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Supplementary Material

Mechanism, Thermochemistry, and Kinetics of the Reversible Reactions:

$C_2H_3 + H_2 \rightleftharpoons C_2H_4 + H \rightleftharpoons C_2H_5$

Thanh Lam Nguyen,[1] David H. Bross,[2] Branko Ruscic,[2] G. Barney Ellison,[3] and John F. Stanton*,[1]

[1]*Quantum Theory Project, Department of Chemistry and Physics, University of Florida, Gainesville, FL 32611 (USA).*

[2]*Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, Illinois 60439, United States.*

[3]*Department of Chemistry, University of Colorado, Boulder, CO 80309 (USA).*

Corresponding author: *johnstanton@ufl.edu*

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E,J-resolved master equation model for a thermally activated reaction

E,J-resolved master equation model for a thermally activated reaction ($C_2H_5 \rightarrow C_2H_4 + H$), which has a well and a product channel, is given by:

$$\frac{\partial C_{C2H5}(E_i,J_i,t)}{\partial t} = \sum_{J_k=0}^{J_{max}} \sum_{E_k=0}^{E_{max}} \omega_{LJ} \cdot P(E_i,J_i|E_k,J_k) \cdot C_{C2H5}(E_k,J_k,t) \cdot \Delta E - \omega_{LJ} \cdot C_{C2H5}(E_i,J_i,t) - k_{C2H5 \rightarrow C2H4+H}(E_i,J_i) \cdot C_{C2} (E_i,J_i,t)$$

(S1)

All terms have been defined in the main text. Here initial energy distribution of C_2H_5 is assumed to be Boltzmann thermal energy distribution function:

$$F_{C_2H_5}(E_i,J_i) = \frac{(2J_i+1) \cdot \rho_{C2H5}(E_i,J_i) \cdot \exp(-E_i/RT)}{\sum_{J_i=0}^{J_{max}} (2J_i+1) \int_{E_i=0}^{E_{max}} \rho_{C2H5}(E_i,J_i) \cdot \exp(-E_i/RT) \cdot dE_i} \qquad \text{(S2)}$$

Eq. (S1) can be cast in the matrix form:

$$\frac{\partial C}{\partial t} = MC \qquad \text{(S3)}$$

The reaction rate coefficient, $k_{uni.}(T,p)$, is equally assigned to the lowest eigenvalue of M.

$$k_{uni.}(T,p) = |\lambda_1| \tag{S4}$$

Table S1: Calculated thermal rate coefficients (in cm^3/s) for the $C_2H_3 + H_2 \rightarrow C_2H_4 + H$ reaction using the SCTST theory.

T (K)	1000/T (1/K)	$k(T)_1$ (cm^3/s)
300	3.33333333	4.12E-18
325	3.07692308	1.05E-17
350	2.85714286	2.39E-17
375	2.66666667	4.94E-17
400	2.5	9.41E-17
425	2.35294118	1.68E-16
450	2.22222222	2.82E-16
475	2.10526316	4.52E-16
500	2	6.94E-16
525	1.9047619	1.03E-15
550	1.81818182	1.48E-15
575	1.73913043	2.06E-15
600	1.66666667	2.81E-15
625	1.6	3.75E-15
650	1.53846154	4.90E-15
675	1.48148148	6.30E-15
700	1.42857143	7.98E-15
725	1.37931034	9.96E-15
750	1.33333333	1.23E-14
775	1.29032258	1.50E-14
800	1.25	1.81E-14
825	1.21212121	2.16E-14
850	1.17647059	2.56E-14
875	1.14285714	3.01E-14
900	1.11111111	3.52E-14
925	1.08108108	4.08E-14
950	1.05263158	4.70E-14

975	1.02564103	5.39E-14
1000	1	6.14E-14
1025	0.97560976	6.96E-14
1050	0.95238095	7.86E-14
1075	0.93023256	8.83E-14
1100	0.90909091	9.88E-14
1125	0.88888889	1.10E-13
1150	0.86956522	1.22E-13
1175	0.85106383	1.35E-13
1200	0.83333333	1.49E-13
1225	0.81632653	1.64E-13
1250	0.8	1.80E-13
1275	0.78431373	1.97E-13
1300	0.76923077	2.15E-13
1325	0.75471698	2.34E-13
1350	0.74074074	2.54E-13
1375	0.72727273	2.76E-13
1400	0.71428571	2.98E-13
1425	0.70175439	3.21E-13
1450	0.68965517	3.46E-13
1475	0.6779661	3.72E-13
1500	0.66666667	3.99E-13
1525	0.6557377	4.27E-13
1550	0.64516129	4.57E-13
1575	0.63492063	4.88E-13
1600	0.625	5.20E-13
1625	0.61538462	5.53E-13
1650	0.60606061	5.88E-13
1675	0.59701493	6.24E-13
1700	0.58823529	6.61E-13
1725	0.57971014	7.00E-13
1750	0.57142857	7.40E-13
1775	0.56338028	7.81E-13
1800	0.55555556	8.24E-13
1825	0.54794521	8.68E-13
1850	0.54054054	9.13E-13
1875	0.53333333	9.60E-13
1900	0.52631579	1.01E-12
1925	0.51948052	1.06E-12

1950	0.51282051	1.11E-12
1975	0.50632911	1.16E-12
2000	0.5	1.21E-12
2025	0.49382716	1.27E-12
2050	0.48780488	1.33E-12
2075	0.48192771	1.38E-12
2100	0.47619048	1.44E-12
2125	0.47058824	1.50E-12
2150	0.46511628	1.56E-12
2175	0.45977011	1.63E-12
2200	0.45454545	1.69E-12
2225	0.4494382	1.76E-12
2250	0.44444444	1.82E-12
2275	0.43956044	1.89E-12
2300	0.43478261	1.96E-12
2325	0.43010753	2.03E-12
2350	0.42553191	2.10E-12
2375	0.42105263	2.17E-12
2400	0.41666667	2.25E-12
2425	0.41237113	2.32E-12
2450	0.40816327	2.40E-12
2475	0.4040404	2.48E-12
2500	0.4	2.55E-12
2525	0.3960396	2.63E-12
2550	0.39215686	2.71E-12
2575	0.38834951	2.79E-12
2600	0.38461538	2.88E-12
2625	0.38095238	2.96E-12
2650	0.37735849	3.04E-12
2675	0.37383178	3.13E-12
2700	0.37037037	3.21E-12
2725	0.36697248	3.30E-12
2750	0.36363636	3.39E-12
2775	0.36036036	3.47E-12
2800	0.35714286	3.56E-12
2825	0.3539823	3.65E-12
2850	0.35087719	3.74E-12
2875	0.34782609	3.83E-12
2900	0.34482759	3.92E-12

2925	0.34188034	4.01E-12
2950	0.33898305	4.10E-12
2975	0.33613445	4.19E-12
3000	0.33333333	4.28E-12
3025	0.33057851	4.37E-12
3050	0.32786885	4.46E-12
3075	0.32520325	4.56E-12
3100	0.32258065	4.65E-12
3125	0.32	4.74E-12
3150	0.31746032	4.83E-12
3175	0.31496063	4.92E-12
3200	0.3125	5.01E-12
3225	0.31007752	5.10E-12
3250	0.30769231	5.19E-12
3275	0.30534351	5.28E-12
3300	0.3030303	5.37E-12
3325	0.30075188	5.46E-12
3350	0.29850746	5.55E-12
3375	0.2962963	5.64E-12
3400	0.29411765	5.72E-12
3425	0.2919708	5.81E-12
3450	0.28985507	5.89E-12
3475	0.28776978	5.98E-12
3500	0.28571429	6.06E-12

Table S2: Calculated thermal rate coefficients (in cm^3/s) for the $C_2H_4 + H \rightarrow C_2H_3 + H_2$ reaction using the SCTST theory and the equilibrium constant (K_{eq}).

T (K)	1000/T (1/K)	k(T)$_{-1}$
1000	1	1.30E-13
1025	0.975609756	1.60E-13
1050	0.952380952	1.96E-13
1075	0.930232558	2.36E-13
1100	0.909090909	2.84E-13
1125	0.888888889	3.38E-13
1150	0.869565217	4.00E-13
1175	0.85106383	4.70E-13
1200	0.833333333	5.50E-13
1225	0.816326531	6.39E-13
1250	0.8	7.39E-13
1275	0.784313725	8.49E-13
1300	0.769230769	9.72E-13
1325	0.754716981	1.11E-12
1350	0.740740741	1.26E-12
1375	0.727272727	1.42E-12
1400	0.714285714	1.60E-12
1425	0.701754386	1.79E-12
1450	0.689655172	2.00E-12
1475	0.677966102	2.23E-12
1500	0.666666667	2.48E-12
1525	0.655737705	2.74E-12
1550	0.64516129	3.02E-12
1575	0.634920635	3.33E-12
1600	0.625	3.65E-12
1625	0.615384615	4.00E-12
1650	0.606060606	4.37E-12
1675	0.597014925	4.76E-12
1700	0.588235294	5.17E-12
1725	0.579710145	5.61E-12
1750	0.571428571	6.07E-12
1775	0.563380282	6.56E-12
1800	0.555555556	7.07E-12

1825	0.547945205	7.61E-12
1850	0.540540541	8.17E-12
1875	0.533333333	8.76E-12
1900	0.526315789	9.38E-12
1925	0.519480519	1.00E-11
1950	0.512820513	1.07E-11
1975	0.506329114	1.14E-11
2000	0.5	1.21E-11
2025	0.49382716	1.29E-11
2050	0.487804878	1.37E-11
2075	0.481927711	1.45E-11
2100	0.476190476	1.53E-11
2125	0.470588235	1.62E-11
2150	0.465116279	1.71E-11
2175	0.459770115	1.80E-11
2200	0.454545455	1.90E-11
2225	0.449438202	2.00E-11
2250	0.444444444	2.10E-11
2275	0.43956044	2.20E-11
2300	0.434782609	2.31E-11
2325	0.430107527	2.42E-11
2350	0.425531915	2.53E-11
2375	0.421052632	2.65E-11
2400	0.416666667	2.77E-11
2425	0.412371134	2.89E-11
2450	0.408163265	3.01E-11
2475	0.404040404	3.14E-11
2500	0.4	3.27E-11
2525	0.396039604	3.40E-11
2550	0.392156863	3.54E-11
2575	0.388349515	3.67E-11
2600	0.384615385	3.81E-11
2625	0.380952381	3.95E-11
2650	0.377358491	4.10E-11
2675	0.373831776	4.25E-11
2700	0.37037037	4.39E-11
2725	0.366972477	4.55E-11
2750	0.363636364	4.70E-11
2775	0.36036036	4.85E-11

2800	0.357142857	5.01E-11
2825	0.353982301	5.17E-11
2850	0.350877193	5.33E-11
2875	0.347826087	5.49E-11
2900	0.344827586	5.66E-11
2925	0.341880342	5.82E-11
2950	0.338983051	5.99E-11
2975	0.336134454	6.16E-11
3000	0.333333333	6.33E-11
3025	0.330578512	6.50E-11
3050	0.327868852	6.68E-11
3075	0.325203252	6.85E-11
3100	0.322580645	7.02E-11
3125	0.32	7.20E-11
3150	0.317460317	7.37E-11
3175	0.31496063	7.55E-11
3200	0.3125	7.73E-11
3225	0.310077519	7.91E-11
3250	0.307692308	8.09E-11
3275	0.305343511	8.26E-11
3300	0.303030303	8.44E-11
3325	0.30075188	8.62E-11
3350	0.298507463	8.80E-11
3375	0.296296296	8.98E-11
3400	0.294117647	9.16E-11
3425	0.291970803	9.34E-11
3450	0.289855072	9.51E-11
3475	0.287769784	9.69E-11
3500	0.285714286	9.87E-11

Table S3: Calculated thermal rate coefficients (in cm^3/s) at the high-pressure limit (i.e. the capture rate constants) for the $C_2H_4 + H \rightarrow C_2H_5$ reaction using the SCTST theory.

T (K)	$k(T)_2$ (cm^3/s)
200	2.08E-13
225	3.30E-13
250	4.96E-13
275	7.10E-13
300	9.76E-13
325	1.29E-12
350	1.67E-12
375	2.10E-12
400	2.58E-12
425	3.12E-12
450	3.71E-12
475	4.36E-12
500	5.05E-12
525	5.80E-12
550	6.59E-12
575	7.43E-12
600	8.32E-12
625	9.25E-12
650	1.02E-11
675	1.12E-11
700	1.23E-11
725	1.34E-11
750	1.45E-11
775	1.57E-11
800	1.69E-11
825	1.81E-11
850	1.94E-11
875	2.07E-11
900	2.20E-11
925	2.34E-11
950	2.48E-11
975	2.62E-11
1000	2.76E-11
1025	2.91E-11

1050	3.06E-11
1075	3.21E-11
1100	3.37E-11
1125	3.52E-11
1150	3.68E-11
1175	3.84E-11
1200	4.00E-11
1225	4.17E-11
1250	4.33E-11
1275	4.50E-11
1300	4.67E-11
1325	4.84E-11
1350	5.02E-11
1375	5.19E-11
1400	5.37E-11
1425	5.55E-11
1450	5.73E-11
1475	5.91E-11
1500	6.09E-11
1525	6.27E-11
1550	6.46E-11
1575	6.64E-11
1600	6.83E-11
1625	7.02E-11
1650	7.21E-11
1675	7.40E-11
1700	7.59E-11
1725	7.79E-11
1750	7.98E-11
1775	8.17E-11
1800	8.37E-11
1825	8.57E-11
1850	8.76E-11
1875	8.96E-11
1900	9.16E-11
1925	9.36E-11
1950	9.56E-11
1975	9.77E-11

2000	9.97E-11
2025	1.02E-10
2050	1.04E-10
2075	1.06E-10
2100	1.08E-10
2125	1.10E-10
2150	1.12E-10
2175	1.14E-10
2200	1.16E-10
2225	1.18E-10
2250	1.20E-10
2275	1.22E-10
2300	1.25E-10
2325	1.27E-10
2350	1.29E-10
2375	1.31E-10
2400	1.33E-10
2425	1.35E-10
2450	1.37E-10
2475	1.39E-10
2500	1.42E-10
2525	1.44E-10
2550	1.46E-10
2575	1.48E-10

Table S4: Calculated reaction rate coefficients (cm^3/s) as functions of temperature and pressure for the $C_2H_4 + H \rightarrow C_2H_5$ reaction using the ME/SCTST approach.

T (K) / P(atm)	0.5	1	5	10	50	100
300	8.84E-13	9.23E-13	9.63E-13	9.69E-13	9.74E-13	9.75E-13
400	2.01E-12	2.20E-12	2.47E-12	2.52E-12	2.57E-12	2.57E-12
500	3.10E-12	3.62E-12	4.49E-12	4.72E-12	4.97E-12	5.01E-12
600	3.77E-12	4.66E-12	6.55E-12	7.15E-12	7.96E-12	8.12E-12
700	3.89E-12	5.10E-12	8.13E-12	9.29E-12	1.12E-11	1.16E-11
800	3.66E-12	5.04E-12	9.05E-12	1.09E-11	1.43E-11	1.53E-11
900	3.14E-12	4.52E-12	9.08E-12	1.14E-11	1.67E-11	1.85E-11
1000	2.54E-12	3.80E-12	8.47E-12	1.12E-11	1.81E-11	2.09E-11
1100	1.96E-12	3.04E-12	7.44E-12	1.03E-11	1.85E-11	2.22E-11
1200	1.47E-12	2.36E-12	6.27E-12	9.01E-12	1.79E-11	2.24E-11
1300	1.09E-12	1.80E-12	5.13E-12	7.64E-12	1.66E-11	2.17E-11
1400	8.15E-13	1.37E-12	4.14E-12	6.36E-12	1.50E-11	2.03E-11
1500	6.07E-13	1.04E-12	3.30E-12	5.20E-12	1.32E-11	1.84E-11
1550	5.29E-13	9.10E-13	2.96E-12	4.71E-12	1.23E-11	1.75E-11
1600	4.61E-13	7.98E-13	2.64E-12	4.25E-12	1.14E-11	1.65E-11
1700	3.56E-13	6.23E-13	2.13E-12	3.49E-12	9.87E-12	1.46E-11
1800	2.80E-13	4.94E-13	1.74E-12	2.89E-12	8.51E-12	1.29E-11
1900	2.23E-13	3.98E-13	1.43E-12	2.40E-12	7.34E-12	1.13E-11
2000	1.82E-13	3.27E-13	1.19E-12	2.03E-12	6.38E-12	1.00E-11
2200	1.27E-13	2.30E-13	8.65E-13	1.49E-12	4.91E-12	7.88E-12
2400	9.42E-14	1.71E-13	6.57E-13	1.14E-12	3.89E-12	6.36E-12
2500	8.28E-14	1.52E-13	5.83E-13	1.02E-12	3.51E-12	5.78E-12
2600	7.34E-14	1.35E-13	5.22E-13	9.17E-13	3.19E-12	5.28E-12
2800	5.95E-14	1.10E-13	4.29E-13	7.58E-13	2.68E-12	4.48E-12
3000	4.98E-14	9.17E-14	3.63E-13	6.45E-13	2.31E-12	3.89E-12
3200	4.28E-14	7.91E-14	3.15E-13	5.61E-13	2.03E-12	3.43E-12
3400	3.76E-14	6.94E-14	2.78E-13	4.96E-13	1.81E-12	3.07E-12
3500	3.53E-14	6.52E-14	2.62E-13	4.68E-13	1.71E-12	2.91E-12

Table S4 (Continued): Calculated reaction rate coefficients (cm^3/s) as functions of temperature and pressure for the C_2H_4 + H $\rightarrow$ C_2H_5 reaction using the ME/SCTST approach.

P (Torr) / T(K)	285 K	298 K	400 K	511 K	604 K
0.1	3.62E-14	3.61E-14	3.26E-14	2.46E-14	1.78E-14
0.2	5.43E-14	5.49E-14	5.33E-14	4.21E-14	3.13E-14
0.3	6.83E-14	6.96E-14	7.05E-14	5.74E-14	4.35E-14
0.4	8.02E-14	8.20E-14	8.58E-14	7.14E-14	5.47E-14
0.5	9.05E-14	9.30E-14	9.98E-14	8.44E-14	6.53E-14
0.6	9.98E-14	1.03E-13	1.13E-13	9.67E-14	7.55E-14
0.7	1.08E-13	1.12E-13	1.25E-13	1.08E-13	8.52E-14
0.8	1.16E-13	1.20E-13	1.36E-13	1.20E-13	9.46E-14
0.9	1.23E-13	1.28E-13	1.47E-13	1.30E-13	1.04E-13
1	1.30E-13	1.36E-13	1.57E-13	1.41E-13	1.12E-13
2	1.83E-13	1.94E-13	2.44E-13	2.30E-13	1.91E-13
3	2.21E-13	2.35E-13	3.11E-13	3.05E-13	2.57E-13
4	2.51E-13	2.69E-13	3.68E-13	3.69E-13	3.17E-13
5	2.76E-13	2.97E-13	4.18E-13	4.28E-13	3.71E-13
6	2.97E-13	3.21E-13	4.62E-13	4.81E-13	4.21E-13
7	3.16E-13	3.42E-13	5.02E-13	5.30E-13	4.69E-13
8	3.32E-13	3.61E-13	5.39E-13	5.76E-13	5.13E-13
9	3.47E-13	3.78E-13	5.73E-13	6.19E-13	5.55E-13
10	3.61E-13	3.94E-13	6.04E-13	6.59E-13	5.95E-13
20	4.53E-13	5.02E-13	8.39E-13	9.80E-13	9.24E-13
30	5.07E-13	5.66E-13	9.96E-13	1.21E-12	1.17E-12
40	5.44E-13	6.11E-13	1.11E-12	1.40E-12	1.38E-12
50	5.72E-13	6.44E-13	1.21E-12	1.55E-12	1.56E-12
60	5.93E-13	6.71E-13	1.28E-12	1.68E-12	1.71E-12
70	6.11E-13	6.92E-13	1.35E-12	1.80E-12	1.85E-12
80	6.25E-13	7.10E-13	1.41E-12	1.90E-12	1.98E-12
90	6.37E-13	7.25E-13	1.46E-12	1.99E-12	2.09E-12
100	6.48E-13	7.39E-13	1.50E-12	2.08E-12	2.20E-12
200	7.07E-13	8.14E-13	1.78E-12	2.66E-12	2.98E-12
300	7.33E-13	8.48E-13	1.93E-12	3.00E-12	3.48E-12
400	7.49E-13	8.68E-13	2.02E-12	3.25E-12	3.85E-12
500	7.59E-13	8.81E-13	2.09E-12	3.43E-12	4.14E-12
600	7.66E-13	8.91E-13	2.14E-12	3.58E-12	4.38E-12
700	7.71E-13	8.98E-13	2.18E-12	3.70E-12	4.59E-12
800	7.75E-13	9.04E-13	2.22E-12	3.80E-12	4.76E-12

900	7.79E-13	9.08E-13	2.24E-12	3.89E-12	4.92E-12
1000	7.81E-13	9.12E-13	2.27E-12	3.96E-12	5.06E-12

Table S5: A comparison of the calculated rate coefficients (cm^3/s) at 800 K as a function of pressure for the $C_2H_4 + H \rightarrow C_2H_5$ reaction using four different ME approaches

T = 800 K

P (Torr)	TAR [a)]	CAR-1 [b)]	CAR-2 [c)]	SSA [d)]
0.1	8.022E-15	8.022E-15	8.020E-15	7.319E-15
0.3	2.091E-14	2.090E-14	2.090E-14	1.918E-14
0.5	3.244E-14	3.241E-14	3.243E-14	2.985E-14
0.7	4.320E-14	4.321E-14	4.320E-14	3.984E-14
1	5.839E-14	5.838E-14	5.839E-14	5.395E-14
3	1.444E-13	1.444E-13	1.444E-13	1.344E-13
5	2.168E-13	2.167E-13	2.168E-13	2.025E-13
7	2.815E-13	2.814E-13	2.815E-13	2.636E-13
10	3.690E-13	3.690E-13	3.691E-13	3.465E-13
30	8.110E-13	8.108E-13	8.111E-13	7.683E-13
50	1.139E-12	1.138E-12	1.139E-12	1.083E-12
70	1.410E-12	1.409E-12	1.410E-12	1.345E-12
100	1.752E-12	1.751E-12	1.752E-12	1.677E-12
300	3.220E-12	3.216E-12	3.221E-12	3.108E-12
500	4.135E-12	4.128E-12	4.135E-12	4.007E-12
700	4.818E-12	4.808E-12	4.819E-12	4.680E-12
1000	5.606E-12	5.605E-12	5.608E-12	5.459E-12

a) Thermally activated reaction model ($C_2H_5 \rightarrow C_2H_4 + H$).
b) Chemically activated reaction model ($C_2H_4 + H \rightleftharpoons C_2H_5$), and $k(T,p) = k_\infty \times (1 - \gamma_H)$ as recommended in the Multiwell software package by John R. Barker.
c) Chemically activated reaction model ($C_2H_4 + H \rightleftharpoons C_2H_5$), and Eq. 20 (see the main text).
d) Steady state approach for a chemically activated reaction, and Eq. 15 (see the main text). This SSA model starts to break down at 800 K, but it remains valid when T < 800 K.

Table S5 (Continued): A comparison of the calculated rate coefficients (cm^3/s) at 1000 K as a function of pressure for the $C_2H_4 + H \rightarrow C_2H_5$ reaction using four different ME approaches

T = 1000 K

P (Torr)	TAR [a)]	CAR-1 [b)]	CAR-2 [c)]	SSA [d)]
1	2.585E-14	2.559E-14	2.586E-14	1.785E-14
3	6.740E-14		6.746E-14	4.713E-14
5	1.040E-13		1.041E-13	7.324E-14
7	1.377E-13		1.378E-13	9.748E-14
10	1.846E-13	1.834E-13	1.848E-13	1.314E-13
30	4.388E-13		4.393E-13	3.188E-13
50	6.430E-13		6.435E-13	4.723E-13
70	8.206E-13		8.212E-13	6.075E-13
100	1.055E-12	1.024E-12	1.056E-12	7.879E-13
300	2.180E-12		2.182E-12	1.678E-12
500	2.975E-12		2.977E-12	2.325E-12
700	3.614E-12		3.617E-12	2.855E-12
1000	4.401E-12	4.367E-12	4.404E-12	3.520E-12
3000	7.590E-12		7.597E-12	6.319E-12
5000	9.454E-12		9.461E-12	8.024E-12
7000	1.079E-11		1.080E-11	9.277E-12
10000	1.228E-11	1.228E-11	1.229E-11	1.070E-11

d). At 1000 K, the SSA model completely breaks down.

T = 2000 K

P (Torr)	TAR [a)]	CAR-1 [b)]	CAR-2 [c)]
1	8.104E-16	8.107E-16	8.111E-16
3	2.304E-15	2.306E-15	2.306E-15
5	3.726E-15	3.729E-15	3.730E-15
7	5.106E-15	5.108E-15	5.109E-15
10	7.108E-15	7.116E-15	7.116E-15
30	1.946E-14	1.948E-14	1.948E-14
50	3.085E-14	3.088E-14	3.087E-14
70	4.165E-14	4.170E-14	4.169E-14
100	5.711E-14	5.719E-14	5.718E-14
300	1.484E-13	1.486E-13	1.486E-13

500	2.291E-13	2.294E-13	2.293E-13
700	3.038E-13	3.042E-13	3.040E-13
1000	4.083E-13	4.087E-13	4.083E-13
3000	9.884E-13	9.900E-13	9.891E-13
5000	1.470E-12	1.472E-12	1.471E-12
7000	1.899E-12	1.902E-12	1.900E-12
10000	2.477E-12	2.481E-12	2.479E-12
30000	5.414E-12	5.424E-12	5.418E-12
50000	7.620E-12	7.635E-12	7.627E-12
70000	9.466E-12	9.481E-12	9.473E-12
100000	1.182E-11	1.183E-11	1.183E-11

T = 3000 K

P (Torr)	TAR a)	CAR-2 c)
1	1.984E-16	1.983E-16
3	5.712E-16	5.707E-16
5	9.299E-16	9.292E-16
7	1.280E-15	1.279E-15
10	1.793E-15	1.791E-15
30	5.006E-15	5.001E-15
50	8.024E-15	8.014E-15
70	1.092E-14	1.091E-14
100	1.512E-14	1.510E-14
300	4.065E-14	4.058E-14
500	6.391E-14	6.380E-14
700	8.587E-14	8.572E-14
1000	1.172E-13	1.169E-13
3000	2.998E-13	2.991E-13
5000	4.595E-13	4.586E-13
7000	6.065E-13	6.056E-13
10000	8.113E-13	8.102E-13
30000	1.939E-12	1.940E-12
50000	2.865E-12	2.872E-12
70000	3.683E-12	3.700E-12
100000	4.778E-12	4.816E-12

Table S6: Calculated tunneling corrections as a function of temperature for the C_2H_3 + H_2 $\rightarrow$ C_2H_4 + H reaction using the SCTST theory.

T(K)	k(T) without tun.	k(T) with tun.	Tun. Correction (κ(T))
300	1.07E-18	4.12E-18	3.84E+00
325	3.36E-18	1.05E-17	3.13E+00
350	8.94E-18	2.39E-17	2.67E+00
375	2.09E-17	4.94E-17	2.36E+00
400	4.42E-17	9.41E-17	2.13E+00
425	8.56E-17	1.68E-16	1.96E+00
450	1.54E-16	2.82E-16	1.83E+00
475	2.62E-16	4.52E-16	1.72E+00
500	4.24E-16	6.94E-16	1.64E+00
525	6.56E-16	1.03E-15	1.57E+00
550	9.77E-16	1.48E-15	1.51E+00
575	1.41E-15	2.06E-15	1.46E+00
600	1.98E-15	2.81E-15	1.42E+00
625	2.70E-15	3.75E-15	1.38E+00
650	3.62E-15	4.90E-15	1.35E+00
675	4.75E-15	6.30E-15	1.33E+00
700	6.13E-15	7.98E-15	1.30E+00
725	7.78E-15	9.96E-15	1.28E+00
750	9.74E-15	1.23E-14	1.26E+00
775	1.20E-14	1.50E-14	1.24E+00
800	1.47E-14	1.81E-14	1.23E+00
825	1.78E-14	2.16E-14	1.22E+00
850	2.13E-14	2.56E-14	1.20E+00
875	2.53E-14	3.01E-14	1.19E+00
900	2.98E-14	3.52E-14	1.18E+00
925	3.49E-14	4.08E-14	1.17E+00
950	4.05E-14	4.70E-14	1.16E+00
975	4.67E-14	5.39E-14	1.15E+00
1000	5.36E-14	6.14E-14	1.15E+00
1025	6.12E-14	6.96E-14	1.14E+00
1050	6.95E-14	7.86E-14	1.13E+00
1075	7.85E-14	8.83E-14	1.13E+00
1100	8.83E-14	9.88E-14	1.12E+00
1125	9.89E-14	1.10E-13	1.11E+00

1150	1.10E-13	1.22E-13	1.11E+00
1175	1.23E-13	1.35E-13	1.10E+00
1200	1.36E-13	1.49E-13	1.10E+00
1225	1.50E-13	1.64E-13	1.10E+00
1250	1.65E-13	1.80E-13	1.09E+00
1275	1.81E-13	1.97E-13	1.09E+00
1300	1.98E-13	2.15E-13	1.08E+00
1325	2.17E-13	2.34E-13	1.08E+00
1350	2.36E-13	2.54E-13	1.08E+00
1375	2.56E-13	2.76E-13	1.08E+00
1400	2.78E-13	2.98E-13	1.07E+00
1425	3.00E-13	3.21E-13	1.07E+00
1450	3.24E-13	3.46E-13	1.07E+00
1475	3.49E-13	3.72E-13	1.06E+00
1500	3.75E-13	3.99E-13	1.06E+00
1525	4.03E-13	4.27E-13	1.06E+00
1550	4.32E-13	4.57E-13	1.06E+00
1575	4.62E-13	4.88E-13	1.06E+00
1600	4.93E-13	5.20E-13	1.05E+00
1625	5.25E-13	5.53E-13	1.05E+00
1650	5.59E-13	5.88E-13	1.05E+00
1675	5.94E-13	6.24E-13	1.05E+00
1700	6.31E-13	6.61E-13	1.05E+00
1725	6.69E-13	7.00E-13	1.05E+00
1750	7.08E-13	7.40E-13	1.04E+00
1775	7.48E-13	7.81E-13	1.04E+00
1800	7.90E-13	8.24E-13	1.04E+00
1825	8.34E-13	8.68E-13	1.04E+00
1850	8.78E-13	9.13E-13	1.04E+00
1875	9.24E-13	9.60E-13	1.04E+00
1900	9.72E-13	1.01E-12	1.04E+00
1925	1.02E-12	1.06E-12	1.04E+00
1950	1.07E-12	1.11E-12	1.03E+00
1975	1.12E-12	1.16E-12	1.03E+00
2000	1.18E-12	1.21E-12	1.03E+00

Optimized geometries of various species

C_2H_3 (C_s, $^2A'$): ae-CCSD(T)/cc-pVQZ // UHF

```
HEAT-345Q
C
C 1 R1*
H 1 R2* 2 A1*
H 1 R3* 2 A2* 3 T180
H 2 R4* 1 A3* 3 T180

R1   =      1.307413290373744
R2   =      1.081723724184898
A1   =    122.057880654972905
R3   =      1.087181560366102
A2   =    121.279851219171391
T180 =    180.000000000000000
R4   =      1.075581119201201
A3   =    137.363322899459064
```

C_2H_4 (D_{2h}, $^1A_1$): ae-CCSD(T)/cc-pVQZ // RHF

```
HEAT-345Q
C
C 1 R1*
H 1 R2* 2 A1*
H 1 R2* 2 A1* 3 D180
H 2 R2* 1 A1* 3 D180
H 2 R2* 1 A1* 5 D180

R1   =      1.330902917626653
R2   =      1.079752371421382
A1   =    121.448016067414059
D180 =    180.000000000000000
```

C_2H_5 (C_s, $^2A'$): ae-CCSD(T)/cc-pVQZ // UHF

```
HEAT-345Q
C
C 1 R1
H 1 R2 2 A1
H 1 R3 2 A2 3 T1
```

```
H 1 R3 2 A2 3 T2
H 2 R4 1 A3 3 T3
H 2 R4 1 A3 3 T4

R1  =     1.484754348094979
R2  =     1.095430448603470
A1  =   111.646939695568605
R3  =     1.088412112085974
A2  =   111.580217293014798
T1  =   119.360318042895344
T2  =  -119.360318042895344
R4  =     1.077652719659850
A3  =   120.813623360314452
T3  =    85.455662573944480
T4  =   -85.455662573944480
```

TS1 (C_s, $^2A'$): ae-CCSD(T)/cc-pVQZ // UHF

```
HEAT-345Q
H
C 1 R1*
C 2 R2* 1 A1*
H 2 R3* 3 A2* 1 T1*
H 2 R3* 3 A2* 1 T2*
H 3 R4* 2 A3* 1 T3*
H 3 R4* 2 A3* 1 T4*

R1  =     1.981950449111066
R2  =     1.341149588425816
A1  =   106.655914053263487
R3  =     1.079445246175276
A2  =   121.248975399909156
T1  =    94.655688607126208
T2  =   -94.655688607126208
R4  =     1.079247392069564
A3  =   121.328812222024141
T3  =    88.799300980087395
T4  =   -88.799300980087395
```

TS1 (C_s, $^2A'$): ae-CCSD(T)/cc-pVQZ // ROHF

```
HEAT-345Q
H
```

```
C 1 R1*
C 2 R2* 1 A1*
H 2 R3* 3 A2* 1 T1*
H 2 R3* 3 A2* 1 T2*
H 3 R4* 2 A3* 1 T3*
H 3 R4* 2 A3* 1 T4*

R1   =     1.982646393556012
R2   =     1.343265335057637
A1   =   106.560181074648682
R3   =     1.079480329790683
A2   =   121.229700627428400
T1   =    94.718156988897547
T2   =   -94.718156988897547
R4   =     1.079315572788190
A3   =   121.315855945123403
T3   =    88.775569747622228
T4   =   -88.775569747622228
```

TS2 (C_s, $^2A'$): ae-CCSD(T)/cc-pVQZ // UHF

```
HEAT-345Q
C
C 1 R1*
H 1 R2* 2 A1*
H 2 R3* 1 A2* 3 T180
H 2 R4* 1 A3* 4 T180
H 1 R5* 2 A4* 3 T180
X 6 R0 1 A5* 3 T180
H 6 R6* 7 A5* 1 T180

R1   =     1.314696068503856
R2   =     1.078080276583277
A1   =   131.559284241466571
R3   =     1.081392379108812
A2   =   121.406021847894522
T180 =   180.000000000000000
R4   =     1.083852697068704
A3   =   121.430010447996494
R5   =     1.446328141095375
A4   =   114.483549666949699
R0   =     1.000000000000000
A5   =    87.390531570229783
R6   =     0.862813820478743
```

TS3 (C_{2v}, $^{2}B_{1}$): ae-CCSD(T)/cc-pVQZ // UHF

```
HEAT-345Q
X
H 1 R0
C 2 R1* 1 A1*
C 2 R1* 1 A1* 3 T180
H 3 R2* 2 A2* 1 T90*
H 3 R2* 2 A2* 1 Tm90*
H 4 R2* 2 A2* 1 T90*
H 4 R2* 2 A2* 1 Tm90*

R0   =      1.000000000000000
R1   =      1.290216448720350
A1   =    144.866813199303550
T180 =    180.000000000000000
R2   =      1.076159762632992
A2   =    112.708317862970560
T90  =     69.290755272482755
Tm90 =    -69.290755272482755
```

Ro-vibrational parameters and anharmonic constants (all in cm^{-1}) for various species

C_2H_3

	ANO2 a)		ANO1 b)								
ω1	723.7815	x11	-3.1037								
ω2	825.7328	x2i	2.5757	1.0783							
ω3	925.1483	x3i	3.8283	-0.0940	-0.2882						
ω4	1070.7801	x4i	-34.9720	0.6219	1.7690	-7.3640					
ω5	1396.2211	x5i	-0.4151	-1.1211	-5.6418	-4.1735	-3.3217				
ω6	1642.3325	x6i	-2.0176	-7.9209	-6.9465	-11.2744	-6.4847	-7.1344			
ω7	3076.9052	x7i	-5.4179	-5.8609	-8.2251	-8.7029	-16.8495	-7.8422	-47.7603		
ω8	3182.3996	x8i	-7.0895	-5.8476	-15.5273	-11.2059	-18.7664	1.9991	-62.4763	-48.9464	
ω9	3252.9634	x9i	0.1749	-10.1917	-3.5752	1.5972	-1.7544	-0.9093	0.6039	2.0052	-61.8138

Three rotational constants (cm^{-1})

A	7.8037
B	1.0880
C	0.9549

a) Obtained at fc-CCSD(T)/ANO2 level of theory
b) Calculated at fc-CCSD(T)/ANO1 level of theory

C_2H_4

Harmonic vib. frequencies (cm^{-1})

	ANO2 (in cm^{-1})
ω1	823.9830
ω2	951.8802
ω3	965.8709
ω4	1051.7872
ω5	1246.7681
ω6	1367.8359
ω7	1476.5674
ω8	1670.8931
ω9	3140.1665
ω10	3158.7995

$\boldsymbol{\omega}$11	3224.1575
$\boldsymbol{\omega}$12	3250.3880

Three rotational constants (cm^{-1})

A (in cm^{-1})	4.9039
B	1.0038
C	0.8333

Anharmonic constants (cm^{-1})

ANO1	**1**	2	3	4
x11	4.3442			
x2i	0.7569	2.3874		
x3i	6.1162	0.6447	0.9274	
x4i	1.2604	-5.8769	-8.3740	-1.8225
x5i	-6.1974	5.0296	1.6302	0.1798
x6i	1.8536	-3.0486	-2.3630	-3.8531
x7i	-3.6984	-3.2823	-4.0933	1.7472
x8i	-7.8406	-7.2307	-7.2805	-3.9021
x9i	-3.6327	-5.1113	-4.4890	-6.7800
x10i	-3.2009	-6.4196	-4.7058	-6.6592
x11i	-4.9923	-9.5793	-7.8258	-5.4790
x12i	-2.8880	-8.8687	-8.2962	-5.9247
	5	6	7	8
x55	-0.2895			
x6i	-2.2715	-0.9409		
x7i	-5.6368	-5.0667	-3.0889	
x8i	-15.1488	-9.2395	-1.9102	-0.8700
x9i	-5.4373	-5.2213	-13.0393	-8.1338
x10i	-6.6838	-5.5998	-3.2687	-22.2981
x11i	-1.2917	-7.2734	-11.5576	3.0821
x12i	-6.2928	-7.1946	-10.2969	-1.9772
	9	10	11	12
x99	-13.7476			
x10i	-55.3970	-13.7848		
x11i	-56.5743	-58.6835	-16.1203	
x12i	-57.8048	-56.4728	-64.9344	-16.0017

C_2H_5

Harmonic vib. frequencies (cm^{-1})

	ANO2 (cm^{-1})
ω1 (**1DHR**)	**120.9308**
ω2	467.7380
ω3	809.3232
ω4	987.4477
ω5	1071.3188
ω6	1201.1202
ω7	1404.5662
ω8	1477.2985
ω9	1492.0082
ω10	1492.0789
ω11	2986.2513
ω12	3068.4187
ω13	3113.6714
ω14	3159.3045
ω15	3265.1512
Rotational constants	
A (in cm^{-1})	3.4689
B	0.7591
C	0.7039

1DHR potential

$$V_{1DHR} = \frac{V_o}{2}(1 - cos3\theta), with\ V_o = 30\ cm^{-1}\ and\ B_{hr} = 16\ cm^{-1}$$

Anharmonic constants (cm^{-1})

	ANO1			
x11	-66.5374			
x2i	-28.3026	16.1158		
x3i	14.3320	15.7641	3.7860	
x4i	-3.1186	1.5941	-0.8608	-1.5916

x5i	-1.2856	-3.7080	-1.6363	-4.2507
x6i	-21.0127	-1.6752	-4.2197	-7.6575
x7i	2.6467	-0.6979	-0.5183	-5.5803
x8i	2.4729	5.2013	-3.4305	-2.6700
x9i	-1.7249	2.5167	-6.7878	-4.2974
x10i	-2.0554	0.2218	-3.2053	-6.1197
x11i	27.0236	8.6438	-0.6061	-10.4427
x12i	-11.0857	0.8991	-2.3042	-0.8768
x13i	-12.8979	-0.5310	-2.3181	-4.1164
x14i	6.3665	-12.4531	-4.2939	-1.5725
x15i	8.0489	-18.9154	-4.9163	0.0350
x55	-5.5251			
x6i	-4.9089	-1.6753		
x7i	-4.8848	-2.6993	-7.9437	
x8i	-2.5616	-5.4478	-2.8990	-4.2150
x9i	-3.2374	-7.3201	-3.6965	-16.3829
x10i	-1.3344	-5.1115	-4.9181	-2.7673
x11i	2.4840	1.4227	2.0284	-5.8662
x12i	0.9516	-5.1087	-2.8412	-1.6679
x13i	0.8205	-3.8459	-6.4572	-8.3597
x14i	-1.1499	-4.0872	-1.0211	2.1353
x15i	-0.0395	-3.6299	-1.2601	-9.7636
x99	-2.1390			
x10i	-2.1252	-1.2562		
x11i	-2.9565	-26.1300	-52.2687	
x12i	-9.0668	-15.9513	-41.9263	-24.5143
x13i	-11.9221	-9.7745	-8.5142	-111.7388
x14i	2.5334	-0.5240	0.0784	0.2501
x15i	-7.6108	-0.5076	0.0427	-0.1926
x1313		-32.9545		
x14i		-0.3972	-28.3601	
x15i		-0.9953	-115.8986	-33.0685

TS1 (H-addition): $C_2H_4 + H = C_2H_5$

Harmonic vib. frequencies (cm^{-1})

	ANO2		**ANO1//ROHF**		**ANO1//UHF**
ωF	767.4551i	xFF	-140.3099	xFF	-135.5767
ω2	370.1676	x2F	96.0464i	x2F	92.2658i
ω3	401.3949	x3F	88.5148i	x3F	84.9941i
ω4	821.8382	x4F	-1.5688i	x4F	-1.4944i
ω5	931.5782	x5F	-8.3165i	x5F	-9.5865i
ω6	989.8053	x6F	15.9583i	x6F	12.5083i
ω7	1044.9995	x7F	-1.5978i	x7F	-3.3770i
ω8	1245.9548	x8F	-0.1202i	x8F	-0.2021i
ω9	1344.0524	x9F	-12.6583i	x9F	-15.4547i
ω10	1473.9225	x10F	-0.6742i	x10F	-0.5546i
ω11	1630.0208	x11F	-16.9948i	x11F	-22.4470i
ω12	3145.5794	x12F	2.0521i	x12F	2.4312i
ω13	3160.1214	x13F	0.3138i	x13F	0.3076i
ω14	3230.7760	x14F	2.4960i	x14F	2.8817i
ω15	3256.2492	x15F	2.2070i	x15F	2.5923i
A	2.5384				
B	0.7655				
C	0.7577				

Anharmonic constants (cm^{-1}) based on ROHF reference

	ANO1			
x2i	16.0345			
x3i	25.7955	10.6079		
x4i	-0.0539	-1.3565	4.0408	
x5i	-4.4511	-5.4092	2.2118	3.0111
x6i	9.6620	9.2680	2.8359	0.7933
x7i	-1.5530	4.4124	1.1411	-5.4453
x8i	0.7593	-0.9412	-5.9654	2.5701
x9i	-5.7409	-4.6132	1.8176	-2.6713
x10i	-0.2677	-1.5669	-3.6771	-3.8530
x11i	-7.1966	-5.2222	-6.6580	-7.5557
x12i	0.1074	-0.3111	-3.6370	-4.9339

x13i	-0.5003	-0.9020	-3.2029	-5.9527
x14i	0.3101	-0.1679	-4.9788	-8.4569
x15i	0.3100	-0.3189	-3.1020	-9.4817
x66	1.4572			
x7i	-7.6258	-1.9319		
x8i	1.4040	-0.1624	-0.4064	
x9i	-3.7231	-4.7518	-2.2220	-1.3253
x10i	-2.3949	0.0813	-5.6425	-3.9907
x11i	-7.1637	-2.8043	-13.8367	-7.2183
x12i	-4.9088	-6.3084	-5.4191	-4.5649
x13i	-4.9268	-6.1624	-6.5206	-4.8564
x14i	-8.6007	-5.2777	-2.4295	-5.6315
x15i	-7.3367	-5.5725	-6.2087	-5.4657
x1010	-3.0954			
x11i	-1.5867	-2.8165		
x12i	-14.5355	-10.4016	-13.8484	
x13i	-3.4441	-9.6859	-55.4792	-13.9026
x14i	-11.5307	0.0240	-57.0367	-58.4871
x15i	-10.3450	-4.0409	-57.4978	-56.9514
X1414			-16.3626	
x15i			-64.3319	-16.2069

Anharmonic constants (cm^{-1}) based on UHF reference

	ANO1			
x2i	15.7947			
x3i	25.3090	10.4867		
x4i	-0.0179	-1.3292	4.0906	
x5i	-4.9511	-5.8622	2.2737	2.8688
x6i	8.9323	8.5877	2.8418	0.9463
x7i	-2.1268	3.7839	1.2487	-4.8542
x8i	0.7381	-0.9331	-5.9797	2.6278
x9i	-5.9965	-4.7933	1.9586	-2.3536
x10i	-0.2259	-1.5438	-3.6674	-3.5257
x11i	-8.1947	-6.1348	-6.7831	-6.7705
x12i	0.1965	-0.2079	-3.6163	-4.7627

x13i	-0.4402	-0.8487	-3.1841	-5.9200
x14i	0.4204	-0.0581	-4.9643	-8.3049
x15i	0.4257	-0.2062	-3.0509	-9.4727
x66	1.2173			
x7i	-7.3940	-1.5914		
x8i	1.4484	0.0098	-0.3843	
x9i	-3.6355	-4.1085	-2.1284	-1.0242
x10i	-2.2048	0.1716	-5.6281	-4.1168
x11i	-7.0087	-2.5882	-13.9444	-6.6733
x12i	-4.9094	-6.2810	-5.3969	-4.6749
x13i	-4.7666	-6.0465	-6.5106	-5.0027
x14i	-8.5971	-5.2354	-2.2469	-5.9405
x15i	-7.1889	-5.5096	-6.1819	-5.7616
x1010	-3.0876			
x11i	-1.5486	-2.7527		
x12i	-14.2314	-9.8997	-13.8472	
x13i	-3.4076	-9.0524	-55.2007	-13.9043
x14i	-11.5034	0.6058	-57.0672	-58.1850
x15i	-10.3234	-3.5844	-57.1863	-56.9863
X1414			-16.3540	
x15i			-64.0215	-16.1983

TS2 (H-abstraction): $C_2H_3 + H_2 = H + C_2H_4$

Harmonic vib. frequencies (cm^{-1})

	ANO2		ANO1
ωF	1324.6845i	xFF	-188.4614
ω2	270.2214	x2F	42.8014i
ω3	369.9700	x3F	47.6905i
ω4	820.5762	x4F	34.1140i
ω5	907.2815	x5F	22.2190i
ω6	945.1807	x6F	97.1985i
ω7	961.1345	x7F	55.9111i

$\boldsymbol{\omega}8$	1090.1186	x8F	126.0746i
$\boldsymbol{\omega}9$	1150.9694	x9F	55.0554i
$\boldsymbol{\omega}10$	1402.9928	x10F	0.6030i
$\boldsymbol{\omega}11$	1634.4538	x11F	-18.7725i
$\boldsymbol{\omega}12$	2020.2071	x12F	-719.5663i
$\boldsymbol{\omega}13$	3113.3153	x13F	8.5032i
$\boldsymbol{\omega}14$	3201.9921	x14F	4.9874i
$\boldsymbol{\omega}15$	3222.0012	x15F	-6.6256i
Rot. Constants (cm^{-1})			
A	2.3160		
B	0.8262		
C	0.6090		

Anharmonic constants (cm^{-1})

	ANO1			
x2i	5.4362			
x3i	8.5864	-0.1263		
x4i	3.9678	6.0822	1.5207	
x5i	2.2262	2.9678	1.2832	0.0693
x6i	4.9963	4.7434	6.2374	1.2240
x7i	3.2705	3.2502	3.9399	2.0405
x8i	10.0911	3.3053	19.5157	5.6041
x9i	8.7286	7.3529	-1.0648	2.6045
x10i	-0.3183	-0.5538	-0.5606	-2.1553
x11i	-2.3541	-2.1965	-8.0171	-7.7348
x12i	-27.0073	-33.3051	-33.1005	-23.7729
x13i	0.9181	-1.0165	-3.4023	-6.8178
x14i	0.7903	-0.1331	-4.0496	-6.6477
x15i	-1.4582	-3.7108	-6.0940	-9.1372
x66	21.4011			
x7i	38.7716	4.3712		
x8i	18.8874	11.7577	86.0359	
x9i	5.3233	3.8397	68.3730	1.9112
x10i	-1.5365	-3.3421	-0.1255	-1.3339
x11i	-15.2214	-11.3350	-15.2662	-10.4470
x12i	-142.4893	-76.1627	-477.6116	-117.7658
x13i	-1.6311	-4.1144	-2.1672	-2.7199

x14i	-4.1193	-9.7395	-1.9704	-3.7469
x15i	-4.0757	-4.3671	-3.9257	-8.9607
x1010	-2.8839			
x11i	-6.1315	-4.1072		
x12i	1.3269	56.7401	309.5159	
x13i	-15.5842	-16.7884	-10.3559	-32.8144
x14i	-17.7090	0.0980	-4.6527	-92.1822
x15i	-2.2859	-0.0883	8.5886	-11.3268
X1414			-35.1459	
x15i			-17.5354	-53.6398

TS3 (self-isomerization): CH_3-CH_2 = CH_2-CH_3

Rot-vibrational parameters

	ANO2		ANO1
ωF	1939.2060i	xFF	-77.6585
ω2	562.6250	x2F	11.4998i
ω3	730.5467	x3F	-22.0354i
ω4	733.6306	x4F	-15.2601i
ω5	781.1570	x5F	-0.7756i
ω6	1133.0625	x6F	6.7879i
ω7	1196.1857	x7F	-1.3776i
ω8	1278.2507	x8F	16.1550i
ω9	1421.9647	x9F	-0.8977i
ω10	1449.9166	x10F	-4.6339i
ω11	2231.5941	x11F	-43.9037i
ω12	3163.9074	x12F	4.4052i
ω13	3171.3154	x13F	4.5035i
ω14	3275.7843	x14F	6.8416i
ω15	3295.9487	x15F	6.7478i
A	3.5921		
B	0.8016		
C	0.7228		

Anharmonic constants (cm^{-1})

	ANO1			
x2i	10.2984			
x3i	19.2086	4.9853		
x4i	11.5131	11.9534	-10.7225	
x5i	4.1715	-1.7772	5.3367	4.3069
x6i	2.4531	-6.6765	-5.3144	-3.2882
x7i	-3.3910	1.1336	-4.3800	-5.5812
x8i	17.0752	-9.7449	-6.3407	-5.7236
x9i	3.7719	-1.6424	-0.2042	-3.2586
x10i	10.7972	0.1842	-0.6640	-6.4331
x11i	-10.5250	-8.4715	-7.8468	-0.0560
x12i	-9.1498	-3.8933	-0.7521	-3.0234
x13i	-10.8910	-5.8204	0.6180	-2.7102
x14i	-11.1958	-8.4254	-4.0015	-4.1864
x15i	-12.6925	-8.7113	-3.8720	-2.8160
x66	-6.4991			
x7i	-5.9018	-1.1844		
x8i	0.2075	-0.8720	-1.0515	
x9i	-4.3152	-5.0396	-1.4878	-2.8963
x10i	-5.7843	-8.0789	0.4570	-15.4395
x11i	-9.9074	-2.0710	-36.4598	-1.3269
x12i	-0.0064	-4.5916	-3.5463	-3.0247
x13i	0.2410	-5.0511	-3.9016	-5.3718
x14i	1.4979	-3.8456	-4.5693	-11.1819
x15i	1.0874	-5.3435	-5.1944	-10.7363
x1010	-4.4882			
x11i	-2.8893	-29.0936		
x12i	-2.7807	0.4836	-14.5841	
x13i	-1.0670	-0.3919	-58.1918	-14.7212
x14i	-9.0928	0.9906	-58.3092	-59.9562
x15i	-10.2561	-0.0835	-59.1982	-57.9707

X1414			-17.1329	
x15i			-67.6014	-16.8619