 1.307030
H 0.215195 0.464839 2.142558
H -0.960273 -0.683110 1.499120

REACTANT 2

C 0.981892 1.640379 0.795309
S 0.981892 0.339913 -0.493232
S -0.981892 -0.339913 -0.493232
C -0.981892 -1.640379 0.795309
H 1.983742 2.076655 0.777378
H 0.247197 2.408969 0.560125
H 0.792582 1.219645 1.782359
H -1.983742 -2.076655 0.777378
H -0.247197 -2.408969 0.560125
H -0.792582 -1.219645 1.782359

PRODUCT 1

C 0.000000 1.276840 -0.259553
C 0.000000 0.000000 0.585554
C 0.000000 -1.276840 -0.259553
H 0.882751 1.322941 -0.905415
H 0.000000 2.173102 0.367188
H -0.882751 1.322941 -0.905415
H -0.875663 0.000000 1.244299
H 0.875663 0.000000 1.244299
H 0.000000 -2.173102 0.367188
H -0.882751 -1.322941 -0.905415
H 0.882751 -1.322941 -0.905415

PRODUCT 2

C 1.765498 0.867708 -0.340662
S 0.911065 -0.570438 0.400827
S -1.015322 -0.425306 -0.442601
C -1.776759 0.824125 0.446336
H 2.766565 0.877945 0.096825

H 1.840163 0.758016 -1.421657
H 1.249320 1.791260 -0.081846
H -2.542678 1.396984 -0.059851
H -1.577687 0.956715 1.500869

TRANSITION STATE

C 0.264711 -0.464881 1.258842
S -1.056366 -1.221749 0.327295
S -1.813542 0.333919 -0.841561
C -3.071409 1.090486 0.252204
C 2.260132 0.443189 -0.336864
C 2.870084 -0.799717 -0.945895
C 3.160208 1.262659 0.561591
H -3.808052 0.348267 0.556185
H -3.559495 1.862918 -0.347238
H -2.610633 1.551522 1.125110
H 0.759086 -1.243552 1.842772
H -0.042221 0.381010 1.872674
H 1.243401 0.004503 0.438732
H 1.709170 1.048553 -1.060228
H 4.008947 1.677764 0.001116
H 2.626414 2.103916 1.012588
H 3.578245 0.653748 1.370496
H 3.676500 -0.543683 -1.646767
H 3.305929 -1.447367 -0.177636
H 2.128876 -1.382732 -1.498828

Frequencies = -1666.93, 14.4284, 28.6741, 59.8707, 87.2866, 146.645, 158.282, 162.244, 193.022, 225.352, 242.656, 262.443, 368.143, 472.498, 487.755, 536.87, 674.625, 723.189, 848.558, 883.749, 930.166, 947.672, 969.971, 971.845, 998.536, 1029.19, 1118.05, 1168.51, 1187.78, 1347.77, 1349.82, 1397.52, 1403.68, 1413.66, 1417.49, 1431.17, 1461.47, 1479.27, 1482.27, 1488.53, 1498.18, 1498.96, 2988.92, 2993.01, 3040.07, 3044.54, 3046.37, 3058.91, 3069.37, 3082.77, 3091.75, 3122.6, 3141.86, 3146.97
cos = .95, .63, -.48, .26, .17
sin = -.16, -.31, .22, 0, 0
barrier = 1.72
Substituted frequency = 14.59 (from rotational profile)
Reduced moment of inertia = 179.415

Reaction84

REACTANT 1

C 0.000000 1.486187 -0.014859
C 0.000000 0.000000 0.149312
C 1.287076 -0.743093 -0.014859
C -1.287076 -0.743093 -0.014859
H 0.000000 1.783483 -1.079233
H 0.886704 1.944418 0.434881
H -0.886704 1.944418 0.434881
H -1.240564 -1.740117 0.434881
H -2.127268 -0.204301 0.434881
H -1.544541 -0.891741 -1.079233
H 1.240564 -1.740117 0.434881
H 1.544541 -0.891741 -1.079233
H 2.127268 -0.204301 0.434881

REACTANT 2

C 0.981892 1.640379 0.795309
S 0.981892 0.339913 -0.493232
S -0.981892 -0.339913 -0.493232
C -0.981892 -1.640379 0.795309
H 1.983742 2.076655 0.777378
H 0.247197 2.408969 0.560125
H 0.792582 1.219645 1.782359
H -1.983742 -2.076655 0.777378
H -0.247197 -2.408969 0.560125
H -0.792582 -1.219645 1.782359

PRODUCT 1

C 0.000000 0.000000 0.371940
C 0.000000 1.461427 -0.095749
C -1.265633 -0.730714 -0.095749
C 1.265633 -0.730714 -0.095749
H 0.000000 0.000000 1.469892
H 0.884045 1.995279 0.265249
H 0.000000 1.519937 -1.189845
H -0.884045 1.995279 0.265249
H -1.285940 -1.763245 0.265249
H -2.169985 -0.232035 0.265249
H -1.316304 -0.759968 -1.189845
H 1.285940 -1.763245 0.265249
H 1.316304 -0.759968 -1.189845
H 2.169985 -0.232035 0.265249

PRODUCT 2

C 1.765498 0.867708 -0.340662
S 0.911065 -0.570438 0.400827
S -1.015322 -0.425306 -0.442601
C -1.776759 0.824125 0.446336
H 2.766565 0.877945 0.096825
H 1.840163 0.758016 -1.421657
H 1.249320 1.791260 -0.081846
H -2.542678 1.396984 -0.059851
H -1.577687 0.956715 1.500869

TRANSITION STATE

C -2.165751 0.237276 -0.008405
C -0.020252 -1.174139 -0.904888
S 1.319682 -1.329212 0.260244
S 1.964807 0.632841 0.572235
C 3.186682 0.878144 -0.768353
H 3.970073 0.123813 -0.711755
H 3.620631 1.866402 -0.597446
H 2.708871 0.860408 -1.747321
H -0.457641 -2.163373 -1.051664
H 0.250546 -0.696992 -1.846021
H -1.079054 -0.432171 -0.411000

C -2.064113 0.241772 1.505052
C -2.026528 1.608443 -0.643369
C -3.329007 -0.576656 -0.545485
H -2.872377 2.253938 -0.366585
H -1.109991 2.107228 -0.317110
H -2.010649 1.545591 -1.735923
H -4.287758 -0.109494 -0.279623
H -3.297685 -0.654162 -1.636712
H -3.336153 -1.589901 -0.132375
H -2.936661 0.741801 1.950227
H -2.027880 -0.773801 1.909821
H -1.172289 0.773614 1.846509

Frequencies = -1641.84, 19.2488, 33.7185, 59.1488, 91.8515, 118.024, 149.243, 156.98, 198.515, 222.384, 229.944, 232.045, 253.129, 325.443, 367.11, 375.205, 471.243, 503.546, 541.202, 675.103, 729.376, 790.182, 940.172, 942.822, 963.605, 969.661, 971.776, 986.747, 998.116, 1015.71, 1041.03, 1183.49, 1244.87, 1247.84, 1347.81, 1394.47, 1396.28, 1404.05, 1415.68, 1422.5, 1430.04, 1460.87, 1474.55, 1478.85, 1482.42, 1484.14, 1498.25, 1501, 1508.99, 2980.94, 2984.16, 2991.17, 3039.09, 3048.93, 3052, 3056.84, 3059.37, 3080.57, 3087.59, 3092.56, 3121.49, 3140.79, 3147.24
cos = .05, .05, 1.09, .04, .07
sin = 0, 0, .18, .01, .02
barrier = 1.24
Substituted frequency = 15.35 (from rotational profile)
Reduced moment of inertia = 266.464

Reaction85

REACTANT 1

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935
C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

REACTANT 2

C 1.085389 1.313238 0.036768
C 0.384580 0.008453 -0.166818
S -1.359504 -0.096411 0.035726
C 1.125045 -1.280188 0.007989
H -1.655216 1.176510 -0.281170
H 1.189097 1.567951 1.104198
H 2.094663 1.272829 -0.385000
H 0.556706 2.144567 -0.439850
H 2.079005 -1.245228 -0.528633
H 1.360984 -1.490121 1.064115
H 0.556743 -2.132957 -0.372915

PRODUCT 1

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000
H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

PRODUCT 2

C -0.416743 0.016648 0.401914
S 1.370091 -0.080624 -0.092069
C -1.092896 1.273450 -0.142201
C -1.091922 -1.265135 -0.089637
H -0.436704 0.030165 1.494167
H 1.749074 1.095395 0.437615
H -0.614345 -2.155502 0.325257
H -2.142662 -1.270770 0.214075
H -1.055862 -1.333473 -1.180727
H -2.143622 1.299170 0.167520
H -0.613112 2.182183 0.228997
H -1.054854 1.293045 -1.234244

TRANSITION STATE

C -2.831102 1.755871 -0.369805
C -2.224837 0.717264 0.223303
C -1.294018 -0.199499 -0.440906
S -1.449514 -1.915826 0.117086
C 1.258238 0.551161 0.180574
C 1.261354 0.529649 1.694793
C 1.403632 1.918342 -0.451425
S 2.348315 -0.729265 -0.476961
H 0.471051 1.182980 2.075739
H 1.085980 -0.474614 2.087801
H 2.215462 0.891984 2.098355
H -0.059278 0.151442 -0.134313
H -1.293779 -0.112465 -1.528782
H 2.249798 -0.389210 -1.774203
H -2.391056 0.543726 1.284743
H -3.470514 2.428979 0.188585
H -2.708647 1.959448 -1.428913
H 2.384971 2.354976 -0.227734
H 1.297095 1.879318 -1.538942
H 0.635544 2.593611 -0.062672
H -0.237029 -2.325442 -0.300871

Frequencies = -1682.55, 29.1053, 61.0642, 89.6105, 103.26, 155.588, 178.794, 193.354, 221.16, 238.413, 265.698, 286.638, 295.452, 322.029, 343.982, 426.884, 507.462, 642.346, 665.462, 767.9, 880.075, 899.637, 910.812, 921.216, 952.685, 965.107, 994.132, 1015.28, 1028.09, 1121.76, 1165.65, 1184.4, 1214.36,

1241.59, 1316.91, 1384.29, 1399.68, 1416.98, 1439.75, 1455.51, 1478.84, 1479.76, 1494.18, 1496.47, 1644.59, 2644.18, 2663.11, 2999.84, 3003.44, 3063.55, 3066.41, 3077.9, 3088.19, 3097.79, 3127.8, 3133.56, 3218.98
cos = 3.03, .85, 3.82, -.09, -.11
sin = .62, .37, -.65, -.26, .14
barrier = 6.74
Substituted frequency = 23.89 (from rotational profile)
Reduced moment of inertia = 320.908

Reaction86

REACTANT 1

C 0.000000 0.000000 1.337862
C 0.000000 0.000000 0.115777
C 0.000000 0.000000 -1.251352
H 0.000000 0.000000 2.400040
H 0.000000 0.929833 -1.806877
H 0.000000 -0.929833 -1.806877

REACTANT 2

C 1.275072 0.157942 -0.000791
C -0.003799 0.840478 0.061607
C 2.332294 -0.411226 -0.034669
H 3.266389 -0.915805 -0.072492
H -0.090502 1.423579 0.979934
H -0.113254 1.531514 -0.777702
S -1.469790 -0.282226 -0.079388
H -1.167393 -1.046849 0.983591

PRODUCT 1

C 2.361273 -0.341462 0.000000
C 1.253535 0.166078 0.000000
C 0.000000 0.724962 0.000000
S -1.495795 -0.181980 0.000000
H 3.330556 -0.775632 0.000000
H -0.140578 1.798264 0.000000
H -0.946110 -1.408414 0.000000

PRODUCT 2

C 0.000000 0.000000 -1.238052
H 0.000000 1.021022 -1.629805
H -0.884231 -0.510511 -1.629805
H 0.884231 -0.510511 -1.629805
C 0.000000 0.000000 0.219184
C 0.000000 0.000000 1.420084
H 0.000000 0.000000 2.482121

TRANSITION STATE

C 1.335382 -1.346404 -0.421577
C -0.800061 0.043176 0.540247
C -1.984336 -0.690974 0.248230
C -2.952137 -1.351389 -0.037266
S -0.751075 1.675064 -0.240864
H 0.471268 2.004604 0.214774
H 0.226018 -0.643257 0.060430
H -0.556395 0.084950 1.602223
H -3.816317 -1.922340 -0.273558
C 2.487838 -0.608309 -0.071831
H 1.214209 -2.308019 0.074744
H 1.088472 -1.371990 -1.481983
C 3.431123 0.072443 0.262093
H 4.283096 0.643768 0.537824

Frequencies = -1717.03, 21.4772, 49.7909, 118.661, 135.6, 182.267, 234.854, 342.363, 365.005, 390.332, 452.778, 503.629, 595.5, 602.638, 624.158, 658.089, 683.094, 742.947, 923.595, 973.275, 1002.92, 1049.26, 1070.39, 1074.55, 1235.3, 1361.85, 1418.25, 1449.13, 2141.34, 2177.63, 2665.53, 3082.01, 3091.02, 3155.8, 3471.94, 3474
cos = 4.61, .94, .13, .09, .06
sin = .35, -.51, .03, -.04, -.03
barrier = 5.35
Substituted frequency = 20.64 (from rotational profile)
Reduced moment of inertia = 145.511

Reaction87

REACTANT 1

C 0.000000 0.000000 1.337862
C 0.000000 0.000000 0.115777
C 0.000000 0.000000 -1.251352
H 0.000000 0.000000 2.400040
H 0.000000 0.929833 -1.806877
H 0.000000 -0.929833 -1.806877

REACTANT 2

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

PRODUCT 1

C 1.748228 0.124075 0.039321
C 0.565049 -0.440481 -0.067799
S -1.053621 0.123840 -0.050080
H 2.653636 -0.427995 -0.197380
H 1.877846 1.151585 0.382815
H -1.553214 -0.806591 0.786707

PRODUCT 2

C 0.000000 0.000000 -1.238052
H 0.000000 1.021022 -1.629805

H -0.884231 -0.510511 -1.629805
H 0.884231 -0.510511 -1.629805
C 0.000000 0.000000 0.219184
C 0.000000 0.000000 1.420084
H 0.000000 0.000000 2.482121

TRANSITION STATE

C 1.404403 1.253575 0.360046
C 2.277692 0.183885 0.003040
C 2.965928 -0.756049 -0.313669
C -1.148092 0.449123 -0.078287
C -2.033791 1.403166 -0.312999
S -1.400257 -1.256853 0.164504
H -1.739371 2.448280 -0.299547
H -3.077311 1.189741 -0.534307
H 0.195352 0.861612 0.150796
H -0.285550 -1.673751 -0.465719
H 1.415253 1.506771 1.420669
H 1.499748 2.139672 -0.268729
H 3.599160 -1.564874 -0.584018

Frequencies = -1531.82, 26.6492, 49.0585, 142.069, 181.221, 242.645, 295.163, 338.651, 417.185, 498.065, 522.628, 623.921, 625.386, 659.223, 741.377, 897.83, 959.487, 991.049, 1060.9, 1071.71, 1088.96, 1311.68, 1405.67, 1415.64, 1449.43, 1657.94, 2171.77, 2645.18, 3067.65, 3099.66, 3132.61, 3179.71, 3474.27
cos = .99, 2.07, .32, .17, .13
sin = .79, -1.00, .31, -.07, 0
barrier = 4.03
Substituted frequency = 29.56 (from rotational profile)
Reduced moment of inertia = 103.694

Reaction88

REACTANT 1

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

REACTANT 2

C -0.416743 0.016648 0.401914
S 1.370091 -0.080624 -0.092069
C -1.092896 1.273450 -0.142201
C -1.091922 -1.265135 -0.089637
H -0.436704 0.030165 1.494167
H 1.749074 1.095395 0.437615
H -0.614345 -2.155502 0.325257
H -2.142662 -1.270770 0.214075
H -1.055862 -1.333473 -1.180727
H -2.143622 1.299170 0.167520
H -0.613112 2.182183 0.228997
H -1.054854 1.293045 -1.234244

PRODUCT 1

C 1.085389 1.313238 0.036768
C 0.384580 0.008453 -0.166818
S -1.359504 -0.096411 0.035726
C 1.125045 -1.280188 0.007989
H -1.655216 1.176510 -0.281170
H 1.189097 1.567951 1.104198
H 2.094663 1.272829 -0.385000
H 0.556706 2.144567 -0.439850
H 2.079005 -1.245228 -0.528633
H 1.360984 -1.490121 1.064115
H 0.556743 -2.132957 -0.372915

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000
H -1.620529 -0.881510 0.000000

TRANSITION STATE

C 1.442404 -0.985385 -0.780411
C 2.340993 0.132673 -0.529823
C 3.130650 0.272712 0.551061
C -1.038807 -0.317728 0.123188
S -1.243034 1.440872 -0.225804
C -0.971811 -0.683929 1.590660
C -1.998046 -1.144653 -0.708656
H -0.772565 -1.754800 1.702772
H -0.177982 -0.138331 2.107085
H -1.918029 -0.460809 2.098410
H 0.223583 -0.630495 -0.364213
H 1.243366 -1.203928 -1.829133
H 1.640841 -1.885259 -0.197484
H -0.313547 1.888844 0.636402
H 2.329727 0.933810 -1.266142
H 3.751675 1.149632 0.689989
H 3.186529 -0.495586 1.316410
H -3.034303 -1.021245 -0.369482
H -1.956152 -0.871946 -1.766199
H -1.746893 -2.205975 -0.621675

Frequencies = -1690.76, 22.5843, 55.726, 97.3769, 143.646, 189.775, 206.806, 222.641, 233.895, 294.365, 311.457, 345.202, 413.279, 495.813, 630.486, 635.974, 672.234, 880.106, 888.796, 923.125, 951.57, 961.63, 992.675, 1000.82, 1022.02, 1071.79, 1127.34, 1185.44, 1204.33, 1215.44, 1316.03, 1394.89, 1398.98, 1418.3,

1428.72, 1436.06, 1477.83, 1481.47, 1482.59, 1493.84, 1498.91, 1629.03, 2660.3, 3001.07, 3005.14, 3061.07, 3063.59, 3070.42, 3088.65, 3093.13, 3123.33, 3128.16, 3149.16, 3214.97
cos = 1.10, 1.53, .86, -.14, .03
sin = .76, -.26, -.02, -.06, .04
barrier = 3.35
Substituted frequency = 21.00 (from rotational profile)
Reduced moment of inertia = 152.171

Reaction89

REACTANT 1

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

REACTANT 2

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935
C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

PRODUCT 1

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000
H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000
H -1.620529 -0.881510 0.000000

TRANSITION STATE

C 1.254952 -1.362991 -0.372201
C -0.922916 0.094769 0.372956
C -2.105871 -0.446541 -0.294484
C -2.966285 -1.309388 0.264472
S -0.535722 1.797128 -0.077031
H 0.727209 1.797023 0.388512
H 0.145688 -0.611814 -0.042941
H -0.893366 -0.080351 1.448584
H -2.250452 -0.150306 -1.331482
H -3.796098 -1.720792 -0.297427
H -2.866150 -1.626741 1.297528
C 2.390572 -0.471262 -0.467668
H 1.267136 -2.076674 0.450850
H 0.888840 -1.789150 -1.304490
C 3.273412 -0.222767 0.523048
H 2.509055 0.063953 -1.407468
H 4.087509 0.480077 0.393406
H 3.208997 -0.730197 1.480685

Frequencies = -1750.04, 33.2077, 61.1064, 94.0139, 130.148, 170.47, 213.935, 251.764, 269.108, 383.795, 416.19, 461.817, 587.601, 634.17, 711.277, 773.475, 888.523, 912.252, 917.925, 949.505, 966.617, 995.929, 1007.08, 1020.76, 1047.07, 1078.01, 1173.35, 1208.71, 1246.47, 1312.43, 1319.34, 1366.42, 1411.85, 1434.79, 1455.4, 1486.34, 1609.78, 1646.68, 2653.36, 3081.44, 3092.54, 3127.4, 3130.18, 3131.51, 3135.43, 3163.72, 3219.29, 3220.95
cos = 2.56, 2.49, .46, .15, .11
sin = -.04, .23, -.25, -.03, -.05
barrier = 4.23
Substituted frequency = 26.70 (from rotational profile)
Reduced moment of inertia = 153.511

Reaction90

REACTANT 1

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

REACTANT 2

C 1.275072 0.157942 -0.000791
C -0.003799 0.840478 0.061607
C 2.332294 -0.411226 -0.034669
H 3.266389 -0.915805 -0.072492
H -0.090502 1.423579 0.979934
H -0.113254 1.531514 -0.777702

S -1.469790 -0.282226 -0.079388
H -1.167393 -1.046849 0.983591

PRODUCT 1

C 2.361273 -0.341462 0.000000
C 1.253535 0.166078 0.000000
C 0.000000 0.724962 0.000000
S -1.495795 -0.181980 0.000000
H 3.330556 -0.775632 0.000000
H -0.140578 1.798264 0.000000
H -0.946110 -1.408414 0.000000

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000
H -1.620529 -0.881510 0.000000

TRANSITION STATE

C 1.262282 -1.385295 -0.160954
C -0.928318 0.048212 0.595692
C -2.087702 -0.672315 0.199525
C -3.032289 -1.324235 -0.172604
S -0.778113 1.669845 -0.189929
H 0.403853 1.985037 0.370002
H 0.153928 -0.667914 0.193433
H -0.778463 0.092240 1.674149
H -3.877258 -1.886798 -0.485463
C 2.300136 -0.437767 -0.508114
H 1.428474 -1.976750 0.738897
H 0.828769 -1.957697 -0.978986
C 3.265353 -0.000849 0.327529
H 2.262382 -0.023345 -1.513104
H 3.997646 0.732943 0.013072
H 3.353701 -0.381747 1.340425

Frequencies = -1744.43, 30.1102, 53.5183, 113.775, 117.382, 178.486, 200.978, 254.831, 368.534, 409.216, 442.303, 464.136, 604.544, 632.503, 678.495, 684.929, 744.256, 894.119, 923.969, 947.854, 974.224, 998.016, 1030.14, 1062.75, 1078.73, 1208.33, 1238.91, 1313.96, 1367.5, 1411.34, 1435.23, 1486.2, 1612.31, 2172.77, 2665.13, 3081.3, 3096.44, 3128.21, 3133.65, 3164.92, 3219.29, 3474.83
cos = 3.28, 1.67, .52, .17, .07
sin = -.03, .10, -.09, -.08, 0
barrier = 4.09
Substituted frequency = 25.32 (from rotational profile)
Reduced moment of inertia = 148.805

Reaction91

REACTANT 1

H 0.000000 0.000000 1.529822
C 0.000000 0.000000 0.441567
C 0.000000 1.227454 -0.195709
C 0.000000 -1.227454 -0.195709
H 0.000000 1.296093 -1.278176
H 0.000000 -1.296093 -1.278176
H 0.000000 2.154667 0.362821
H 0.000000 -2.154667 0.362821

REACTANT 2

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

PRODUCT 1

C 1.748228 0.124075 0.039321
C 0.565049 -0.440481 -0.067799
S -1.053621 0.123840 -0.050080
H 2.653636 -0.427995 -0.197380
H 1.877846 1.151585 0.382815
H -1.553214 -0.806591 0.786707

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000
H -1.620529 -0.881510 0.000000

TRANSITION STATE

C 1.354420 1.202792 0.326917
C -1.238251 0.465915 -0.090671
C -2.102488 1.447790 -0.286113
S -1.538685 -1.237014 0.125883
H -1.777203 2.483676 -0.260537
H -3.157268 1.269249 -0.485640
H 0.152505 0.846294 0.146918
H -0.456680 -1.678377 -0.543299
H 1.290968 1.799793 1.237137
C 2.174212 -0.008000 0.439090
H 1.567214 1.817850 -0.548445
C 2.886916 -0.554136 -0.557372
H 2.162791 -0.511120 1.403923
H 3.452126 -1.467876 -0.415872

H 2.935655 -0.093431 -1.539424

Frequencies = -1422.82, 34.1666, 45.4969, 98.9452, 162.102, 212.686, 249.39, 297.391, 408.9, 482.774, 560.089, 625.66, 640.505, 752.502, 897.044, 917.284, 950.171, 959.338, 985.119, 1022.04, 1065.28, 1100.77, 1201.44, 1320.89, 1338.47, 1401.43, 1410.94, 1439.38, 1481.16, 1651.12, 1657.88, 2643.49, 3067.06, 3095.61, 3122.77, 3129, 3144.33, 3175.95, 3215.28
cos = .65, 2.59, .23, .21, .18
sin = .41, -.90, .36, -.10, .05
barrier = 3.73
Substituted frequency = 31.04 (from rotational profile)
Reduced moment of inertia = 108.057

Reaction92

REACTANT 1

C 0.048305 -0.585330 0.000000
C 0.048305 0.719129 0.000000
H -0.879766 -1.164226 0.000000
H 0.968792 -1.165682 0.000000
H -0.668691 1.527114 0.000000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

H 0.000000 0.922461 1.234284
C 0.000000 0.000000 0.663526
C 0.000000 0.000000 -0.663526
H 0.000000 -0.922461 1.234284
H 0.000000 -0.922461 -1.234284
H 0.000000 0.922461 -1.234284

TRANSITION STATE

C -0.682471 1.060512 -0.098893
S -1.642651 -0.454619 -0.028294
C 1.966759 0.524099 0.114915
C 2.290168 -0.734871 -0.087920
H -1.452580 -0.718440 1.276241
H -0.936371 1.772865 0.685064
H -0.805984 1.498833 -1.088476
H 0.559987 0.829299 0.015691
H 2.609917 1.366098 0.351025
H 3.321128 -1.086878 -0.031553
H 1.539587 -1.486308 -0.323894

Frequencies = -1438.41, 57.7378, 80.2392, 189.809, 264.307, 293.521, 502.931, 515.181, 727.967, 834.387,, 858, 908.362, 959.865, 1051.89, 1113.19, 1175.13, 1339.23, 1400.17, 1418.31, 1435.55, 1653.01, 2665.62, 3068.56, 3075.65, 3147.75, 3158.02, 3167.96
cos = .46, 1.81, .73, .21, .02
sin = -.09, .30, -.10, -.04, -.02
barrier = 2.73
Substituted frequency = 56.43 (from rotational profile)
Reduced moment of inertia = 28.347

Reaction93

REACTANT 1

C -1.182767 -0.471341 0.000000
C 0.000000 0.399631 0.000000
H -0.891421 -1.533355 0.000000
H -1.806266 -0.294883 0.882076
H -1.806266 -0.294883 -0.882076
C 1.305795 0.329023 0.000000
H 1.827779 -0.633804 0.000000
H 1.938007 1.213050 0.000000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 1.136405 -0.506718 0.000000
C 0.000000 0.472962 0.000000
C -1.290338 0.153308 0.000000
H 0.777133 -1.538473 0.000000
H 1.776312 -0.367396 0.878460
H 1.776312 -0.367396 -0.878460
H 0.279136 1.525424 0.000000
H -2.064770 0.912040 0.000000

H -1.620529 -0.881510 0.000000

TRANSITION STATE

C 0.941071 -0.993827 -0.236723
S 2.248241 0.200721 0.047467
C -1.504763 0.155093 -0.033714
C -2.639699 -0.787339 0.150932
C -1.464336 1.469883 -0.123436
H 2.033063 0.382803 1.362104
H 0.954670 -1.830698 0.460603
H 1.004004 -1.333750 -1.269674
H -0.233696 -0.451120 -0.128614
H -2.369940 2.076636 -0.060239
H -0.530479 2.006347 -0.265469
H -2.518524 -1.383285 1.061873
H -3.593644 -0.249671 0.222382
H -2.710951 -1.491655 -0.684788

Frequencies = -1581.1, 36.5354, 77.765, 127.034, 162.921, 215.569, 264.012, 321.386, 490.5, 522.013, 615.57, 730.019, 837.74, 917.612, 919.115, 960.698, 1049.94, 1053.68, 1112.74, 1168.06, 1327.99, 1397.55, 1416.64, 1422.27, 1442.57, 1467.52, 1481.99, 1715.98, 2663.51, 2994.78, 3055.98, 3062.51, 3062.99, 3073.63, 3157.8, 3163.02
cos = -.41, 1.74, .89, .06, .04
sin = -.27, .25, -.15, -.01, -.01
barrier = 2.27
Substituted frequency = 33.99 (from rotational profile)
Reduced moment of inertia = 71.669

Reaction94

REACTANT 1

C 1.748228 0.124075 0.039321
C 0.565049 -0.440481 -0.067799
S -1.053621 0.123840 -0.050080
H 2.653636 -0.427995 -0.197380
H 1.877846 1.151585 0.382815
H -1.553214 -0.806591 0.786707

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 1.680075 0.267096 0.000000
C 0.586966 -0.490668 0.000000
S -1.105145 0.025375 0.000000
H 2.661414 -0.191945 0.000164
H 1.640534 1.350512 0.000000
H 0.656735 -1.573893 0.000115
H -0.878618 1.350755 0.000199

TRANSITION STATE

C 1.375354 1.119593 0.092857
S 2.390438 -0.340478 -0.094912
C -1.253327 0.508828 -0.058269
C -2.099759 1.527326 -0.040148
S -1.630114 -1.195268 0.062516
H -1.733827 2.548352 0.016412
H -3.178505 1.395680 -0.086822
H 0.109030 0.802922 0.006599
H -0.683945 -1.632992 -0.789567
H 1.499885 1.625288 1.048632
H 1.557395 1.786133 -0.748890
H 2.131179 -0.887942 1.105310

Frequencies = -1576.97, 40.0358, 58.3562, 139.681, 177.535, 241.055, 268.495, 308.509, 462.763, 508.072, 636.122, 722.549, 744.406, 842.838, 901.796, 956.295, 1045.11, 1077.36, 1117.54, 1325.82, 1402.17, 1420.07, 1421.43, 1655.18, 2642.35, 2665.37, 3080.38, 3099.8, 3167.02, 3178.47
cos = 2.44, 2.98, .42, .28, .02
sin = .63, -1.04, .31, -.06, .04
barrier = 5.68
Substituted frequency = 39.47 (from rotational profile)
Reduced moment of inertia = 74.447

Reaction95

REACTANT 1

C -0.616735 1.784664 0.000000
C 0.000000 0.641728 0.000000
C 0.646237 -0.542325 0.000000
C 0.043298 -1.798157 0.000000
H -0.891354 2.291206 0.924852
H -0.891354 2.291206 -0.924852
H 1.734854 -0.498138 0.000000
H 0.645043 -2.696969 0.000000
H -1.033984 -1.902762 0.000000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000

H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.601003 1.747736 0.000000
C 0.601003 0.410866 0.000000
C -0.601003 -0.410866 0.000000
C -0.601003 -1.747736 0.000000
H 1.522634 2.317119 0.000000
H -0.325173 2.314048 0.000000
H 1.549525 -0.122615 0.000000
H -1.549525 0.122615 0.000000
H -1.522634 -2.317119 0.000000
H 0.325173 -2.314048 0.000000

TRANSITION STATE

H 2.420177 0.155492 1.358253
S 2.563009 -0.046518 0.036803
C 1.055936 -0.984791 -0.216639
H 0.919645 -1.790343 0.503518
H 1.048661 -1.357339 -1.240156
H 0.012812 -0.235904 -0.124057
C -1.108663 0.642786 -0.044866
C -0.770533 1.924320 -0.080572
C -2.412824 0.030524 0.066831
H -1.520175 2.715234 -0.020720
H 0.263581 2.241914 -0.173980
C -2.658925 -1.284054 0.075783
H -3.253659 0.724058 0.147871
H -3.668292 -1.667643 0.161138
H -1.860849 -2.013905 -0.003931

Frequencies = -1535.63, 35.6222, 76.658, 86.1747, 131.911, 186.484, 259.536, 288.387, 426.879, 468.957, 544.698, 564.892, 730.032, 747.548, 838.661, 892.574, 916.576, 936.446, 1005.8, 1007.5, 1052.7, 1114.06, 1210.96, 1307.66, 1336.65, 1406.69, 1416.98, 1427.05, 1459.69, 1650.39, 1696.48, 2664.29, 3067.56, 3072.41, 3075.75, 3141.41, 3160.02, 3171.46, 3226.1
cos = 1.16, 2.39, .58, .33, .01
sin = -.32, .85, -.39, -.02, .04
barrier = 4.05
Substituted frequency = 35.30 (from rotational profile)
Reduced moment of inertia = 86.196

Reaction96

REACTANT 1

C 0.000000 0.563285 0.000000
C 0.002126 1.868593 0.000000
C -0.001292 -0.753901 0.000000
H 0.927691 2.444135 0.000000
H -0.921527 2.447183 0.000000
C -0.000179 -1.985314 0.000000
H -0.010096 -3.047296 0.000000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.577564 -0.556077 0.000000
C -0.120844 -1.696256 0.000000
H 1.664407 -0.591983 0.000000
H 0.382899 -2.655113 0.000000
H -1.204289 -1.698261 0.000000
C 0.000000 0.743701 0.000000
C -0.453376 1.859580 0.000000
H -0.863076 2.839673 0.000000

TRANSITION STATE

H 2.378944 0.000195 1.416393
S 2.545788 -0.043319 0.083021
C 1.086180 -0.990570 -0.303055
H 0.922412 -1.850752 0.343389
H 1.101803 -1.262534 -1.356872
H -0.027155 -0.268603 -0.172294
C -1.149802 0.503856 -0.065532
C -0.879340 1.803454 -0.090699
C -2.333563 -0.216478 0.050277
H -1.660459 2.556125 -0.009259
H 0.141154 2.159121 -0.194026
C -3.295006 -0.947357 0.144905
H -4.160126 -1.557880 0.228949

Frequencies = -1624.12, 31.5373, 71.3045, 125.271, 178.937, 248.493, 269.415, 356.524, 407.153, 536.772, 592.206, 616.896, 644.683, 682.697, 744.735, 841.899, 908.237, 934.123, 1033.85, 1108.73, 1124.58, 1292.03, 1414.56,

1419.71, 1447.06, 1685.84, 2139.87, 2665.97, 3083.43, 3100.97, 3172.91, 3186.78, 3474.03
cos = .94, 1.95, .60, .15, .01
sin = .57, -.10, -.03, -.05, 0
barrier = 3.33
Substituted frequency = 30.26 (from rotational profile)
Reduced moment of inertia = 91.309

Reaction97

REACTANT 1

C -2.422806 0.046950 0.000000
C -1.114572 -0.372300 0.000000
C -0.006888 0.473095 0.000000
S 1.672518 -0.005683 0.000000
H -3.237222 -0.665268 0.000000
H -2.680066 1.100113 0.000000
H -0.925605 -1.444297 0.000000
H -0.130203 1.550370 0.000201
H 1.478396 -1.336458 0.000273

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C -2.236947 -0.294381 -0.225760
C -1.154167 0.042786 0.469935
C 0.022427 0.761788 -0.107523
S 1.590314 -0.212815 0.004217
H 1.149804 -1.281795 -0.681292
H 0.248918 1.667388 0.462132
H -0.151649 1.051179 -1.144544
H -1.079709 -0.218775 1.522430
H -3.066248 -0.818818 0.234521
H -2.334011 -0.055295 -1.280633

TRANSITION STATE

C -1.318559 -1.292094 0.026729
S -2.749958 -0.244052 -0.027609
C 1.010799 0.078679 -0.408215
C 2.062374 -0.554583 0.400148
C 2.976824 -1.407980 -0.075019
S 0.704451 1.804905 0.052099
H -0.441986 1.950792 -0.636599
H -0.102524 -0.548025 -0.179219
H 1.154227 -0.042807 -1.482796
H 2.046496 -0.332992 1.465642
H 3.694575 -1.887507 0.579838
H 3.036327 -1.651172 -1.131186
H -1.141115 -1.781300 0.982096
H -1.334149 -1.985789 -0.811236
H -2.572359 0.361004 1.159766

Frequencies = -1630.53, 25.2268, 64.7219, 103.848, 142.852, 189.645, 215.267, 262.039, 288.339, 393.753, 447.687, 531.254, 666.399, 753.388, 766.818, 847.506, 904.092, 924.096, 964.911, 1012.34, 1014.84, 1045.58, 1115.88, 1163.6, 1241.81, 1320.54, 1375.66, 1415.08, 1434.34, 1456.28, 1659.74, 2660.93, 2661.6, 3084.37, 3085.04, 3126.91, 3133.5, 3179.89, 3218.62
cos = 2.40, 2.05, .94, -.01, -.03
sin = -.32, .24, -.36, -.08, .04
barrier = 3.94
Substituted frequency = 30.58 (from rotational profile)
Reduced moment of inertia = 96.516

Reaction98

REACTANT 1

C -0.947193 -2.121756 0.000000
C 0.426022 -1.859686 0.000000
C 0.896906 -0.557327 0.000000
C 0.000000 0.547670 0.000000
C -1.392629 0.251430 0.000000
C -1.850963 -1.052950 0.000000
C 0.445002 1.888991 0.000000
C 1.878925 2.311111 0.000000
H -2.099790 1.074512 0.000000
H -2.917822 -1.247932 0.000000
H -1.308617 -3.143390 0.000000
H 1.131203 -2.683834 0.000000
H 1.965165 -0.376385 0.000000
H -0.313695 2.664718 0.000000
H 1.969642 3.398457 0.000000
H 2.418744 1.934479 0.879000
H 2.418744 1.934479 -0.879000

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.233464 -2.323390 0.000000
C 0.234516 -1.621334 1.203430
C 0.234516 -0.228378 1.200443
C 0.232665 0.490135 0.000000
C 0.234516 -0.228378 -1.200443
C 0.234516 -1.621334 -1.203430
C 0.193136 2.002902 0.000000
C -1.238505 2.566349 0.000000
H 0.241341 0.310332 -2.143183
H 0.240197 -2.158580 -2.145613
H 0.236924 -3.407588 0.000000
H 0.240197 -2.158580 2.145613
H 0.241341 0.310332 2.143183
H 0.728687 2.380336 -0.877063
H 0.728687 2.380336 0.877063
H -1.228538 3.660050 0.000000
H -1.790892 2.231970 -0.882270
H -1.790892 2.231970 0.882270

TRANSITION STATE

S -2.777010 -1.336507 -0.305981
C -2.453496 -0.213632 1.034991
C -0.431114 1.505733 0.386966
H -0.349905 2.092296 1.305060
C -1.008735 2.305847 -0.766594
H -3.311576 0.438611 1.183300
H -2.113102 -0.685155 1.954438
H -1.643381 -2.053124 -0.211150
H -1.385361 0.672244 0.706618
C 0.771230 0.674224 0.161696
C 1.119395 0.175664 -1.106483
C 2.231671 -0.644278 -1.274721
C 3.024297 -0.993769 -0.183135
C 2.693234 -0.510736 1.083461
C 1.584915 0.309735 1.251308
H 0.519046 0.435282 -1.970126
H 2.481839 -1.010091 -2.264752
H 3.891187 -1.630739 -0.316831
H 3.305699 -0.770113 1.940293
H 1.340529 0.686259 2.239917
H -0.272883 3.005828 -1.179116
H -1.346846 1.661318 -1.582517
H -1.871475 2.888752 -0.434360

Frequencies = -1609.65, 28.6035, 40.758, 59.5512, 93.1344, 154.491, 183.088, 229.924, 247.888, 300.685, 413.442, 414.948, 447.632, 495.594, 546.123, 569.783, 634.178, 709.334, 749.135, 763.738, 786.068, 847.811, 851.562, 872.508, 918.89, 976.215, 997.101, 1004.13, 1017.57, 1049.42, 1056.8, 1067.19, 1103.9, 1119.75, 1130.68, 1180.71, 1202.65, 1229.63, 1315.5, 1346.72, 1363.26, 1403.66, 1413, 1420.49, 1423.33, 1484.18, 1492.75, 1502.02, 1524.02, 1611.09, 1635.34, 2665.99, 3012.39, 3065.22, 3072.02, 3083.87, 3093.51, 3150.92, 3161.39, 3170.49, 3177.99, 3183.09, 3190.51
cos = 1.59, 1.86, .73, .07, 0
sin = -.50, .29, .26, -.02, -.03
barrier = 3.83
Substituted frequency = 22.34 (from rotational profile)
Reduced moment of inertia = 168.766

Reaction99

REACTANT 1

C 1.204480 1.947859 0.000000
C 0.000000 2.655851 0.000000
C -1.204550 1.947870 0.000000
C -1.210360 0.562927 0.000000
C 0.000000 -0.185830 0.000000
C 1.210328 0.562914 0.000000
C 0.000000 -1.613421 0.000000
C -1.292355 -2.379901 0.000000
H 2.159845 0.042987 0.000000
H 2.146614 2.485446 0.000000
H 0.000000 3.739549 0.000000
H -2.146693 2.485442 0.000000
H -2.159862 0.042983 0.000000
C 1.292457 -2.379780 0.000000
H -1.113817 -3.456217 0.000000
H -1.908904 -2.148888 0.878614
H -1.908904 -2.148888 -0.878614
H 1.113988 -3.456104 0.000000
H 1.908872 -2.148625 -0.878644
H 1.908872 -2.148625 0.878644

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 1.146472 -0.234671 0.000000
C -0.212351 0.106357 0.000000
C -1.149373 -0.931186 0.000000

C -0.749050 -2.266575 0.000000
C 0.604946 -2.589098 0.000000
C 1.552118 -1.566192 0.000000
C -0.665622 1.559652 0.000000
C -0.212351 2.303218 1.269454
C -0.212351 2.303218 -1.269454
H -2.207845 -0.689745 0.000000
H -1.495863 -3.053096 0.000000
H 0.920818 -3.626292 0.000000
H 2.609838 -1.806508 0.000000
H 1.898687 0.547305 0.000000
H -1.761619 1.550108 0.000000
H -0.604785 3.324495 -1.278812
H -0.604785 3.324495 1.278812
H -0.562986 1.794828 -2.171034
H -0.562986 1.794828 2.171034
H 0.878452 2.365622 -1.324421
H 0.878452 2.365622 1.324421

TRANSITION STATE

S 2.786583 -1.603001 -0.209288
C 2.408653 -0.047691 -0.985602
C 0.391172 1.307008 0.275046
C 0.364712 2.621659 -0.493503
C 0.937625 1.479736 1.689495
H 3.252753 0.630145 -0.877000
H 2.055335 -0.124738 -2.011613
H 1.675856 -2.260357 -0.585234
H 1.330442 0.628890 -0.317779
C -0.820914 0.439810 0.149949
C -0.941731 -0.743474 0.905757
C -2.039514 -1.585182 0.767957
C -3.059641 -1.274346 -0.130205
C -2.961628 -0.110447 -0.887501
C -1.860086 0.730742 -0.752192
H -0.162674 -1.013652 1.607527
H -2.099918 -2.487520 1.366974
H -3.917530 -1.928577 -0.235804
H -3.748790 0.149797 -1.587033
H -1.820178 1.631506 -1.351060
H 0.227706 2.033671 2.316085
H 1.142319 0.528132 2.182437
H 1.874079 2.044142 1.669886
H -0.412288 3.295710 -0.111508
H 1.323120 3.137468 -0.391187
H 0.182553 2.476506 -1.561284

Frequencies = -1581.64, 20.5981, 35.0339, 57.5968, 84.6499, 153.694, 157.669, 190.474, 219.119, 245.635, 268.457, 316.011, 361.227, 415.526, 430.027, 460.714, 483.496, 546.591, 599.927, 634.646, 709.592, 740.105, 752.829, 782.166, 850.377, 852.043, 908.477, 923.264, 951.799, 978.129, 990.605, 998.25, 1011.98, 1035.99, 1051.61, 1099.05, 1110.67, 1117.35, 1143.81, 1180.45, 1184.46, 1213.6, 1280.22, 1319.69, 1358.65, 1400.32, 1400.6, 1411.52, 1418.76, 1421.37, 1474.15, 1485.89, 1494.09, 1500.3, 1512.05, 1528.96, 1611.37, 1636.56, 2664.66, 3004.37, 3009.75, 3067.15, 3072.01, 3084.34, 3091.25, 3106.01, 3158.36, 3166.28, 3177.76, 3183.12, 3193.27, 3197.22
cos = 1.56, 1.12, .81, .09, .08
sin = -.60, .35, .43, -.04, -.03
barrier = 3.43
Substituted frequency = 22.40 (from rotational profile)
Reduced moment of inertia = 167.241

Reaction100

REACTANT 1

C 0.257358 -2.083274 0.000000
C 0.733479 -0.787214 0.000000
C 0.000000 0.398983 0.000000
C -1.499325 0.444678 0.000000
C 0.696711 1.727848 0.000000
H 0.943168 -2.920686 0.000000
H -0.799592 -2.318264 0.000000
H 1.816210 -0.670869 0.000000
H 1.783302 1.620820 0.000000
H -1.958204 -0.543545 0.000000
H -1.872158 0.987818 0.878018
H -1.872158 0.987818 -0.878018
H 0.415048 2.325393 0.877522
H 0.415048 2.325393 -0.877522

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C -0.039118 -2.155117 0.000000
C 0.468489 -0.926272 0.000000
C -0.328860 0.352844 0.000000
C -0.039118 1.176572 1.267632
C -0.039118 1.176572 -1.267632
H -1.111703 -2.326848 0.000000
H 0.594781 -3.034933 0.000000
H 1.552036 -0.801120 0.000000
H -1.392759 0.086675 0.000000
H -0.625702 2.100094 -1.275359
H -0.625702 2.100094 1.275359
H -0.281411 0.610329 -2.170251

H -0.281411 0.610329 2.170251
H 1.019109 1.453891 -1.319421
H 1.019109 1.453891 1.319421

TRANSITION STATE

C -1.080130 -0.403133 -0.095833
C -1.203963 -1.436447 -1.211105
C 1.504081 -0.732746 0.765943
S 2.622712 0.280038 -0.168864
H 2.219226 1.471353 0.306363
H 0.143938 -0.533717 0.287469
H 1.437923 -0.494168 1.824909
H 1.703768 -1.784191 0.572819
C -1.148899 0.992948 -0.569391
C -1.890765 -0.744858 1.145197
H -2.229753 -1.475739 -1.597734
H -0.542927 -1.198837 -2.049301
H -0.948678 -2.437879 -0.852020
H -2.966618 -0.659886 0.950264
H -1.692117 -1.771493 1.465266
H -1.653476 -0.084054 1.983021
C -1.671539 2.045315 0.076534
H -0.692972 1.168568 -1.542804
H -1.642298 3.037577 -0.358659
H -2.152129 1.955388 1.044168

Frequencies = -1534.06, 22.4499, 59.7149, 92.3905, 152.156, 164.748, 209.411, 223.014, 231.853, 287.161, 323.954, 370.435, 463.691, 508.005, 551.403, 679.955, 755.419, 785.379, 847.946, 909.146, 947.81, 954.331, 991.809, 1026.2, 1031.78, 1054.45, 1109.19, 1131.04, 1195.99, 1259.63, 1331.89, 1385.9, 1396.14, 1407.67, 1413.51, 1418.25, 1453.21, 1486.45, 1488.35, 1501.58, 1509.04, 1650.66, 2660.47, 3004.33, 3010.6, 3062.06, 3068.47, 3086.24, 3087.78, 3089.42, 3116.58, 3139.08, 3183, 3217.82
cos = 1.99, 1.23, .71, -.11, -.02
sin = -.25, .39, -.10, .09, -.01
barrier = 3.09
Substituted frequency = 22.30 (from rotational profile)
Reduced moment of inertia = 111.353

Reaction101

REACTANT 1

C 0.821897 -0.025137 0.000086
C -0.378047 -0.711838 -0.000009
S -1.929833 -0.032719 -0.000199
H -0.315203 -1.799063 0.000046
C 0.921964 1.466291 0.000032
C 2.115592 -0.784099 0.000254
H 1.483398 1.807508 -0.877872
H -0.059619 1.936413 -0.000109
H 1.483179 1.807583 0.878048
H 2.717700 -0.518090 -0.876885
H 2.717517 -0.518016 0.877498
H 1.961914 -1.864141 0.000284

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

C 0.132027 -0.835770 0.000000
C -0.358696 0.583412 0.000000
S 0.548402 1.925752 0.000000
H -1.449374 0.681652 0.000000
H 1.225030 -0.815693 0.000000
C -0.358696 -1.557557 1.271321
C -0.358696 -1.557557 -1.271321
H -0.004581 -2.591851 1.273036
H 0.013651 -1.067890 2.173865
H -1.451930 -1.576841 1.318633
H -0.004581 -2.591851 -1.273036
H -1.451930 -1.576841 -1.318633
H 0.013651 -1.067890 -2.173865

TRANSITION STATE

C -0.791967 0.867858 -0.086682
C -1.070809 -0.435201 -0.690132
S -1.718980 -1.760246 0.033733
C -0.731726 2.019235 -1.091513
C -1.518086 1.211216 1.206781
H -0.753441 -0.526648 -1.731389
H -0.152641 1.748580 -1.978497
H -1.738716 2.297946 -1.419697
H -0.274666 2.905332 -0.642969
H -1.094225 2.113272 1.656604
H -2.578851 1.398295 1.009969
H -1.460969 0.393722 1.926134
H 0.394140 0.718761 0.263191
C 1.828598 0.608254 0.799915
H 2.212817 1.615798 0.672945
H 1.628622 0.315464 1.825578
S 2.681422 -0.548743 -0.203043
H 2.122785 -1.664880 0.296891

Frequencies = -1088.71, 28.8771, 48.8133, 83.0695, 142.583, 166.079, 188.242, 222.898, 242.818, 266.844, 352.656, 387.624, 466.399, 529.866, 561.301, 777.221, 781.532, 852.265,

876.027, 947.97, 953.497, 999.072, 1011.27, 1100.47, 1103.67, 1136.92, 1163.32, 1255.81, 1330.59, 1367.93, 1386.03, 1402.02, 1417.25, 1427.19, 1479.95, 1487.25, 1499.82, 1509.31, 2669.07, 3018.3, 3026.3, 3072.73, 3077.48, 3082.44, 3093.92, 3109.06, 3117.64, 3213.8
cos = 4.17, 2.05, .63, -.02, .03
sin = .84, -.66, .06, -.09, -.01
barrier = 5.96
Substituted frequency = 26.51 (from rotational profile)
Reduced moment of inertia = 130.896

Reaction102

REACTANT 1

C 0.000000 0.000000 1.043643
C 0.000000 0.000000 2.265132
C 0.000000 0.000000 -0.332748
H 0.000000 0.000000 3.326998
C 0.000000 1.288872 -1.104719
C 0.000000 -1.288872 -1.104719
H 0.000000 2.156753 -0.445259
H 0.879523 1.352850 -1.759006
H -0.879523 1.352850 -1.759006
H 0.000000 -2.156753 -0.445259
H -0.879523 -1.352850 -1.759006
H 0.879523 -1.352850 -1.759006

REACTANT 2

S 0.047809 -0.669761 0.000000
C 0.047809 1.162317 0.000000
H -1.285585 -0.835583 0.000000
H -0.430914 1.557520 0.895039
H 1.095613 1.462810 0.000000
H -0.430914 1.557520 -0.895039

PRODUCT 1

H 1.682966 -0.909640 0.000950
C 1.142492 0.024163 -0.030038
H 1.645501 0.965195 0.127774
S -0.582672 -0.088931 0.008630
H -0.860671 1.222358 -0.086577

PRODUCT 2

H -1.494578 0.497337 0.000000
C -0.402762 0.385740 0.000000
C -0.112137 -1.050895 0.000000
C 0.141538 -2.226011 0.000000
H 0.361479 -3.265166 0.000000
C 0.141538 1.060591 1.274591
C 0.141538 1.060591 -1.274591
H -0.121966 2.121770 1.281913
H -0.271032 0.595988 2.172321
H 1.230409 0.976104 1.318597
H -0.121966 2.121770 -1.281913
H 1.230409 0.976104 -1.318597
H -0.271032 0.595988 -2.172321

TRANSITION STATE

C -1.398890 -0.744169 -0.797997
S -2.551548 0.174593 0.191919
C 1.157563 -0.316863 0.067382
C 1.343543 1.101583 -0.050260
C 1.452368 2.298129 -0.170145
C 2.020263 -1.143715 -0.884288
H -0.065238 -0.509853 -0.345467
C 1.138504 -0.830190 1.505392
H -1.557072 -1.811333 -0.657831
H -1.354222 -0.451559 -1.844820
H -2.191507 1.402962 -0.219539
H 1.570653 3.349329 -0.265501
H 0.848526 -1.884632 1.529587
H 2.130342 -0.742755 1.963395
H 0.433213 -0.264508 2.117106
H 1.712123 -2.193185 -0.865015
H 1.942261 -0.778377 -1.910532
H 3.075589 -1.098240 -0.592597

Frequencies = -1604.34, 34.5468, 61.0151, 98.2098, 159.446, 183.77, 196.153, 208.387, 239.188, 269.249, 346.778, 422.101, 515.306, 558.383, 583.743, 616.216, 666.182, 754.729, 770.702, 852.205, 954.396, 964.076, 990.604, 1038.46, 1111.86, 1133.89, 1169.83, 1238.17, 1396.48, 1401.23, 1408.96, 1416.13, 1419.7, 1482.22, 1486.44, 1496.76, 1504.89, 2165.83, 2666.95, 3011.89, 3015.38, 3071.05, 3073.55, 3084.68, 3100.79, 3106.75, 3178.96, 3474.53
cos = 1.78, .76, .82, .06, .11
sin = -.64, .33, .26, -.05, .02
barrier = 3.07
Substituted frequency = 26.26 (from rotational profile)
Reduced moment of inertia = 114.160