

Electronic Supplementary Information
for
Cleavage of an aromatic ring and radical migration

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Table S1. Calculated rate constants (s^{-1}) for unimolecular isomerization and decomposition reactions of naphthalenyl ($C_{10}H_7$, (a)), acetanaphthylenyl ($C_{12}H_7$, (b)), and pyrenyl ($C_{16}H_9$, (c)) radicals at pressures of 30 Torr, 1, 10, and 100 atm.

a) naphthalenyl radicals, $C_{10}H_7$

Pressure = 30 Torr					
T(K)	n1→n-p1	n1→n-p2	n1→n-p3	n1→n-p4	n1→n2
500	1.06E-27	1.44E-26	2.53E-20	1.02E-24	8.74E-13
600	3.68E-20	2.39E-19	1.57E-14	5.26E-18	1.36E-08
700	8.63E-15	3.49E-14	2.20E-10	4.63E-13	1.58E-05
800	8.48E-11	2.45E-10	2.89E-07	2.78E-09	3.36E-03
900	9.94E-08	2.21E-07	7.71E-05	2.45E-06	2.22E-01
1000	2.62E-05	4.72E-05	6.74E-03	5.19E-04	6.35E+00
1125	6.15E-03	9.10E-03	5.78E-01	9.30E-02	1.70E+02
1250	4.08E-01	5.28E-01	1.90E+01	4.73E+00	2.06E+03
1375	1.01E+01	1.20E+01	2.90E+02	9.19E+01	1.30E+04
1500	1.27E+02	1.41E+02	2.55E+03	9.32E+02	5.12E+04
1650	1.17E+03	1.23E+03	1.73E+04	6.88E+03	1.58E+05
1800	5.60E+03	5.73E+03	6.64E+04	2.77E+04	3.37E+05
2000	***	***	***	***	***
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 1 atm					
T(K)	n1→n-p1	n1→n-p2	n1→n-p3	n1→n-p4	n1→n2
500	4.16E-28	6.99E-27	2.53E-20	4.03E-26	8.74E-13
600	1.33E-20	9.15E-20	1.57E-14	2.12E-19	1.36E-08
700	3.68E-15	1.36E-14	2.22E-10	1.99E-14	1.59E-05
800	4.98E-11	1.21E-10	2.92E-07	1.38E-10	3.37E-03
900	8.32E-08	1.54E-07	7.84E-05	1.59E-07	2.25E-01
1000	3.03E-05	4.65E-05	6.89E-03	4.88E-05	6.60E+00
1125	9.97E-03	1.30E-02	6.04E-01	1.53E-02	1.95E+02
1250	9.03E-01	1.04E+00	2.14E+01	1.42E+00	2.88E+03
1375	3.14E+01	3.28E+01	3.85E+02	5.07E+01	2.45E+04
1500	5.16E+02	5.03E+02	4.01E+03	8.33E+02	1.32E+05
1650	6.68E+03	6.13E+03	3.58E+04	1.03E+04	5.95E+05
1800	5.42E+04	4.76E+04	2.19E+05	7.72E+04	1.87E+06
2000	3.63E+05	3.06E+05	1.12E+06	4.53E+05	4.97E+06
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 10 atm					
T(K)	n1→n-p1	n1→n-p2	n1→n-p3	n1→n-p4	n1→n2

500	3.70E-28	6.56E-27	2.53E-20	4.03E-27	8.74E-13
600	1.03E-20	7.81E-20	1.57E-14	2.13E-20	1.36E-08
700	2.36E-15	9.76E-15	2.22E-10	2.00E-15	1.59E-05
800	2.68E-11	7.14E-11	2.92E-07	1.42E-11	3.37E-03
900	4.20E-08	8.01E-08	7.88E-05	1.69E-08	2.25E-01
1000	1.63E-05	2.44E-05	6.97E-03	5.62E-06	6.63E+00
1125	6.64E-03	8.07E-03	6.16E-01	2.09E-03	1.98E+02
1250	7.95E-01	8.44E-01	2.21E+01	2.51E-01	3.02E+03
1375	3.67E+01	3.55E+01	4.08E+02	1.25E+01	2.79E+04
1500	7.97E+02	7.20E+02	4.54E+03	3.01E+02	1.72E+05
1650	1.45E+04	1.23E+04	4.77E+04	6.19E+03	9.82E+05
1800	1.32E+05	1.07E+05	3.04E+05	6.09E+04	3.70E+06
2000	1.42E+06	1.12E+06	2.26E+06	6.55E+05	1.39E+07
2250	8.69E+06	6.60E+06	1.10E+07	3.92E+06	3.80E+07
2500	***	***	***	***	***
Pressure = 100 atm					
T(K)	n1→n-p1	n1→n-p2	n1→n-p3	n1→n-p4	n1→n2
500	3.52E-28	6.15E-27	2.53E-20	4.03E-28	8.74E-13
600	9.79E-21	7.41E-20	1.57E-14	2.13E-21	1.36E-08
700	2.16E-15	9.16E-15	2.22E-10	2.00E-16	1.59E-05
800	2.27E-11	6.31E-11	2.92E-07	1.42E-12	3.37E-03
900	3.13E-08	6.35E-08	7.88E-05	1.71E-09	2.25E-01
1000	1.05E-05	1.67E-05	6.98E-03	5.79E-07	6.63E+00
1125	3.71E-03	4.69E-03	6.21E-01	2.26E-04	1.99E+02
1250	4.32E-01	4.61E-01	2.25E+01	2.99E-02	3.05E+03
1375	2.21E+01	2.08E+01	4.23E+02	1.74E+00	2.87E+04
1500	5.85E+02	5.07E+02	4.83E+03	5.23E+01	1.86E+05
1650	1.45E+04	1.17E+04	5.39E+04	1.53E+03	1.18E+06
1800	1.85E+05	1.42E+05	3.87E+05	2.32E+04	5.27E+06
2000	2.37E+06	1.75E+06	3.06E+06	3.68E+05	2.45E+07
2250	2.05E+07	1.47E+07	1.91E+07	3.69E+06	9.10E+07
2500	1.33E+08	9.40E+07	8.07E+07	2.18E+07	2.21E+08
Pressure = 30 Torr					
T(K)	n2→n-p1	n2→n-p2	n2→n-p3	n2→n-p4	n2→n1
500	1.03E-29	6.63E-29	2.13E-20	3.83E-21	7.26E-13
600	1.13E-21	4.05E-21	1.36E-14	3.67E-15	1.17E-08
700	7.04E-16	1.76E-15	1.96E-10	7.04E-11	1.38E-05
800	1.51E-11	2.97E-11	2.62E-07	1.15E-07	2.96E-03
900	3.18E-08	5.29E-08	7.12E-05	3.55E-05	1.98E-01
1000	1.26E-05	1.86E-05	6.31E-03	3.33E-03	5.69E+00
1125	4.06E-03	5.33E-03	5.47E-01	2.87E-01	1.54E+02

1250	3.21E-01	3.88E-01	1.82E+01	9.13E+00	1.87E+03
1375	8.89E+00	1.01E+01	2.84E+02	1.36E+02	1.19E+04
1500	1.11E+02	1.21E+02	2.40E+03	1.12E+03	4.74E+04
1650	1.03E+03	1.08E+03	1.60E+04	7.46E+03	1.48E+05
1800	5.02E+03	5.09E+03	6.16E+04	2.88E+04	3.23E+05
2000	2.28E+04	2.25E+04	2.18E+05	9.90E+04	***
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 1 atm					
T(K)	n2→n-p1	n2→n-p2	n2→n-p3	n2→n-p4	n2→n1
500	1.68E-31	1.20E-30	2.13E-20	3.83E-21	7.26E-13
600	1.99E-23	6.76E-23	1.36E-14	3.68E-15	1.17E-08
700	1.86E-17	3.96E-17	1.96E-10	7.08E-11	1.38E-05
800	7.17E-13	1.15E-12	2.62E-07	1.17E-07	2.97E-03
900	2.88E-09	3.87E-09	7.13E-05	3.77E-05	2.00E-01
1000	2.17E-06	2.58E-06	6.35E-03	3.81E-03	5.93E+00
1125	1.48E-03	1.58E-03	5.66E-01	3.77E-01	1.76E+02
1250	2.32E-01	2.30E-01	2.03E+01	1.43E+01	2.61E+03
1375	1.20E+01	1.13E+01	3.70E+02	2.61E+02	2.24E+04
1500	2.65E+02	2.40E+02	3.92E+03	2.67E+03	1.21E+05
1650	4.47E+03	3.90E+03	3.68E+04	2.38E+04	5.52E+05
1800	3.64E+04	3.08E+04	2.03E+05	1.26E+05	1.78E+06
2000	2.53E+05	2.09E+05	1.02E+06	6.20E+05	4.94E+06
2250	1.44E+06	1.17E+06	3.93E+06	2.04E+06	***
2500	***	***	***	***	***
Pressure = 10 atm					
T(K)	n2→n-p1	n2→n-p2	n2→n-p3	n2→n-p4	n2→n1
500	1.41E-32	1.05E-31	2.13E-20	3.83E-21	7.26E-13
600	1.42E-24	5.17E-24	1.36E-14	3.68E-15	1.17E-08
700	1.10E-18	2.48E-18	1.96E-10	7.08E-11	1.38E-05
800	3.96E-14	6.43E-14	2.62E-07	1.18E-07	2.97E-03
900	1.78E-10	2.30E-10	7.13E-05	3.78E-05	2.01E-01
1000	1.74E-07	1.93E-07	6.35E-03	3.85E-03	5.95E+00
1125	1.84E-04	1.80E-04	5.67E-01	3.91E-01	1.79E+02
1250	4.69E-02	4.24E-02	2.06E+01	1.57E+01	2.75E+03
1375	3.96E+00	3.38E+00	3.87E+02	3.14E+02	2.54E+04
1500	1.39E+02	1.14E+02	4.38E+03	3.67E+03	1.58E+05
1650	3.96E+03	3.15E+03	4.75E+04	3.98E+04	9.04E+05
1800	5.07E+04	3.93E+04	3.17E+05	2.60E+05	3.43E+06
2000	5.99E+05	4.53E+05	2.15E+06	1.71E+06	1.36E+07
2250	4.33E+06	3.19E+06	1.09E+07	8.52E+06	3.87E+07

2500	2.28E+07	1.68E+07	3.16E+07	1.87E+07	***
Pressure = 100 atm					
T(K)	n2→n-p1	n2→n-p2	n2→n-p3	n2→n-p4	n2→n1
500	1.01E-33	7.40E-33	2.13E-20	3.83E-21	7.26E-13
600	1.09E-25	3.99E-25	1.36E-14	3.68E-15	1.17E-08
700	8.42E-20	1.94E-19	1.96E-10	7.08E-11	1.38E-05
800	2.82E-15	4.73E-15	2.62E-07	1.18E-07	2.97E-03
900	1.14E-11	1.52E-11	7.13E-05	3.78E-05	2.01E-01
1000	1.03E-08	1.16E-08	6.35E-03	3.85E-03	5.95E+00
1125	1.12E-05	1.08E-05	5.67E-01	3.93E-01	1.80E+02
1250	3.47E-03	3.03E-03	2.06E+01	1.59E+01	2.77E+03
1375	4.02E-01	3.27E-01	3.89E+02	3.27E+02	2.62E+04
1500	2.08E+01	1.61E+01	4.49E+03	4.03E+03	1.70E+05
1650	9.83E+02	7.36E+02	5.12E+04	4.86E+04	1.08E+06
1800	2.10E+04	1.53E+04	3.81E+05	3.72E+05	4.86E+06
2000	4.58E+05	3.26E+05	3.22E+06	3.17E+06	2.27E+07
2250	6.27E+06	4.38E+06	2.28E+07	2.24E+07	8.55E+07
2500	3.49E+07	2.40E+07	8.89E+07	8.73E+07	2.36E+08

b) acetanaphthylenyl radicals, C₁₂H₇

Pressure = 30 Torr					
T(K)	an1→an3	an1→an4	an1→an5	an1→an7	an1→an-p1
500	3.34E-13	4.32E-17	5.56E-19	1.37E-22	9.81E-37
700	2.91E-17	1.80E-18	2.49E-19	4.69E-12	1.20E-23
800	5.48E-13	9.07E-14	3.14E-14	1.09E-08	2.52E-18
900	1.32E-09	4.41E-10	2.14E-10	4.75E-06	3.80E-14
1000	8.47E-07	4.14E-07	2.29E-08	6.22E-04	8.33E-11
1125	3.49E-04	2.68E-04	1.77E-04	7.98E-02	1.75E-07
1250	4.51E-02	4.21E-02	2.94E-02	3.53E+00	7.54E-05
1375	2.01E+00	2.08E+00	1.50E+00	6.62E+01	9.96E-03
1500	3.85E+01	4.21E+01	3.09E+01	6.24E+02	5.16E-01
1650	5.50E+02	6.16E+02	4.61E+02	4.62E+03	2.15E+01
1750	2.10E+03	2.36E+03	1.79E+03	1.28E+04	1.53E+02
1800	3.67E+03	7.30E+03	***	1.98E+04	3.57E+02
2000	***	8.14E+04	***	***	7.00E+03
2250	***	2.76E+05	***	***	6.87E+04
2500	***	***	***	***	***
Pressure = 1 atm					
T(K)	an1→an3	an1→an4	an1→an5	an1→an7	an1→an-p1
500	5.18E-13	-2.39E-16	7.30E-15	1.34E-22	4.41E-37

600	1.55E-10	8.41E-15	4.66E-15	1.69E-16	-7.78E-31
900	1.21E-10	3.94E-12	4.43E-13	4.76E-06	2.19E-15
1000	6.64E-08	5.75E-09	1.20E-09	6.31E-04	6.58E-12
1125	4.34E-05	8.72E-06	2.93E-06	8.50E-02	2.14E-08
1250	8.00E-03	2.84E-03	1.31E-03	4.31E+00	1.37E-05
1375	5.37E-01	2.84E-01	1.58E-01	1.04E+02	2.59E-03
1500	1.60E+01	1.12E+01	7.00E+00	1.37E+03	1.90E-01
1650	3.96E+02	3.44E+02	2.35E+02	1.57E+04	1.25E+01
1750	2.18E+03	2.08E+03	1.47E+03	5.67E+04	1.26E+02
1800	4.60E+03	4.51E+03	3.24E+03	9.92E+04	3.52E+02
2000	4.80E+04	5.03E+04	3.76E+04	5.85E+05	1.02E+04
2250	***	1.43E+06	***	***	2.53E+05
2500	***	4.00E+06	***	***	1.70E+06
Pressure = 10 atm					
T(K)	an1→an3	an1→an4	an1→an5	an1→an7	an1→an-p1
500	4.96E-14	8.39E-13	1.20E-13	7.28E-23	2.90E-36
1125	8.70E-06	2.80E-07	2.67E-08	8.54E-02	2.64E-09
1250	1.56E-03	1.35E-04	2.46E-05	4.38E+00	2.09E-06
1375	1.23E-01	2.12E-02	5.90E-03	1.10E+02	5.12E-04
1500	4.69E+00	1.34E+00	5.04E-01	1.60E+03	4.91E-02
1650	1.63E+02	7.23E+01	3.51E+01	2.22E+04	4.38E+00
1750	1.13E+03	6.29E+02	3.44E+02	9.48E+04	5.38E+01
1800	2.66E+03	1.63E+03	9.36E+02	1.81E+05	1.66E+02
2000	4.37E+04	3.50E+04	2.30E+04	1.50E+06	7.38E+03
2250	4.66E+05	4.31E+05	3.07E+05	9.21E+06	2.22E+05
2500	***	1.04E+07	***	***	3.36E+06
Pressure = 100 atm					
T(K)	an1→an3	an1→an4	an1→an5	an1→an7	an1→an-p1
500	7.24E-14	1.93E-12	6.18E-13	1.38E-23	-2.93E-36
1000	2.13E-07	2.64E-08	2.03E-08	4.72E-04	6.65E-14
1125	3.81E-06	1.04E-08	1.67E-09	7.13E-02	2.49E-10
1250	4.00E-04	2.98E-06	7.18E-08	3.73E+00	1.80E-07
1375	2.79E-02	6.80E-04	4.15E-05	1.11E+02	6.11E-05
1500	9.85E-01	5.69E-02	6.48E-03	1.65E+03	6.87E-03
1650	3.89E+01	4.83E+00	9.27E-01	2.42E+04	7.86E-01
1750	3.19E+02	5.88E+01	1.47E+01	1.11E+05	1.16E+01
1800	8.30E+02	1.81E+02	5.08E+01	2.22E+05	3.95E+01
2000	2.08E+04	7.74E+03	3.12E+03	2.35E+06	2.60E+03
2250	3.69E+05	2.10E+05	1.12E+05	2.05E+07	1.30E+05
2500	2.52E+06	1.79E+06	1.10E+06	9.24E+07	2.12E+06

Pressure = 30 Torr					
T(K)	an3→an1	an3→an4	an3→an5	an3→an7	an3→an-p1
700	1.72E-18	5.12E-06	3.52E-10	6.22E-14	4.30E-21
800	4.60E-14	1.26E-03	8.17E-07	2.01E-10	2.12E-16
900	1.46E-10	9.70E-02	3.77E-04	1.07E-07	8.86E-13
1000	7.51E-07	3.17E+00	4.91E-02	1.56E-05	6.81E-10
1125	6.75E-05	9.85E+01	5.26E+00	2.03E-03	5.42E-07
1250	9.25E-03	1.34E+03	1.65E+02	8.58E-02	1.19E-04
1375	4.74E-01	9.26E+03	1.98E+03	1.57E+00	9.99E-03
1500	1.03E+01	3.79E+04	1.15E+04	1.55E+01	3.87E-01
1650	1.67E+02	1.25E+05	4.92E+04	1.37E+02	1.36E+01
1750	6.93E+02	2.26E+05	9.89E+04	4.61E+02	9.58E+01
1800	1.26E+03	4.13E+05	***	7.95E+02	2.24E+02
2000	***	***	***	***	***
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 1 atm					
T(K)	an3→an1	an3→an4	an3→an5	an3→an7	an3→an-p1
500	9.39E-26	3.26E-13	1.17E-21	4.61E-25	3.27E-36
700	9.64E-18	5.12E-06	1.41E-11	6.25E-14	5.14E-21
800	8.29E-15	1.26E-03	3.42E-08	2.04E-10	2.98E-16
900	1.34E-11	9.77E-02	1.83E-05	1.14E-07	1.49E-12
1000	9.14E-09	3.28E+00	3.18E-03	1.81E-05	1.32E-09
1125	1.97E-05	1.12E+02	5.92E-01	2.85E-03	1.08E-06
1250	1.68E-03	1.87E+03	3.68E+01	1.56E-01	2.15E-04
1375	1.27E-01	1.77E+04	9.30E+02	3.80E+00	1.54E-02
1500	4.27E+00	1.04E+05	1.11E+04	4.87E+01	5.41E-01
1650	1.20E+02	5.16E+05	9.82E+04	5.37E+02	1.92E+01
1750	7.15E+02	1.17E+06	2.87E+05	1.97E+03	1.47E+02
1800	1.56E+03	1.65E+06	4.50E+05	3.53E+03	3.71E+02
2000	1.91E+04	4.88E+06	1.76E+06	2.55E+04	8.58E+03
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 10 atm					
T(K)	an3→an1	an3→an4	an3→an5	an3→an7	an3→an-p1
500	2.80E-25	3.26E-13	1.17E-22	4.61E-25	3.27E-36
700	1.28E-17	5.12E-06	1.41E-12	6.25E-14	5.19E-21
800	6.48E-15	1.26E-03	3.44E-09	2.05E-10	3.06E-16
900	5.59E-12	9.77E-02	1.86E-06	1.14E-07	1.59E-12
1000	2.39E-09	3.28E+00	3.35E-04	1.82E-05	1.49E-09
1125	1.49E-06	1.13E+02	7.00E-02	2.96E-03	1.38E-06

1250	2.87E-04	1.95E+03	5.50E+00	1.74E-01	3.16E-04
1375	2.90E-02	2.01E+04	1.97E+02	4.77E+00	2.54E-02
1500	1.25E+00	1.36E+05	3.62E+03	7.25E+01	9.26E-01
1650	4.94E+01	8.60E+05	5.64E+04	1.01E+03	3.13E+01
1750	3.71E+02	2.31E+06	2.38E+05	4.25E+03	2.28E+02
1800	9.07E+02	3.56E+06	4.41E+05	8.06E+03	5.62E+02
2000	1.72E+04	1.42E+07	2.99E+06	6.78E+04	1.30E+04
2250	2.25E+05	4.51E+07	1.37E+07	4.91E+05	2.70E+05
2500	***	***	***	***	***
Pressure = 100 atm					
T(K)	an3→an1	an3→an4	an3→an5	an3→an7	an3→an-p1
500	5.97E-26	3.26E-13	1.17E-23	2.96E-25	3.27E-36
600	1.95E-20	4.05E-09	6.61E-18	1.37E-18	2.34E-27
700	6.61E-17	5.12E-06	1.41E-13	6.25E-14	5.19E-21
800	6.97E-15	1.26E-03	3.44E-10	2.05E-10	3.07E-16
900	4.68E-12	9.77E-02	1.86E-07	1.14E-07	1.60E-12
1000	1.72E-09	3.28E+00	3.37E-05	1.83E-05	1.52E-09
1125	6.58E-07	1.13E+02	7.19E-03	2.97E-03	1.45E-06
1250	8.38E-05	1.97E+03	5.97E-01	1.77E-01	3.49E-04
1375	6.50E-03	2.05E+04	2.41E+01	5.00E+00	3.07E-02
1500	2.63E-01	1.45E+05	5.48E+02	8.09E+01	1.25E+00
1650	1.18E+01	1.02E+06	1.23E+04	1.28E+03	4.87E+01
1750	1.05E+02	3.05E+06	7.02E+04	6.07E+03	3.81E+02
1800	2.84E+02	5.00E+06	1.53E+05	1.23E+04	9.67E+02
2000	8.23E+03	2.63E+07	1.97E+06	1.33E+05	2.33E+04
2250	1.76E+05	1.16E+08	1.75E+07	1.20E+06	4.90E+05
2500	1.49E+06	3.19E+08	7.18E+07	5.95E+06	4.95E+06
Pressure = 30 Torr					
T(K)	an4→an1	an4→an3	an4→an5	an4→an7	an4→an-p1
700	8.67E-20	4.35E-06	2.65E-05	2.14E-16	5.92E-22
800	6.52E-15	1.08E-03	5.19E-03	2.84E-12	5.64E-17
900	4.19E-11	8.34E-02	3.25E-01	4.64E-09	3.94E-13
1125	3.69E-05	8.53E+01	2.28E+02	4.59E-04	4.60E-07
1250	7.44E-03	1.16E+03	2.62E+03	3.39E-02	1.14E-04
1375	4.29E-01	8.05E+03	1.56E+04	9.02E-01	9.91E-03
1500	9.80E+00	3.29E+04	5.56E+04	1.13E+01	3.88E-01
1650	1.64E+02	1.09E+05	1.62E+05	1.17E+02	1.36E+01
1750	6.82E+02	1.97E+05	2.77E+05	4.16E+02	9.50E+01
1800	1.29E+03	2.09E+05	***	7.49E+02	2.35E+02
2000	1.18E+04	***	***	***	3.88E+03
2250	5.20E+04	***	***	***	3.94E+04

2500	***	***	***	***	1.88E+05
Pressure = 1 atm					
T(K)	an4→an1	an4→an3	an4→an5	an4→an7	an4→an-p1
500	6.86E-25	2.70E-13	1.96E-12	1.67E-30	3.23E-39
700	2.46E-17	4.36E-06	2.65E-05	9.16E-18	4.62E-23
800	3.47E-15	1.08E-03	5.20E-03	1.45E-13	7.03E-18
900	3.75E-13	8.41E-02	3.27E-01	3.22E-10	8.10E-14
1000	6.83E-10	2.83E+00	9.17E+00	1.69E-07	1.43E-10
1250	4.64E-04	1.62E+03	3.71E+03	1.24E-02	8.07E-05
1375	5.82E-02	1.54E+04	3.08E+04	6.13E-01	8.74E-03
1500	2.60E+00	9.06E+04	1.61E+05	1.34E+01	4.03E-01
1650	9.15E+01	4.50E+05	7.07E+05	2.34E+02	1.72E+01
1750	6.00E+02	1.02E+06	1.49E+06	1.07E+03	1.39E+02
1800	1.36E+03	1.44E+06	2.05E+06	2.10E+03	3.57E+02
2000	1.79E+04	4.25E+06	5.52E+06	1.93E+04	8.45E+03
2250	2.71E+05	***	***	***	1.52E+05
2500	1.01E+06	***	***	***	1.02E+06
Pressure = 10 atm					
T(K)	an4→an1	an4→an3	an4→an5	an4→an7	an4→an-p1
500	2.20E-24	2.70E-13	1.96E-12	1.62E-31	3.20E-40
700	3.31E-17	4.36E-06	2.65E-05	9.15E-19	4.85E-24
800	1.58E-15	1.08E-03	5.20E-03	1.47E-14	8.09E-19
900	9.84E-14	8.41E-02	3.27E-01	3.41E-11	1.09E-14
1000	1.87E-11	2.83E+00	9.19E+00	1.96E-08	2.44E-11
1125	4.16E-08	9.81E+01	2.62E+02	1.29E-05	5.75E-08
1250	2.49E-05	1.70E+03	3.87E+03	2.44E-03	2.83E-05
1375	4.38E-03	1.74E+04	3.48E+04	1.75E-01	4.26E-03
1500	3.11E-01	1.19E+05	2.11E+05	5.71E+00	2.58E-01
1650	1.92E+01	7.49E+05	1.19E+06	1.61E+02	1.40E+01
1750	1.82E+02	2.02E+06	3.01E+06	9.77E+02	1.30E+02
1800	4.90E+02	3.11E+06	4.49E+06	2.17E+03	3.53E+02
2000	1.23E+04	1.23E+07	1.62E+07	2.95E+04	1.06E+04
2250	1.90E+05	3.93E+07	4.74E+07	3.05E+05	2.51E+05
2500	2.64E+06	***	***	***	2.46E+06
Pressure = 100 atm					
T(K)	an4→an1	an4→an3	an4→an5	an4→an7	an4→an-p1
500	7.01E-25	2.70E-13	1.96E-12	1.26E-32	2.79E-41
600	8.80E-20	3.41E-09	2.55E-08	3.07E-25	6.64E-32
800	8.79E-15	1.08E-03	5.20E-03	1.42E-15	7.90E-20
900	-3.23E-13	8.41E-02	3.27E-01	3.37E-12	1.11E-15

1000	-4.96E-12	2.83E+00	9.19E+00	1.98E-09	2.66E-12
1125	1.20E-09	9.82E+01	2.63E+02	1.37E-06	7.23E-09
1250	5.42E-07	1.71E+03	3.89E+03	2.91E-04	4.42E-06
1375	2.24E-04	1.78E+04	3.56E+04	2.51E-02	8.76E-04
1500	1.34E-02	1.26E+05	2.25E+05	1.06E+00	7.16E-02
1650	1.28E+00	8.87E+05	1.41E+06	4.37E+01	5.57E+00
1750	1.70E+01	2.66E+06	3.95E+06	3.51E+02	6.41E+01
1800	5.43E+01	4.36E+06	6.29E+06	8.96E+02	1.93E+02
2000	2.72E+03	2.29E+07	2.99E+07	2.06E+04	8.21E+03
2250	9.15E+04	1.01E+08	1.20E+08	3.50E+05	2.77E+05
2500	9.92E+05	2.78E+08	3.12E+08	2.56E+06	3.63E+06
Pressure = 30 Torr					
T(K)	an5→an1	an5→an3	an5→an4	an5→an7	an5→an-p1
700	3.13E-20	5.64E-10	4.99E-05	1.61E-17	3.19E-22
800	3.99E-15	1.23E-06	9.17E-03	5.45E-13	4.32E-17
900	3.42E-11	5.44E-04	5.45E-01	1.66E-09	3.70E-13
1000	5.95E-06	6.82E-02	1.43E+01	8.49E-07	4.59E-10
1125	3.48E-05	7.07E+00	3.54E+02	3.32E-04	5.03E-07
1250	7.82E-03	2.15E+02	3.94E+03	2.90E-02	1.25E-04
1375	4.52E-01	2.53E+03	2.28E+04	8.45E-01	1.07E-02
1500	1.03E+01	1.44E+04	7.98E+04	1.11E+01	4.15E-01
1650	1.73E+02	6.04E+04	2.28E+05	1.19E+02	1.46E+01
1750	7.29E+02	1.20E+05	3.84E+05	4.30E+02	1.04E+02
1800	***	***	***	***	***
2000	***	***	***	***	***
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 1 atm					
T(K)	an5→an1	an5→an3	an5→an4	an5→an7	an5→an-p1
500	1.35E-24	2.26E-21	4.57E-12	2.37E-34	2.11E-41
700	2.93E-17	2.25E-11	4.99E-05	3.81E-20	2.38E-24
800	5.79E-15	5.18E-08	9.18E-03	2.27E-15	8.27E-19
900	7.07E-14	2.64E-05	5.49E-01	1.48E-11	1.82E-14
1000	2.29E-10	4.43E-03	1.48E+01	1.77E-08	5.25E-11
1250	3.43E-04	4.80E+01	5.58E+03	4.58E-03	6.02E-05
1375	4.76E-02	1.19E+03	4.51E+04	3.19E-01	7.72E-03
1500	2.34E+00	1.39E+04	2.31E+05	8.80E+00	3.91E-01
1650	8.81E+01	1.20E+05	9.93E+05	1.85E+02	1.75E+01
1750	5.94E+02	3.49E+05	2.07E+06	9.17E+02	1.44E+02
1800	1.36E+03	5.44E+05	2.83E+06	1.85E+03	3.71E+02
2000	1.85E+04	2.09E+06	7.48E+06	1.85E+04	8.99E+03

2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 10 atm					
T(K)	an5→an1	an5→an3	an5→an4	an5→an7	an5→an-p1
500	3.27E-24	2.26E-22	4.57E-12	2.33E-36	2.10E-43
700	3.93E-17	2.25E-12	4.99E-05	3.90E-22	2.78E-26
800	7.63E-15	5.19E-09	9.18E-03	2.50E-17	1.22E-20
1000	2.19E-12	4.66E-04	1.48E+01	3.12E-10	1.81E-12
1125	6.14E-09	9.41E-02	4.07E+02	5.86E-07	8.89E-09
1250	4.63E-05	7.17E+00	5.82E+03	2.50E-04	7.69E-06
1375	1.77E-03	2.51E+02	5.10E+04	3.30E-02	1.77E-03
1500	1.69E-01	4.53E+03	3.03E+05	1.70E+00	1.45E-01
1650	1.31E+01	6.92E+04	1.68E+06	7.10E+01	1.02E+01
1750	1.38E+02	2.88E+05	4.18E+06	5.25E+02	1.06E+02
1800	3.90E+02	5.32E+05	6.21E+06	1.26E+03	3.02E+02
2000	1.11E+04	3.56E+06	2.19E+07	2.18E+04	1.02E+04
2250	1.85E+05	1.61E+07	6.30E+07	2.65E+05	2.56E+05
2500	***	***	***	***	***
Pressure = 100 atm					
T(K)	an5→an1	an5→an3	an5→an4	an5→an7	an5→an-p1
500	1.04E-24	2.26E-23	4.57E-12	1.94E-38	1.79E-45
600	1.15E-19	1.14E-17	5.25E-08	2.75E-30	1.31E-35
700	2.08E-16	2.25E-13	4.99E-05	3.74E-24	2.64E-28
800	6.94E-15	5.19E-10	9.18E-03	2.47E-19	1.23E-22
1125	2.64E-11	9.66E-03	4.07E+02	7.73E-09	1.62E-10
1250	2.13E-08	7.79E-01	5.85E+03	4.45E-06	2.16E-07
1375	1.03E-05	3.08E+01	5.21E+04	8.86E-04	8.17E-05
1500	2.13E-03	6.85E+02	3.23E+05	7.43E-02	1.14E-02
1650	3.46E-01	1.51E+04	1.98E+06	5.91E+00	1.47E+00
1750	5.89E+00	8.50E+04	5.49E+06	6.74E+01	2.23E+01
1800	2.10E+01	1.84E+05	8.70E+06	2.01E+02	7.55E+01
2000	1.49E+03	2.34E+06	4.05E+07	7.60E+03	4.68E+03
2250	6.55E+04	2.05E+07	1.60E+08	1.92E+05	2.10E+05
2500	8.21E+05	8.30E+07	4.09E+08	1.76E+06	3.19E+06
Pressure = 30 Torr					
T(K)	an7→an1	an7→an3	an7→an4	an7→an5	an7→an-p1
500	4.89E-13	8.70E-14	9.65E-18	1.46E-20	4.04E-27
600	8.01E-09	1.76E-09	1.32E-12	1.28E-14	2.76E-20
700	9.93E-06	2.24E-06	9.03E-09	3.62E-10	2.31E-15
800	2.23E-03	4.87E-04	8.04E-06	8.74E-07	1.20E-11

900	1.55E-01	3.17E-02	1.60E-03	3.39E-04	9.20E-09
1000	4.70E+00	8.54E-01	1.01E-01	3.53E-02	1.78E-06
1125	1.39E+02	2.06E+01	5.37E+00	2.50E+00	3.17E-04
1250	1.89E+03	2.25E+02	1.02E+02	5.82E+01	1.95E-02
1375	1.35E+04	1.36E+03	8.98E+02	5.74E+02	6.06E-01
1500	5.74E+04	5.31E+03	4.46E+03	3.05E+03	1.13E+01
1650	1.92E+05	1.88E+04	1.84E+04	1.33E+04	2.21E+02
1750	3.38E+05	3.76E+04	3.90E+04	2.89E+04	1.24E+03
1800	4.25E+05	5.14E+04	9.58E+04	***	2.75E+03
2000	***	***	***	***	***
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 1 atm					
T(K)	an7→an1	an7→an3	an7→an4	an7→an5	an7→an-p1
500	4.78E-13	8.70E-14	3.81E-19	2.43E-23	4.04E-27
600	7.99E-09	1.76E-09	5.31E-14	2.23E-17	2.76E-20
700	9.87E-06	2.25E-06	3.88E-10	8.55E-13	2.33E-15
800	2.20E-03	4.96E-04	4.10E-07	3.64E-09	1.24E-11
900	1.56E-01	3.36E-02	1.11E-04	3.03E-06	1.02E-08
1000	4.76E+00	9.90E-01	1.07E-02	6.97E-04	2.26E-06
1125	1.48E+02	2.88E+01	1.05E+00	1.49E-01	5.02E-04
1250	2.30E+03	4.09E+02	3.76E+01	9.20E+00	3.66E-02
1375	2.12E+04	3.29E+03	6.10E+02	2.17E+02	1.15E+00
1500	1.26E+05	1.67E+04	5.27E+03	2.42E+03	1.95E+01
1650	6.50E+05	7.33E+04	3.66E+04	2.06E+04	3.31E+02
1750	1.50E+06	1.59E+05	9.90E+04	6.10E+04	1.73E+03
1800	2.14E+06	2.23E+05	1.52E+05	9.72E+04	3.75E+03
2000	6.28E+06	7.01E+05	6.10E+05	4.31E+05	5.97E+04
2250	***	***	***	***	***
2500	***	***	***	***	***
Pressure = 10 atm					
T(K)	an7→an1	an7→an3	an7→an4	an7→an5	an7→an-p1
500	2.69E-13	8.70E-14	3.95E-20	3.46E-22	4.00E-27
600	6.29E-09	1.76E-09	5.25E-15	1.33E-19	2.75E-20
700	9.01E-06	2.25E-06	3.87E-11	8.75E-15	2.33E-15
800	2.12E-03	4.96E-04	4.16E-08	4.01E-11	1.24E-11
900	1.49E-01	3.37E-02	1.17E-05	3.97E-08	1.03E-08
1000	4.47E+00	1.00E+00	1.25E-03	1.23E-05	2.30E-06
1125	1.48E+02	3.00E+01	1.50E-01	4.42E-03	5.29E-04
1250	2.35E+03	4.55E+02	7.37E+00	5.02E-01	4.16E-02
1375	2.26E+04	4.13E+03	1.74E+02	2.24E+01	1.47E+00

1500	1.47E+05	2.49E+04	2.26E+03	4.66E+02	2.80E+01
1650	9.21E+05	1.38E+05	2.52E+04	7.92E+03	5.06E+02
1750	2.51E+06	3.42E+05	9.01E+04	3.49E+04	2.57E+03
1800	3.91E+06	5.09E+05	1.57E+05	6.63E+04	5.39E+03
2000	1.61E+07	1.84E+06	9.16E+05	5.01E+05	7.24E+04
2250	5.14E+07	5.80E+06	4.13E+06	2.69E+06	1.06E+06
2500	***	***	***	***	***
Pressure = 100 atm					
T(K)	an7→an1	an7→an3	an7→an4	an7→an5	an7→an-p1
500	4.50E-14	4.78E-14	-1.32E-18	-1.20E-19	3.69E-27
600	1.53E-09	1.76E-09	4.77E-16	-1.00E-17	2.61E-20
700	3.24E-06	2.25E-06	3.65E-12	7.53E-17	2.25E-15
800	1.07E-03	4.96E-04	4.03E-09	3.96E-13	1.21E-11
900	9.70E-02	3.38E-02	1.16E-06	4.07E-10	1.01E-08
1000	3.44E+00	1.00E+00	1.26E-04	1.36E-07	2.27E-06
1125	1.16E+02	3.01E+01	1.60E-02	5.83E-05	5.28E-04
1250	1.82E+03	4.62E+02	8.77E-01	8.94E-03	4.21E-02
1375	2.28E+04	4.33E+03	2.50E+01	6.02E-01	1.54E+00
1500	1.51E+05	2.78E+04	4.18E+02	2.05E+01	3.09E+01
1650	1.01E+06	1.75E+05	6.84E+03	6.58E+02	6.15E+02
1750	2.95E+06	4.88E+05	3.24E+04	4.49E+03	3.35E+03
1800	4.80E+06	7.74E+05	6.49E+04	1.05E+04	7.25E+03
2000	2.53E+07	3.59E+06	6.40E+05	1.74E+05	1.03E+05
2250	1.15E+08	1.39E+07	4.65E+06	1.93E+06	1.34E+06
2500	3.23E+08	3.55E+07	1.74E+07	9.20E+06	1.02E+07

c) pyrenyl radicals, C₁₆H₉

Pressure = 30 Torr				
T(K)	pyr1→pyr4	pyr1→pyr2	pyr1→pyr6	pyr1→pyr-p1
500	8.85E-15	2.94E-13	5.68E-31	3.47E-45
600	8.07E-11	4.56E-09	1.89E-23	8.56E-35
700	1.17E-07	5.87E-06	4.64E-18	2.30E-27
800	3.49E-05	1.39E-03	5.23E-14	8.24E-22
900	3.25E-03	1.02E-01	7.42E-11	1.60E-17
1000	1.27E-01	3.25E+00	2.40E-08	4.10E-14
1125	5.11E+00	1.04E+02	7.06E-06	1.04E-10
1250	9.51E+01	1.57E+03	5.75E-04	5.84E-08
1375	9.47E+02	1.25E+04	1.80E-02	1.09E-05
1500	5.65E+03	5.73E+04	2.79E-01	8.77E-04
1650	2.83E+04	2.05E+05	3.87E+00	7.13E-02
1800	9.17E+04	4.92E+05	***	2.75E+00

2000	***	***	***	***
2250	***	***	***	***
2500	***	***	***	***
Pressure = 1 atm				
T(K)	pyr1→pyr4	pyr1→pyr2	pyr1→pyr6	pyr1→pyr-p1
500	8.85E-15	2.94E-13	5.69E-31	3.50E-45
600	8.07E-11	4.56E-09	1.89E-23	8.80E-35
700	1.17E-07	5.87E-06	4.64E-18	2.48E-27
800	3.49E-05	1.39E-03	5.26E-14	9.84E-22
900	3.25E-03	1.02E-01	7.61E-11	2.24E-17
1000	1.28E-01	3.26E+00	2.59E-08	6.73E-14
1125	5.22E+00	1.06E+02	8.81E-06	1.93E-10
1250	1.04E+02	1.75E+03	9.11E-04	1.05E-07
1375	1.19E+03	1.70E+04	3.81E-02	1.69E-05
1500	8.86E+03	1.08E+05	7.82E-01	1.15E-03
1650	6.08E+04	6.10E+05	1.42E+01	8.10E-02
1800	2.70E+05	2.17E+06	1.45E+02	2.94E+00
2000	1.18E+06	7.00E+06	1.74E+03	1.57E+02
2250	***	***	***	***
2500	***	***	***	***
Pressure = 10 atm				
T(K)	pyr1→pyr4	pyr1→pyr2	pyr1→pyr6	pyr1→pyr-p1
500	8.85E-15	2.94E-13	5.69E-31	3.50E-45
600	8.07E-11	4.56E-09	1.89E-23	8.81E-35
700	1.17E-07	5.87E-06	4.64E-18	2.49E-27
800	3.49E-05	1.39E-03	5.26E-14	9.94E-22
900	3.25E-03	1.02E-01	7.62E-11	2.29E-17
1000	1.28E-01	3.26E+00	2.60E-08	7.14E-14
1125	5.22E+00	1.06E+02	8.97E-06	2.22E-10
1250	1.04E+02	1.76E+03	9.64E-04	1.36E-07
1375	1.22E+03	1.76E+04	4.40E-02	2.50E-05
1500	9.52E+03	1.19E+05	1.04E+00	1.82E-03
1650	7.33E+04	7.91E+05	2.30E+01	1.24E-01
1800	3.84E+05	3.58E+06	2.81E+02	3.99E+00
2000	2.15E+06	1.62E+07	3.97E+03	1.82E+02
2250	1.01E+07	5.77E+07	5.25E+04	8.64E+03
2500	***	***	***	***
Pressure = 100 atm				
T(K)	pyr1→pyr4	pyr1→pyr2	pyr1→pyr6	pyr1→pyr-p1
500	8.85E-15	2.94E-13	6.47E-31	3.51E-45

600	8.07E-11	4.56E-09	1.89E-23	8.82E-35
700	1.17E-07	5.87E-06	4.64E-18	2.49E-27
800	3.49E-05	1.39E-03	5.26E-14	9.95E-22
900	3.25E-03	1.02E-01	7.62E-11	2.30E-17
1000	1.28E-01	3.26E+00	2.60E-08	7.19E-14
1125	5.23E+00	1.07E+02	8.98E-06	2.26E-10
1250	1.04E+02	1.76E+03	9.71E-04	1.43E-07
1375	1.22E+03	1.76E+04	4.50E-02	2.78E-05
1500	9.63E+03	1.21E+05	1.10E+00	2.22E-03
1650	7.62E+04	8.33E+05	2.66E+01	1.72E-01
1800	4.27E+05	4.13E+06	3.70E+02	6.18E+00
2000	2.77E+06	2.31E+07	6.32E+03	2.89E+02
2250	1.65E+07	1.15E+08	9.77E+04	1.21E+04
2500	6.20E+07	3.53E+08	8.26E+05	2.28E+05
Pressure = 30 Torr				
T(K)	pyr2→pyr4	pyr2→pyr1	pyr2→pyr6	pyr2→pyr-p1
500	3.09E-24	1.58E-13	4.24E-33	1.67E-47
600	4.81E-18	2.70E-09	2.09E-27	1.39E-36
700	2.30E-13	3.70E-06	4.01E-21	1.13E-28
800	1.08E-09	9.18E-04	2.22E-16	1.04E-22
900	9.81E-07	6.99E-02	1.26E-12	4.29E-18
1000	2.60E-04	2.29E+00	1.26E-09	1.91E-14
1125	7.05E-02	7.53E+01	1.10E-06	7.45E-11
1250	5.43E+00	1.16E+03	1.92E-04	5.06E-08
1375	1.48E+02	9.43E+03	9.76E-03	1.01E-05
1500	1.72E+03	4.39E+04	2.00E-01	8.32E-04
1650	1.38E+04	1.59E+05	3.28E+00	6.79E-02
1800	5.65E+04	3.87E+05	***	2.55E+00
2000	2.30E+05	***	***	1.25E+02
2250	***	***	***	4.03E+03
2500	***	***	***	3.93E+04
Pressure = 1 atm				
T(K)	pyr2→pyr4	pyr2→pyr1	pyr2→pyr6	pyr2→pyr-p1
500	1.22E-25	1.58E-13	4.87E-37	6.69E-49
600	1.90E-19	2.70E-09	1.08E-28	5.84E-38
700	9.09E-15	3.70E-06	1.59E-22	5.37E-30
800	4.28E-11	9.18E-04	9.23E-18	6.43E-24
900	3.96E-08	7.00E-02	5.85E-14	4.02E-19
1000	1.12E-05	2.30E+00	7.50E-11	2.99E-15
1125	3.72E-03	7.71E+01	1.08E-07	2.24E-11
1250	4.26E-01	1.29E+03	3.71E-05	2.61E-08

1375	2.06E+01	1.29E+04	4.04E-03	7.53E-06
1500	4.72E+02	8.31E+04	1.72E-01	7.58E-04
1650	8.69E+03	4.74E+05	5.79E+00	6.85E-02
1800	7.42E+04	1.71E+06	8.65E+01	2.74E+00
2000	5.33E+05	5.58E+06	1.34E+03	1.49E+02
2250	3.25E+06	***	***	7.41E+03
2500	***	***	***	1.25E+05
Pressure = 10 atm				
T(K)	pyr2→pyr4	pyr2→pyr1	pyr2→pyr6	pyr2→pyr-p1
500	1.22E-26	1.58E-13	4.70E-38	6.65E-50
600	1.90E-20	2.70E-09	1.08E-29	5.83E-39
700	9.09E-16	3.70E-06	1.59E-23	5.40E-31
800	4.28E-12	9.18E-04	9.24E-19	6.59E-25
900	3.96E-09	7.00E-02	5.90E-15	4.32E-20
1000	1.12E-06	2.30E+00	7.73E-12	3.54E-16
1125	3.80E-04	7.72E+01	1.20E-08	3.29E-12
1250	4.61E-02	1.30E+03	4.85E-06	5.29E-09
1375	2.55E+00	1.33E+04	6.98E-04	2.23E-06
1500	7.43E+01	9.14E+04	4.36E-02	3.28E-04
1650	2.08E+03	6.15E+05	2.50E+00	4.33E-02
1800	2.94E+04	2.82E+06	6.28E+01	2.24E+00
2000	4.08E+05	1.29E+07	1.69E+03	1.45E+02
2250	3.67E+06	4.66E+07	3.41E+04	7.98E+03
2500	2.17E+07	***	***	1.79E+05
Pressure = 100 atm				
T(K)	pyr2→pyr4	pyr2→pyr1	pyr2→pyr6	pyr2→pyr-p1
500	3.23E-22	1.58E-13	1.37E-32	2.64E-50
600	1.93E-21	2.70E-09	1.07E-30	5.60E-40
700	9.09E-17	3.70E-06	1.59E-24	5.26E-32
800	4.28E-13	9.18E-04	9.22E-20	6.48E-26
900	3.96E-10	7.00E-02	5.89E-16	4.29E-21
1000	1.12E-07	2.30E+00	7.74E-13	3.57E-17
1125	3.81E-05	7.72E+01	1.21E-09	3.47E-13
1250	4.66E-03	1.30E+03	5.05E-07	6.09E-10
1375	2.63E-01	1.33E+04	7.78E-05	2.99E-07
1500	8.15E+00	9.27E+04	5.54E-03	5.48E-05
1650	2.65E+02	6.47E+05	4.12E-01	1.02E-02
1800	4.87E+03	3.25E+06	1.48E+01	7.64E-01
2000	1.11E+05	1.84E+07	6.94E+02	7.84E+01
2250	2.00E+06	9.26E+07	2.59E+04	6.36E+03
2500	1.48E+07	2.88E+08	3.72E+05	1.70E+05

Pressure = 30 Torr				
T(K)	pyr4→pyr1	pyr4→pyr2	pyr4→pyr6	pyr4→pyr-p1
500	5.72E-15	3.70E-24	4.36E-34	1.25E-48
600	5.55E-11	5.60E-18	4.89E-26	1.15E-37
700	8.38E-08	2.63E-13	3.56E-20	1.07E-29
800	2.60E-05	1.21E-09	9.83E-16	1.21E-23
900	2.48E-03	1.09E-06	2.96E-12	6.86E-19
1000	9.92E-02	2.87E-04	1.86E-09	4.56E-15
1125	4.06E+00	7.72E-02	1.15E-06	3.00E-11
1250	7.67E+01	5.91E+00	1.75E-04	3.12E-08
1375	7.75E+02	1.60E+02	8.81E-03	8.19E-06
1500	4.67E+03	1.86E+03	1.87E-01	7.72E-04
1650	2.37E+04	1.48E+04	3.21E+00	6.73E-02
1800	7.76E+04	6.03E+04	***	2.60E+00
2000	***	4.42E+05	***	1.24E+02
2250	***	***	***	***
2500	***	***	***	***
Pressure = 1 atm				
T(K)	pyr4→pyr1	pyr4→pyr2	pyr4→pyr6	pyr4→pyr-p1
500	5.72E-15	1.46E-25	4.35E-34	5.00E-50
600	5.55E-11	2.21E-19	4.87E-26	4.71E-39
700	8.38E-08	1.04E-14	3.53E-20	4.74E-31
800	2.60E-05	4.81E-11	9.69E-16	6.25E-25
900	2.48E-03	4.40E-08	2.88E-12	4.37E-20
1000	9.95E-02	1.23E-05	1.78E-09	3.73E-16
1125	4.15E+00	4.07E-03	1.13E-06	3.52E-12
1250	8.36E+01	4.64E-01	1.99E-04	5.59E-09
1375	9.74E+02	2.23E+01	1.34E-02	2.32E-06
1500	7.33E+03	5.09E+02	4.18E-01	3.35E-04
1650	5.08E+04	9.33E+03	1.13E+01	4.34E-02
1800	2.28E+05	7.93E+04	1.48E+02	2.20E+00
2000	1.01E+06	5.66E+05	2.03E+03	1.41E+02
2250	***	6.25E+06	***	7.32E+03
2500	***	***	***	***
Pressure = 10 atm				
T(K)	pyr4→pyr1	pyr4→pyr2	pyr4→pyr6	pyr4→pyr-p1
500	5.72E-15	1.47E-26	4.35E-34	4.97E-51
600	5.55E-11	2.21E-20	4.87E-26	4.70E-40
700	8.38E-08	1.04E-15	3.53E-20	4.75E-32
800	2.60E-05	4.81E-12	9.69E-16	6.35E-26

900	2.48E-03	4.41E-09	2.88E-12	4.57E-21
1000	9.96E-02	1.24E-06	1.78E-09	4.13E-17
1125	4.15E+00	4.16E-04	1.13E-06	4.40E-13
1250	8.40E+01	5.02E-02	2.00E-04	8.30E-10
1375	9.98E+02	2.76E+00	1.39E-02	4.24E-07
1500	7.87E+03	8.02E+01	4.77E-01	7.84E-05
1650	6.13E+04	2.24E+03	1.58E+01	1.42E-02
1800	3.24E+05	3.15E+04	2.72E+02	1.01E+00
2000	1.83E+06	4.35E+05	5.32E+03	9.37E+01
2250	8.74E+06	3.88E+06	8.14E+04	6.77E+03
2500	***	4.15E+07	***	1.74E+05
Pressure = 100 atm				
T(K)	pyr4→pyr1	pyr4→pyr2	pyr4→pyr6	pyr4→pyr-p1
500	5.72E-15	-3.95E-17	7.36E-29	1.45E-47
600	5.54E-11	2.15E-17	-7.06E-22	9.47E-42
700	8.38E-08	1.04E-16	3.53E-20	4.62E-33
800	2.60E-05	4.81E-13	9.69E-16	6.23E-27
900	2.48E-03	4.41E-10	2.88E-12	4.52E-22
1000	9.96E-02	1.24E-07	1.78E-09	4.14E-18
1125	4.15E+00	4.17E-05	1.13E-06	4.53E-14
1250	8.41E+01	5.07E-03	2.00E-04	9.00E-11
1375	1.00E+03	2.85E-01	1.40E-02	5.01E-08
1500	7.96E+03	8.80E+00	4.85E-01	1.05E-05
1650	6.37E+04	2.85E+02	1.69E+01	2.31E-03
1800	3.60E+05	5.22E+03	3.22E+02	2.10E-01
2000	2.36E+06	1.19E+05	7.96E+03	2.86E+01
2250	1.42E+07	2.12E+06	1.75E+05	3.28E+03
2500	5.35E+07	1.55E+07	1.76E+06	1.15E+05
Pressure = 30 Torr				
T(K)	pyr6→pyr4	pyr6→pyr1	pyr6→pyr2	pyr6→pyr-p1
500	6.14E-12	5.17E-09	2.01E-13	4.86E-24
600	5.56E-08	1.48E-05	3.63E-09	1.15E-17
700	4.71E-05	4.41E-03	6.03E-06	4.27E-13
800	8.08E-03	3.20E-01	2.06E-03	1.17E-09
900	4.65E-01	8.87E+00	2.19E-01	5.49E-07
1000	1.22E+01	1.23E+02	9.35E+00	7.16E-05
1125	3.14E+02	1.54E+03	3.32E+02	8.00E-03
1250	3.77E+03	9.99E+03	4.49E+03	2.66E-01
1375	2.36E+04	3.94E+04	2.84E+04	3.43E+00
1500	8.82E+04	1.08E+05	1.03E+05	2.20E+01
1650	2.65E+05	2.67E+05	2.97E+05	1.15E+02

1800	***	***	***	***
2000	***	***	***	***
2250	***	***	***	***
2500	***	***	***	***
Pressure = 1 atm				
T(K)	pyr6→pyr4	pyr6→pyr1	pyr6→pyr2	pyr6→pyr-p1
500	6.13E-12	5.17E-09	8.21E-15	4.86E-24
600	5.54E-08	1.48E-05	1.43E-10	1.15E-17
700	4.68E-05	4.42E-03	2.41E-07	4.28E-13
800	7.97E-03	3.22E-01	8.54E-05	1.19E-09
900	4.52E-01	9.10E+00	1.02E-02	5.74E-07
1000	1.17E+01	1.32E+02	5.44E-01	8.16E-05
1125	3.11E+02	1.92E+03	3.25E+01	1.16E-02
1250	4.29E+03	1.58E+04	8.70E+02	5.90E-01
1375	3.59E+04	8.36E+04	1.17E+04	1.36E+01
1500	1.98E+05	3.05E+05	8.79E+04	1.62E+02
1650	9.38E+05	9.84E+05	5.20E+05	1.57E+03
1800	2.88E+06	2.38E+06	1.83E+06	8.41E+03
2000	7.85E+06	5.94E+06	5.88E+06	4.61E+04
2250	***	***	***	***
2500	***	***	***	***
Pressure = 10 atm				
T(K)	pyr6→pyr4	pyr6→pyr1	pyr6→pyr2	pyr6→pyr-p1
500	6.13E-12	5.17E-09	7.93E-16	4.86E-24
600	5.54E-08	1.48E-05	1.43E-11	1.15E-17
700	4.68E-05	4.42E-03	2.41E-08	4.28E-13
800	7.97E-03	3.22E-01	8.55E-06	1.19E-09
900	4.52E-01	9.11E+00	1.03E-03	5.75E-07
1000	1.17E+01	1.33E+02	5.60E-02	8.21E-05
1125	3.09E+02	1.95E+03	3.60E+00	1.19E-02
1250	4.31E+03	1.68E+04	1.14E+02	6.36E-01
1375	3.74E+04	9.64E+04	2.03E+03	1.64E+01
1500	2.25E+05	4.05E+05	2.23E+04	2.40E+02
1650	1.32E+06	1.60E+06	2.24E+05	3.27E+03
1800	5.32E+06	4.62E+06	1.32E+06	2.57E+04
2000	2.11E+07	1.34E+07	7.26E+06	2.04E+05
2250	6.42E+07	3.70E+07	3.05E+07	1.33E+06
2500	***	***	***	***
Pressure = 100 atm				
T(K)	pyr6→pyr4	pyr6→pyr1	pyr6→pyr2	pyr6→pyr-p1

500	5.59E-12	5.17E-09	7.43E-17	4.82E-24
700	4.68E-05	4.42E-03	2.39E-09	4.27E-13
800	7.97E-03	3.22E-01	8.53E-07	1.18E-09
900	4.52E-01	9.11E+00	1.03E-04	5.74E-07
1000	1.17E+01	1.33E+02	5.61E-03	8.20E-05
1125	3.09E+02	1.96E+03	3.64E-01	1.19E-02
1250	4.31E+03	1.69E+04	1.18E+01	6.41E-01
1375	3.75E+04	9.86E+04	2.26E+02	1.68E+01
1500	2.29E+05	4.29E+05	2.83E+03	2.56E+02
1650	1.40E+06	1.85E+06	3.68E+04	3.87E+03
1800	6.30E+06	6.11E+06	3.11E+05	3.62E+04
2000	3.16E+07	2.14E+07	2.95E+06	3.95E+05
2250	1.41E+08	6.79E+07	2.25E+07	3.69E+06
2500	3.95E+08	1.64E+08	9.25E+07	1.90E+07

Input file for MESS calculations for acetanaphthylenyl C₁₂H₇

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TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1750. 1800. 2000. 2250. 2500.
PressureList[atm]           0.03947368 1. 10. 100.
EnergyStepOverTemperature   0.2          #Ratio of discretization
energy step to T
ExcessEnergyOverTemperature 100
ModelEnergyLimit[kcal/mol]  900
WellCutoff                  10
ChemicalEigenvalueMax      0.2
ChemicalEigenvalueMin      1.e-6          #only for direct
diagonalization method
CalculationMethod           direct
EigenvalueOutput            eigenvalue.out
Reactant p0 #ground energy of bimolecular species will be used as a
reference.
Model
EnergyRelaxation
Exponential
Factor[1/cm]                424      ! Jasper calc N2
Power                        0.62
ExponentCutoff              15
End
CollisionFrequency
LennardJones
Epsilons[1/cm]              390. 390.    ! N2 , A3/A3a/A6 ! from new Jasper calc
11/22/2015
Sigmas[angstrom]            4.46 4.46    ! N2 , A3/A3a/A6 ! from new Jasper calc
11/22/2015
End
OutputTemperatureStep[K]    100
OutputTemperatureSize       20
OutputReferenceEnergy[kcal/mol] 0.
!-----
-----
!-----acenaphthyl_r1-----
Well          r1
Species
RRHO
Geometry[angstrom]  19
C  -7.181696E-4  0.1435829247  0.0
C  -0.0022138539 -1.2508989365  0.0
C  1.2795848959  -1.8760814616  0.0
C  2.4231964015  -1.1026278286  0.0
C  2.3872671119  0.3220807881  0.0
C  1.1632254154  0.953615526   0.0
C  -1.1741020156 0.9453582479  0.0
C  -2.3985522807 0.3159759915  0.0
C  -2.4304637694 -1.1061536675  0.0
```

```

C -1.2821088291 -1.8756454309 0.0
C 0.693693617 2.3606539277 0.0
C -0.6535341127 2.3098696137 0.0
H 1.3552589179 -2.9582184066 0.0
H 3.3906452688 -1.5925634837 0.0
H 3.3185404911 0.8783282952 0.0
H -3.3269994117 0.8756467813 0.0
H -3.3956523455 -1.6000491436 0.0
H -1.3559796286 -2.9579994708 0.0
H 1.3241382972 3.2379477337 0.0
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
158.0710 211.6969 234.7778
365.9744 422.2033 455.6565
485.1063 516.1505 552.7046
554.0561 618.2513 642.5834
671.1068 688.2660 754.1094
770.3678 796.7588 812.9834
839.9674 872.6851 920.8921
928.7725 976.3406 986.7715
1012.2674 1031.6820 1056.2176
1090.2221 1167.5662 1194.6249
1205.5967 1235.8709 1252.5743
1263.5522 1373.4543 1401.4680
1447.5953 1448.8568 1471.5426
1512.8806 1520.6319 1629.9215
1643.4957 1654.9728 3161.1479
3163.9318 3171.9540 3176.4411
3184.3486 3188.3929 3223.4979
ZeroEnergy[kcal/mol] 4.12
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----acenaphthyl_r2-----
Well r2
Species
RRHO
Geometry[angstrom] 19
C 0.0 0.0019761092 -0.1448036619
C 0.0 0.0064044823 1.251016489
C 0.0 1.1637766989 -0.9714381007
C 0.0 -1.1578260868 -0.9552866917
C 0.0 2.3357344401 -0.2812477774
C 0.0 -2.3832209095 -0.3210360726
C 0.0 2.437907745 1.1182711139
C 0.0 -2.4207908479 1.1006636102

```

```

C 0.0 1.2825585628 1.8871021642
C 0.0 -1.2747226617 1.8737533405
C 0.0 0.6768149646 -2.3581108212
C 0.0 -0.6846062214 -2.3471296489
H 0.0 1.3109278774 -3.233061325
H 0.0 -1.3235993472 -3.2195474395
H 0.0 -3.3142556515 -0.8782856269
H 0.0 3.4101425532 1.5985161277
H 0.0 -3.3873480651 1.5919593234
H 0.0 1.3539196615 2.9700947145
H 0.0 -1.3511493037 2.9558812822
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
162.1411 215.6859 223.6765
376.3819 427.7729 464.1174
471.8980 517.9078 556.0147
571.9585 608.4848 667.4815
669.6252 691.8142 733.6112
761.0282 788.2923 806.8620
836.4440 872.5436 922.6499
934.7380 954.8575 982.5604
1019.2727 1042.3579 1078.5341
1103.5450 1126.9311 1166.5715
1201.6016 1235.6751 1253.6049
1309.6430 1339.6364 1396.1015
1434.0218 1441.5528 1480.1225
1493.9906 1534.0507 1605.1169
1630.9804 1649.3440 3160.3959
3161.1777 3169.5571 3177.5608
3185.0777 3208.3877 3230.3486
ZeroEnergy[kcal/mol] 0.16
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----acenaphthyl_r3-----
Well r3
Species
RRHO
Geometry[angstrom] 19
C 0.0 0.0039417783 -0.1367277615
C 0.0 -0.0023575553 1.2596950531
C 0.0 1.1627493909 -0.9532511296
C 0.0 -1.1558544216 -0.946196373
C 0.0 2.4010854911 -0.3313021172
C 0.0 -2.3841340466 -0.3207526409
C 0.0 2.3683852359 1.0708880709

```

```

C 0.0 -2.4265464544 1.1018680847
C 0.0 1.2846463671 1.8952896836
C 0.0 -1.2846437591 1.8803813062
C 0.0 0.6810288767 -2.3452214167
C 0.0 -0.6795993455 -2.3400065167
H 0.0 1.3142764616 -3.2216755346
H 0.0 -1.3166806598 -3.2140189788
H 0.0 3.3373716367 -0.879184689
H 0.0 -3.3128383324 -0.881479214
H 0.0 -3.3951237739 1.5896528761
H 0.0 1.3760848441 2.9764923794
H 0.0 -1.3648167339 2.9620909181
Core RigidRotor
SymmetryFactor 1.0
End
Frequencies[1/cm] 51
162.0936 215.2115 226.7142
368.2147 422.0645 463.2916
470.3589 516.2825 558.4451
559.7193 602.6398 665.7470
667.7912 690.4240 730.4871
771.1028 800.4515 809.7866
853.1106 871.6318 884.2082
922.7464 936.3854 982.1307
1026.9503 1035.9694 1049.8317
1098.2924 1105.2787 1186.1405
1205.2073 1214.6736 1258.4951
1320.8538 1348.4557 1390.7478
1410.1140 1454.2976 1466.1424
1501.5230 1537.1915 1590.9339
1641.2609 1650.1730 3161.4360
3164.0802 3168.0891 3171.8805
3184.6159 3203.8687 3223.9657
ZeroEnergy[kcal/mol] 0.00
ElectronicLevels[1/cm] 1
0 2
End
End
!-----
!-----acenaphthyl_r4-----
Well r4
Species
RRHO
Geometry[angstrom] 19
C 0.0 3.96774E-5 -0.1368658817
C 0.0 -0.0140147665 1.2655318374
C 0.0 1.1629814968 -0.9444930601
C 0.0 -1.1611051002 -0.9469791407
C 0.0 2.39577719 -0.325848674
C 0.0 -2.3880881519 -0.3189103252

```



```

C 0.0 2.4454932641 1.1057836919
C 0.0 -2.4328931655 1.1041336603
C 0.0 1.2818876951 1.814486037
C 0.0 -1.2947582424 1.8872663853
C 0.0 0.6813654552 -2.3361080927
C 0.0 -0.6796630273 -2.3381869762
H 0.0 1.3162163352 -3.2116438619
H 0.0 -1.3133931935 -3.2144222641
H 0.0 3.3241957076 -0.8879899169
H 0.0 -3.3170178097 -0.8794144426
H 0.0 3.4080448597 1.6060298141
H 0.0 -3.4028638425 1.5887905066
H 0.0 -1.3712953815 2.9680537034

```

Core RigidRotor

SymmetryFactor 1.0

End

Frequencies[1/cm] 51

157.2825	213.5453	237.2940
381.9429	428.9109	449.2605
472.3204	509.1968	559.6401
564.6478	609.5205	671.1112
674.3249	690.6572	734.1413
779.8698	798.7868	808.9582
834.4591	868.1226	923.8605
933.4268	945.3124	984.4662
1016.2160	1032.9910	1061.0394
1101.0921	1119.6881	1187.6259
1210.8697	1219.0778	1259.9443
1326.8316	1357.8954	1377.0539
1415.2627	1444.3457	1480.0577
1490.0693	1536.5344	1607.0549
1635.0590	1652.1661	3158.8629
3163.8443	3173.3513	3177.0919
3192.0788	3204.2050	3224.0658

ZeroEnergy[kcal/mol] 0.81

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----acenaphthyl_i1-----

Well i1

Species

RRHO

Geometry[angstrom] 19

```

C -0.0056221435 -0.6324571341 0.0
C -0.0059859306 -2.0700791607 0.0
C 1.2393583668 -2.7487025659 0.0
C 2.4221507738 -2.0484339481 0.0
C 2.425403286 -0.6393533042 0.0

```

```

C  1.2390257966   0.0765261518   0.0
C  -1.2643732144  -0.0246390531   0.0
C  -2.4639201198  -0.6548521258   0.0
C  -2.4449007176  -2.078276247    0.0
C  -1.2502079527  -2.7570685516   0.0
C  1.2477968344   1.502000949     0.0
C  1.2614978649   2.7061251041    0.0
H  1.2429772248  -3.8336760706   0.0
H  3.3673287938  -2.5790591746   0.0
H  3.3649092359  -0.1004684864   0.0
H  -3.4041457466  -0.1144254698   0.0
H  -3.3836441609  -2.6218884533   0.0
H  -1.2414382289  -3.8416483581   0.0
H  1.2701350378   3.7683828984    0.0
Core RigidRotor
SymmetryFactor  1.0
End
Frequencies[1/cm]  51
105.6687           126.0675           171.8135
202.2382           339.7239           363.3411
444.6261           455.0156           478.6658
489.7461           543.2679           579.4884
592.6596           627.9893           646.1774
689.5120           703.1422           752.2892
765.5702           798.9627           820.3050
868.9895           886.2369           927.6995
974.4424           989.5170           1022.4014
1053.1950          1089.0520          1165.3628
1188.6548          1197.1373          1239.5904
1263.0605          1343.9982          1359.4477
1399.9266          1454.3466          1466.1515
1509.4071          1585.8509          1625.3259
1653.5401          2205.7135          3158.7792
3163.1490          3170.0666          3180.0092
3182.3132          3195.3574          3477.0847
ZeroEnergy[kcal/mol]  29.35
ElectronicLevels[1/cm]  1
0  2
End
End
!-----
!-----acenaphthyl_i2-----
Well          i2
Species
RRHO
Geometry[angstrom]  19
C  -0.0401167242  -0.3343888995   0.0405278859
C  0.0063103719  -1.7872452727   0.0428599882
C  1.2582320634  -2.486131433    0.0471996818
C  2.4892226909  -1.847633367    0.0497143512

```

C	2.3181087499	-0.4571416136	0.0465936742
C	1.2665339039	0.1886245544	0.0427893678
C	-1.2769779841	0.3593921473	0.0361678993
C	-2.4488468956	-0.383612169	0.0342251416
C	-2.4229894124	-1.7875387272	0.036384751
C	-1.2293450837	-2.4780402372	0.0405549804
H	1.2321157702	-3.5713355205	0.0487140499
H	3.4283396546	-2.3843114326	0.0527780583
H	-3.399641903	0.1370565352	0.0310376052
H	-3.3594995354	-2.3335605733	0.0346242597
H	-1.2277553981	-3.5624159349	0.0422357178
C	-1.264552382	1.8312994256	0.0337914838
C	-2.3016593941	2.6367533064	0.0293138311
H	-0.2623502286	2.2772423041	0.0359114362
H	-2.4920692637	3.6983779075	0.0267348367

Core RigidRotor

SymmetryFactor 0.5

End

Frequencies[1/cm] 51

72.0879	160.3424	170.9057
171.4423	252.3447	341.6937
402.0598	409.9412	452.5020
467.5367	519.8303	529.0010
558.4427	579.0052	654.4460
665.3755	741.3116	742.0290
769.3223	826.7543	844.5243
852.6752	865.2394	928.4539
946.4782	972.5330	988.6501
1087.2156	1111.5344	1139.3180
1193.8569	1224.4995	1230.7638
1273.7164	1309.9108	1336.0541
1370.8246	1424.9611	1473.1763
1518.5610	1574.5395	1627.0811
1651.4722	2046.7782	3012.5853
3162.2808	3166.5387	3176.5506
3188.6626	3204.2052	3255.0372

ZeroEnergy[kcal/mol] 74.37

ElectronicLevels[1/cm] 1

0 2

End

End

!-----

!-----acenaphthyl_i3-----

Well i3

Species

RRHO

Geometry[angstrom] 19

C	0.0304428489	-0.6288328041	0.0
C	0.0113882782	-2.061247495	0.0
C	1.2378177698	-2.7800171177	0.0

C 2.4505192937 -2.1226759437 0.0
 C 2.4051531427 -0.7301057671 0.0
 C 1.291185988 0.0399976138 0.0
 C -1.2170146488 0.0812649248 0.0
 C -2.4086238813 -0.6277081984 0.0
 C -2.4174371633 -2.0351939026 0.0
 C -1.236182669 -2.7365421026 0.0
 C -1.2391622861 1.5075150463 0.0
 C -1.2621269439 2.7119470079 0.0
 H 1.2062613045 -3.8651308853 0.0
 H 3.3869608483 -2.6684274444 0.0
 H 1.3229689213 1.1233767505 0.0
 H -3.3436177017 -0.0809288247 0.0
 H -3.3651696198 -2.5608008769 0.0
 H -1.2418152927 -3.821291436 0.0
 H -1.2893811888 3.7738904549 0.0

Core RigidRotor
 SymmetryFactor 1.0
 End

Frequencies[1/cm] 51
 102.5876 137.3277 173.1163
 206.3585 355.6932 360.6494
 435.5744 445.5733 480.5900
 491.1716 551.7720 568.5820
 587.4727 625.8361 646.3011
 692.4168 698.2124 749.0005
 769.4050 791.9603 829.0511
 862.4413 874.1095 927.1973
 961.0303 987.3124 1030.6602
 1053.8638 1094.3499 1149.9527
 1191.4773 1215.9950 1240.7400
 1277.2987 1325.8473 1356.3818
 1386.9402 1446.8879 1472.7911
 1514.3450 1595.2408 1614.7758
 1638.2334 2201.4816 3156.9860
 3165.3539 3178.0216 3181.0678
 3181.9597 3196.1216 3475.2122

ZeroEnergy[kcal/mol] 28.38
 ElectronicLevels[1/cm] 1
 0 2

End
 End

!-----
 !-----c2h2_c10h5_p1-----
 Bimolecular p1
 Fragment c10h5
 RRHO

Geometry[angstrom] 15
 C -0.0487577884 1.3542619665 0.0
 C -0.0061738276 -0.112813919 0.0

```

C 1.2484439964 -0.8033235483 0.0
C 2.4769986136 -0.1586501421 0.0
C 2.3079034105 1.2324871526 0.0
C 1.2540093771 1.8735721328 0.0
C -1.3084658409 1.9404007606 0.0
C -2.495273682 1.2821623162 0.0
C -2.4500607971 -0.1377145729 0.0
C -1.2455727994 -0.8045987489 0.0
H 1.2271110589 -1.8886559438 0.0
H 3.4169855869 -0.6941772612 0.0
H -3.4463037318 1.803189305 0.0
H -3.3801944199 -0.6953428578 0.0
H -1.2342351562 -1.8889146398 0.0
Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 39
167.1714 197.9686 372.4928
409.0559 426.9181 429.2902
508.9979 515.0208 561.5798
573.5679 695.9853 704.8748
749.4885 791.8887 815.3099
859.7586 892.7443 945.3313
974.5645 1046.0693 1073.4487
1105.4442 1144.6783 1176.7437
1225.6745 1286.0502 1303.4783
1373.7373 1425.0186 1452.3470
1486.3949 1529.3948 1647.3203
2053.9533 3161.0307 3163.9788
3172.1643 3185.0983 3201.9104
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1
0 2
End
Fragment c2h2
RRHO
Geometry[angstrom] 4
C 0.0 0.0 0.5990703976
C 0.0 0.0 -0.5990703976
H 0.0 0.0 1.6619081422
H 0.0 0.0 -1.6619081422
Core RigidRotor
SymmetryFactor 2
End
Frequencies[1/cm] 7
642.0679 642.0679 772.6955
772.6955 2069.5209 3420.9273
3523.7963
ZeroEnergy[kcal/mol] 0.0
ElectronicLevels[1/cm] 1

```

```

0 1
End
GroundEnergy[kcal/mol] 116.62
End
!-----acenaphthyl_ts1-----
Barrier      ts1  r1  r2
RRHO
Geometry[angstrom]  19
C  0.5087908702  -0.0485492822  0.0413850346
C  0.2734338046  -0.0179258381  1.4131676388
C  0.5146234656  1.1386476936  -0.7173163293
C  0.2227400135  -1.1477086493  -0.8263692827
C  0.1083636368  2.3877746298  -0.28787245
C  -0.0083124144  -2.3806726531  -0.2114964046
C  -0.0845564804  2.4285365833  1.1443276877
C  -0.0283560052  -2.4284094885  1.1985722432
C  0.0558185499  1.3051152865  1.9536603013
C  0.0667484149  -1.2895260767  2.0053914079
C  0.1137207257  0.897944511  -2.0427827661
C  -0.0097301707  -0.5619427789  -2.1297980148
H  -0.2385322629  -3.2739701377  -0.7815368291
H  -0.3847998176  3.3545663461  1.6265396696
H  -0.2100715584  -3.3835198762  1.6782759684
H  -0.1055198951  1.4061561132  3.0238942436
H  -0.0738871093  -1.3858142154  3.0770116312
H  -0.2644117955  2.2990231658  -1.7959893373
H  -0.2830919715  -1.1193113334  -3.0174924123
Core RigidRotor
SymmetryFactor  0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]  2034.9601
WellDepth[kcal/mol]  100.45
WellDepth[kcal/mol]  104.41
End
Frequencies[1/cm]  50
137.3007          172.9491
214.8533          327.8003          392.4195
418.7264          488.6662          504.4655
526.7878          565.2806          574.1623
621.4360          682.2573          716.7540
757.9489          762.4247          807.3244
822.8810          844.4122          867.1362
919.7835          959.6237          984.1430
1000.2450         1025.8936         1042.8817
1061.0907         1082.2462         1152.5994
1183.5819         1204.6570         1232.9696
1251.6744         1281.8005         1334.8657
1376.5091         1398.3007         1420.0002
1443.6833         1497.2020         1534.8837

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1599.8660          1607.2878          1704.2619
3139.2962          3156.9325          3164.2170
3174.5240          3187.4136          3197.0827
ZeroEnergy[kcal/mol] 104.57
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----acenaphthyl_ts2-----
Barrier      ts2  r2  r3
RRHO
Geometry[angstrom] 19
C -5.219764E-4  0.0635455789  -0.0253580528
C -6.788874E-4  0.0639719588  1.3809751845
C -8.650319E-4  1.2047187753  -0.8785870336
C -4.43515E-5   -1.107505588   -0.8248845344
C -0.0012015879 2.3787570685   -0.1486372193
C 2.720524E-4   -2.3312756277  -0.192541284
C -0.0013360179 2.4057659656   1.2027833327
C 1.351305E-4   -2.3688080834  1.2303916886
C -0.0011706732 1.3252662453   2.060687805
C -3.202199E-4  -1.2231834073  1.9996098676
C -5.854956E-4  0.7078485759  -2.2556063077
C -9.99163E-5   -0.6539311157  -2.2244469302
H -0.0019710545 3.5445754381   0.4981144652
H 6.239907E-4   -3.2617552039  -0.7507058089
H 4.004984E-4   -3.3345940473  1.7233014139
H -0.0014055112 1.390706225    3.1417661598
H -4.051406E-4  -1.297470693   3.0817980423
H -7.762811E-4  1.3282708025   -3.1403288843
H 2.264735E-4   -1.3071688677  -3.0863459044
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 2356.9433
WellDepth[kcal/mol] 63.11
WellDepth[kcal/mol] 63.27
End
Frequencies[1/cm] 50
117.0698          167.8315
215.6303          286.6819          425.4744
431.1124          469.5959          480.6520
504.7287          559.1887          576.1852
614.7243          662.3279          664.2973
688.5281          740.3038          740.6844
772.5622          827.8136          864.9948
876.0601          924.7050          937.2622
981.8874          1021.9148         1043.7621
1079.9922         1102.5602         1121.3079

```

```

1190.9504          1218.9583          1239.4824
1299.2713          1324.5688          1364.0236
1418.3081          1451.6238          1468.4473
1510.7338          1534.1625          1559.0298
1644.7373          1664.6142          2051.5770
3161.5677          3170.7394          3185.1772
3189.5713          3207.3616          3229.1183
ZeroEnergy[kcal/mol] 63.27
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----acenaphthyl_ts3-----
Barrier      ts3  r3  r4
RRHO
Geometry[angstrom] 19
C 0.0764607947 0.0137860799 0.0210425128
C 0.079135097 -0.0176746232 1.4173300366
C 0.0445497662 1.1912817826 -0.8025671227
C 0.0344867873 -1.1381179477 -0.7927188117
C 0.0114204051 2.4341506178 -0.2145708605
C -0.0205438735 -2.3719084154 -0.1724002989
C 0.179579778 2.4011755249 1.2129633945
C -0.0297312457 -2.4279654934 1.2451392995
C 0.2105766491 1.3092041558 1.9732801301
C 0.0177464444 -1.2894216248 2.034482898
C 0.0063873459 0.7014958124 -2.1913117986
C 0.0022916933 -0.6577731038 -2.1854098072
H -0.1056425093 3.3558591566 -0.7721619284
H -0.0655848804 -3.2937315683 -0.7426128741
H -0.4769899497 2.3638594376 2.3514687736
H -0.0717247073 -3.3996330139 1.7245417282
H 0.0223642197 -1.3682689513 3.1153564254
H -0.0190941501 1.3341575519 -3.0675934445
H -0.0373016648 -1.2943903777 -3.0590932523
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm] 1940.819
WellDepth[kcal/mol] 59.31
WellDepth[kcal/mol] 58.5
End
Frequencies[1/cm] 50
158.2420          209.2210
229.6907          365.6465          387.4228
448.4206          454.1154          470.9328
530.4633          537.8568          576.6762
605.2743          659.9312          669.6251
674.8749          739.8932          776.2644

```


786.9382	832.5436	846.2537
892.3878	928.8683	945.3406
988.0707	1003.7999	1037.7466
1059.3445	1087.6455	1108.2901
1185.6886	1206.6618	1242.1643
1268.6741	1332.1413	1353.1776
1416.6732	1454.0631	1480.6763
1514.2185	1552.8827	1606.4302
1640.6742	1691.9940	2152.4347
3164.4381	3177.2329	3182.2220
3190.4041	3204.7567	3225.5556

ZeroEnergy[kcal/mol] 59.31

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----acenaphthyl_ts4-----

Barrier ts4 r1 i1

RRHO

Geometry[angstrom] 19

C	-0.4581092763	-0.01999462	0.0913066819
C	-0.5824134776	-0.0109823064	1.5036671314
C	-0.4027821134	1.1925347701	-0.6617768059
C	-0.3875222445	-1.2378710273	-0.5928938258
C	-0.4712070366	2.4022874583	-0.0107382053
C	-0.4315333862	-2.4472585405	0.0281195257
C	-0.5955559795	2.4205847197	1.4017978084
C	-0.556372569	-2.4435321769	1.4502677128
C	-0.6499136415	1.2592742634	2.1407742915
C	-0.6294483901	-1.2684845361	2.1651270124
H	-0.4309605009	3.3317242673	-0.5656266143
H	-0.3762934551	-3.3875511171	-0.5089403171
H	-0.6488303721	3.3776761768	1.9081035649
H	-0.5938315199	-3.3943754319	1.9716325469
H	-0.7452847822	1.3057229267	3.2205986007
H	-0.7241207193	-1.2957467997	3.245406825
C	-0.2772093983	0.8644853314	-2.0575212155
C	-0.2128940075	-0.2128536704	-2.6713805972
H	-0.13397413	-0.8816246873	-3.4988531205

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 439.3123

WellDepth[kcal/mol] 40.69

WellDepth[kcal/mol] 15.46

End

Frequencies[1/cm] 50

162.4185	166.0560	
198.1064	351.6216	403.3921

453.5575	464.7149	481.6486
497.1026	543.9695	582.6755
585.0480	625.5706	636.4377
699.9409	741.0525	757.2322
770.7830	801.6895	819.8283
880.6909	893.5021	922.4709
973.4753	987.5260	1024.5476
1048.7610	1070.1379	1163.9178
1192.7981	1203.8986	1237.5309
1253.6965	1350.0144	1386.0636
1412.7465	1450.4093	1456.6037
1510.3286	1589.3614	1633.8986
1651.1918	1899.7646	3156.7080
3162.6953	3171.0942	3179.4200
3180.7053	3194.3664	3413.9347

ZeroEnergy[kcal/mol] 44.81

ElectronicLevels[1/cm] 1

0 2

End

!-----

!-----acenaphthyl_ts5-----

Barrier ts5 r2 i2

RRHO

Geometry[angstrom] 19

C	-0.0012340598	0.2487451677	-0.0531284689
C	-0.0241217675	0.1234395233	1.396132199
C	-0.0517332264	1.6055774373	-0.4119630101
C	0.0628855766	-0.8981163554	-0.879782205
C	-0.1035175675	2.5813708309	0.3409014908
C	0.1033473151	-2.1450598397	-0.2865870632
C	-0.1316866322	2.5795445257	1.7432872545
C	0.084525806	-2.2870993793	1.1160549807
C	-0.0872228014	1.2836373834	2.2355050502
C	0.0212806892	-1.1852473595	1.9376779296
C	1.1086324797	-0.5325414025	-3.1063756277
C	0.0513361801	-0.743363604	-2.3667977707
H	0.155794308	-3.0282240659	-0.9130103101
H	-0.1772390027	3.4475674349	2.3876951627
H	0.1223403426	-3.2809108912	1.5474271891
H	-0.098320032	1.1301501301	3.3101571955
H	0.0061463953	-1.3099521545	3.0149223826
H	1.3387074028	-0.3857043619	-4.1511835224
H	-0.9331084059	-0.8067490195	-2.8478158569

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 127.9651

WellDepth[kcal/mol] 78.3

WellDepth[kcal/mol] 4.09

```

End
Frequencies[1/cm] 50
113.9393      168.1807
196.7696      212.3188      341.9112
398.2903      420.7841      446.0364
459.7540      498.0721      523.8359
545.1052      623.7793      636.9352
679.7055      740.8006      745.1895
770.2531      820.6279      833.4588
847.5044      874.5960      928.2950
947.0255      986.0956      991.7875
1080.5476     1112.9235     1141.0282
1192.3756     1225.8337     1238.1257
1251.7302     1299.4997     1333.7106
1367.8084     1425.8203     1471.0770
1521.8028     1576.4658     1631.6071
1671.7279     2054.9570     3004.2525
3160.8026     3165.0754     3175.5951
3188.5428     3199.2447     3239.2421
ZeroEnergy[kcal/mol] 78.46
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----acenaphthyl_ts6-----
Barrier      ts6  i2  i3
RRHO
Geometry[angstrom] 19
C  -0.1380813398  -0.4688925405  0.0602027452
C  -0.0391197322  -1.8873089325  0.0476452421
C   1.2643121491  -2.4722048327  0.0492472433
C   2.4114614126  -1.6927305545  0.0627586527
C   2.1945869379  -0.3012961255  0.074589684
C   1.0524866041  0.2778402943  0.0738362871
C  -1.3652510105  0.2236852238  0.0599050912
C  -2.5416777645  -0.4982346416  0.0470327244
C  -2.4736998335  -1.911669606  0.0344126146
C  -1.2711790804  -2.5934690133  0.0345211532
H   1.3571279995  -3.5536501337  0.0395946226
H   3.3953760066  -2.1463338831  0.0637922633
H  -3.502987982  0.0010547897  0.0465173574
H  -3.4000383173  -2.4750662176  0.0243339161
H  -1.2658238351  -3.678213208  0.0246039702
C  -1.1278479367  1.673781449  0.0742000791
C  -1.7705864039  2.7648086842  0.0792726047
H   0.1297652439  1.6618387587  0.0811294357
H  -1.8645171178  3.8296594891  0.0872303131
Core RigidRotor
SymmetryFactor 1.0
End

```

```

Tunneling      Eckart
ImaginaryFrequency[1/cm]  1538.8938
WellDepth[kcal/mol]  13.97
WellDepth[kcal/mol]  59.96
End
Frequencies[1/cm]  50
113.7020          171.8118
226.9024          229.4351          346.7337
380.8078          420.5834          467.2336
487.2996          502.7867          528.4533
557.6358          565.2911          611.4008
639.9610          664.4546          718.1782
754.8171          769.6486          771.3952
833.2270          867.6980          910.2201
931.5847          955.4747          984.8251
995.4392          1067.0995         1104.1858
1145.8064         1189.3677         1236.7653
1249.4382         1317.2636         1367.2780
1381.3368         1424.9051         1484.7963
1500.6268         1555.8542         1578.9264
1645.7058         1767.1763         1825.0658
3161.0237         3164.0025         3178.9132
3184.1410         3192.7984         3381.2580
ZeroEnergy[kcal/mol]  88.34
ElectronicLevels[1/cm]  1
0 2
End
!-----
!-----acenaphthyl_ts7-----
Barrier      ts7  i2  p1
RRHO
Geometry[angstrom]  19
C  -0.298853125  -0.2323869543  0.1009401229
C  -0.1005111251  -1.6827560222  0.0913161248
C  1.1789046284  -2.2461187592  0.4036896352
C  2.2895607785  -1.4826114682  0.7282025411
C  1.9897749575  -0.1111006975  0.7077989089
C  0.8991093884  0.4102400737  0.443261013
C  -1.5668623106  0.2423851899  -0.2122114776
C  -2.6340927211  -0.5396160641  -0.5261100735
C  -2.4455043592  -1.9470626125  -0.5364726434
C  -1.2185430376  -2.4939886325  -0.2371811802
H  1.2730598079  -3.3273543191  0.3823957252
H  3.2497112965  -1.9238457709  0.9618373664
H  -3.6069875176  -0.1211760694  -0.7640665783
H  -3.2819007408  -2.5919111582  -0.7838412519
H  -1.0932071837  -3.571090588  -0.2501035251
C  -1.6879968812  2.663230424  -0.1409523699
C  -0.5971656951  3.0889405126  0.1638404285
H  -2.7124223727  2.5744943892  -0.4139778998

```

```

H 0.3915592125 3.3691845269 0.4357561339
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 227.7052
WellDepth[kcal/mol] 43.53
WellDepth[kcal/mol] 1.28
End
Frequencies[1/cm] 50
44.3920 65.8807
69.2015 167.1660 199.4051
224.9429 380.5807 410.9002
434.1061 449.0144 493.9640
519.9857 540.2121 576.2710
601.8366 641.3494 687.9119
710.4687 744.7914 752.1263
760.8721 806.8362 815.3111
859.9125 889.4000 945.0353
972.4339 1048.8432 1073.2010
1103.1327 1147.2727 1180.9789
1224.8988 1291.4014 1308.3801
1375.5751 1424.3391 1452.9435
1486.7056 1530.2517 1646.0167
1970.4795 1993.0126 3151.5940
3161.2468 3166.3798 3181.9282
3197.1505 3410.4226 3500.3220
ZeroEnergy[kcal/mol] 117.90
ElectronicLevels[1/cm] 1
0 2
End
!-----
!-----acenaphthyl_ts8-----
Barrier ts8 i1 i3
RRHO
Geometry[angstrom] 19
C -0.0010464004 -0.5551444447 -0.099946363
C 0.0114827289 -1.986492504 -0.070376564
C 1.2609891202 -2.6996196248 -0.0200575585
C 2.4760248336 -2.0674458618 0.0029004484
C 2.4235600413 -0.6549161912 -0.2062838975
C 1.2921007215 0.0353317534 -0.2536598791
C -1.233161449 0.1499746655 -0.0210038313
C -2.4212484671 -0.5721159431 0.0456132562
C -2.4122019967 -1.9753076936 0.0297981532
C -1.223727794 -2.6730007695 -0.027793924
C -1.2505656446 1.5755166078 -0.0202241568
C -1.2810406987 2.7789448268 -0.0144623384
H 1.214401054 -3.7837074304 0.0344293333
H 3.4028718772 -2.6130851374 0.1296837818

```

```

H 2.3256370004 0.5003209172 0.4105306728
H -3.3608004138 -0.0362744414 0.1009508083
H -3.353388598 -2.5114593642 0.070248792
H -1.2253790067 -3.7578553291 -0.0251972465
H -1.2999719081 3.8410389646 -0.0151494867
Core RigidRotor
SymmetryFactor 0.5
End
Tunneling Eckart
ImaginaryFrequency[1/cm] 1957.7983
WellDepth[kcal/mol] 59.85
WellDepth[kcal/mol] 60.82
End
Frequencies[1/cm] 50
104.6569 127.8711
167.8444 199.0486 334.4684
361.9788 405.0088 451.3533
458.3418 468.9576 490.8846
539.5496 580.7284 590.3138
638.0075 653.7278 678.7252
688.8987 764.0879 770.3619
784.9060 842.9337 850.3003
929.2673 976.8321 988.3076
992.9736 1059.2877 1092.8371
1161.9047 1195.1661 1225.9012
1263.8383 1267.8991 1346.1594
1389.7266 1424.9093 1483.9313
1517.7100 1594.0600 1620.3188
1712.6741 2157.1504 2208.4772
3149.7423 3164.5601 3180.9248
3189.4391 3196.2711 3477.6812
ZeroEnergy[kcal/mol] 89.20
ElectronicLevels[1/cm] 1
0 2
End
!-----
End

```

Input file for MESS calculations for pyrenyl C₁₆H₉

```
TemperatureList[K]          500. 600. 700. 800. 900. 1000. 1125.
1250. 1375. 1500. 1650. 1800. 2000. 2250. 2500.
PressureList[atm]          0.03947368 1. 10. 100.
EnergyStepOverTemperature  0.2          #Ratio of discretization
energy step to T
ExcessEnergyOverTemperature 100
ModelEnergyLimit[kcal/mol] 800
WellCutoff                 10
ChemicalEigenvalueMax     0.2
ChemicalEigenvalueMin     1.e-6          #only for direct
diagonalization method
CalculationMethod          direct
EigenvalueOutput           eigenvalue.out
Reactant                   #ground energy of bimolecular species will be used as a
reference.
Model
  EnergyRelaxation
    Exponential
      Factor[1/cm]         424      ! Jasper calc N2
      Power                0.62
      ExponentCutoff       15
    End
  CollisionFrequency
    LennardJones
      Epsilons[1/cm]      101.5  834.9  ! N2 pyrene-Frenklach
      Sigmas[angstrom]    3.6154  7.24  ! N2 pyrene-Frenklach
      Masses[amu]         28.   203.
    End
  OutputTemperatureStep[K] 100
  OutputTemperatureSize   20
  OutputReferenceEnergy[kcal/mol] 0.
  Well                    pyr1 # pyr1
  Species
    RRHO
      Geometry[angstrom]  25
C -2.8293761222 -1.2065335493 0.
C -1.4271332095 -1.227846425 0.
C -0.7136987279 0.0079990604 0.
C -1.4372243567 1.2399577044 0.
C -2.8376573021 1.2109573929 0.
C -3.5221882777 -0.0009882164 0.
C 0.7132604721 0.0006593923 0.
C 1.4443043271 1.2348253215 0.
C 0.6484660276 2.4061757077 0.
C -0.6885964848 2.47936499 0.
C -0.6795657824 -2.454527866 0.
C 0.6784922683 -2.4580839194 0.
C 1.4284689677 -1.2330561538 0.
```

```

C 2.8306248588 -1.2078488057 0.
C 3.5254472596 -0.0023886817 0.
C 2.8452300865 1.2112998378 0.
H -3.3719416009 -2.1458892708 0.
H -3.386510486 2.1465455112 0.
H -4.6065237795 -0.0040643845 0.
H -1.2251754646 3.423077232 0.
H -1.2288413689 -3.3902324065 0.
H 1.2247140653 -3.3956582682 0.
H 3.3739612885 -2.146847526 0.
H 4.609589003 -0.0083971531 0.
H 3.3879853387 2.1489414764 0.
  Core RigidRotor
  SymmetryFactor 1
  End
  Frequencies[1/cm] 69
    96.9223 151.6968 217.4529
    247.1686 260.9874 355.3444
    397.1868 407.4517 461.5248
    485.5974 504.2874 507.1622
    516.8146 550.4680 552.1204
    582.1549 596.7204 663.3012
    700.4377 726.9564 741.8096
    765.4403 782.6726 809.9931
    820.7758 826.8848 837.8492
    860.8493 906.5237 917.0637
    976.4228 976.6329 984.1501
    990.1959 1011.9907 1088.7748
    1108.7237 1113.5338 1166.3300
    1184.6300 1197.6340 1219.1252
    1230.2505 1252.6396 1262.3681
    1312.9131 1342.4714 1365.8114
    1391.5694 1424.5287 1444.9749
    1451.6513 1455.9598 1516.2112
    1529.0852 1594.8510 1608.6617
    1630.3907 1642.4817 1660.9135
    3155.3034 3157.0621 3160.5860
    3162.7907 3169.2115 3175.8583
    3177.7073 3184.5889 3192.1812
  ZeroEnergy[kcal/mol] 0.2
  ElectronicLevels[1/cm] 1
    0 2
  End
  End
  Well pyr2 # pyr2
  Species
  RRHO
  Geometry[angstrom] 25
C 2.742448 -1.303944 -0.0
C 1.340799 -1.270342 -0.0

```


C	0.681175	-0.005311	-0.0
C	1.447233	1.198317	0.0
C	2.846490	1.111687	0.0
C	3.482512	-0.125804	0.0
C	-0.741697	0.053554	-0.0
C	-1.397162	1.329511	-0.0
C	0.539928	-2.462702	-0.0
C	-0.817100	-2.404298	-0.0
C	-1.513876	-1.147508	0.0
C	-2.914868	-1.071034	0.0
C	-3.566440	0.167904	0.0
C	-2.779587	1.291498	0.0
H	3.248314	-2.263623	-0.0
H	3.432670	2.024457	0.0
H	4.565757	-0.172522	0.0
H	1.046173	-3.422252	-0.0
H	-1.403806	-3.316948	-0.0
H	-3.498313	-1.986246	0.0
H	-4.649343	0.224259	0.0
C	-0.601283	2.524839	-0.0
C	0.755313	2.457674	-0.0
H	-1.110950	3.481032	-0.0
H	1.346176	3.367595	-0.0

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 69

98.1047	154.3538	211.0769
252.3144	259.7625	361.4225
406.0632	410.7827	462.2890
485.9760	501.6923	510.2935
514.4748	538.8922	551.8566
572.2429	596.4491	684.8786
700.0267	714.5526	744.8815
764.4403	782.8291	802.8498
821.9377	831.3428	836.5110
855.9252	910.0799	940.3117
971.9682	977.4787	982.1570
990.3947	1005.3817	1095.6105
1117.7055	1135.0311	1163.9011
1175.8280	1197.1216	1205.6575
1239.7491	1259.3853	1266.5174
1325.3918	1334.5850	1386.6532
1399.5450	1422.3930	1440.1092
1450.0664	1469.6300	1486.1255
1525.8426	1585.1100	1604.5764
1629.7949	1640.6447	1665.1913
3156.7831	3159.0565	3160.2547
3163.8735	3168.8002	3175.1647
3177.2141	3184.9132	3188.8180

```

ZeroEnergy[kcal/mol]          0.6
ElectronicLevels[1/cm]      1
    0  2
End
End
Well      pyr3 # pyr3
Species
RRHO
    Geometry[angstrom]      25
C -2.7789294925 -1.187789014 0.
C -1.376692435 -1.1993176254 0.
C -0.6726190631 0.0413145942 0.
C -1.4016976495 1.2675591447 0.
C -2.8031031614 1.2275442117 0.
C -3.481159067 0.0128709962 0.
C 0.7532517573 0.0556959601 0.
C 1.4500843286 1.3030386644 0.
C 0.6885846547 2.5204612467 0.
C -0.6696348468 2.5027183542 0.
C -0.6200709617 -2.4193257591 0.
C 0.7383339546 -2.409719815 0.
C 1.4745769549 -1.1772292662 0.
C 2.885823156 -1.1478373664 0.
C 3.4888500614 0.0830883937 0.
C 2.8604662869 1.3019492939 0.
H -3.3144919713 -2.1311688199 0.
H -3.3580318411 2.1597014857 0.
H -4.5652411039 0.0021801174 0.
H 1.2255459626 3.4629904595 0.
H -1.2289126995 3.4324518384 0.
H -1.1604185299 -3.360208792 0.
H 1.2945018575 -3.3410374821 0.
H 3.4504392677 -2.0740477539 0.
H 3.4070315804 2.239026933 0.
    Core RigidRotor
    SymmetryFactor          1
    End
    Frequencies[1/cm]      69
100.9611          149.9303          214.4928
244.9302          271.7799          362.4372
393.2100          413.3439          460.8665
494.9190          504.6772          507.8689
515.7089          526.3619          550.1192
565.7222          594.7570          673.9236
697.1454          713.8679          751.5820
764.6863          798.0538          800.3010
800.5081          832.0940          842.2496
865.2133          867.5033          912.4985
976.3291          979.7803          984.3364
988.8318          1007.6456         1084.8090

```

1105.6248	1130.0137	1165.7153
1166.8176	1201.2425	1207.7484
1250.1620	1253.6515	1266.6504
1319.4899	1344.6445	1371.7052
1413.8117	1415.0886	1443.8938
1448.7105	1476.3372	1501.1295
1527.9445	1544.5178	1618.7269
1620.1164	1646.3184	1665.1793
3158.1939	3158.4234	3161.2432
3164.2951	3165.8856	3168.7876
3177.4120	3177.6825	3185.8037

ZeroEnergy[kcal/mol] 0.0

ElectronicLevels[1/cm] 1

0 2

End

End

Well i1 # i1

Species

RRHO

Geometry[angstrom] 25

C	2.8720490145	-1.5064626125	0.
C	1.4591008137	-1.4939694575	0.
C	0.7675139571	-0.2397672045	0.
C	1.5788432304	0.8905031274	0.
C	2.9405369083	0.9121887587	0.
C	3.6043485987	-0.3363368315	0.
C	-0.6792924169	-0.209032863	0.
C	-1.4264293073	1.0071417222	0.
C	0.6950671439	-2.7060155877	0.
C	-0.6615443033	-2.6789368398	0.
C	-1.3894321445	-1.4418644076	0.
C	-2.7999458733	-1.4405095651	0.
C	-3.5058796803	-0.2557922327	0.
C	-2.8205860258	0.9634169564	0.
C	-0.8000144298	2.2899297631	0.
C	-0.3792583254	3.4203105808	0.
H	3.381084497	-2.4643621104	0.
H	3.5028284195	1.8398192105	0.
H	4.6887264582	-0.369344577	0.
H	1.2266642425	-3.6519496964	0.
H	-1.2285352897	-3.6037925666	0.
H	-3.3223988872	-2.3911614192	0.
H	-4.5896002126	-0.2623621413	0.
H	-3.3693324031	1.8970249749	0.
H	0.0310070156	4.4000560187	0.

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 69

60.4542	106.0521	133.6960
---------	----------	----------

153.3281	212.8789	226.0283
248.5844	374.6357	377.3653
410.9389	430.0401	489.3215
501.5688	510.3718	533.8078
544.6358	570.1415	584.1235
624.1625	642.0509	666.8631
675.2802	712.8282	722.5486
754.8459	777.0242	800.1124
814.8753	842.4180	849.3153
889.2925	925.1853	969.3047
979.1880	988.0391	993.7410
1014.8094	1064.1567	1105.4421
1143.0927	1172.0539	1188.5011
1192.9347	1230.1950	1253.2456
1264.5359	1308.6172	1341.4636
1356.5782	1410.1542	1432.6525
1447.2956	1469.8390	1510.0695
1523.7958	1587.3554	1623.7507
1644.8137	1653.9107	2188.2231
3155.9601	3157.6392	3165.2809
3166.6062	3176.2281	3180.4115
3182.2759	3197.3882	3477.0915

ZeroEnergy[kcal/mol] 50.6

ElectronicLevels[1/cm] 1

0 2

End

End

Well i2 # i2

Species

RRHO

Geometry[angstrom] 25

C	2.6788137076	1.1259509632	0.
C	1.2604822685	1.2112907944	0.
C	0.4988823293	0.0026141284	0.
C	1.17347827	-1.256066726	0.
C	2.5613205379	-1.2853275836	0.
C	3.3117158229	-0.0952853559	0.
C	-0.9363514462	0.0590765347	0.
C	-1.7186513404	-1.1829295516	0.
C	-0.9748305016	-2.4268204623	0.
C	0.3746403024	-2.4635768198	0.
C	0.5897042068	2.4610669375	0.
C	-0.7926892017	2.5195831678	0.
C	-1.4813611009	1.3176819314	0.
C	-4.7454057381	0.8049201206	0.
C	-3.9459169938	-0.1030202434	0.
C	-3.0878602355	-1.216135004	0.
H	3.2564803665	2.0439555311	0.
H	3.0710452331	-2.2431451537	0.
H	4.3945258902	-0.1460064573	0.

```

H -1.543827894 -3.3503597379 0.
H 0.8935525513 -3.4164727631 0.
H 1.176346656 3.3743755745 0.
H -1.3126173768 3.4713178165 0.
H -5.4264597494 1.6197864499 0.
H -3.5711915642 -2.1889960915 0.
  Core RigidRotor
  SymmetryFactor 1
  End
  Frequencies[1/cm] 69
  47.6178 102.3428 137.2050
  172.0542 197.7887 237.1399
  251.8347 347.0020 358.3223
  442.6540 455.7713 466.4439
  473.2978 492.9545 508.0194
  537.7519 539.9544 594.4125
  598.9372 610.8981 643.4180
  664.9495 683.8995 759.7479
  762.9936 783.1776 786.6634
  788.6896 825.9580 838.4887
  855.4433 912.2468 955.4846
  975.7191 980.8450 990.2904
  1052.0515 1058.0338 1105.5972
  1139.7934 1147.3402 1182.5831
  1203.0915 1232.9535 1244.5018
  1260.5690 1324.5343 1357.2096
  1384.1588 1412.2210 1432.7334
  1455.6272 1479.4171 1509.2980
  1565.1970 1586.4176 1619.0329
  1628.7333 1660.4197 2164.6779
  3145.7240 3157.1436 3158.8694
  3161.5740 3169.0721 3174.6564
  3178.3205 3187.0200 3477.2396
  ZeroEnergy[kcal/mol] 63.3
  ElectronicLevels[1/cm] 1
  0 2
  End
  End
  Well i3 # i3
  Species
  RRHO
  Geometry[angstrom] 25
  C 2.168886 -2.007671 -0.0
  C 0.832316 -1.559970 0.0
  C 0.551162 -0.159477 0.0
  C 1.643219 0.763551 0.0
  C 2.943813 0.267622 0.0
  C 3.210390 -1.104116 -0.0
  C -0.833992 0.238650 0.0
  C -1.397446 1.513171 -0.0

```

C	-0.243256	-2.507284	-0.0
C	-1.544819	-2.120922	-0.0
C	-1.904127	-0.734169	0.0
C	-3.271937	-0.334017	-0.0
C	-3.684712	0.996405	-0.0
C	-2.587619	1.862466	-0.0
H	2.363347	-3.074643	-0.0
H	3.763923	0.976565	0.0
H	4.237140	-1.451983	-0.0
H	0.010933	-3.561788	-0.0
H	-2.335456	-2.863040	-0.0
H	-4.025639	-1.115398	-0.0
H	-4.728672	1.281760	-0.0
C	2.344971	3.164542	-0.0
C	1.431943	2.222114	0.0
H	2.377246	4.242803	-0.0
H	0.384427	2.560364	0.0
Core RigidRotor			
SymmetryFactor		1	
End			
Frequencies[1/cm]		69	
31.8801	77.3079	114.5381	
147.1615	187.6593	238.4967	
275.4204	275.6735	363.3435	
403.0475	418.3284	464.2994	
464.4270	480.1403	520.8721	
526.8741	559.0602	559.9119	
586.6323	644.5122	653.5566	
681.9443	697.6663	773.2252	
774.2899	774.8068	798.7057	
816.6861	842.0186	857.9403	
864.0536	928.8674	944.9455	
959.2933	978.8780	991.2089	
1013.4984	1091.4138	1112.3543	
1138.9168	1168.2226	1193.4834	
1217.5708	1229.3182	1243.7831	
1277.5435	1290.4378	1324.5513	
1352.2416	1396.4750	1425.7183	
1437.5655	1459.6671	1489.5381	
1537.1230	1577.4783	1630.0485	
1641.4518	1652.6691	1966.4515	
2906.0862	3160.0989	3163.2264	
3164.9642	3174.5373	3181.3293	
3187.9357	3196.0937	3253.1900	
ZeroEnergy[kcal/mol]		98.1	
ElectronicLevels[1/cm]		1	
0	2		
End			
End			
Well	i4	# i4	

Species

RRHO

Geometry[angstrom] 25

C 3.0732447159 1.0545182404 0.
C 1.6904806067 1.1584724323 0.
C 0.8905067821 -0.0300724741 0.
C 1.544249542 -1.3002685653 0.
C 2.9617257023 -1.3547566276 0.
C 3.7085168571 -0.2004197832 0.
C -0.5349923372 0.0468615726 0.
C -1.2787109981 -1.1437755773 0.
C -0.6129760325 -2.3983798188 0.
C 0.7538202624 -2.4759233679 0.
C 1.027654151 2.4467176031 0.
C -0.3129887831 2.5530963972 0.
C -1.1854747135 1.3758617552 0.
C -2.5108756737 1.5343546876 0.
C -3.9021608222 -1.2863505509 0.
C -2.7019484732 -1.1537189041 0.
H 3.6708810224 1.9598422157 0.
H 3.4457169754 -2.3253267218 0.
H 4.7914203596 -0.2522631157 0.
H -1.2160067043 -3.2979537749 0.
H 1.2460264305 -3.4422816569 0.
H 1.6472708154 3.3376385139 0.
H -0.7897280712 3.5263836728 0.
H -3.1738495565 2.3874215133 0.
H -4.9622780577 -1.3535156656 0.

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 69

66.4750	86.1367	144.5852
177.2857	206.8182	232.7042
264.5294	332.6827	378.3113
412.6786	422.2884	426.7874
474.9499	497.4186	527.1147
528.5952	553.3363	566.2199
602.5303	620.6973	634.2468
666.4789	681.6557	701.1790
709.2720	746.7574	766.9913
806.0464	813.7459	819.7204
852.8903	853.6462	908.8157
937.1141	971.0301	972.1800
980.1680	988.9281	1093.3098
1121.6305	1153.4650	1182.9310
1200.5845	1221.3755	1252.0237
1260.8171	1280.6508	1368.2082
1372.9156	1397.4115	1426.2649
1465.9284	1468.3763	1528.9487

1549.9358	1604.3483	1626.7888
1632.3578	1666.8754	2177.9990
3158.2428	3161.7184	3168.7369
3171.1360	3184.1152	3186.4751
3194.2305	3229.3695	3475.6767

ZeroEnergy[kcal/mol] 65.7

ElectronicLevels[1/cm] 1

0 2

End

End

Well i5 # i5

Species

RRHO

Geometry[angstrom] 25

C	2.8185565168	-1.8810383217	0.
C	1.4047692148	-1.8796399112	0.
C	0.6717765652	-0.6492083138	0.
C	1.4392376967	0.5508472548	0.
C	2.7955765202	0.4588722238	0.
C	3.5457374268	-0.7033516488	0.
C	-0.7905376571	-0.6865280733	0.
C	-1.6573502802	0.4589788484	0.
C	0.7083011061	-3.1294966822	0.
C	-0.6434533632	-3.1700383219	0.
C	-1.4256514187	-1.9693359568	0.
C	-2.8312421888	-2.085803845	0.
C	-3.6369806492	-0.9708459415	0.
C	-3.0454019175	0.2922344372	0.
C	-1.2411830363	1.8277597181	0.
C	-1.0327125894	3.0148189918	0.
H	3.3341665613	-2.836533034	0.
H	0.9536426876	1.5132286227	0.
H	4.6294932628	-0.7045332715	0.
H	1.2898129514	-4.0451430634	0.
H	-1.1685690057	-4.1189225938	0.
H	-3.2658295968	-3.0795041404	0.
H	-4.7165760532	-1.064144343	0.
H	-3.6641175567	1.1807555372	0.
H	-0.8136991969	4.0544518282	0.

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 69

28.2114	92.4583	152.9392
167.7202	232.9919	243.4794
255.3457	370.4696	375.3082
405.0002	411.2864	492.4621
508.1461	515.8477	517.2003
549.0583	572.7216	593.3622
621.6078	637.1267	667.9206

686.9503	712.5901	724.7751
768.9295	775.5067	799.1155
819.3139	838.2112	848.7738
871.3654	927.6383	952.5628
978.2979	989.6077	995.7899
1001.0739	1079.6692	1115.9714
1142.9616	1174.5578	1190.1062
1214.5002	1224.9054	1254.7430
1272.2384	1293.5517	1336.0496
1345.4543	1404.7817	1411.4796
1453.1801	1460.3593	1507.7010
1539.8138	1593.5322	1615.4772
1628.7007	1665.3454	2192.4888
3154.2868	3160.6886	3166.7797
3179.5137	3181.2796	3183.6332
3198.2713	3234.5958	3473.7867

ZeroEnergy[kcal/mol] 54.6

ElectronicLevels[1/cm] 1

0 2

End

End

Well i6 # i6

Species

RRHO

Geometry[angstrom] 25

C	2.5569446896	1.0911571693	0.
C	1.1429894649	1.1856517458	0.
C	0.3611716297	-0.0093615624	0.
C	1.0322395376	-1.2695336515	0.
C	2.4365296432	-1.3123869643	0.
C	3.1905778354	-0.1392143457	0.
C	-1.0689881839	0.0666776211	0.
C	-1.8339131008	-1.16872336	0.
C	-1.1183388622	-2.3985547364	0.
C	0.2485393364	-2.4593096381	0.
C	0.4871453754	2.438858401	0.
C	-0.8927420832	2.5047339004	0.
C	-1.6654941101	1.3417283845	0.
C	-5.1669648019	0.5174778396	0.
C	-4.2147904722	-0.3251703094	0.
C	-3.256155328	-1.2845108152	0.
H	3.1397048837	2.0057721257	0.
H	2.9318383654	-2.2772219839	0.
H	4.2728764779	-0.192894924	0.
H	-1.6926533422	-3.318388305	0.
H	0.7525456082	-3.4194948657	0.
H	1.0832861573	3.345037123	0.
H	-1.3910484832	3.4670537828	0.
H	-2.7430248793	1.4220549612	0.
H	-3.6087223577	-2.3172875927	0.

```

Core RigidRotor
SymmetryFactor 1
End
Frequencies[1/cm] 69
44.3884 124.3933 132.6210
160.7698 203.1549 219.1808
273.2745 295.9100 358.7724
365.3807 437.1636 470.7392
474.0591 494.0489 497.0149
528.1671 538.5800 597.0550
611.1152 645.5741 678.5274
761.6995 769.4615 781.6948
802.7547 813.8198 833.2992
854.9408 901.1952 918.5105
952.8994 973.1135 981.7332
991.5508 1017.5201 1065.9376
1099.6816 1127.6993 1139.6976
1158.9746 1187.2161 1209.6704
1223.5168 1237.8795 1247.5241
1275.8766 1352.8311 1371.0921
1390.5371 1431.8235 1449.6218
1458.9638 1464.2420 1506.2502
1531.7556 1586.1813 1594.2287
1597.3926 1614.7446 2014.3085
3085.6651 3167.1023 3168.4489
3170.2597 3175.7426 3184.4207
3189.1784 3192.6713 3212.9163
ZeroEnergy[kcal/mol] 70.5
ElectronicLevels[1/cm] 1
0 2
End
End
Well i8 # i8
Species
RRHO
Geometry[angstrom] 25
C 2.5118921345 1.0880104851 0.0189825455
C 1.0919575206 1.1681612055 0.0217602356
C 0.3305156816 -0.041134198 0.020866794
C 1.0150171426 -1.2987955206 0.0185801646
C 2.3954791112 -1.3241531728 0.014885416
C 3.1461571223 -0.1285091535 0.0142239663
C -1.0878970261 0.0313584182 0.0173682862
C -1.927734947 -1.254732667 0.0122994721
C -1.1074714412 -2.5329127762 0.0352205793
C 0.2278917794 -2.5255456159 0.027720367
C 0.4120021333 2.4098394002 0.0276903488
C -0.9618508517 2.4541562872 0.0293593725
C -1.7110424357 1.2616919726 0.0216024265

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C -4.6308124508 -2.0370974288 -2.8309830456
C -3.7388617388 -1.6958189109 -1.9179730049
C -2.9037258041 -1.2917459507 -1.0696225712
H 3.0853395008 2.008608162 0.0220142323
H 2.909621189 -2.2794117535 0.0137441254
H 4.2289180654 -0.1786739124 0.0116770526
H -2.5547325251 -1.2483539073 0.9230916263
H -1.6685346338 -3.4597102181 0.0409549697
H 0.7676679553 -3.4674269239 0.0376698381
H 0.9926146828 3.3259951779 0.0290824628
H -1.4779950844 3.4072172687 0.0322110619
H -2.7946960802 1.3142217323 0.0054742783
  Core RigidRotor
  SymmetryFactor 1
  End
  Frequencies[1/cm] 69
    26.6013 38.3555 106.1338
    156.6942 191.8795 194.7956
    259.9122 278.9345 339.2650
    365.0768 392.2029 438.7742
    467.2092 475.3020 477.4771
    502.5046 530.3980 570.6145
    597.1276 643.3531 660.5928
    734.5222 758.6583 788.7769
    793.8547 803.1977 821.0914
    851.9514 855.6597 914.3216
    929.5351 973.0521 984.1555
    992.6614 999.7884 1045.0965
    1074.1304 1102.6970 1120.4529
    1169.8110 1185.0848 1198.5890
    1207.0191 1234.8628 1245.0948
    1258.5233 1283.4206 1364.1148
    1373.8185 1393.3808 1416.6806
    1421.3103 1465.2450 1498.1721
    1542.6974 1621.8728 1634.3654
    1648.1514 1700.2059 1948.7760
    2923.7597 3157.3972 3162.0813
    3163.3283 3168.8330 3171.1296
    3187.8611 3188.6632 3189.2468
  ZeroEnergy[kcal/mol] 108.2
  ElectronicLevels[1/cm] 1
    0 2
  End
  End
  Bimolecular P2 # phenanthrynyl + C2H2
  Fragment C14H7
  RRHO
  Geometry[angstrom] 21
C 2.785159 0.874853 0.00
C 1.371008 0.832869 -0.00

```

C	0.716966	-0.439717	-0.00
C	1.549555	-1.555053	-0.00
C	2.908581	-1.549480	0.00
C	3.539938	-0.279607	0.00
C	-0.715012	-0.496794	-0.00
C	-1.551854	-1.614858	-0.00
C	0.566963	2.018426	-0.00
C	-0.793178	1.962903	-0.00
C	-1.499204	0.713229	-0.00
C	-2.923938	0.666221	0.00
C	-3.649574	-0.523999	0.00
C	-2.788615	-1.621689	0.00
H	3.276426	1.841816	0.00
H	3.495280	-2.461137	0.00
H	4.623221	-0.224213	0.00
H	1.070738	2.979314	-0.00
H	-1.370303	2.881182	-0.00
H	-3.464895	1.607389	0.00
H	-4.731227	-0.548178	0.00

Core RigidRotor

SymmetryFactor 1

End

Frequencies[1/cm] 57

97.5233	130.9593	217.6501
235.2771	242.7574	380.8247
415.2875	446.6019	450.8809
462.1908	470.0646	512.4947
548.8311	584.1860	594.3175
661.0581	665.3065	726.0083
748.4073	761.3440	769.6862
806.5268	844.6845	875.2896
890.3231	940.9563	970.0704
981.1091	982.6918	1054.0355
1067.0967	1132.6549	1144.7551
1171.1460	1189.5766	1219.9747
1229.6604	1267.5846	1325.9037
1343.1816	1387.3664	1413.6586
1435.2096	1450.8579	1492.7488
1509.7869	1536.9604	1630.1257
1648.0069	2035.6063	3158.8859
3161.0099	3164.1619	3172.4776
3178.7450	3183.8469	3201.1039

ZeroEnergy[kcal/mol] 0.

ElectronicLevels[1/cm] 1

0 2

End

Fragment C2H2

RRHO

Geometry[angstrom] 4

H	0.000000	0.000000	-1.660312
---	----------	----------	-----------

```

C      0.000000      0.000000      -0.598105
C      0.000000      0.000000      0.598105
H      0.000000      0.000000      1.660312
      Core      RigidRotor
      SymmetryFactor      2
      End
      Frequencies[1/cm]      7
664. 664. 766. 766. 2066. 3406. 3509.
      ZeroEnergy[kcal/mol]      0.
      ElectronicLevels[1/cm]      1
      0 1
      End
      GroundEnergy[kcal/mol]      137.2
      End
      Bimolecular      P4      # phenalenyl + C3
      Fragment      C13H9
      RRHO
      Geometry[angstrom]      22
C 1.8178437237 1.1500188787 0.
C 0.4040855703 1.2412879264 0.
C -0.3640161484 0.0360546041 0.
C 0.295563854 -1.2318435257 0.
C 1.7118740006 -1.2646995826 0.
C 2.4508937258 -0.0874345432 0.
C -1.7918260148 0.098727446 0.
C -2.528374262 -1.1115156275 0.
C -1.8784521875 -2.3401953576 0.
C -0.4902923267 -2.4106033848 0.
C -0.2755210298 2.4843133519 0.
C -1.6645240354 2.5358058695 0.
C -2.419580164 1.3688101005 0.
H 2.4033242798 2.0629913578 0.
H 2.2152127511 -2.2253606116 0.
H 3.5342507668 -0.134934309 0.
H -3.6120000495 -1.0670710706 0.
H -2.4613062677 -3.2546236916 0.
H 0.0077871102 -3.3739995395 0.
H 0.3049218644 3.4004248442 0.
H -2.1651020143 3.4977366206 0.
H -3.5029601465 1.4194902442 0.
      Core      RigidRotor
      SymmetryFactor      6
      End
      Frequencies[1/cm]      60
161.5667      161.6962      210.0358
285.7289      429.6145      430.2224
480.4549      480.5152      486.3764
490.4889      491.2758      585.1701
624.0981      644.5109      644.9080
752.5599      753.7435      768.8897

```

788.3498	834.1765	834.2711
852.9716	853.4431	888.7918
890.2833	971.3642	971.9654
980.5023	1056.0280	1056.3452
1112.5786	1123.2460	1123.4518
1167.4182	1203.0883	1203.2645
1218.5071	1252.3280	1252.4588
1347.1764	1347.2744	1408.3229
1424.0597	1446.7136	1446.8425
1498.1788	1548.8329	1577.4406
1577.5901	1590.2508	1590.3250
3159.9117	3159.9725	3162.0532
3168.7826	3171.6580	3171.9310
3184.0389	3184.1436	3186.3543

ZeroEnergy[kcal/mol] 0.

ElectronicLevels[1/cm] 1

0 2

End

Fragment C3

RRHO

Geometry[angstrom] 3

C 1.291048 -0. 0.000000

C 0.000000 0. 0.000000

C -1.291048 -0. 0.000000

Core RigidRotor

SymmetryFactor 2

End

Frequencies[1/cm] 4

106.2317 106.2317 1237.5978 2148.2082

ZeroEnergy[kcal/mol] 0.

ElectronicLevels[1/cm] 1

0 1

End

GroundEnergy[kcal/mol] 137.8

End

Barrier ts1 pyr1 i1 # ts1

RRHO

Geometry[angstrom] 25 #

C 2.889741 -1.165753 0.00

C 1.478119 -1.188715 0.00

C 0.748789 0.045699 0.00

C 1.525993 1.211156 -0.00

C 2.892095 1.249098 -0.00

C 3.590605 0.023287 -0.00

C -0.702947 0.010476 0.00

C -1.510447 1.192409 0.00

C 0.759981 -2.428978 0.00

C -0.595872 -2.457237 -0.00

C -1.367645 -1.247958 -0.00

C -2.777815 -1.297689 -0.00

C	-3.533614	-0.143039	-0.00
C	-2.899175	1.103162	0.00
H	3.422577	-2.110625	0.00
H	3.436806	2.188017	-0.00
H	4.675655	0.019342	-0.00
H	1.329420	-3.352717	0.00
H	-1.126847	-3.403214	-0.00
H	-3.262854	-2.268042	-0.00
H	-4.615973	-0.197287	-0.00
H	-3.481820	2.016247	0.00
C	-0.839183	2.445248	0.00
C	0.141035	3.169442	-0.00
H	0.825078	3.984629	-0.00

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 346.5878

WellDepth[kcal/mol] 55.0

WellDepth[kcal/mol] 4.6

End

Frequencies[1/cm] 68

78.5810	113.8852	
157.3723	226.4136	241.5056
262.1357	373.4840	388.1286
426.5528	435.7769	485.3459
491.4354	504.2754	529.1462
553.3771	562.5446	573.3974
610.5481	636.8783	655.0103
717.7867	718.2544	744.1022
757.0497	778.9266	800.3637
817.4256	843.7118	852.7529
889.9778	922.9726	970.0332
979.6023	988.6441	996.1459
1011.6756	1071.9145	1100.6417
1142.7452	1172.2959	1191.9110
1196.2848	1228.2905	1251.9256
1266.0870	1304.8987	1338.5873
1359.1957	1407.5231	1423.3232
1448.2239	1459.6003	1512.4236
1525.3674	1584.0900	1624.6009
1640.4236	1654.0484	2088.3193
3149.0504	3156.2459	3161.6837
3164.5592	3175.4262	3178.4044
3181.0309	3195.3314	3448.8030

ZeroEnergy[kcal/mol] 55.2

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts2 pyr3 i2 # ts2

```

RRHO
  Geometry[angstrom]  25      #
C      2.878030      1.184896    -0.00
C      1.460792      1.241648     0.00
C      0.718607      0.021177     0.00
C      1.420642     -1.222982    -0.00
C      2.810770     -1.225765    -0.00
C      3.537355     -0.024176    -0.00
C     -0.718366      0.053375     0.00
C     -1.463436     -1.212885     0.00
C     -0.697521     -2.440072    -0.00
C      0.653004     -2.447457    -0.00
C      0.767000      2.480174     0.00
C     -0.612315      2.513059     0.00
C     -1.304694      1.305469     0.00
C     -3.721024      1.136367    -0.00
C     -3.576871     -0.078468     0.00
C     -2.838867     -1.267383     0.00
H      3.437088      2.114480     0.00
H      3.337675     -2.174275    -0.00
H      4.620976     -0.052737    -0.00
H     -1.248414     -3.374646    -0.00
H      1.193628     -3.388302    -0.00
H      1.339307      3.402897     0.00
H     -1.140426      3.461216     0.00
H     -4.078353      2.138309    -0.00
H     -3.340120     -2.228801     0.00
  Core      RigidRotor
  SymmetryFactor      1
  End
  Tunneling      Eckart
  ImaginaryFrequency[1/cm]  326.8111
  WellDepth[kcal/mol]      67.1
  WellDepth[kcal/mol]      3.8
  End
  Frequencies[1/cm]      68
  70.0118      131.4262
  188.6729      203.4686      231.9579
  264.0973      348.7896      386.9108
  436.5821      454.3957      462.4112
  477.9408      494.6130      505.6620
  529.8547      545.4330      560.8047
  595.2112      612.8544      646.8174
  684.3019      719.7686      758.0925
  762.9913      777.9237      787.5593
  790.5819      826.0168      837.5606
  852.5085      911.8772      958.4921
  979.5056      980.1584      989.4057
  1045.4655     1080.0058     1106.0047
  1138.5694     1153.0514     1180.6970

```


1201.8599	1232.3998	1241.4709
1261.1047	1329.6098	1350.8346
1382.8547	1408.6530	1430.7872
1443.7973	1477.5357	1507.7708
1530.6909	1587.2605	1607.7782
1623.3459	1659.2512	2056.4807
3148.9181	3156.6770	3160.7505
3165.2422	3166.1301	3168.7269
3176.4630	3186.6178	3451.8873

ZeroEnergy[kcal/mol] 67.1

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts3 pyr2 i3 # ts3

RRHO

Geometry[angstrom] 25 #

C	2.513096	-1.655210	0.038140
C	1.122182	-1.415505	0.044236
C	0.640143	-0.076542	-0.042773
C	1.577108	0.989860	-0.136258
C	2.933245	0.708791	-0.150983
C	3.404857	-0.610787	-0.059425
C	-0.782818	0.131303	-0.048546
C	-1.515665	1.308507	-0.133385
C	0.190061	-2.500620	0.130118
C	-1.153644	-2.296556	0.119499
C	-1.706446	-0.977667	0.024741
C	-3.115776	-0.766309	0.002894
C	-3.697688	0.495189	-0.088999
C	-2.737705	1.515425	-0.150207
H	2.868116	-2.677760	0.108318
H	3.639648	1.527867	-0.224322
H	4.472172	-0.800295	-0.064816
H	0.586870	-3.507793	0.200489
H	-1.832808	-3.139814	0.181769
H	-3.758294	-1.639447	0.063438
H	-4.771863	0.633004	-0.102642
C	0.726908	3.164070	0.738932
C	1.138931	2.415216	-0.252937
H	0.373821	4.174093	0.884034
H	1.201597	2.855159	-1.256535

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 138.4933

WellDepth[kcal/mol] 99.4

WellDepth[kcal/mol] 1.9

End

Frequencies[1/cm] 68

63.2252	112.9780	
153.7867	159.0190	234.4296
240.2077	295.2679	357.3470
396.1520	427.7678	453.8260
463.8637	471.3902	503.8551
527.3153	540.7268	578.2631
618.6717	622.9349	680.0957
683.3468	694.6341	774.1426
774.7040	780.4494	796.5641
825.3196	834.4200	852.6322
879.5597	926.5129	947.2647
965.6238	976.4314	988.3459
1027.6951	1091.9483	1115.8070
1135.8787	1167.4576	1190.5499
1214.3862	1232.2045	1239.8363
1262.6842	1275.7677	1326.8198
1349.6411	1400.4661	1426.3826
1438.6636	1458.3868	1496.6625
1537.8569	1578.2984	1633.1005
1645.6008	1662.2874	2013.1998
3003.7248	3157.6761	3161.6515
3164.1273	3174.3038	3179.7667
3187.1634	3188.7654	3242.6261

ZeroEnergy[kcal/mol] 100.0

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts4 pyr2 i4 # ts4

RRHO

Geometry[angstrom] 25 #

C	2.852131	1.105272	0.0
C	1.466342	1.185964	0.0
C	0.686501	-0.015271	-0.0
C	1.361936	-1.275753	-0.0
C	2.778457	-1.305280	0.0
C	3.506727	-0.137414	0.0
C	-0.740822	0.037212	-0.0
C	-1.454530	-1.178385	-0.0
C	-0.771934	-2.420995	-0.0
C	0.595211	-2.469533	-0.0
C	0.780679	2.459725	0.0
C	-0.562576	2.538767	-0.0
C	-1.420081	1.351453	-0.0
C	-2.754745	1.522542	-0.0
H	3.433928	2.020840	0.0
H	3.279815	-2.267030	0.0
H	4.590348	-0.172251	0.0
H	-1.358977	-3.331417	-0.0
H	1.109907	-3.424053	-0.0
H	1.382329	3.362852	0.0

H	-1.054721	3.504601	-0.0
H	-3.329177	2.441665	-0.0
C	-3.965980	-0.588369	0.0
C	-2.866904	-1.111887	-0.0
H	-4.995912	-0.323492	0.0

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 320.1717

WellDepth[kcal/mol] 68.7

WellDepth[kcal/mol] 3.6

End

Frequencies[1/cm] 68

84.1857	108.5569	
181.8077	208.9317	229.8046
340.2698	353.0975	383.3735
424.0774	428.2775	431.5073
476.4204	494.1944	529.5233
530.5133	550.3078	570.9358
596.9490	598.8909	639.7168
684.9110	706.3727	710.1730
725.6639	754.0248	767.2910
810.2145	818.2157	822.7197
853.5425	902.4983	907.8478
945.9905	972.7342	973.5517
980.1171	988.8174	1095.8447
1123.0403	1153.2803	1182.6573
1201.1101	1233.6588	1258.6152
1262.0424	1280.7582	1367.6996
1370.9121	1390.3936	1428.3235
1455.5777	1468.1616	1525.4821
1535.7671	1592.2201	1625.2402
1632.7810	1666.9083	2100.7464
3157.5261	3161.3010	3167.9216
3170.7075	3180.7174	3185.1156
3186.0909	3191.4483	3458.5837

ZeroEnergy[kcal/mol] 69.3

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts6 i3 P2 # ts6

RRHO

Geometry[angstrom] 25 #

C	2.170438	-2.103922	0.020685
C	0.826904	-1.663199	0.025517
C	0.554369	-0.260090	-0.048248
C	1.659189	0.594109	-0.130277
C	2.959528	0.180736	-0.127854

C	3.216070	-1.208242	-0.053750
C	-0.811975	0.181016	-0.037091
C	-1.326213	1.477013	-0.093503
C	-0.269103	-2.582503	0.102352
C	-1.562232	-2.159929	0.106975
C	-1.898335	-0.766802	0.037975
C	-3.256702	-0.334203	0.043764
C	-3.634084	1.005763	-0.021572
C	-2.510921	1.832976	-0.085674
C	1.961074	3.482043	0.576165
C	1.474743	2.915985	-0.382110
H	2.368359	-3.168877	0.078093
H	3.777266	0.890519	-0.183577
H	4.240808	-1.564617	-0.055373
H	-0.044324	-3.642663	0.156596
H	-2.368111	-2.883471	0.164483
H	-4.030880	-1.092952	0.103546
H	-4.669385	1.320590	-0.016725
H	2.402116	3.824565	1.481206
H	1.007639	2.772395	-1.328383

Core RigidRotor
SymmetryFactor 0.5

End

Tunneling Eckart
ImaginaryFrequency[1/cm] 312.4934
WellDepth[kcal/mol] 41.3
WellDepth[kcal/mol] 2.2

End

Frequencies[1/cm]			68
31.9814	41.2221		
101.1023	118.0465	132.3821	
201.7788	234.4560	236.5591	
253.5205	383.0452	416.5115	
443.4784	452.5266	461.7332	
472.2720	516.7275	540.8275	
554.1821	586.3416	594.6350	
641.6106	658.1027	671.4914	
703.8964	759.0591	761.2835	
763.4966	770.5510	778.6303	
811.3941	847.6057	876.2099	
901.1739	942.0926	972.2346	
981.3188	982.4890	1062.1250	
1064.0514	1132.0515	1144.4772	
1171.0267	1193.5141	1220.7383	
1229.3459	1268.2552	1324.5621	
1346.4653	1387.3516	1410.1000	
1435.6500	1449.2451	1490.0082	
1517.3065	1536.5871	1632.1294	
1642.5062	1941.3488	2035.4632	
3157.2645	3158.6743	3162.6503	

3171.1519 3178.2923 3181.4578
3197.6281 3398.5225 3485.1802

ZeroEnergy[kcal/mol] 139.4

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts7 i1 i5 # ts7

RRHO

Geometry[angstrom] 25 #

C	3.123018	-0.739097	0.063229
C	1.712754	-0.963453	-0.033936
C	0.794631	0.128726	-0.059043
C	1.447855	1.385278	-0.172546
C	2.761053	1.575628	-0.095365
C	3.679766	0.517616	0.129216
C	-0.626165	-0.104083	-0.017665
C	-1.605645	0.940583	0.003873
C	1.199833	-2.298147	-0.045934
C	-0.138946	-2.528824	-0.032334
C	-1.085776	-1.455961	-0.005128
C	-2.469084	-1.735784	0.027726
C	-3.393685	-0.716015	0.048759
C	-2.960834	0.614766	0.037037
C	-1.280546	2.331114	-0.001741
C	-1.141391	3.528032	0.001103
H	3.763448	-1.615235	0.115547
H	1.918002	2.444918	0.432464
H	4.739070	0.668014	0.297599
H	1.900801	-3.126188	-0.052205
H	-0.519769	-3.544543	-0.034222
H	-2.791078	-2.771482	0.036515
H	-4.454761	-0.935060	0.074308
H	-3.684007	1.420542	0.054132
H	-0.972733	4.576757	-0.007654

Core RigidRotor

SymmetryFactor 0.5

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2044.3978

WellDepth[kcal/mol] 62.0

WellDepth[kcal/mol] 58.0

End

Frequencies[1/cm] 68

53.6453	101.4376	
141.3265	154.0910	220.3646
226.4185	241.7998	369.3969
375.8217	394.7494	416.3117
427.3296	486.4604	507.2686
515.7480	531.7418	545.4810
569.7419	581.4682	627.8841

644.2826	666.8375	677.4072
708.3487	714.8106	775.5439
786.6085	795.5272	817.3156
833.0974	857.1283	929.3571
965.9424	971.5676	981.1523
990.7581	1001.1257	1082.8780
1103.8710	1144.3796	1173.4917
1191.9938	1215.6554	1218.3641
1258.5526	1269.7942	1348.8700
1355.0269	1396.0825	1411.7026
1437.4052	1462.3769	1495.2236
1534.7874	1587.1276	1627.9599
1647.5897	1705.3007	2163.2572
2195.4058	3147.1447	3159.6064
3166.0392	3178.1054	3182.9485
3187.7481	3198.3493	3476.0620

ZeroEnergy[kcal/mol] 112.6

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts8 i3 i5 # ts8

RRHO

Geometry[angstrom] 25 #

C	-3.216523	-0.453141	0.0
C	-1.846661	-0.835313	0.0
C	-0.822603	0.165487	0.0
C	-1.340255	1.462090	-0.0
C	-2.565185	1.786892	-0.0
C	-3.628145	0.876397	0.0
C	0.570425	-0.178457	0.0
C	1.587875	0.817638	-0.0
C	-1.431044	-2.208160	0.0
C	-0.112899	-2.545728	0.0
C	0.925773	-1.555116	0.0
C	2.290840	-1.909839	0.0
C	3.268927	-0.934690	0.0
C	2.920610	0.421897	-0.0
C	1.215743	2.236993	-0.0
C	1.892394	3.335230	-0.0
H	-3.967904	-1.236932	0.0
H	0.046139	2.357057	-0.0
H	-4.676847	1.147031	0.0
H	-2.191192	-2.981945	0.0
H	0.179764	-3.590326	0.0
H	2.562775	-2.959918	0.0
H	4.315890	-1.216082	0.0
H	3.691998	1.183122	-0.0
H	1.783735	4.404914	-0.0

Core RigidRotor

SymmetryFactor 1

```

End
Tunneling      Eckart
  ImaginaryFrequency[1/cm]    710.5553
  WellDepth[kcal/mol]         3.7
  WellDepth[kcal/mol]         47.2
End
Frequencies[1/cm]      68
  70.9695      111.9981
  163.8014      237.0523      255.2889
  271.2572      301.2110      314.7421
  383.0827      421.4499      444.2043
  475.8488      497.9059      512.1660
  527.9670      554.7680      569.6187
  571.1332      580.9238      655.8645
  683.8873      699.2120      756.8300
  772.7245      776.2535      776.5046
  798.6507      819.7388      848.4667
  863.3160      928.4218      950.2943
  966.1387      976.6080      978.7743
  989.8099      1015.1550      1093.1845
  1137.1578      1162.3011      1176.3430
  1192.8446      1224.1341      1238.4976
  1264.6134      1284.7663      1342.2733
  1348.7084      1401.5533      1418.1553
  1436.7768      1461.7097      1486.1891
  1535.5819      1541.9127      1579.5277
  1635.3497      1645.6353      1755.1825
  1999.8110      3157.9296      3160.8540
  3163.6591      3176.8087      3178.9871
  3186.3254      3189.5510      3299.8048
  ZeroEnergy[kcal/mol]        101.8
  ElectronicLevels[1/cm]      1
    0    2
End
Barrier      ts9    i2    i6    #    ts9
RRHO
Geometry[angstrom]      25    #
C      2.904672    1.080695    0.018660
C      1.492288    1.194990    0.004886
C      0.689407    0.011220    -0.007359
C      1.345871    -1.259974    -0.006377
C      2.735835    -1.319678    0.005289
C      3.513642    -0.153932    0.018439
C      -0.753015    0.099766    -0.018000
C      -1.530160    -1.153624    0.002927
C      -0.802450    -2.402413    -0.014656
C      0.544660    -2.458875    -0.018324
C      0.866507    2.467509    0.005897
C      -0.503511    2.568991    -0.016934
C      -1.261517    1.395324    -0.047996

```

C	-3.645225	1.252739	0.033548
C	-3.600061	0.002147	0.030274
C	-2.910896	-1.204610	0.026099
H	3.499017	1.987649	0.028439
H	3.219034	-2.290851	0.003438
H	4.594954	-0.228523	0.027735
H	-1.387065	-3.315878	-0.015954
H	1.054227	-3.416324	-0.024064
H	1.481892	3.360912	0.019079
H	-0.992734	3.536337	-0.023270
H	-2.572938	1.810852	-0.123007
H	-3.412672	-2.165820	0.009361

Core RigidRotor
SymmetryFactor 0.5

End

Tunneling Eckart
ImaginaryFrequency[1/cm] 1131.0779
WellDepth[kcal/mol] 32.8
WellDepth[kcal/mol] 25.6

End

Frequencies[1/cm]		68
64.6972	117.0689	
175.1517	205.3783	222.9669
271.7722	293.5258	337.7460
392.0570	408.4802	445.3232
457.4496	473.5761	494.0867
502.8367	534.0813	545.6443
551.4650	607.1810	616.8764
653.5707	680.8413	759.3974
760.4500	777.5745	780.3355
783.0963	824.1952	838.3498
854.4478	911.3274	962.4137
975.2409	981.1901	990.4154
1046.0109	1083.6591	1111.7774
1135.4432	1160.5989	1182.9343
1201.6447	1228.4168	1236.4802
1263.1989	1322.1620	1342.6276
1377.2867	1402.3346	1430.9953
1436.6195	1472.1194	1508.4491
1516.1576	1581.4640	1604.7382
1625.2120	1662.8843	1819.9322
2064.1643	3160.9146	3163.2043
3164.6894	3166.1883	3171.8340
3180.8776	3182.6279	3188.9055

ZeroEnergy[kcal/mol] 96.1

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts11 i6 i8 # ts11

RRHO


```

Geometry[angstrom]      25      #
C      3.082130      0.949699      0.011999
C      1.677004      1.158763      0.012803
C      0.807542      0.027874      0.015115
C      1.371091     -1.283949     -0.013556
C      2.748666     -1.438588     -0.018977
C      3.604908     -0.321568      0.000687
C      -0.605305      0.229529      0.015750
C      -1.498757     -0.964117      0.052577
C      -0.862412     -2.286081     -0.026536
C      0.475363     -2.421700     -0.055959
C      1.113996      2.458058      0.000377
C      -0.250671      2.631650     -0.018848
C      -1.111785      1.520609     -0.010353
C      -4.991472      0.675871     -0.079978
C      -3.929979     -0.050228     -0.027337
C      -2.903855     -0.866911     -0.001039
H      3.737544      1.813775      0.014003
H      3.169597     -2.438019     -0.043260
H      4.678365     -0.469701     -0.002076
H      -1.519591     -3.146069     -0.066801
H      0.912784     -3.411879     -0.127982
H      1.777237      3.316372      0.000453
H      -0.674485      3.628569     -0.037674
H      -2.182871      1.678225     -0.017945
H      -2.257353     -1.084729      1.140930
Core      RigidRotor
SymmetryFactor      0.5
End
Tunneling      Eckart
ImaginaryFrequency[1/cm]      1127.4394
WellDepth[kcal/mol]      57.6
WellDepth[kcal/mol]      19.9
End
Frequencies[1/cm]      68
46.8167      85.3315
141.2304      164.1529      201.1144
219.9164      288.3476      328.1294
345.0211      430.7518      442.2098
457.6076      477.6692      481.6941
500.6792      531.8707      548.8204
565.6565      602.4911      649.1125
696.8188      708.7794      764.3619
784.0987      799.0244      811.0553
825.5219      853.2008      919.3498
923.2744      952.4306      957.4057
989.7133      1001.6334      1010.1996
1059.2619      1073.1447      1114.5580
1125.2506      1142.4330      1181.8871
1205.9673      1232.0921      1243.4327

```

1262.7231	1301.2131	1374.5395
1393.0501	1417.2915	1428.2243
1465.7497	1494.3317	1514.9306
1540.4746	1615.9532	1625.1386
1636.4322	1678.0558	1921.9071
2000.4000	3166.0924	3168.6376
3169.8184	3173.7515	3188.6844
3191.7530	3195.2069	3201.4640

ZeroEnergy[kcal/mol] 128.1

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts17 pyr1 pyr2 # ts17

RRHO

Geometry[angstrom] 25 #

C	-2.815474	1.204629	-0.0
C	-1.413957	1.246064	0.0
C	-0.713283	0.011512	0.0
C	-1.379596	-1.262733	0.0
C	-2.781490	-1.235153	-0.0
C	-3.475346	-0.022944	-0.0
C	0.694256	0.061426	0.0
C	1.353430	-1.154286	0.0
C	0.733695	-2.405093	0.0
C	-0.616668	-2.519586	-0.0
C	-0.624886	2.458739	0.0
C	0.743129	2.467039	0.0
C	1.485302	1.232944	0.0
C	2.891988	1.065385	-0.0
C	3.534851	-0.198041	-0.0
C	2.711072	-1.318055	0.0
H	-3.385575	2.127526	-0.0
H	-3.334585	-2.168351	-0.0
H	-4.559693	-0.040271	-0.0
H	-1.160132	-3.457142	-0.0
H	-1.159191	3.403481	0.0
H	1.275432	3.412577	-0.0
H	3.521090	1.950555	-0.0
H	4.616819	-0.246363	-0.0
H	2.223690	-2.773098	0.0

Core RigidRotor

SymmetryFactor 1

End

Tunneling Eckart

ImaginaryFrequency[1/cm] 2599.2692

WellDepth[kcal/mol] 67.4

WellDepth[kcal/mol] 67.0

End

Frequencies[1/cm] 68

84.5580 144.9262

179.7749	233.7415	285.9298
360.5352	408.2610	416.5171
439.3409	470.3386	492.6142
495.8395	523.7072	524.2289
553.8998	568.6851	604.7384
655.7324	700.9241	716.9509
727.4322	763.7184	783.8121
801.3416	829.0609	832.7928
839.0616	870.1667	908.0093
914.2003	947.6928	976.7378
978.9783	987.0601	1010.5822
1082.3692	1106.9633	1120.1046
1158.3240	1188.1154	1200.0956
1221.6646	1241.8065	1254.6524
1284.7941	1316.7490	1374.5188
1392.5286	1416.5529	1441.0048
1455.1662	1466.2857	1502.8670
1531.8011	1568.0315	1576.7896
1606.1030	1637.2214	1673.4850
1731.4242	3154.8467	3156.7045
3159.8185	3169.1889	3174.8500
3180.7733	3183.7332	3190.6610

ZeroEnergy[kcal/mol] 67.6

ElectronicLevels[1/cm] 1

0 2

End

Barrier ts18 pyr2 pyr3 # ts18

RRHO

Geometry[angstrom] 25 #

C	-2.739786	-1.281677	0.020284
C	-1.341433	-1.259566	0.021637
C	-0.664784	-0.002866	0.019838
C	-1.422954	1.206365	-0.009392
C	-2.826976	1.131477	-0.011383
C	-3.473334	-0.095863	0.008279
C	0.761198	0.048595	0.025054
C	1.406617	1.323575	0.025645
C	0.629609	2.517249	-0.034600
C	-0.730980	2.459529	-0.048521
C	-0.555870	-2.464082	0.006377
C	0.798778	-2.425813	-0.020539
C	1.522342	-1.179914	-0.016854
C	2.922609	-1.154686	-0.079468
C	3.501263	0.109346	0.088718
C	2.813959	1.252000	0.143627
H	-3.253392	-2.237206	0.022871
H	-3.402811	2.050489	-0.032607
H	-4.556763	-0.134599	0.007187
H	1.149085	3.468227	-0.046546
H	-1.318074	3.371313	-0.081223

```

H          -1.076090  -3.416255   0.005193
H          1.372224  -3.346262  -0.043501
H          3.489513  -2.067690  -0.218197
H          3.994759   1.209966  -0.445389
  Core      RigidRotor
    SymmetryFactor    0.5
  End
  Tunneling      Eckart
    ImaginaryFrequency[1/cm]    2107.5613
    WellDepth[kcal/mol]        61.8
    WellDepth[kcal/mol]        62.4
  End
    Frequencies[1/cm]    68
    99.0822              147.2121
    209.1812             241.7853              264.1037
    349.9881             375.6121              394.5488
    412.9380             458.9583              491.7479
    506.5437             516.5646              521.0825
    536.6689             555.3142              576.4601
    595.7439             662.2867              687.2976
    717.1655             736.0816              768.9009
    769.9623             814.4767              826.1888
    829.5671             852.8482              876.2554
    914.3356             970.7003              980.5307
    985.8288             992.4045              993.2847
    1094.4712            1116.7944             1131.5464
    1156.6809            1178.8453             1202.0874
    1235.6561            1250.9511             1265.6253
    1296.6683            1330.5055             1353.7226
    1378.9895            1419.5272             1433.9439
    1442.5112            1455.1044             1500.7286
    1527.5223            1569.2980             1614.2585
    1633.1208            1660.6523             1693.6111
    2122.2327            3158.8861             3161.5478
    3164.5370            3169.8674             3177.0397
    3180.2074            3186.2933             3188.5368
    ZeroEnergy[kcal/mol]    62.4
    ElectronicLevels[1/cm]  1
      0  2
  End
  Barrier      vts   i8   P4   # barrierless C3 loss
  RRHO
    Stoichiometry C16H9
    Core      PhaseSpaceTheory
      FragmentGeometry[angstrom]    22
C 1.8178437237 1.1500188787 0.
C 0.4040855703 1.2412879264 0.
C -0.3640161484 0.0360546041 0.
C 0.295563854 -1.2318435257 0.
C 1.7118740006 -1.2646995826 0.

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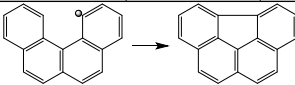
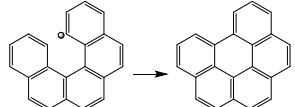
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C  2.4508937258  -0.0874345432  0.
C  -1.7918260148  0.098727446  0.
C  -2.528374262  -1.1115156275  0.
C  -1.8784521875  -2.3401953576  0.
C  -0.4902923267  -2.4106033848  0.
C  -0.2755210298  2.4843133519  0.
C  -1.6645240354  2.5358058695  0.
C  -2.419580164  1.3688101005  0.
H  2.4033242798  2.0629913578  0.
H  2.2152127511  -2.2253606116  0.
H  3.5342507668  -0.134934309  0.
H  -3.6120000495  -1.0670710706  0.
H  -2.4613062677  -3.2546236916  0.
H  0.0077871102  -3.3739995395  0.
H  0.3049218644  3.4004248442  0.
H  -2.1651020143  3.4977366206  0.
H  -3.5029601465  1.4194902442  0.
      FragmentGeometry[angstrom]      3
C              1.291048  -0.  0.000000
C              0.000000  0.  0.000000
C             -1.291048  -0.  0.000000
      SymmetryFactor                    1
      PotentialPrefactor[au]            1.0E0
      PotentialPowerExponent            6.
End
      Frequencies[1/cm]                 64
161.5667      161.6962      210.0358
285.7289      429.6145      430.2224
480.4549      480.5152      486.3764
490.4889      491.2758      585.1701
624.0981      644.5109      644.9080
752.5599      753.7435      768.8897
788.3498      834.1765      834.2711
852.9716      853.4431      888.7918
890.2833      971.3642      971.9654
980.5023      1056.0280      1056.3452
1112.5786     1123.2460      1123.4518
1167.4182     1203.0883      1203.2645
1218.5071     1252.3280      1252.4588
1347.1764     1347.2744      1408.3229
1424.0597     1446.7136      1446.8425
1498.1788     1548.8329      1577.4406
1577.5901     1590.2508      1590.3250
3159.9117     3159.9725      3162.0532
3168.7826     3171.6580      3171.9310
3184.0389     3184.1436      3186.3543
106.2317  106.2317  1237.5978      2148.2082
      ElectronicLevels[1/cm]           1
              0              2
      ZeroEnergy[kcal/mol]             137.8

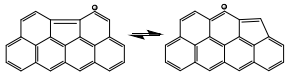
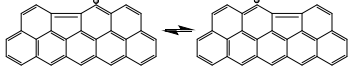
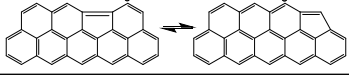
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End
End

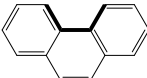
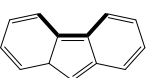
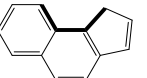
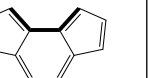
Table S2. Reaction model, rate coefficients, and computed reaction event frequencies.


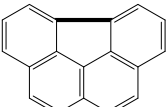
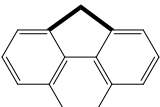
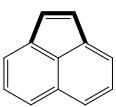
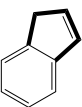
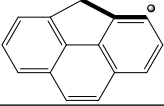
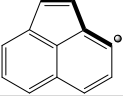
Rxn ID	Reaction ^a	Rate constant ^b			Source	Rxn frequency ^c	
		1400 K	1600 K	1800 K		C3H08	XSF1.88
111	$Z + H \rightarrow Z\bullet + H_2$	2.77E+11	6.94E+11	1.45E+12	[1]	689.30	3159.19
112	reverse of 111	6.54E+11	1.12E+12	1.78E+12		440.49	2601.04
113	$Z\bullet + H \rightarrow Z$	1.25E+14	1.27E+14	1.29E+14	[2]	168.52	342.95
121	$A + H \rightarrow A\bullet + H_2$	1.97E+11	4.90E+11	1.02E+12	[1]	249.95	1395.57
122	reverse of 121	3.16E+11	5.77E+11	9.58E+11		120.95	942.92
123	$A\bullet + H \rightarrow A$	1.12E+14	1.14E+14	1.17E+14	[2]	55.23	205.12
131	$Z + OH \rightarrow Z^* + H_2O$	1.32E+11	2.19E+11	3.39E+11	[1]	17.12	36.00
141	$A + OH \rightarrow A^* + H_2O$	1.56E+11	2.51E+11	3.80E+11	[1]	10.96	25.00
151	${}^2R5 + H \rightarrow {}^2R5\bullet + H_2$	6.31E+10	1.82E+11	4.25E+11	[3]	122.77	580.74
152	reverse of 151	4.88E+11	8.19E+11	1.28E+12		68.58	461.16
153	${}^2R5\bullet + H \rightarrow {}^2R5$	1.65E+14	1.70E+14	1.74E+14	[2]	48.30	111.46
204	closure forming R5  probability = 1					1.69	18.39
205	closure forming R6  probability = 1					1.72	23.05
211	$Z^* + C_2H_2 \rightarrow {}^2R5 + H$	1.16E+12	1.49E+12	1.71E+12	[4]	49.96	298.07
212	reverse of 211	4.58E+09	3.19E+10	1.34E+11		31.03	167.65
221	$6-6-6^* + C_2H_2 \rightarrow A + H$	4.13E+11	6.66E+11	9.52E+11	[4]	9.22	87.08
225	$6-5-6^* + C_2H_2 \rightarrow A + H$	9.48E+11	9.80E+11	8.73E+11	[5]	2.19	15.14
231	$Z^* + C_3H_4 \rightarrow A2A + H$	8.19E+11	9.22E+11	9.46E+11	[6]	0.07	0.26
233	${}^3R5^* + CH_3 \rightarrow A + H + H$	2.37E+12	2.52E+12	2.63E+12	[7]	0.01	0.03
235	${}^2R5^* + CH_3 \rightarrow A2A + H + H$	3.04E+13	2.47E+13	2.00E+13	[8]	7.94	18.30
237	${}^1R5 + CH_3 \rightarrow A + H + H$	2.37E+11	2.51E+11	2.63E+11	= 0.1 ^d *k ₂₃₃	17.42	85.04
241	${}^1R5-A^* + C_2H_2 \rightarrow A + H$	3.89E+09	1.13E+10	1.11E+10	[9]	0.04	0.24
251	$5-6-6^* + C_2H_2 \rightarrow A + H$	9.48E+11	9.80E+11	8.73E+11	=k ₂₂₅	2.91	19.90
253	$6-6-5^* + C_2H_2 \rightarrow A + H$	9.48E+11	9.80E+11	8.73E+11	=k ₂₂₅	1.07	8.27
255	$5-5-5^* + C_2H_2 \rightarrow A + H$	9.48E+11	9.80E+11	8.73E+11	=k ₂₂₅	0.99	4.91
257	${}^1R5-6-6^* + C_2H_2 \rightarrow A + H$	9.48E+11	9.80E+11	8.73E+11	=k ₂₂₅	0.83	5.48
259	${}^1R5-6-5^* + C_2H_2 \rightarrow A + H$	9.48E+11	9.80E+11	8.73E+11	=k ₂₂₅	0.25	1.36

311	$Z^* + C_2H_2 \rightarrow ZC_2H + H$	7.30E+10	1.96E+11	4.09E+11	[4]	10.01	89.48
312	reverse of 311	1.37E+11	5.04E+11	1.31E+12		2.66	22.73
314	$R5C2H+H \rightarrow R5^*+C_2H_2$	1.37E+11	5.04E+11	1.31E+12	$=k_{312}$	0.81	3.66
321	$A^* + C_2H_2 \rightarrow AC2H + H$	1.38E+12	2.08E+12	2.52E+12	[4]	25.26	114.71
322	reverse of 321	2.11E+12	4.38E+12	6.69E+12		30.43	144.57
351	$^2R5-A^*+C_2H_2 \rightarrow R5AC2H+H$	2.68E+11	4.48E+11	6.28E+11	[3]	12.38	52.26
352	reverse of 351	8.30E+11	1.78E+12	2.96E+12		3.85	19.56
411	$AC2H^* + C_2H_2 \rightarrow A^*1$	3.75E+11	2.96E+11	2.07E+11	[10]	0.17	0.94
412	reverse of 411	5.81E+01	3.05E+03	5.42E+04		0.10	1.17
421	$AC2H^* + C_2H_2 \rightarrow A^*2$	1.68E+11	1.98E+11	1.46E+11	[10]	0.11	0.63
422	reverse of 421	2.38E+01	1.91E+03	3.64E+04		0.06	0.80
431	$AC2H^* + C_2H_2 \rightarrow AC2HC2H+H$	3.96E+10	1.42E+11	3.26E+11	[10]	0.19	1.70
432	reverse of 431	2.19E+11	1.00E+12	2.70E+12		0.11	1.34
501	$A^*1 \rightarrow A^*2$	3.56E+04	3.78E+05	1.87E+06	[10]	8.58	32.70
502	$A^*2 \rightarrow A^*1$	3.25E+04	3.49E+05	1.78E+06	[10]	4.59	28.10
511	$ZZC2H + H \rightarrow R5 + H$	2.83E+12	4.13E+12	5.17E+12	[4]	5.07	36.82
513	$Z^*ZC2H \rightarrow R5^*$	1.00E+08	1.00E+08	1.00E+08	guess	1.89	20.37
521	$6-6-6C2H + H \rightarrow A + H$	4.13E+11	6.66E+11	9.52E+11	[4]	0.22	1.92
531	$AC2HC2H + H \rightarrow A^*1$	2.13E+12	1.94E+12	1.51E+12	[10]	0.06	0.65
532	reverse of 531	5.98E+01	2.85E+03	4.76E+04		0.12	1.06
533	$AC2HC2H + H \rightarrow A^*2$	8.66E+11	1.23E+12	1.03E+12	[10]	0.05	0.23
534	reverse of 533	2.22E+01	1.69E+03	3.09E+04		0.06	0.45
536	$A1^* \rightarrow$ cleavage	2.22E+01	1.69E+03	3.09E+04	[10]	0.03	1.36
551	$^2R5-AC2H + H \rightarrow A^*2$	1.64E+11	3.42E+11	3.96E+11	[3]	1.09	3.53
552	reverse of 551	6.12E+03	1.71E+05	1.55E+06		0.38	1.51
561	$5-6-6C2H + H \rightarrow A + H$	6.04E+12	3.53E+12	2.32E+12	[11]	0.13	0.91
563	$^1R5-6-6C2H+H \rightarrow A+H$	6.04E+12	3.53E+12	2.32E+12	[11]	0.07	0.41
565	$^1R5-R6C2H + H \rightarrow A+H$	6.08E+09	2.50E+10	3.60E+10	[9]	0.01	0.01
567	$R5C2H_{6-5} + H \rightarrow A+H$ $R5C2H_{6-6} + H \rightarrow A+H$	6.04E+12	3.53E+12	2.32E+12	[11]	0.03	0.22
571	$^3R5 + H \rightarrow A2A + H$	4.52E+11	1.10E+12	2.71E+12	[6]	0.67	1.53
572	reverse of 571	1.30E+11	3.93E+11	1.15E+12		0.00	0.00
601	$^2R5 + H \rightarrow ^2R5 + H$	4.18E+11	4.58E+11	4.20E+11	[12]	13.26	58.16
603	$^2R5-^2R5$ collision	7.38E+11	1.08E+12	1.39E+12	[13] [14]	2.20	17.15

605	² R5-R6 collision	7.38E+11	1.08E+12	1.39E+12	[13] [14]	5.44	41.51
611	embedded-R5 migration ^e	K_{eq}	K_{eq}	K_{eq}	[15]	71.15	306.75
		7.29	4.78	3.44			
		1	1	1			
		3.61	2.82	2.33			
621	² R5-R6 flip	Equilibrium constant = 1			[14]	11.25	97.67
711	A1* + O ₂ → A1O + O	1.53E+13	1.68E+13	1.80E+13	[16] S46 in [17])	357.59	339.90
713	A2* + O ₂ → A2O + O	1.34E+13	1.54E+13	1.70E+13	[16] (S48 in [17])	10.97	13.81
717	A* + OH → R5 + CO	1.00E+14	1.00E+14	1.00E+14	[18]	3.63	8.48
721	A1*2O → R5 + CO	3.71E+05	4.05E+06	2.72E+07	[19] (S51 in [17])	59.41	64.29
723	A1*1O → AR5 + CO	5.57E+04	9.00E+05	8.34E+06	[19] (S52 in [17])	46.17	37.43
725	A2*1O → AR5 + CO	7.96E+04	1.23E+06	1.05E+07	[19] (S53 in [17])	5.56	8.54
	A2*2O → AR5 + CO						
731	AO + H ₂ → AOH + H	1.74E+11	4.12E+11	8.05E+11	[20,21]	124.47	152.17
735	AOH + H → A* + H ₂ O	2.97E+13	3.77E+13	4.54E+13	[22]	115.94	144.73
745	¹ R5 + O → Z* + CO	1.10E+12	1.21E+12	1.32E+12	0.1 ^d *k([17])	0.23	0.08
811	² R5* + O ₂ → ² R5O+O	1.86E+07	7.52E+07	2.31E+08	[23]	0.00	0.00
813	³ R5* + O ₂ → A* + CO + ...	5.20E+06	1.83E+07	4.94E+07	[23]	0.00	0.00
815	² R5* + OH → ² R5O + H	6.40E+12	8.91E+12	9.77E+12	[24]	0.79	1.50
821	² R5O + H → CO + ...	3.83E+13	4.97E+13	5.87E+13	[25]	0.22	0.15

^aReaction site designation:

A	armchair
Z	zigzag
R5	five-membered ring
R6	six-membered ring
bays	<div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div style="text-align: center;">6-6-6 </div> <div style="text-align: center;">6-5-6 </div> <div style="text-align: center;">6-6-5 </div> <div style="text-align: center;">5-6-5 </div> </div>

A2A	phenalene 
R5 (see paper)	⁰ R5  ¹ R5  ² R5  ³ R5 
¹ R5-A*	
² R5-A*	
A*1	1-naphthyl
A*2	2-naphthyl

^bThe rate-constant values are for a pressure of 1 atm, in the units of s⁻¹ for unimolecular reactions and cm³ mol⁻¹ s⁻¹ for bimolecular reactions.

^cReaction event frequency (in s⁻¹) is calculated as the total number of reaction events occurred during a kMC simulation run, divided by the 0.01 s time interval of the run, and averaged over the number of kMC runs.

^dThe multiplier 0.1 accounts for the fraction of radicals of partially-embedded five-membered rings, ¹R5, at the conditions of the present calculations: temperature range 1400–1800 K and the flame concentrations at these temperatures of H and H₂. The calculations were done using $k_1(\text{c-C}_5\text{H}_6 \rightarrow \text{c-C}_5\text{H}_5 + \text{H}_2)$ and $k_2(\text{c-C}_5\text{H}_6 + \text{H} \rightarrow \text{c-C}_5\text{H}_5 + \text{H}_2)$ and its reverse, k_{-2} , of Robinson and Lindstedt [26] and $k_3(\text{c-C}_5\text{H}_5 + \text{H} \rightarrow \text{c-C}_5\text{H}_6)$ of Harding *et al.* [27]. Assuming steady-state for the c-C₅H₅ radical and considering that $k_{-2}[\text{H}_2]$

$\ll k_3[\text{H}]$ at the simulation conditions, we obtain that $[\text{c-C}_5\text{H}_5]/[\text{c-C}_5\text{H}_6] \approx \frac{k_2}{k_3} \approx 0.1$.

^eThe embedded migration was assumed to be in a state of partial equilibrium, ensued upon a reactant site being encountered; the product state was determined by probabilities computed from the equilibrium constants, unless the migration step forms two side-by-side five-membered rings, in which case no migration took place.

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