High pressure effects on the mutual sensitization of the oxidation of NO and CH_4-C_2H_6 blends

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I. Experimental Data – HPST and JSR CH_4 and NGB Experiments

Table S1: NGB experiments in the UIC HPST, 49 atm, Φ=0.5, [CH_4] = 409 ppm, [C_2H_6] = 44 ppm. All species mole fractions in ppm.

Shock Number	Reaction Time/ s	T_5 / K	P_5/ atm	CH_4	C_2H_6	C_2H_4	C_2H_2	CO	CO_2
4	0.00218	1110.1	50.4	406.66	43.87	0.07	0.00	0.63	0.00
1	0.00185	1119.5	49.4	400.31	43.12	0.04	0.00	0.00	0.00
3	0.00202	1165.7	51.1	405.74	43.54	0.22	0.00	0.91	0.00
8	0.00201	1193.9	45.6	401.26	43.09	0.17	0.00	0.79	0.36
2	0.00187	1198.7	51.7	403.37	43.28	0.55	0.08	0.00	0.00
6	0.00177	1224.8	52.8	406.56	43.35	0.60	0.02	1.26	0.24
7	0.00178	1226.1	51.1	406.81	43.48	0.50	0.03	1.30	0.13
11	0.00158	1275.0	52.4	408.68	42.79	2.08	0.03	1.40	1.10
5	0.00164	1277.1	57.9	406.66	41.69	3.60	0.15	3.46	1.89
13	0.00167	1283.9	44.9	405.75	42.63	1.56	0.03	1.34	0.09
9	0.00158	1301.1	53.8	397.40	40.67	4.16	0.10	2.50	1.16
14	0.00148	1323.0	44.9	401.33	40.80	5.32	0.14	2.66	0.02
10	0.00154	1341.0	52.8	390.10	37.33	10.98	0.41	6.09	3.81
24	0.00159	1368.0	40.8	391.57	38.32	9.92	0.44	5.36	3.48
16	0.00131	1398.3	47.7	339.42	29.66	22.08	2.64	23.68	4.87
12	0.00137	1401.3	53.1	352.07	30.75	21.71	2.23	20.39	4.41
15	0.00133	1402.8	50.4	322.47	27.48	25.27	4.10	36.68	5.36
25	0.00143	1420.4	43.6	343.35	29.91	25.50	3.84	31.98	5.59
23	0.00131	1421.6	45.6	319.99	27.66	28.07	5.14	48.42	8.02
22	0.00142	1423.2	45.9	316.33	27.20	27.17	5.00	43.05	7.45
20	0.00129	1426.4	45.9	306.66	25.99	27.39	5.24	50.35	7.78
26	0.00119	1447.4	45.9	176.73	14.95	17.24	5.02	146.17	85.72
19	0.00120	1456.5	49.4	94.11	7.80	10.16	3.43	155.63	179.84

21	0.00127	1468.8	49.4	87.80	7.28	9.69	3.41	153.88	183.59
17	0.00131	1471.6	51.1	47.82	4.00	5.11	2.01	137.09	266.85
18	0.00119	1516.0	51.7	18.49	1.72	1.66	0.72	92.97	344.88

Table S2: NGB-NO experiments in the UIC HPST, 46 atm, Φ=0.5, [CH_4] = 346 ppm, [C_2H_6] = 37 ppm, [NO] = 44 ppm. All species mole fractions in ppm.

Shock Number	Reaction Time/ s	T_5 / K	P_5/ atm	CH_4	NO	C_2H_6	C_2H_4	C_2H_2	CO	CO_2
1	0.00221	1070.0	47.0	338.36	44.2	36.96	0.68	0.00	0.00	0.00
4	0.00210	1090.7	51.1	345.13	42.4	40.07	0.43	0.00	0.40	0.00
2	0.00244	1112.0	47.0	339.33	43.6	37.03	0.85	0.00	0.43	0.00
5	0.00224	1127.4	44.6	345.13	--	36.59	1.42	0.00	0.96	0.00
3	0.00243	1128.2	45.6	338.75	--	36.79	1.07	0.00	0.72	0.00
6	0.00199	1161.9	45.9	333.21	--	33.87	3.95	0.02	3.01	0.00
7	0.00220	1176.3	44.2	331.62	43.5	32.93	4.83	0.02	3.65	0.00
8	0.00209	1209.1	44.2	321.87	--	29.73	8.25	0.06	7.49	0.00
9	0.00204	1231.9	44.2	306.68	43.5	26.33	12.55	0.21	13.73	0.00
12	0.00183	1239.8	43.6	309.19	41.3	26.73	12.55	0.18	13.71	3.10
10	0.00193	1277.5	44.2	290.94	45.3	23.05	17.03	0.47	23.88	4.57
13	0.00183	1279.5	43.6	299.33	--	25.07	15.58	0.53	18.43	3.52
11	0.00182	1287.9	42.5	295.33	43.5	24.57	16.62	0.56	20.08	3.36
16	0.00179	1311.1	42.5	290.07	--	23.68	19.35	1.04	25.38	3.67
14	0.00176	1320.4	43.9	285.52	41.9	23.18	20.13	1.24	27.67	3.75
19	0.00175	1343.9	42.5	278.32	42.6	22.22	22.88	1.71	32.59	4.08
15	0.00167	1363.4	45.9	192.83	--	13.78	24.44	4.30	101.63	15.22
25	0.00152	1364.1	45.6	253.09	39.4	19.49	26.05	3.20	47.11	5.19
17	0.00160	1370.6	44.6	247.40	39.7	19.06	26.36	3.52	49.64	5.73
26	0.00157	1389.6	45.9	219.81	38.1	16.23	27.79	5.44	70.54	8.08
22	0.00141	1399.6	51.7	168.27	37.7	11.30	22.68	5.50	120.35	18.70
23	0.00154	1403.0	46.6	165.01	--	11.58	23.51	7.13	125.34	20.74
24	0.00146	1411.0	49.0	142.51	--	9.89	19.81	6.03	143.60	35.69
18	0.00159	1411.7	45.9	115.39	39.3	7.96	16.46	5.07	156.82	60.27

28	0.00156	1418.1	41.2	145.02	38.9	10.15	20.40	5.93	141.16	32.80
20	0.00147	1440.2	47.0	53.52	36.3	3.51	7.70	3.01	159.55	153.34
27	0.00142	1452.4	47.7	44.58	34.7	2.91	6.36	2.58	160.24	162.92
21	0.00148	1495.9	52.8	16.98	33.4	1.38	1.72	0.77	99.26	270.49

Table S3: NGB experiments in the CNRS JSR, 10 atm, Φ=0.5, t=800 ms, [CH_4] = 2283 ppm, [C_2H_6] = 217 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O	O_2
950	2050.00	170.00	27.00	17.00	23.00	798.00	17.00	9480.00
1010	1800.00	105.00	91.00	267.00	39.00	1410.00	39.00	12600.00
1040	1590.00	83.00	101.00	505.00	81.00	2030.00	41.00	12200.00
1070	1190.00	58.00	87.00	898.00	248.00	3090.00	37.00	11700.00
1100	717.00	33.00	50.00	1180.00	640.00	4070.00	26.00	10500.00
1130	413.00	22.00	25.00	1090.00	1240.00	4990.00	17.00	9960.00

Table S4: NGB-NO experiments in the CNRS JSR, 10 atm, Φ=0.5, t=800 ms, [CH_4] = 2283 ppm, [C_2H_6] = 217 ppm, [NO] = 200 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O	O_2	NO	NO_2
800.0	2070.00	179.00	3.00	7.00	28.00	859.00	28.00	12300.00	157.00	37.00
830.0	1970.00	140.00	15.00	142.00	34.00	1230.00	75.00	12400.00	112.00	72.00
860.0	1610.00	71.00	32.00	568.00	105.00	2170.00	84.00	11600.00	92.00	70.00
890.0	1040.00	35.00	25.00	1020.00	375.00	3530.00	58.00	10600.00	115.00	55.00
920.0	666.00	25.00	18.00	1130.00	835.00	4520.00	36.00	9850.00	147.00	40.00
980.0	468.00	22.00	12.00	966.00	1270.00	5080.00	23.00	9410.00	158.00	27.00
1040.0	365.00	19.00	11.00	758.00	1600.00	5340.00	19.00	9300.00	169.00	20.00
1100.0	291.00	11.00	18.00	478.00	1920.00	5460.00	23.00	9160.00	177.00	13.00
1160.0	202.00	0.00	19.00	362.00	2140.00	5760.00	19.00	8890.00	178.00	7.00

Table S5: NGB-NO experiments in the CNRS JSR, 10 atm, Φ=1.0, t=800 ms, [CH_4] = 2283 ppm, [C_2H_6] = 217 ppm, [NO] = 200 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O	O_2	NO	NO_2	HCN
800	2050.00	172.00	2.00	2.00	18.00	658.00	16.00	8970.00	173.00	20.00	0.00
830	2000.00	157.00	9.00	49.00	20.00	799.00	56.00	8140.00	156.00	36.00	0.70
860	1750.00	89.00	27.00	388.00	48.00	1480.00	90.00	7740.00	139.00	39.00	1.40
890	1380.00	51.00	29.00	816.00	157.00	2480.00	77.00	6980.00	151.00	26.00	2.00
920	1090.00	39.00	27.00	1080.00	304.00	3220.00	60.00	6830.00	170.00	16.00	2.50
950	904.00	33.00	28.00	1200.00	435.00	3650.00	48.00	6570.00	178.00	10.00	3.50
980	759.00	30.00	31.00	1270.00	570.00	4010.00	39.00	6300.00	180.00	6.00	5.00
1010	678.00	29.00	32.00	1260.00	677.00	4180.00	32.00	6260.00	180.00	4.00	6.00
1040	591.00	26.00	33.00	1260.00	832.00	4500.00	28.00	6270.00	178.00	3.00	8.00
1070	509.00	23.00	34.00	1210.00	993.00	4660.00	24.00	5990.00	176.00	2.00	10.00
1100	421.00	18.00	32.00	1150.00	1200.00	4970.00	20.00	5760.00	165.00	2.00	13.00
1130	347.00	15.00	28.00	1020.00	1440.00	5220.00	15.00	5580.00	155.00	2.00	16.00
1160	296.00	13.00	25.00	821.00	16.70	5300.00	12.00	5740.00	135.00	2.00	18.00

Table S6: NGB-NO experiments in the CNRS JSR, 10 atm, Φ=1.5, t=800 ms, [CH_4] = 2283 ppm, [C_2H_6] = 217 ppm, [NO] = 200 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O	O_2	NO	NO_2	HCN
800	2180.00	210.00	0.00	0.16	0.00	685.00	4.03	3500.00	193.00	6.00	0.00
830	2050.00	150.00	7.20	91.00	2.20	946.00	89.00	3300.00	161.00	19.60	0.00
860	1900.00	99.90	13.90	370.00	23.00	1490.00	111.00	2800.00	162.00	15.20	0.00
890	1700.00	74.50	23.20	580.00	53.70	1800.00	112.00	2500.00	170.00	10.50	0.00
920	1580.00	64.50	36.40	719.00	76.00	2080.00	105.00	2300.00	181.00	7.27	0.00
950	1460.00	58.80	54.10	797.00	96.90	2260.00	105.00	2200.00	181.00	5.52	0.00
980	1350.00	53.00	69.30	871.00	122.00	2370.00	100.00	2000.00	179.00	4.34	0.00
1010	1230.00	50.00	79.20	975.00	140.00	2540.00	88.00	1900.00	176.00	3.51	6.00
1040	1100.00	47.00	86.80	1050.00	185.00	2740.00	75.20	1700.00	174.00	2.90	10.00
1070	962.00	43.00	88.70	1150.00	216.00	2950.00	63.00	1500.00	169.00	2.42	14.10
1100	810.00	40.60	89.50	1230.00	294.00	3170.00	50.20	1300.00	162.00	2.02	25.60

1130	680.00	35.00	86.80	1310.00	345.00	3430.00	38.70	1100.00	150.00	1.67	36.60
1160	580.00	30.00	80.90	1330.00	444.00	3650.00	21.00	970.00	134.00	1.36	47.50

Table S7: NGB-NO experiments in the CNRS JSR, 10 atm, Φ=0.3, t=800 ms, [CH_4] = 2283 ppm, [C_2H_6] = 217 ppm, [NO] = 200 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O	O_2	NO	NO_2
800	2000.00	172.00	0.00	1.00	21.00	765.00	6.00	17800.00	188.00	17.00
830	2000.00	169.00	2.00	2.00	22.00	775.00	14.00	18300.00	176.00	33.00
860	1970.00	163.00	5.00	11.00	23.00	817.00	32.00	18200.00	162.00	50.00
890	1840.00	115.00	29.00	186.00	35.00	1220.00	89.00	18100.00	127.00	69.00
920	1350.00	38.00	45.00	744.00	133.00	2450.00	94.00	17200.00	113.00	70.00
980	400.00	7.00	18.00	1270.00	967.00	4860.00	30.00	15600.00	148.00	55.00
1010	237.00	6.00	11.00	1090.00	1370.00	5310.00	18.00	15200.00	158.00	47.00
1040	160.00	5.00	8.00	888.00	1650.00	5620.00	13.00	14700.00	165.00	38.00
1070	122.00	5.00	8.00	716.00	1870.00	5700.00	12.00	14700.00	171.00	32.00
1100	110.00	4.00	7.00	570.00	2000.00	5710.00	11.00	14700.00	179.00	24.00
1130	95.00	3.00	7.00	460.00	2120.00	5730.00	11.00	14700.00	182.00	23.00
1160	79.00	2.00	7.00	362.00	2260.00	5860.00	10.00	15300.00	186.00	17.00

Table S8: CH_4 experiments in the CNRS JSR, 10 atm, Φ=0.5, t=800 ms, [CH_4] = 2500 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O
1000	2225.00	0.00	0.00	1.00	1.00	199.00	5.00
1020	2205.00	4.00	0.00	4.00	1.00	166.00	9.00
1040	2176.00	25.00	1.00	16.00	1.00	189.00	15.00
1060	2100.00	35.00	4.00	49.00	2.00	254.00	21.00
1080	1906.00	26.00	14.00	134.00	6.00	474.00	28.00
1100	1706.00	33.00	32.00	298.00	25.00	860.00	32.00
1120	1237.00	48.00	50.00	691.00	144.00	1908.00	33.00
1140	739.00	24.00	43.00	1048.00	504.00	3315.00	26.00
1160	292.00	0.00	21.00	1050.00	976.00	4180.00	15.00
1180	145.00	0.00	10.00	876.00	1411.00	4632.00	9.00

Table S9: CH_4-NO experiments in the CNRS JSR, 10 atm, Φ=0.5, t=800 ms, [CH_4] = 2500 ppm, [NO] = 200 ppm. All species mole fractions in ppm.

T/K	CH_4	CO	CO_2	H_2O	CH_2O	NO	NO_2
830	2171	1	1	151	10	180	29
860	1860	192	11	612	65	167	62
890	1268	734	129	1962	66	167	60
920	684	1078	442	3254	41	194	47
950	339	1131	881	4205	23	214	38
980	157	995	1296	4657	12	217	30
1010	82	839	1643	4965	7	220	26
1040	54	700	1848	5051	5	203	22
1070	23	485	2229	5308	3	190	21
1100	15	354	2381	5356	2	184	18

Table S10: CH_4 experiments in the CNRS JSR, 10 atm, Φ=1.0, t=800 ms, [CH_4] = 2500 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_6	C_2H_4	CO	CO_2	H_2O	CH_2O
1050	2181.00	10.00	0.00	2.00	1.00	116.00	4.00
1100	2118.00	29.00	2.00	16.00	1.00	150.00	11.00
1120	2074.00	10.00	5.00	43.00	2.00	213.00	14.00
1140	1930.00	38.00	16.00	107.00	5.00	358.00	18.00
1160	1660.00	41.00	36.00	293.00	49.00	825.00	20.00
1180	1303.00	33.00	43.00	514.00	207.00	1593.00	18.00
1200	1040.00	24.00	46.00	642.00	438.00	2279.00	15.00

Table S11: CH_4-NO experiments in the CNRS JSR, 10 atm, Φ=1.0, t=800 ms, [CH_4] = 2500 ppm, [NO] = 200 ppm. All species mole fractions in ppm.

T/K	CH_4	C_2H_4	CO	CO_2	H_2O	CH_2O	NO	NO_2	HCN
800	2171.00	0.00	0.00	1.00	133.00	0.00	150.00	9.00	0.00
830	2167.00	0.00	0.00	1.00	106.00	2.00	228.00	13.00	0.00

860	2082.00	0.00	47.00	3.00	265.00	45.00	223.00	31.00	0.00
890	1610.00	0.00	462.00	43.00	1187.00	74.00	221.00	31.00	0.00
920	1210.00	2.00	830.00	138.00	2084.00	63.00	236.00	21.00	1.00
950	1000.00	4.00	991.00	212.00	2493.00	53.00	240.00	15.00	1.00
980	902.00	7.00	1070.00	263.00	2707.00	47.00	239.00	12.00	1.00
1010	770.00	12.00	1159.00	335.00	3014.00	40.00	234.00	9.00	1.00
1040	667.00	19.00	1165.00	401.00	3147.00	34.00	213.00	7.00	2.00
1070	655.00	26.00	1187.00	501.00	3325.00	26.00	210.00	7.00	3.00
1100	499.00	30.00	1206.00	626.00	3615.00	22.00	199.00	5.00	4.00
1130	450.00	34.00	1172.00	757.00	3837.00	18.00	192.00	5.00	6.00
1160	378.00	34.00	1081.00	927.00	3960.00	13.00	190.00	4.00	8.00
1190	269.00	31.00	1005.00	1092.00	4135.00	10.00	172.00	3.00	11.00

II. HPNGB Reaction Mechanism

The reaction mechanism is given in CHEMKIN format. Units: A (mole-cm-sec), E (cal/mole).

S.No.	Reaction	A	n	E_a
1.	OH+H2=H+H2O	1.73E+08	1.5	3430.0
2.	H+O2=O+OH	2.64E+16	-0.7	17041.0
3.	O+H2=H+OH	4.59E+04	2.7	6260.0
4.	H+O2(+M)=HO2(+M)	5.12E+12	0.4	0.0
	Low pressure limit: 0.63280E+20 -0.14000E+01 0.00000E+00			
	TROE centering: 0.50000E+00 0.10000E-29 0.10000E+31			
	O2 Enhanced by 8.500E-01			
	H2O Enhanced by 1.189E+01			
	CO Enhanced by 1.090E+00			
	CO2 Enhanced by 2.180E+00			
	AR Enhanced by 4.000E-01			
	HE Enhanced by 4.600E-01			
	H2 Enhanced by 7.500E-01			
5.	HO2+OH=O2+H2O	1.41E+18	-1.8	59.6
	Declared duplicate reaction...			
6.	HO2+OH=O2+H2O	1.12E+85	-22.3	26900.0
	Declared duplicate reaction...			

7.	HO2+OH=O2+H2O			5.37E+70	-16.7	32900.8
	Declared duplicate reaction...					
8.	HO2+OH=O2+H2O			1.00+136	-40.0	34800.3
	Declared duplicate reaction...					
9.	HO2+OH=O2+H2O			2.51E+12	2.0	40000.3
	Declared duplicate reaction...					
10.	HO2+H=OH+OH			7.48E+13	0.0	295.0
11.	H2+O2=HO2+H			5.92E+05	2.4	53502.0
12.	HO2+H=O+H2O			3.97E+12	0.0	671.0
13.	HO2+O=OH+O2			4.00E+13	0.0	0.0
14.	OH+OH=O+H2O			3.97E+04	2.4	-2110.0
15.	H+H+M=H2+M			1.78E+18	-1.0	0.0
	H2	Enhanced by	0.000E+00			
	H2O	Enhanced by	0.000E+00			
	CO2	Enhanced by	0.000E+00			
	AR	Enhanced by	6.300E-01			
	HE	Enhanced by	6.300E-01			
16.	H+H+H2=H2+H2			9.00E+16	-0.6	0.0
17.	H+H+H2O=H2+H2O			5.62E+19	-1.2	0.0
18.	H+H+CO2=H2+CO2			5.50E+20	-2.0	0.0
19.	H+OH+M=H2O+M			4.40E+22	-2.0	0.0
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	6.300E+00			
	CO	Enhanced by	1.750E+00			
	CO2	Enhanced by	3.600E+00			
	AR	Enhanced by	3.800E-01			
	HE	Enhanced by	3.800E-01			
20.	O+H+M=OH+M			9.43E+18	-1.0	0.0
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	1.200E+01			
	CO	Enhanced by	1.750E+00			
	CO2	Enhanced by	3.600E+00			
	AR	Enhanced by	7.000E-01			
	HE	Enhanced by	7.000E-01			
21.	O+O+M=O2+M			1.20E+17	-1.0	0.0
	H2	Enhanced by	2.400E+00			
	H2O	Enhanced by	1.540E+01			
	CO	Enhanced by	1.750E+00			

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    CO2             Enhanced by    3.600E+00
    AR              Enhanced by    8.300E-01
    HE              Enhanced by    8.300E-01
22. HO2+HO2=O2+H2O2                                 1.30E+11    0.0    -1630.0
    Declared duplicate reaction...
23. HO2+HO2=O2+H2O2                                 3.66E+14    0.0    12000.0
    Declared duplicate reaction...
24. OH+OH(+M)=H2O2(+M)                              1.11E+14   -0.4        0.0
    Low pressure limit:  0.20100E+18 -0.58400E+00 -0.22930E+04
    TROE centering:      0.73460E+00  0.94000E+02  0.17560E+04  0.51820E+04
    H2              Enhanced by    2.000E+00
    H2O             Enhanced by    6.000E+00
    CO              Enhanced by    1.750E+00
    CO2             Enhanced by    3.600E+00
    AR              Enhanced by    7.000E-01
    HE              Enhanced by    7.000E-01
25. H2O2+H=HO2+H2                                   6.05E+06    2.0     5200.0
26. H2O2+H=OH+H2O                                   2.41E+13    0.0     3970.0
27. H2O2+O=OH+HO2                                   9.63E+06    2.0     3970.0
28. H2O2+OH=HO2+H2O                                 2.00E+12    0.0      427.0
    Declared duplicate reaction...
29. H2O2+OH=HO2+H2O                                 2.67E+41   -7.0    37600.0
    Declared duplicate reaction...
30. C2H6(+M)=CH3+CH3(+M)                            8.03E+28   -3.5    95346.0
    Low pressure limit:  0.28000E+73 -0.15100E+02  0.10774E+06
    TROE centering:      0.21100E+00  0.10000E-29  0.10000E+31
    H2              Enhanced by    2.860E+00
    H2O             Enhanced by    8.570E+00
    CH4             Enhanced by    4.230E+00
    CO              Enhanced by    2.140E+00
    CO2             Enhanced by    2.860E+00
    C2H6            Enhanced by    4.230E+00
    N2              Enhanced by    1.000E+00
    HE              Enhanced by    1.000E+00
31. CH4(+M)=CH3+H(+M)                               2.40E+16    0.0   104913.6
    Low pressure limit:  0.45165E+18  0.00000E+00  0.90806E+05
    TROE centering:      0.10000E+01  0.10000E+31  0.13500E+04  0.78340E+04
    H2              Enhanced by    2.860E+00
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    H2O             Enhanced by    8.570E+00
    CH4             Enhanced by    4.230E+00
    CO              Enhanced by    2.140E+00
    CO2             Enhanced by    2.860E+00
    C2H6            Enhanced by    4.230E+00
    N2              Enhanced by    1.430E+00
    HE              Enhanced by    1.000E+00
32. CH4+O2=CH3+HO2                                  5.58E+05    2.6    52185.9
33. CH4+H=CH3+H2                                    1.77E+14    0.0    13777.9
34. CH4+OH=CH3+H2O                                  1.37E+06    2.2     2682.5
35. CH4+O=CH3+OH                                    4.40E+05    2.5     6577.0
36. CH4+HO2=CH3+H2O2                                4.70E+04    2.5    21002.6
37. CH3+HO2=CH3O+OH                                 1.00E+13    0.0        0.0
38. CH3+O=CH2O+H                                    6.74E+13    0.0        0.0
39. CH3+O=H2+CO+H                                   1.69E+13    0.0        0.0
40. CH3+O2=CH3O+O                                   7.55E+12    0.0    28296.9
41. CH3+O2=CH2O+OH                                  2.25E+11    0.0     9841.6
42. CH3+O2(+M)=CH3O2(+M)                            7.80E+08    1.2        0.0
    Low pressure limit:  0.54000E+26 -0.33000E+01  0.00000E+00
    H2O             Enhanced by    1.000E+01
43. CH3O2+H=CH3O+OH                                 1.00E+14    0.0        0.0
44. CH3O2+O=CH3O+O2                                 3.60E+13    0.0        0.0
45. CH3O2+OH=CH3OH+O2                               6.00E+13    0.0        0.0
46. CH3O2+HO2=CH3OOH+O2                             2.50E+11    0.0    -1570.0
47. CH3O2+H2O2=CH3OOH+HO2                           2.40E+12    0.0     9940.0
48. CH3O2+CH2O=CH3OOH+HCO                           2.00E+12    0.0    11665.0
49. CH3O2+CH4=CH3OOH+CH3                            1.80E+11    0.0    18500.0
50. CH3O2+CH3=CH3O+CH3O                             2.40E+13    0.0        0.0
51. CH3O2+CH3O=CH2O+CH3OOH                          3.00E+11    0.0        0.0
52. CH3O2+CH2OH=CH2O+CH3OOH                         1.20E+13    0.0        0.0
53. CH3O2+CH3OH=CH3OOH+CH2OH                        1.80E+12    0.0    13700.0
54. CH3O2+CH3O2=CH3O+CH3O+O2                        1.00E+11    0.0      300.0
55. CH3O2+CH3O2=CH3OH+CH2O+O2                       4.00E+09    0.0    -2210.0
56. CH3OOH=CH3O+OH                                  6.30E+14    0.0    42300.0
57. CH3OOH+H=CH3O2+H2                               8.80E+10    0.0     1860.0
58. CH3OOH+H=CH3O+H2O                               8.20E+10    0.0     1860.0
59. CH3OOH+O=CH3O2+OH                               1.00E+12    0.0     3000.0
60. CH3OOH+OH=CH3O2+H2O                             1.80E+12    0.0     -378.0
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61. CH2OH+H=CH3+OH                                    1.00E+14    0.0        0.0
62. CH3O+H=CH3+OH                                     1.00E+14    0.0        0.0
63. CH3+OH=CH2+H2O                                    1.11E+03    3.0     2782.0
64. CH3+HCO=CH4+CO                                    1.20E+14    0.0        0.0
65. CH3+H=CH2+H2                                      9.00E+13    0.0    15100.0
66. CH3+OH(+M)=CH3OH(+M)                              6.30E+13    0.0        0.0
    Low pressure limit:  0.18900E+39 -0.63000E+01  0.31000E+04
    TROE centering:      0.21050E+00  0.83500E+02  0.53980E+04  0.83700E+04
    H2O             Enhanced by    8.580E+00
    CO2             Enhanced by    3.000E+00
    CO              Enhanced by    2.000E+00
    H2              Enhanced by    2.000E+00
67. CH3OH+OH=CH2OH+H2O                                5.30E+04    2.5      960.0
68. CH3OH+OH=CH3O+H2O                                 1.32E+04    2.5      960.0
69. CH3OH+O=CH2OH+OH                                  3.88E+05    2.5     3080.0
70. CH3OH+H=CH2OH+H2                                  1.70E+07    2.1     4868.0
71. CH3OH+H=CH3O+H2                                   4.24E+06    2.1     4868.0
72. CH3OH+HO2=CH2OH+H2O2                              9.64E+10    0.0    12578.0
73. CH2O+H(+M)=CH3O(+M)                               5.40E+11    0.5     2600.0
    Low pressure limit:  0.15400E+31 -0.48000E+01  0.55600E+04
    TROE centering:      0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
    H2O             Enhanced by    8.580E+00
    CO              Enhanced by    2.000E+00
    H2              Enhanced by    2.000E+00
    CO2             Enhanced by    3.000E+00
74. H+CH2O(+M)=CH2OH(+M)                              5.40E+11    0.5     3600.0
    Low pressure limit:  0.91000E+32 -0.48200E+01  0.65300E+04
    TROE centering:      0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
    H2O             Enhanced by    8.580E+00
    CO              Enhanced by    2.000E+00
    CO2             Enhanced by    3.000E+00
    H2              Enhanced by    2.000E+00
75. CH3O+H=CH2O+H2                                    2.00E+13    0.0        0.0
76. CH2OH+H=CH2O+H2                                   2.00E+13    0.0        0.0
77. CH3O+OH=CH2O+H2O                                  1.00E+13    0.0        0.0
78. CH2OH+OH=CH2O+H2O                                 1.00E+13    0.0        0.0
79. CH3O+O=CH2O+OH                                    1.00E+13    0.0        0.0
80. CH2OH+O=CH2O+OH                                   1.00E+13    0.0        0.0
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81.	CH3O+O2=CH2O+HO2	6.30E+10	0.0	2600.0
82.	CH2OH+O2=CH2O+HO2	1.57E+15	-1.0	0.0
	Declared duplicate reaction...			
83.	CH2OH+O2=CH2O+HO2	7.23E+13	0.0	3577.0
	Declared duplicate reaction...			
84.	CH2+H=CH+H2	1.00E+18	-1.6	0.0
85.	CH2+OH=CH+H2O	1.13E+07	2.0	3000.0
86.	CH2+OH=CH2O+H	2.50E+13	0.0	0.0
87.	CH+O2=HCO+O	3.30E+13	0.0	0.0
88.	CH+O=CO+H	5.70E+13	0.0	0.0
89.	CH+OH=HCO+H	3.00E+13	0.0	0.0
90.	CH+OH=C+H2O	4.00E+07	2.0	3000.0
91.	CH+CO2=HCO+CO	3.40E+12	0.0	690.0
92.	CH+H=C+H2	1.50E+14	0.0	0.0
93.	CH+H2O=CH2O+H	5.72E+12	0.0	-751.0
94.	CH+CH2O=CH2CO+H	9.46E+13	0.0	-515.0
95.	CH+C2H2=C3H2+H	1.00E+14	0.0	0.0
96.	CH+CH2=C2H2+H	4.00E+13	0.0	0.0
97.	CH+CH3=C2H3+H	3.00E+13	0.0	0.0
98.	CH+CH4=C2H4+H	6.00E+13	0.0	0.0
99.	C+O2=CO+O	2.00E+13	0.0	0.0
100.	C+OH=CO+H	5.00E+13	0.0	0.0
101.	C+CH3=C2H2+H	5.00E+13	0.0	0.0
102.	C+CH2=C2H+H	5.00E+13	0.0	0.0
103.	CH2+CO2=CH2O+CO	1.10E+11	0.0	1000.0
104.	CH2+O=CO+H+H	5.00E+13	0.0	0.0
105.	CH2+O=CO+H2	3.00E+13	0.0	0.0
106.	CH2+O2=CO+H2O	2.20E+22	-3.3	2867.0
107.	CH2+O2=CO2+H+H	3.29E+21	-3.3	2867.0
108.	CH2+O2=CH2O+O	3.29E+21	-3.3	2867.0
109.	CH2+O2=CO2+H2	2.63E+21	-3.3	2867.0
110.	CH2+O2=CO+OH+H	1.64E+21	-3.3	2867.0
111.	CH2+CH2=C2H2+H+H	4.00E+13	0.0	0.0
112.	CH2+HCCO=C2H3+CO	3.00E+13	0.0	0.0
113.	CH2+C2H2=H2CCCH+H	1.20E+13	0.0	6600.0
114.	CH2+CH4=CH3+CH3	4.30E+12	0.0	10030.0
115.	CH2O+OH=HCO+H2O	3.43E+09	1.2	-447.0
116.	CH2O+H=HCO+H2	1.30E+08	1.6	2166.0

117.	CH2O+M=HCO+H+M			3.31E+16	0.0	81000.0
	H2	Enhanced by	2.000E+00			
	CO	Enhanced by	2.000E+00			
	CO2	Enhanced by	3.000E+00			
	H2O	Enhanced by	5.000E+00			
118.	CH2O+O=HCO+OH			1.80E+13	0.0	3080.0
119.	CH2O+CH3=HCO+CH4			7.80E-08	6.1	1967.0
120.	CH2O+HO2=HCO+H2O2			3.00E+12	0.0	13000.0
121.	CH2O+O2=HCO+HO2			6.00E+13	0.0	40660.0
122.	HCO+OH=CO+H2O			3.02E+13	0.0	0.0
123.	HCO+M=CO+H+M			1.87E+17	-1.0	17000.0
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	0.000E+00			
	CO	Enhanced by	1.750E+00			
	CO2	Enhanced by	3.600E+00			
124.	HCO+H=CO+H2			1.20E+14	0.0	0.0
125.	HCO+O=CO+OH			3.00E+13	0.0	0.0
126.	HCO+O=CO2+H			3.00E+13	0.0	0.0
127.	HCO+O2=CO+HO2			1.20E+10	0.8	-727.0
128.	HCO+H2O=CO+H+H2O			2.24E+18	-1.0	17000.0
129.	CO+O(+M)=CO2(+M)			1.36E+10	0.0	2384.0
	Low pressure limit:	0.11730E+25	-0.27900E+01	0.41910E+04		
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	1.200E+01			
	CO	Enhanced by	1.750E+00			
	CO2	Enhanced by	3.600E+00			
	AR	Enhanced by	7.000E-01			
	HE	Enhanced by	7.000E-01			
130.	CO+OH=CO2+H			8.00E+11	0.1	7352.0
	Declared duplicate reaction...					
131.	CO+OH=CO2+H			8.78E+10	0.0	-16.0
	Declared duplicate reaction...					
132.	CO+O2=CO2+O			1.12E+12	0.0	47700.0
133.	CO+HO2=CO2+OH			3.01E+13	0.0	23000.0
134.	C2H6+CH3=C2H5+CH4			1.72E+12	0.8	20117.7
135.	C2H6+H=C2H5+H2			2.68E+07	2.0	6324.6
136.	C2H6+O=C2H5+OH			1.81E+05	2.8	5802.0
137.	C2H6+OH=C2H5+H2O			9.15E+06	2.0	993.5

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138. C2H6+O2=C2H5+HO2                                  7.50E+05    2.5    49158.4
139. C2H6+HO2=C2H5+H2O2                                1.30E+13    0.0    20460.0
140. C2H4+H=C2H3+H2                                    1.64E+06    2.5    12240.0
141. C2H4+O=CH3+HCO                                    8.10E+06    1.9      180.0
142. C2H4+O=CH2HCO+H                                   4.70E+06    1.9      180.0
143. C2H4+O=CH2CO+H2                                   6.80E+05    1.9      180.0
144. C2H4+OH=C2H3+H2O                                  3.02E+13    0.0     5955.0
145. C2H4+O2=CH2HCO+OH                                 2.00E+08    1.5    39000.0
146. C2H4+HO2=CH3HCO+OH                                2.20E+12    0.0    17200.0
147. C2H4+CH3=C2H3+CH4                                 5.00E+11    0.0    15000.0
148. CH2+CH3=C2H4+H                                    4.00E+13    0.0        0.0
149. C2H4+H(+M)=C2H5(+M)                               1.08E+12    0.5     1822.0
     Low pressure limit:  0.11120E+35 -0.50000E+01  0.44480E+04
     TROE centering:      0.50000E+00  0.95000E+02  0.95000E+02  0.20000E+03
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
150. CH3+CH3=C2H5+H                                    5.42E+13    0.0    16054.9
151. H+C2H5(+M)=C2H6(+M)                               5.20E+17   -1.0     1580.0
     Low pressure limit:  0.20000E+42 -0.70800E+01  0.66850E+04
     TROE centering:      0.84220E+00  0.12500E+03  0.22190E+04  0.68820E+04
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
152. C2H5+O2(+M)=C2H5O2(+M)                            2.02E+10    1.0      -63.6
     Low pressure limit:  0.84900E+30 -0.42900E+01  0.22000E+03
     TROE centering:      0.10300E+00  0.60100E+03  0.10000E-09
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
153. C2H5+O2(+M)=C2H4+HO2(+M)                          1.41E+07    1.1    -1975.0
     High pressure limit:  0.68500E-11  0.65300E+01 -0.83400E+03
     TROE centering:      0.45000E+00  0.10000E-09  0.10000E+11
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
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     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
154. C2H5O2(+M)=C2H4+HO2(+M)                        7.14E+04    2.3    27955.0
     Low pressure limit:  0.83100E+22 -0.65100E+00  0.22890E+05
     TROE centering:      0.00000E+00  0.10600E+03  0.10600E+03
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
155. C2H5+O2=C2H4+HO2                               5.81E+06    1.6    20578.0
156. C2H5+O=CH3+CH2O                                4.20E+13    0.0        0.0
157. C2H5+O=CH3HCO+H                                5.30E+13    0.0        0.0
158. C2H5+O=C2H4+OH                                 3.00E+13    0.0        0.0
159. C2H5+OH=C2H4+H2O                               2.40E+13    0.0        0.0
160. C2H5+HCO=C2H6+CO                               1.20E+14    0.0        0.0
161. C2H5+CH2O=C2H6+HCO                             5.50E+03    2.8     5860.0
162. C2H5+CH3=C2H4+CH4                              1.10E+12    0.0        0.0
163. C2H5+C2H5=C2H6+C2H4                            1.50E+12    0.0        0.0
164. C2H2+O=CH2+CO                                  6.10E+06    2.0     1900.0
165. C2H2+O=HCCO+H                                  1.43E+07    2.0     1900.0
166. H2+C2H=C2H2+H                                  4.09E+05    2.4      864.3
167. H+C2H2<=>C2H3                                  2.22E+08    1.7     2420.0
168. C2H3+H=C2H2+H2                                 4.00E+13    0.0        0.0
169. C2H3+O=CH2CO+H                                 3.00E+13    0.0        0.0
170. C2H3+O2=CH2O+HCO                               9.16E+16   -1.4     1015.0
171. C2H3+O2=CH2HCO+O                               3.03E+11   -0.3       10.7
172. C2H3+O2=C2H2+HO2                               1.34E+06    1.6     -383.5
173. C2H3+OH=C2H2+H2O                               2.00E+13    0.0        0.0
174. C2H3+CH2=C3H4+H                                3.00E+13    0.0        0.0
175. C2H3+C2H=C2H2+C2H2                             3.00E+13    0.0        0.0
176. C2H3+C2H=H2CCCCH+H                             3.00E+13    0.0        0.0
177. C2H3+CH3=C2H2+CH4                              2.10E+13    0.0        0.0
178. C2H3+CH2O=C2H4+HCO                             5.40E+03    2.8     5860.0
179. C2H3+HCO=C2H4+CO                               9.00E+13    0.0        0.0
180. C2H3+C2H3=CH2CHCCH2+H                          9.00E+12    0.0        0.0
181. C2H3+C2H3=H2CCCH+CH3                           1.80E+13    0.0        0.0
182. C2H3+C2H3=C2H4+C2H2                            6.30E+13    0.0        0.0
183. C2H3+CH=CH2+C2H2                               5.00E+13    0.0        0.0
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184.	OH+C2H2=C2H+H2O	3.37E+07	2.0	14000.0
185.	OH+C2H2=HCCOH+H	5.04E+05	2.3	13500.0
186.	OH+C2H2=CH2CO+H	2.18E-04	4.5	-1000.0
187.	OH+C2H2=CH3+CO	4.83E-04	4.0	-2000.0
188.	OH+C2H2(+M)=C2H2OH(+M)	1.52E+08	1.7	1000.0
	Low pressure limit: 0.18100E+24 -0.20000E+01 0.00000E+00			
	H2 Enhanced by 2.000E+00			
	CO Enhanced by 2.000E+00			
	CO2 Enhanced by 3.000E+00			
	H2O Enhanced by 5.000E+00			
189.	HO2+C2H2=CH2HCO+O	3.00E+12	0.0	10000.0
190.	HO2+C2H2=CH2O+HCO	3.00E+12	0.0	10000.0
191.	HCCOH+H=HCCO+H2	3.00E+07	2.0	1000.0
192.	HCCOH+OH=HCCO+H2O	1.00E+07	2.0	1000.0
193.	HCCOH+O=HCCO+OH	2.00E+07	3.0	1900.0
194.	C2H2+O=C2H+OH	3.16E+15	-0.6	15000.0
195.	C2H2OH+H=CH2HCO+H	5.00E+13	0.0	0.0
196.	C2H2OH+O=OCHCHO+H	5.00E+13	0.0	0.0
197.	C2H2OH+O2=OCHCHO+OH	1.00E+12	0.0	5000.0
198.	CH2HCO+H=CH3+HCO	1.00E+14	0.0	0.0
199.	CH2HCO+H=CH3CO+H	3.00E+13	0.0	0.0
200.	CH2HCO+O=CH2O+HCO	5.00E+13	0.0	0.0
201.	CH2HCO+OH=CH2CO+H2O	2.00E+13	0.0	0.0
202.	CH2HCO+OH=CH2OH+HCO	1.00E+13	0.0	0.0
203.	CH2HCO+CH3=C2H5+HCO	5.00E+13	0.0	0.0
204.	CH2HCO+CH2=C2H4+HCO	5.00E+13	0.0	0.0
205.	CH2HCO+CH=C2H3+HCO	1.00E+14	0.0	0.0
206.	CH2HCO+O2=OH+OCHCHO	2.22E+11	0.0	1500.0
207.	OCHCHO+M=HCO+HCO+M	1.00E+17	0.0	58000.0
208.	OCHCHO+H=CH2O+HCO	3.00E+13	0.0	0.0
209.	CH2HCO+M=CH3+CO+M	2.00E+16	0.0	42000.0
	H2 Enhanced by 2.000E+00			
	CO Enhanced by 2.000E+00			
	CO2 Enhanced by 3.000E+00			
	H2O Enhanced by 5.000E+00			
210.	CH3HCO+OH=CH3CO+H2O	2.30E+10	0.7	-1110.0
211.	CH3HCO+H=CH3CO+H2	4.10E+09	1.2	2400.0
212.	CH3HCO+CH3=CH3CO+CH4	2.00E-06	5.6	2464.0

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213. CH3CO(+M)=CH3+CO(+M)                             2.80E+13    0.0    17100.0
     Low pressure limit:  0.21000E+16  0.00000E+00  0.14000E+05
     TROE centering:      0.50000E+00  0.10000E-29  0.10000E+31
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
214. CH3CO+H=CH3+HCO                                  2.10E+13    0.0        0.0
215. CH3CO+H=CH2CO+H2                                 1.20E+13    0.0        0.0
216. CH3CO+O=CH3+CO2                                  1.50E+14    0.0        0.0
217. CH3CO+O=CH2CO+OH                                 4.00E+13    0.0        0.0
218. CH3CO+OH=CH2CO+H2O                               1.20E+13    0.0        0.0
219. CH3HCO=CH3+HCO                                   7.10E+15    0.0    81280.0
220. CH3HCO+O=CH3CO+OH                                5.80E+12    0.0     1800.0
221. CH3HCO+O2=CH3CO+HO2                              3.00E+13    0.0    39000.0
222. CH3HCO+HO2=CH3CO+H2O2                            3.00E+12    0.0    12000.0
223. CH2CO+O=CO2+CH2                                  1.75E+12    0.0     1350.0
224. CH2CO+H=CH3+CO                                   3.28E+10    0.9     2839.0
225. CH2CO+H=HCCO+H2                                  3.00E+07    2.0    10000.0
226. CH2CO+O=HCCO+OH                                  2.00E+07    2.0    10000.0
227. CH2CO+OH=HCCO+H2O                                1.00E+07    2.0     3000.0
228. CH2CO+OH=CH2OH+CO                                7.20E+12    0.0        0.0
229. CH2CO+OH=CH3+CO2                                 3.00E+12    0.0        0.0
230. CH2+CO(+M)=CH2CO(+M)                             8.10E+11    0.5     4510.0
     Low pressure limit:  0.18800E+34 -0.51100E+01  0.70950E+04
     TROE centering:      0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    8.580E+00
231. C2H+O2=CO+CO+H                                   2.52E+13    0.0        0.0
232. C2H+C2H2=C4H2+H                                  2.47E+12    0.5     -391.0
233. C2H+CH4=CH3+C2H2                                 7.23E+12    0.0      976.0
234. CH+CO(+M)=HCCO(+M)                               5.00E+13    0.0        0.0
     Low pressure limit:  0.18800E+29 -0.37400E+01  0.19360E+04
     TROE centering:      0.57570E+00  0.23700E+03  0.16520E+04  0.50690E+04
     H2O             Enhanced by    8.580E+00
     CO              Enhanced by    2.000E+00
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	CO2	Enhanced by	3.000E+00			
	H2	Enhanced by	2.000E+00			
235.	HCCO+C2H2=H2CCCH+CO			1.00E+11	0.0	3000.0
236.	H+HCCO=CH2(S)+CO			1.00E+14	0.0	0.0
237.	O+HCCO=H+CO+CO			1.00E+14	0.0	0.0
238.	HCCO+O2=CO2+CO+H			1.40E+07	1.7	1000.0
239.	HCCO+O2=CO+CO+OH			2.88E+07	1.7	1000.0
240.	CH+HCCO=C2H2+CO			5.00E+13	0.0	0.0
241.	HCCO+HCCO=C2H2+CO+CO			1.00E+13	0.0	0.0
242.	HCCO+OH=C2O+H2O			6.00E+13	0.0	0.0
243.	C2O+H=CH+CO			1.00E+13	0.0	0.0
244.	C2O+O=CO+CO			5.00E+13	0.0	0.0
245.	C2O+OH=CO+CO+H			2.00E+13	0.0	0.0
246.	C2O+O2=CO+CO+O			2.00E+13	0.0	0.0
247.	CH2(S)+M=CH2+M			1.00E+13	0.0	0.0
	H	Enhanced by	0.000E+00			
	H2O	Enhanced by	0.000E+00			
	C2H2	Enhanced by	0.000E+00			
	C6H6	Enhanced by	0.000E+00			
	AR	Enhanced by	0.000E+00			
248.	CH2(S)+CH4=CH3+CH3			4.00E+13	0.0	0.0
249.	CH2(S)+C2H6=CH3+C2H5			1.20E+14	0.0	0.0
250.	CH2(S)+O2=CO+OH+H			7.00E+13	0.0	0.0
251.	CH2(S)+H2=CH3+H			7.00E+13	0.0	0.0
252.	CH2(S)+H2O=CH3+OH			3.01E+15	-0.6	0.0
253.	CH2(S)+H2O=CH2+H2O			3.00E+13	0.0	0.0
254.	CH2(S)+C2H2=H2CCCH+H			1.80E+14	0.0	0.0
255.	CH2(S)+C2H2=CH2+C2H2			4.00E+13	0.0	0.0
256.	CH2(S)+H=CH2+H			2.00E+14	0.0	0.0
257.	CH2(S)+O=CO+H+H			3.00E+13	0.0	0.0
258.	CH2(S)+OH=CH2O+H			3.00E+13	0.0	0.0
259.	CH2(S)+H=CH+H2			3.00E+13	0.0	0.0
260.	CH2(S)+CO2=CH2O+CO			3.00E+12	0.0	0.0
261.	CH2(S)+CH3=C2H4+H			2.00E+13	0.0	0.0
262.	CH2(S)+CH2CO=C2H4+CO			1.60E+14	0.0	0.0
263.	CH2(S)+C6H6=C6H5+CH3			1.70E+14	0.0	0.0
264.	CH2(S)+C6H6=CH2+C6H6			7.00E+13	0.0	0.0
265.	CH2(S)+AR=CH2+AR			1.45E+13	0.0	884.0

266.	C2H+O=CH+CO	5.00E+13	0.0	0.0
267.	C2H+OH=HCCO+H	2.00E+13	0.0	0.0
268.	C2H+OH=C2+H2O	4.00E+07	2.0	8000.0
269.	C2+H2=C2H+H	4.00E+05	2.4	1000.0
270.	C2+O2=CO+CO	5.00E+13	0.0	0.0
271.	C2+OH=C2O+H	5.00E+13	0.0	0.0
272.	C4H2+OH=H2C4O+H	6.66E+12	0.0	-410.0
273.	C3H2+O2=HCCO+CO+H	2.00E+12	0.0	1000.0
274.	C3H2+O=C2H2+CO	1.00E+14	0.0	0.0
275.	C3H2+OH=C2H2+HCO	5.00E+13	0.0	0.0
276.	C3H2+CH2=H2CCCCH+H	3.00E+13	0.0	0.0
277.	C3H2+CH3=CH2CHCCH+H	2.00E+13	0.0	0.0
278.	C3H2+C2H2=HCCCHCCH+H	5.00E+12	0.0	5000.0
279.	C3H2+H2CCCH=C6H4+H	1.00E+13	0.0	0.0
280.	C3H2+HCCO=HCCHCCH+CO	3.00E+13	0.0	0.0
281.	C3H2+CH2(S)=H2CCCCH+H	5.00E+13	0.0	0.0
282.	H2C4O+OH=C2H2+CO+HCO	1.00E+13	0.0	0.0
283.	H2CCCH+O2=CH2CO+HCO	3.00E+10	0.0	2868.0
284.	H2CCCH+O=CH2O+C2H	1.40E+14	0.0	0.0
285.	H2CCCH+H=C3H2+H2	5.00E+13	0.0	1000.0
286.	H2CCCH+OH=C3H2+H2O	2.00E+13	0.0	0.0
287.	H2CCCH+CH2=CH2CHCCH+H	4.00E+13	0.0	0.0
288.	H2CCCH+CH=HCCHCCH+H	7.00E+13	0.0	0.0
289.	H2CCCH+CH=H2CCCCH+H	7.00E+13	0.0	0.0
290.	CH2CHCCH+OH=HCCHCCH+H2O	7.50E+06	2.0	5000.0
291.	CH2CHCCH+H=HCCHCCH+H2	2.00E+07	2.0	15000.0
292.	CH2CHCCH+OH=H2CCCCH+H2O	1.00E+07	2.0	2000.0
293.	H+HCCHCCH=H2CCCCH+H	1.00E+14	0.0	0.0
294.	H2CCCCH+O2=CH2CO+HCCO	1.00E+12	0.0	0.0
295.	H2CCCCH+OH=C4H2+H2O	3.00E+13	0.0	0.0
296.	H2CCCCH+O=CH2CO+C2H	2.00E+13	0.0	0.0
297.	H2CCCCH+O=H2C4O+H	2.00E+13	0.0	0.0
298.	H2CCCCH+H=C4H2+H2	5.00E+13	0.0	0.0
299.	H2CCCCH+CH2=C3H4+C2H	2.00E+13	0.0	0.0
300.	CH2CHCCH+H=H2CCCCH+H2	3.00E+07	2.0	5000.0
301.	CH2CHCHCH+OH=CH2CHCCH+H2O	2.00E+07	2.0	1000.0
302.	CH2CHCHCH+H=CH2CHCCH+H2	3.00E+07	2.0	1000.0
303.	C6H6+H=C6H5+H2	3.00E+07	2.0	8000.0

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304. C6H6+OH=C6H5+H2O                                 7.50E+06    2.0     5000.0
305. C6H6+O=C6H5+OH                                   2.40E+13    0.0     4700.0
306. C2H3+C2H2=CH2CHCCH+H                             1.32E+12    0.2     8312.0
307. C2H2+CH2CHCHCH=C6H6+H                            8.21E+08    0.8     6348.0
308. HCCHCCH+C2H2=C6H5                                1.67E+10    0.4     7719.3
309. C3H4+H=C3H4P+H                                   1.00E+13    0.0     5000.0
310. C3H4+H=H2CCCH+H2                                 3.00E+07    2.0     5000.0
311. C3H4+OH=H2CCCH+H2O                               2.00E+07    2.0     1000.0
312. C3H4P+H=H2CCCH+H2                                3.00E+07    2.0     5000.0
313. C3H4P+H=CH3+C2H2                                 1.00E+14    0.0     4000.0
314. C3H4P+OH=H2CCCH+H2O                              2.00E+07    2.0     1000.0
315. C6H5+OH=C6H5O+H                                  5.00E+13    0.0        0.0
316. C6H5+OH=C6H4+H2O                                 1.00E+07    2.0     1000.0
317. C6H5+O2=C6H5O+O                                  2.60E+13    0.0     6120.0
     Declared duplicate reaction...
318. C6H5+O2=C6H5O+O                                  3.00E+13    0.0     8981.0
     Declared duplicate reaction...
319. C6H5O=C5H5+CO                                    7.40E+11    0.0    43853.0
320. CH2+C4H2=H2CCCCCH+H                              1.30E+13    0.0     4326.0
321. CH+C4H2=C5H2+H                                   1.00E+14    0.0        0.0
322. CH2(S)+C4H2=H2CCCCCH+H                           3.00E+13    0.0        0.0
323. C4H2+O=C3H2+CO                                   1.20E+12    0.0        0.0
324. C4H+H2=C4H2+H                                    2.00E+13    0.0     5000.0
325. C4H+H2O=C4H2+OH                                  2.00E+13    0.0     2000.0
326. C4H+O2=CO+CO+C2H                                 1.20E+12    0.0        0.0
327. C4H2+C2H=C6H2+H                                  4.00E+13    0.0        0.0
328. C2H2+O2=HCO+HCO                                  2.00E+08    1.5    30100.0
329. C2H2+M=C2H+H+M                                   9.08E+30   -3.7   127138.0
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
330. C2H4(+M)<=>H2+C2H2(+M)                           6.00E+12    0.4    86770.0
     Low pressure limit:  0.15800E+52 -0.93000E+01  0.97800E+05
     TROE centering:      0.73450E+00  0.18000E+03  0.10350E+04  0.54170E+04
     H2              Enhanced by    2.000E+00
     H2O             Enhanced by    6.000E+00
     CH4             Enhanced by    2.000E+00
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     CO              Enhanced by    1.500E+00
     CO2             Enhanced by    2.000E+00
     C2H6            Enhanced by    3.000E+00
     AR              Enhanced by    7.000E-01
331. C2H3+H(+M)=C2H4(+M)                          6.10E+12    0.3      280.0
     Low pressure limit:  0.98000E+30 -0.38600E+01  0.33200E+04
     TROE centering:      0.78200E+00  0.20750E+03  0.26630E+04  0.60950E+04
     H2              Enhanced by    2.850E+00
     CO              Enhanced by    2.100E+00
     CO2             Enhanced by    2.850E+00
     H2O             Enhanced by    7.140E+00
     CH4             Enhanced by    2.850E+00
     C2H6            Enhanced by    4.290E+00
332. C2H3+C2H4=CH2CHCHCH2+H                       6.31E+11    0.0     3100.0
333. CH2CHCHCH2+H=CH2CHCHCH+H2                    3.00E+07    2.0    13000.0
334. CH2CHCHCH2+H=CH2CHCCH2+H2                    3.00E+07    2.0     6000.0
335. CH2CHCHCH2+OH=CH2CHCHCH+H2O                  2.00E+07    2.0     5000.0
336. CH2CHCHCH2+OH=CH2CHCCH2+H2O                  2.00E+07    2.0     2000.0
337. CH2CHCHCH+H=CH2CHCCH2+H                      1.00E+14    0.0        0.0
338. CH2CHCCH2+H=CH3+H2CCCH                       1.00E+14    0.0        0.0
339. CH2CHCCH2+OH=CH2CHCCH+H2O                    3.00E+13    0.0        0.0
340. H2CCCCH(+M)=C4H2+H(+M)                       1.00E+14    0.0    55000.0
     Low pressure limit:  0.20000E+16  0.00000E+00  0.48000E+05
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
341. HCCHCCH(+M)=C4H2+H(+M)                       1.00E+14    0.0    36000.0
     Low pressure limit:  0.10000E+15  0.00000E+00  0.30000E+05
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
342. CH2CHCCH2(+M)=CH2CHCCH+H(+M)                 1.00E+14    0.0    50000.0
     Low pressure limit:  0.20000E+16  0.00000E+00  0.42000E+05
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
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     H2O             Enhanced by    5.000E+00
343. CH2CHCHCH(+M)=CH2CHCCH+H(+M)                  1.00E+14    0.0    37000.0
     Low pressure limit:  0.10000E+15  0.00000E+00  0.30000E+05
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
344. H+C6H5=C6H6                                   5.00E+13    0.0        0.0
345. H+C6H5=C6H4+H2                                2.00E+07    2.0     1000.0
346. C6H5(+M)=C6H4+H(+M)                           4.30E+12    0.6    77294.0
     Low pressure limit:  0.10000E+85 -0.18870E+02  0.90091E+05
     TROE centering:      0.90200E+00  0.69600E+03  0.35800E+03  0.38560E+04
     H2              Enhanced by    2.000E+00
     CO              Enhanced by    2.000E+00
     CO2             Enhanced by    3.000E+00
     H2O             Enhanced by    5.000E+00
347. C6H4=C4H2+C2H2                                1.20E+18   -0.3    87825.0
348. H2CCCH+H(+M)=C3H4(+M)                         1.00E+17   -0.8      315.0
     Low pressure limit:  0.35000E+34 -0.48800E+01  0.22250E+04
     TROE centering:      0.70860E+00  0.13400E+03  0.17840E+04  0.57400E+04
     H2              Enhanced by    2.860E+00
     H2O             Enhanced by    8.570E+00
     CH4             Enhanced by    2.860E+00
     CO              Enhanced by    2.140E+00
     CO2             Enhanced by    2.860E+00
     C2H6            Enhanced by    4.290E+00
349. H2CCCH+H(+M)=C3H4P(+M)                        1.00E+17   -0.8      315.0
     Low pressure limit:  0.35000E+34 -0.48800E+01  0.22250E+04
     TROE centering:      0.70860E+00  0.13400E+03  0.17840E+04  0.57400E+04
     H2              Enhanced by    2.860E+00
     H2O             Enhanced by    8.570E+00
     CH4             Enhanced by    2.860E+00
     CO              Enhanced by    2.140E+00
     CO2             Enhanced by    2.860E+00
     C2H6            Enhanced by    4.290E+00
350. CH2(S)+C2H4=CH2CHCH2+H                        1.30E+14    0.0        0.0
351. C2H3+CH3=CH2CHCH2+H                           2.86E+21   -2.1    11841.8
352. C2H3+CH3=C3H6                                 3.69E+30   -5.0     7691.9
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353.	C3H6=CH3CHCH+H	1.58E+73	-17.0	120057.9
354.	C3H6=CH3CCH2+H	1.58E+73	-17.0	120057.9
355.	C3H6=C2H2+CH4	2.50E+12	0.0	70000.0
356.	C3H6=C3H4+H2	3.00E+13	0.0	80000.0
357.	C3H6+HO2=CH2CHCH2+H2O2	9.64E+03	2.6	13910.0
358.	C3H6+OH+O2=CH3HCO+CH2O+OH	3.00E+10	0.0	-8280.0
359.	C3H6+OH=CH2CHCH2+H2O	3.12E+06	2.0	-298.0
360.	C3H6+OH=CH3CCH2+H2O	1.11E+06	2.0	1451.0
361.	C3H6+OH=CH3CHCH+H2O	2.11E+06	2.0	2778.0
362.	C3H6+O=C2H5+HCO	1.58E+07	1.8	-1216.0
363.	C3H6+O=CH2CHCH2+OH	5.24E+11	0.7	5884.0
364.	C3H6+O=CH3CHCH+OH	1.20E+11	0.7	8959.0
365.	C3H6+O=CH3CCH2+OH	6.03E+10	0.7	7632.0
366.	C3H6+H=C2H4+CH3	7.23E+12	0.0	1302.0
367.	C3H6+H=CH2CHCH2+H2	1.73E+05	2.5	2492.0
368.	C3H6+H=CH3CCH2+H2	4.09E+05	2.5	9794.0
369.	C3H6+H=CH3CHCH+H2	8.04E+05	2.5	12284.0
370.	CH3CHCH+HO2=C3H6+O2	2.00E+12	0.0	0.0
371.	CH3CCH2+HO2=C3H6+O2	1.00E+12	0.0	0.0
372.	CH2CHCH2+HO2=C3H6+O2	3.00E+12	0.0	0.0
373.	C3H6+CH3=CH2CHCH2+CH4	2.22E+00	3.5	5675.0
374.	C3H6+CH3=CH3CCH2+CH4	8.43E-01	3.5	11656.0
375.	C3H6+CH3=CH3CHCH+CH4	1.35E+00	3.5	12848.0
376.	C3H6+HCO=CH2CHCH2+CH2O	1.08E+07	1.9	17010.0
377.	CH2CHCH2+O2=C3H4+HO2	4.99E+15	-1.4	22428.0
378.	CH2CHCH2+O2=CH2HCO+CH2O	1.06E+10	0.3	12838.0
379.	CH2CHCH2+O2=C2H2+CH2O+OH	2.78E+25	-4.8	15468.0
380.	CH2CHCH2+OH=C3H4+H2O	1.00E+13	0.0	0.0
381.	CH2CHCH2+H=C3H4+H2	5.00E+13	0.0	0.0
382.	C3H6=CH2CHCH2+H	1.58E+73	-17.0	120057.9
383.	CH2CHCH2+CH3=C3H4+CH4	3.02E+12	-0.3	-131.0
384.	CH3CHCH+O2=CH3HCO+HCO	1.09E+23	-3.3	3892.0
385.	CH3CHCH+H=C3H4P+H2	2.00E+13	0.0	0.0
386.	CH3CHCH+OH=C3H4P+H2O	1.00E+13	0.0	0.0
387.	CH3CHCH+H=CH2CHCH2+H	1.00E+14	0.0	0.0
388.	CH3CCH2+H=CH2CHCH2+H	1.00E+14	0.0	0.0
389.	CH3CCH2+O2=CH3CO+CH2O	1.09E+22	-3.3	3892.0
390.	CH3CCH2+O=CH2CO+CH3	1.00E+14	0.0	0.0

391.	CH3CCH2+H=C3H4P+H2	4.00E+13	0.0	0.0
392.	CH3CCH2+OH=C3H4P+H2O	2.00E+13	0.0	0.0
393.	C3H4P+H(+M)=CH3CCH2(+M)	6.50E+12	0.0	2000.0
	Low pressure limit: 0.84500E+40 -0.72700E+01 0.65770E+04			
394.	C3H4+H(+M)=CH2CHCH2(+M)	1.20E+11	0.7	3007.0
	Low pressure limit: 0.55600E+34 -0.50000E+01 0.44480E+04			
395.	C3H4+H(+M)=CH3CCH2(+M)	8.49E+12	0.0	2000.0
	Low pressure limit: 0.11100E+35 -0.50000E+01 0.44480E+04			
396.	CH2CHCHCH2+O=HCO+CH2CHCH2	6.02E+08	1.4	-858.0
397.	C6H5+O=C5H5+CO	9.00E+13	0.0	0.0
398.	H+C6H5O=C5H6+CO	1.06E+42	-7.6	35349.0
399.	C5H6+HO2=C5H5+H2O2	1.99E+12	0.0	11660.0
400.	C5H6+O2=C5H5+HO2	2.00E+13	0.0	25000.0
401.	C5H6+O2=C5H5O+OH	1.00E+13	0.0	20712.0
402.	C5H6+O=C5H5+OH	1.81E+13	0.0	3080.0
403.	H+C5H6=CH2CHCH2+C2H2	1.00E+13	0.0	12000.0
404.	C5H5+H=C5H6	2.92E+29	-4.7	6148.0
405.	C5H5=C5H5(L)	4.09E+47	-10.4	54874.0
406.	H2CCCH+C2H2=C5H5(L)	5.62E+32	-7.3	6758.0
407.	CH2CHCHCH+CO=C5H5O	6.11E-01	1.9	31067.0
408.	C5H5+OH=C5H4OH+H	3.00E+13	0.0	0.0
409.	C5H5+O=CH2CHCHCH+CO	1.00E+14	0.0	0.0
410.	C5H5+HO2=C5H5O+OH	3.00E+13	0.0	0.0
411.	H2CCCH+C2H2=C5H5	7.39E+53	-12.5	57313.0
412.	C5H5+O=C5H5O	1.24E+25	-3.7	4763.0
413.	C5H4O+H=C5H4OH	5.27E+27	-4.2	10863.0
414.	C5H4O=CO+C2H2+C2H2	1.00E+15	0.0	78000.0
415.	H2CCCH+C2H3=C5H5+H	9.63E+40	-7.8	28820.0
416.	C5H6+OH=C5H5+H2O	3.43E+09	1.2	-447.0
417.	C5H6+H=C5H5+H2	2.19E+08	1.8	3000.0
418.	C5H5+O=C5H4O+H	1.00E+14	0.0	0.0
419.	C3H2+H=C3H+H2	1.00E+13	0.0	0.0
420.	C3H+O2=HCCO+CO	1.00E+13	0.0	0.0
421.	C3H+O=C2H+CO	1.00E+13	0.0	0.0
422.	H2CCCCCH+H=C5H2+H2	1.00E+13	0.0	0.0
423.	HCCCHCCH+H=C5H2+H2	1.00E+13	0.0	0.0
424.	HCCCHCCH+H=H2CCCCCH+H	1.00E+13	0.0	0.0
425.	H2CCCH+H2CCCH=C6H5+H	5.00E+12	0.0	0.0

426.	H2CCCH+H2CCCH=FULVENE	4.50E+12	0.0	0.0
427.	H2CCCH+H2CCCH=HCCCHCCH+CH3	5.00E+11	0.0	0.0
428.	FULVENE=C6H6	7.59E+13	0.0	73853.0
429.	H2CCCH+CH2CHCH2=FULVENE+H+H	5.56E+20	-2.5	1692.0
430.	C6H5+C2H2=C6H5C2H+H	2.47E+06	1.8	2289.0
431.	FULVENE+H=C6H6+H	3.00E+12	0.5	2000.0
432.	C6H7=C6H6+H	6.64E+46	-11.1	34478.0
433.	CH2CHCHCH+C2H2=C6H7	1.96E+19	-3.4	4910.0
434.	CH3+C5H5=C6H7+H	2.44E+41	-8.0	39259.0
435.	C6H7+H=C6H6+H2	1.00E+13	0.0	0.0
436.	C6H7+C6H5=2C6H6	1.00E+12	0.0	0.0
437.	C2H3+CH2CHCHCH=C6H813	5.50E+15	-1.7	1470.0
438.	C2H3+CH2CHCHCH2=C6H813+H	1.14E+12	-0.2	9920.0
439.	C2H3+CH2CHCHCH2=C6H814+H	1.14E+12	-0.2	9920.0
440.	CH2CHCHCH2+C2H2=C6H814	2.30E+12	0.0	35000.0
441.	C6H813=C6H7+H	2.42E+59	-13.3	96147.0
442.	C6H814=C6H7+H	1.21E+59	-13.3	96147.0
443.	C6H813+O2=C6H7+HO2	8.13E+11	0.0	24840.0
444.	2C6H7=C6H813+C6H6	2.82E+13	0.0	0.0
445.	2C6H7=C6H814+C6H6	1.39E+13	0.0	0.0
446.	C6H814+H=C6H7+H2	4.00E+13	0.0	3000.0
447.	C6H813=C6H6+H2	4.39E+37	-7.3	71949.0
448.	C6H814=C6H6+H2	1.28E+28	-4.9	49309.0
449.	C10H7S+O2=C10H7O+O	1.00E+13	0.0	0.0
450.	C10H7S+OH=C10H7O+H	5.00E+13	0.0	0.0
451.	C10H7P+O2=C10H7O+O	1.00E+13	0.0	0.0
452.	C10H7P+OH=C10H7O+H	5.00E+13	0.0	0.0
453.	C10H7O=INDENE*+CO	7.40E+11	0.0	43850.0
454.	INDENE+H=INDENE*+H2	2.19E+08	1.8	3000.0
455.	INDENE+OH=INDENE*+H2O	3.43E+09	1.2	-447.0
456.	INDENE+O=INDENE*+OH	1.81E+13	0.0	3080.0
457.	INDENE*+H=INDENE	2.00E+14	0.0	0.0
458.	C7H7+C2H2=INDENE+H	3.20E+11	0.0	7000.0
459.	C10H7O+H=C10H7OH	2.53E+14	0.0	0.0
460.	C10H7OH+H=C10H7O+H2	1.15E+14	0.0	12400.0
461.	C10H7OH+H=C10H8+OH	2.23E+13	0.0	7929.0
462.	C10H7OH+OH=C10H7O+H2O	6.00E+12	0.0	0.0
463.	H2CCCH+C7H7=C10H8+2H	6.03E+11	0.0	0.0

464.	2C5H5=C10H8+H+H	2.00E+12	0.0	4000.0
465.	C6H5+HCCHCCH=C10H8	2.22E+43	-9.1	14810.0
466.	C6H5+HCCHCCH=C10H7P+H	1.36E+22	-2.3	18485.0
467.	C10H7P+H=C10H8	1.00E+14	0.0	0.0
468.	C10H7S+H=C10H8	1.00E+14	0.0	0.0
469.	C10H8+C2H3=C10H7P+C2H4	5.00E+13	0.0	16000.0
470.	C10H8+C2H=C10H7P+C2H2	5.00E+13	0.0	16000.0
471.	C10H8+C2H3=C10H7S+C2H4	5.00E+13	0.0	16000.0
472.	C10H8+C2H=C10H7S+C2H2	5.00E+13	0.0	16000.0
473.	C10H8+H=C10H7S+H2	2.50E+14	0.0	16000.0
474.	C10H8+H=C10H7P+H2	2.50E+14	0.0	16000.0
475.	C10H8+OH=C10H7S+H2O	2.10E+13	0.0	4600.0
476.	C10H8+OH=C10H7P+H2O	2.10E+13	0.0	4600.0
477.	C6H5C2H+H=A1YNE*+H2	2.50E+14	0.0	16000.0
478.	C6H5C2H+OH=A1YNE*+H2O	2.10E+13	0.0	4600.0
479.	C6H5C2H+CH3=A1YNE*+CH4	1.67E+12	0.0	15057.0
480.	A1YNE*+C2H2=C10H7S	3.98E+13	0.0	10100.0
481.	C8H10+OH=C8H8+H2O+H	8.34E+12	0.0	2583.0
482.	C8H10+H=C8H8+H2+H	8.00E+13	0.0	8235.0
483.	C8H10+O2=C8H8+HO2+H	2.00E+14	0.0	41400.0
484.	C7H7+CH3=C8H10	2.10E+37	-7.4	12269.0
485.	C7H7+CH3=C8H8+H2	4.68E+24	-3.2	27018.0
486.	C8H10=C8H8+H2	5.01E+12	0.0	64000.0
487.	C8H10+H=C6H6+C2H5	1.20E+13	0.0	5100.0
488.	C6H5+C2H3=C8H8	2.67E+19	-2.1	2187.0
489.	C6H5+CH2CHCCH=C8H8+C2H	3.20E+11	0.0	1900.0
490.	C6H5+CH2CHCHCH2=C8H8+C2H3	3.20E+11	0.0	1900.0
491.	CH2CHCCH+CH2CHCCH=C8H8	5.47E+40	-8.0	51241.0
492.	CH2CHCHCH+CH2CHCCH=C8H8+H	3.16E+11	0.0	600.0
493.	C8H8+H=C6H5C2H+H2+H	6.92E+14	0.0	14500.0
494.	C6H6+C2H=C6H5C2H+H	1.00E+12	0.0	0.0
495.	C6H5+C2H=C6H5C2H	2.54E+17	-1.5	1541.0
496.	C6H5+C4H2=C6H5C2H+C2H	2.00E+13	0.0	0.0
497.	C6H5+CH2CHCCH=C6H5C2H+C2H3	3.20E+11	0.0	1350.0
498.	CH2CHCHCH+C4H2=C6H5C2H+H	3.16E+11	0.0	1800.0
499.	C7H7+H=C7H8	4.81E+20	-2.1	1986.0
500.	C6H5+CH3=C7H8	2.00E+22	-3.0	2304.0
501.	C7H8+O2=C7H7+HO2	3.00E+14	0.0	41400.0

502.	C7H8+OH=C7H7+H2O	1.26E+13	0.0	2583.0
503.	C7H8+H=C7H7+H2	1.20E+14	0.0	8235.0
504.	C7H8+H=C6H6+CH3	1.20E+13	0.0	5148.0
505.	C7H8+CH3=C7H7+CH4	3.16E+11	0.0	9500.0
506.	C7H8+C6H5=C7H7+C6H6	2.10E+12	0.0	4400.0
507.	C7H8+C2H3=C7H7+C2H4	3.98E+12	0.0	8000.0
508.	CH2CHCHCH+C3H4=C7H8+H	2.00E+11	0.0	3700.0
509.	CH2CHCHCH+C3H4P=C7H8+H	3.16E+11	0.0	3700.0
510.	C7H8O+H=C7H8+OH	2.21E+13	0.0	7910.0
511.	C7H8O+H=C6H5OH+CH3	1.20E+13	0.0	5148.0
512.	C6H5O+CH3=C7H8O	1.00E+12	0.0	0.0
513.	C7H7+C6H5OH=C7H8+C6H5O	1.05E+11	0.0	9500.0
514.	C6H5+CH3=C7H7+H	5.00E+13	0.0	0.0
515.	C7H7+OH=C6H5O+CH3	2.33E+59	-13.0	35964.0
516.	C5H5+C2H2=C7H7	1.73E+17	-1.9	10231.0
517.	CH2CHCCH+H2CCCH=C7H7	9.25E+11	-1.3	-14295.0
518.	C7H7+HO2=C6H5+CH2O+OH	5.00E+12	0.0	0.0
519.	HCCHCCH+C2H3=FULVENE	4.00E+12	0.0	0.0
520.	HCCHCCH+C2H3=C6H5+H	1.60E+13	0.0	0.0
521.	HCCHCCH+C2H3=C4H2+C2H4	1.00E+12	0.0	5000.0
522.	HCCHCCH+C2H3=CH2CHCCH+C2H2	2.00E+12	0.0	5000.0
523.	CH2CHCHCH+C2H=FULVENE	4.00E+12	0.0	0.0
524.	CH2CHCHCH+C2H=C6H5+H	1.60E+13	0.0	0.0
525.	CH2CHCHCH+C2H=CH2CHCCH+C2H2	3.00E+12	0.0	5000.0
526.	H2CCCCH+C2H3=FULVENE	1.00E+13	0.0	0.0
527.	H2CCCCH+C2H3=C6H5+H	6.00E+12	0.0	0.0
528.	H2CCCCH+C2H3=2H2CCCH	4.00E+12	0.0	0.0
529.	H2CCCCH+C2H3=C4H2+C2H4	1.00E+12	0.0	5000.0
530.	H2CCCCH+C2H3=CH2CHCCH+C2H2	2.00E+12	0.0	5000.0
531.	CH2CHCCH2+C2H=FULVENE	1.00E+13	0.0	0.0
532.	CH2CHCCH2+C2H=C6H5+H	6.00E+12	0.0	0.0
533.	CH2CHCCH2+C2H=2H2CCCH	4.00E+12	0.0	0.0
534.	CH2CHCCH2+C2H=CH2CHCCH+C2H2	3.00E+12	0.0	5000.0
535.	H2CCCCCH+CH3=FULVENE	1.40E+13	0.0	0.0
536.	H2CCCCCH+CH3=C6H5+H	6.00E+12	0.0	0.0
537.	H2CCCCCH+CH3=C5H2+CH4	3.00E+12	0.0	5000.0
538.	HCCCHCCH+CH3=FULVENE	1.00E+13	0.0	0.0
539.	HCCCHCCH+CH3=C6H5+H	1.00E+13	0.0	0.0

540.	HCCCHCCH+CH3=C5H2+CH4			3.00E+12	0.0	5000.0
541.	N2+M=N+N+M			1.89E+18	-0.8	224950.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
542.	N+O+M=NO+M			7.60E+14	-0.1	-1770.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
543.	N2+O=N+NO			1.00E+14	0.0	75490.0
544.	N+NO2=N2O+O			1.80E+12	0.0	0.0
545.	N+O2=NO+O			6.40E+09	1.0	6280.0
546.	N+OH=NO+H			3.80E+13	0.0	0.0
547.	NH+O2=HNO+O			4.60E+05	2.0	6500.0
548.	NH+O2=NO+OH			1.30E+06	1.5	100.0
549.	NH+OH=HNO+H			2.00E+13	0.0	0.0
550.	NH+OH=N+H2O			5.00E+11	0.5	2000.0
551.	NH+OH=NO+H2			2.00E+13	0.0	0.0
552.	NH+H=N+H2			3.00E+13	0.0	0.0
553.	NH+O=NO+H			9.20E+13	0.0	0.0
554.	NH+N=N2+H			3.00E+13	0.0	0.0
555.	NH+NH=N2+H+H			2.54E+13	0.0	0.0
556.	NH+NO=N2O+H			4.30E+14	-0.5	0.0
557.	NH+NO=N2+OH			2.20E+13	-0.2	0.0
558.	NH+NO2=N2O+OH			1.00E+13	0.0	0.0
559.	NH2+O2=HNO+OH			4.50E+12	0.0	25000.0
560.	NH2+O=NH+OH			6.80E+12	0.0	0.0
561.	NH2+O=H2+NO			1.30E+08	1.0	-627.0
562.	NH2+O=HNO+H			6.60E+14	-0.5	0.0
563.	NH2+OH=NH+H2O			4.00E+06	2.0	1000.0
564.	NH2+H=NH+H2			4.00E+13	0.0	3650.0
565.	NH2+NO=NNH+OH			2.80E+13	-0.6	0.0
566.	NH2+NO=N2+H2O			5.00E+12	0.0	0.0
567.	NH2+NO=N2O+H2			3.90E+13	0.0	20160.0

568.	NH2+N=N2+H+H			7.20E+13	0.0	0.0
569.	NH2+NH=N2H2+H			5.00E+13	0.0	0.0
570.	NH2+NH2=N2H2+H2			8.50E+11	0.0	0.0
571.	NH2+NH2=NH3+NH			4.00E+13	0.0	10000.0
572.	NH2+HO2=H2NO+OH			5.00E+13	0.0	0.0
573.	NH2+HO2=NH3+O2			1.00E+13	0.0	0.0
574.	NH2+NO2=N2O+H2O			3.20E+18	-2.2	0.0
575.	NH3+M=NH+H2+M			6.31E+14	0.0	93400.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
576.	NH3+M=NH2+H+M			2.51E+16	0.0	93800.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
577.	NH3+OH=NH2+H2O			2.04E+06	2.0	566.0
578.	NH3+H=NH2+H2			6.36E+05	2.4	10171.0
579.	NH3+O=NH2+OH			9.40E+06	1.9	6460.0
580.	NH3+HO2=NH2+H2O2			3.00E+11	0.0	22000.0
581.	NNH+M=N2+H+M			2.00E+14	0.0	20000.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
582.	NNH+NO=N2+HNO			5.00E+13	0.0	0.0
583.	NNH+H=N2+H2			1.00E+14	0.0	0.0
584.	NNH+OH=N2+H2O			5.00E+13	0.0	0.0
585.	NNH+NH2=N2+NH3			5.00E+13	0.0	0.0
586.	NNH+NH=N2+NH2			5.00E+13	0.0	0.0
587.	NNH+O=N2O+H			1.00E+14	0.0	0.0
588.	NNH+O=N2+OH			8.00E+13	0.0	0.0
589.	NNH+O=NH+NO			5.00E+13	0.0	0.0
590.	NNH+O2=N2+HO2			2.00E+14	0.0	0.0

591.	NNH+O2=N2+O2+H			5.00E+13	0.0	0.0
592.	HNO+O=NO+OH			1.00E+13	0.0	0.0
593.	HNO+OH=NO+H2O			3.60E+13	0.0	0.0
594.	HNO+H=NO+H2			4.40E+11	0.7	650.0
595.	HNO+NH2=NO+NH3			2.00E+13	0.0	1000.0
596.	HNO+N=NO+NH			1.00E+13	0.0	1990.0
597.	HNO+NO2=NO+HONO			6.00E+11	0.0	2000.0
598.	HNO+HNO=N2O+H2O			3.95E+12	0.0	5000.0
599.	HNO+NO=N2O+OH			2.00E+12	0.0	26000.0
600.	N2H2+M=NNH+H+M			5.00E+16	0.0	50000.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
601.	N2H2+H=NNH+H2			5.00E+13	0.0	1000.0
602.	N2H2+O=NH2+NO			1.00E+13	0.0	1000.0
603.	N2H2+O=NNH+OH			2.00E+13	0.0	1000.0
604.	N2H2+OH=NNH+H2O			1.00E+13	0.0	1000.0
605.	N2H2+NO=N2O+NH2			3.00E+12	0.0	0.0
606.	N2H2+NH=NNH+NH2			1.00E+13	0.0	1000.0
607.	N2H2+NH2=NH3+NNH			1.00E+13	0.0	1000.0
608.	NO2+OH=NO+HO2			1.36E+13	0.0	7612.2
	Reverse Arrhenius coefficients:			3.11E+12	0.0	516.6
609.	NO+OH(+M)=HONO(+M)			2.00E+12	-0.1	-721.0
	Low pressure limit:	0.50800E+24	-0.25100E+01	-0.67600E+02		
	TROE centering:	0.62000E+00	0.10000E+02	0.10000E+06		
	H2O	Enhanced by	1.000E+01			
	O2	Enhanced by	2.000E+00			
	H2	Enhanced by	2.000E+00			
	H2O	Enhanced by	5.000E+00			
610.	NO+H+M=HNO+M			4.00E+20	-1.8	0.0
	H2O	Enhanced by	4.100E+00			
	H2	Enhanced by	1.250E+00			
	N2	Enhanced by	1.600E+00			
611.	NO+HCO=HNO+CO			7.20E+12	0.0	0.0
612.	NO2+H2=HONO+H			2.40E+13	0.0	29000.0
613.	NO2+H=NO+OH			1.00E+14	0.0	362.0

614.	NO2+O=NO+O2			1.00E+13	0.0	600.0
615.	NO2+M=NO+O+M			1.10E+16	0.0	66000.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
616.	NO2+NO2=NO+NO+O2			2.00E+12	0.0	26825.0
617.	NO2+HO2=HONO+O2			6.30E+08	1.2	5000.0
618.	NO2+HCO=CO+NO+OH			9.45E+12	0.0	-430.0
619.	NO2+HCO=H+CO2+NO			5.55E+12	0.0	-430.0
620.	NO2+CO=NO+CO2			2.19E+13	0.0	29200.0
621.	NO2+NO=N2O+O2			1.00E+12	0.0	60000.0
622.	NO2+CH2=NO+CH2O			5.90E+13	0.0	0.0
623.	NO2+CH=NO+HCO			1.00E+14	0.0	0.0
624.	N2O+OH=N2+HO2			2.00E+12	0.0	40000.0
625.	N2O+H=N2+OH			2.08E-06	5.6	1820.0
626.	N2O+M=N2+O+M			3.00E+14	0.0	55500.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
627.	N2O+O=N2+O2			1.40E+12	0.0	10800.0
628.	N2O+O=NO+NO			2.90E+13	0.0	23150.0
629.	N2O+N=N2+NO			1.00E+13	0.0	19870.0
630.	N2O+CO=N2+CO2			2.70E+11	0.0	20237.0
631.	N2O+NO=NO2+N2			5.30E+05	2.2	46281.0
632.	N2O+CH=HCN+NO			1.90E+13	0.0	-511.0
633.	C+N2O=CN+NO			5.10E+12	0.0	0.0
634.	C+NO=CN+O			2.00E+13	0.0	0.0
635.	C+NO=CO+N			2.80E+13	0.0	0.0
636.	CH+NO=HCN+O			4.80E+13	0.0	0.0
637.	CH+NO=HCO+N			3.40E+13	0.0	0.0
638.	CH+NO=NCO+H			1.90E+13	0.0	0.0
639.	CH2(S)+NO=CH2+NO			1.00E+14	0.0	0.0
640.	CH2(S)+NO=HCN+OH			2.00E+13	0.0	0.0
641.	CH2+NO=HCNO+H			1.30E+12	0.0	-378.0

642.	CH2+NO=HCN+OH	2.20E+12	0.0	-378.0
643.	CH3+NO=HCN+H2O	1.50E-01	3.5	3950.0
644.	CH3+NO=H2CN+OH	1.50E-01	3.5	3950.0
645.	C2H3+NO=C2H2+HNO	1.00E+12	0.0	1000.0
646.	C2H+NO=CN+HCO	2.10E+13	0.0	0.0
647.	HCCO+NO=HCNO+CO	4.89E+12	0.1	-584.0
648.	HCCO+NO=HCN+CO2	1.64E+13	-0.3	-707.0
649.	HCNO+H=HCN+OH	5.70E+12	0.0	0.0
650.	HCNO+O=NO+HCO	7.00E+13	0.0	0.0
651.	HCNO+OH=NO+CH2O	2.00E+13	0.0	0.0
652.	HOCN+OH=NCO+H2O	6.40E+05	2.0	2560.0
653.	HOCN+O=NCO+OH	1.50E+04	2.6	4000.0
654.	HOCN+H=HNCO+H	2.00E+07	2.0	2000.0
655.	HOCN+H=NCO+H2	2.00E+07	2.0	2000.0
656.	HNCO+M=NH+CO+M	1.10E+16	0.0	86000.0
657.	HNCO+HO2=NCO+H2O2	3.00E+11	0.0	29000.0
658.	HNCO+O2=HNO+CO2	1.00E+12	0.0	35000.0
659.	HNCO+NH2=NH3+NCO	5.00E+12	0.0	6200.0
660.	HNCO+NH=NH2+NCO	3.00E+13	0.0	23700.0
661.	HNCO+H=NH2+CO	2.20E+07	1.7	3800.0
662.	HNCO+CN=NCO+HCN	2.50E+12	0.0	0.0
663.	HNCO+O=NCO+OH	2.20E+06	2.1	11430.0
664.	HNCO+O=CO2+NH	9.65E+07	1.4	8520.0
665.	HNCO+O=HNO+CO	1.50E+08	1.6	44012.0
666.	HNCO+OH=NCO+H2O	4.20E+05	2.0	2560.0
667.	HCN+OH=CN+H2O	3.20E+06	1.8	10300.0
668.	HCN+OH=HOCN+H	5.85E+04	2.4	12500.0
669.	HCN+OH=HNCO+H	4.00E-03	4.0	1000.0
670.	HCN+OH=NH2+CO	7.83E-04	4.0	4000.0
671.	HCN+O=NCO+H	1.38E+04	2.6	4980.0
672.	HCN+O=NH+CO	3.45E+03	2.6	4980.0
673.	HCN+O=CN+OH	2.70E+09	1.6	29200.0
674.	CN+OH=NH+CO	6.00E+12	0.0	0.0
675.	CN+OH=HNCO	6.00E+12	0.0	0.0
676.	CN+OH=NCO+H	6.00E+13	0.0	0.0
677.	CN+NO=NCO+N	9.64E+13	0.0	42100.0
678.	CN+NO=CO+N2	9.64E+13	0.0	42100.0
679.	CN+HNO=HCN+NO	1.80E+13	0.0	0.0

680.	CN+HONO=HCN+NO2			1.20E+13	0.0	0.0
681.	CN+H2=HCN+H			3.00E+05	2.5	2237.0
682.	CN+O=CO+N			7.70E+13	0.0	0.0
683.	CN+O2=NCO+O			7.50E+12	0.0	-389.0
684.	CN+N=C+N2			1.04E+15	-0.5	0.0
685.	CN+HCN=C2N2+H			1.50E+07	1.7	1530.0
686.	CN+NO2=NCO+NO			5.30E+15	-0.8	344.0
687.	CN+NO2=CO+N2O			4.90E+14	-0.8	344.0
688.	CN+NO2=N2+CO2			3.70E+14	-0.8	344.0
689.	CN+N2O=NCO+N2			1.00E+13	0.0	0.0
690.	CN+N2O=NCN+NO			3.80E+03	2.6	3700.0
691.	CN+CO2=NCO+CO			3.70E+06	2.2	26900.0
692.	CN+CH2O=HCN+HCO			4.22E+13	0.0	0.0
693.	C2N2+O=NCO+CN			4.57E+12	0.0	8880.0
694.	C2N2+OH=HOCN+CN			1.86E+11	0.0	2900.0
695.	NCO+H=NH+CO			5.00E+13	0.0	0.0
696.	NCO+CH2O=HNCO+HCO			6.02E+12	0.0	0.0
697.	NCO+HCO=HNCO+CO			3.62E+13	0.0	0.0
698.	NCO+NO=N2O+CO			5.23E+17	-1.7	763.0
699.	NCO+NO=CO2+N2			4.11E+17	-1.7	763.0
700.	NCO+NO2=CO+NO+NO			1.39E+13	0.0	0.0
701.	NCO+NO2=CO2+N2O			5.40E+12	0.0	0.0
702.	NCO+HNO=HNCO+NO			1.80E+13	0.0	0.0
703.	NCO+HONO=HNCO+NO2			3.60E+12	0.0	0.0
704.	NCO+N2O=N2+NO+CO			9.00E+13	0.0	27800.0
705.	NCO+NCO=N2+CO+CO			1.80E+13	0.0	0.0
706.	NCO+O=NO+CO			2.00E+13	0.0	0.0
707.	NCO+N=N2+CO			2.00E+13	0.0	0.0
708.	NCO+OH=HCO+NO			5.00E+12	0.0	15000.0
709.	NCO+M=N+CO+M			3.10E+16	-0.5	48000.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
710.	NCO+H2=HNCO+H			7.60E+02	3.0	4000.0
711.	NCO+O2=NO+CO2			2.00E+12	0.0	20000.0
712.	NCO+CN=NCN+CO			1.80E+13	0.0	0.0

713.	NCN+H=HCN+N			1.00E+14	0.0	0.0
714.	NCN+O=CN+NO			1.00E+14	0.0	0.0
715.	NCN+OH=HCN+NO			5.00E+13	0.0	0.0
716.	NCN+O2=NO+NCO			1.00E+13	0.0	0.0
717.	H2NO+O=NH2+O2			2.00E+14	0.0	0.0
718.	H2NO+M=H2+NO+M			7.83E+27	-4.3	60300.0
	H2O	Enhanced by	1.000E+01			
719.	H2NO+M=HNO+H+M			2.80E+24	-2.8	64915.0
	H2O	Enhanced by	1.000E+01			
720.	H2NO+HO2=HNO+H2O2			2.90E+04	2.7	-1600.0
721.	H2NO+O2=HNO+HO2			3.00E+12	0.0	25000.0
722.	H2NO+H=HNO+H2			3.00E+07	2.0	2000.0
723.	H2NO+H=NH2+OH			5.00E+13	0.0	0.0
724.	H2NO+O=HNO+OH			3.00E+07	2.0	2000.0
725.	H2NO+OH=HNO+H2O			2.00E+07	2.0	1000.0
726.	H2NO+NO=HNO+HNO			2.00E+04	2.0	13000.0
727.	H2NO+NH2=HNO+NH3			3.00E+12	0.0	1000.0
728.	HONO+O=NO2+OH			1.20E+13	0.0	6000.0
729.	HONO+OH=NO2+H2O			1.30E+10	1.0	135.0
730.	HONO+NH2=NO2+NH3			7.11E+01	3.0	-4941.0
731.	CH2+N2=HCN+NH			1.00E+13	0.0	74000.0
732.	CH+N2=HCN+N			3.00E+11	0.0	13600.0
733.	CH2+N=HCN+H			5.00E+13	0.0	0.0
734.	CH+N=CN+H			1.30E+13	0.0	0.0
735.	CO2+N=CO+NO			1.90E+11	0.0	3400.0
736.	CH3+N=H2CN+H			3.00E+13	0.0	0.0
737.	C2H3+N=HCN+CH2			2.00E+13	0.0	0.0
738.	H2CCCH+N=HCN+C2H2			1.00E+13	0.0	0.0
739.	H2CN+N=N2+CH2			2.00E+13	0.0	0.0
740.	H2CN+M=HCN+H+M			3.00E+14	0.0	22000.0
	H2O	Enhanced by	1.625E+01			
	CO	Enhanced by	1.875E+00			
	CO2	Enhanced by	3.750E+00			
	CH4	Enhanced by	1.625E+01			
	C2H6	Enhanced by	1.625E+01			
741.	CH2O+NO2=HCO+HONO			8.00E+02	2.8	13730.0
742.	HCO+HNO=CH2O+NO			6.00E+11	0.0	2000.0
743.	HONO+HONO=H2O+NO+NO2			3.49E-01	3.6	12140.0

744.	NCO+CH4=HNCO+CH3	1.00E+13	0.0	8126.0
745.	NCO+C2H6=HNCO+C2H5	1.45E-09	6.9	2916.0
746.	CH3O+HNO=CH3OH+NO	3.16E+13	0.0	0.0
747.	CH2HCO+NO2=CH2O+HCO+NO	8.90E+12	0.0	-159.0
748.	C3H8+NO=NC3H7+HNO	5.00E+13	0.0	51000.0
749.	C3H8+NO=IC3H7+HNO	5.00E+13	0.0	51000.0
750.	C3H8+CN=NC3H7+HCN	2.32E+11	0.8	-217.0
751.	C3H8+CN=IC3H7+HCN	2.00E+11	0.6	-648.0
752.	NCO+HO2=HNCO+O2	5.00E+13	0.0	0.0
753.	NCO+HOCN=HNCO+NCO	5.00E+13	0.0	0.0
754.	CH3+NO(+M)=CH3NO(+M)	2.20E+11	0.6	0.0
	Low pressure limit: 0.20600E+28 -0.35000E+01 0.00000E+00			
755.	CH3NO2(+M)=CH3+NO2(+M)	1.78E+16	0.0	59000.0
	Low pressure limit: 0.12600E+18 0.00000E+00 0.42000E+05			
756.	CH3+NO2=CH3O+NO	1.51E+13	0.0	0.0
757.	CH3O+NO2=CH2O+HONO	6.02E+12	0.0	2285.0
758.	CH3O+NO2(+M)=CH3ONO2(+M)	1.20E+13	0.0	0.0
	Low pressure limit: 0.14000E+31 -0.45000E+01 0.00000E+00			
759.	CH3O+NO=CH2O+HNO	1.30E+14	-0.7	0.0
760.	CH3O2+NO=CH3O+NO2	2.53E+12	0.0	-358.5
761.	CH3NO2+O=H2CNO2+OH	1.51E+13	0.0	5350.0
762.	CH3NO2+OH=H2CNO2+H2O	1.49E+13	0.0	5740.0
763.	CH3NO2+OH=CH3OH+NO2	2.00E+10	0.0	-1000.0
764.	CH3NO2+O2=H2CNO2+HO2	2.00E+13	0.0	57000.0
765.	CH3NO2+CH2(S)=CH3+H2CNO2	1.20E+14	0.0	0.0
766.	CH3NO2+CH2=CH3+H2CNO2	6.50E+12	0.0	7900.0
767.	CH3NO2+H=H2CNO2+H2	7.50E+12	0.0	10000.0
768.	CH3NO2+H=HONO+CH3	3.27E+12	0.0	3730.0
769.	CH3NO2+H=CH3NO+OH	1.40E+12	0.0	3730.0
770.	CH3NO2+CH3=H2CNO2+CH4	7.08E+11	0.0	11140.0
771.	CH3NO2+CH3O=H2CNO2+CH3OH	3.00E+11	0.0	7000.0
772.	CH3NO2+C2H5=H2CNO2+C2H6	3.00E+11	0.0	11700.0
773.	CH3NO2+HO2=H2CNO2+H2O2	1.50E+11	0.0	15000.0
774.	H2CNO2=CH2O+NO	1.00E+13	0.0	36000.0
775.	H2CNO2+HONO=CH3NO2+NO2	1.00E+12	0.0	0.0
776.	H2CNO2+H=CH3+NO2	5.00E+13	0.0	0.0
777.	H2CNO2+O=CH2O+NO2	5.00E+13	0.0	0.0
778.	H2CNO2+OH=CH2OH+NO2	1.00E+13	0.0	0.0

779.	H2CNO2+OH=CH2O+HONO	1.00E+13	0.0	0.0
780.	CH3O+NO(+M)=CH3ONO(+M)	1.21E+13	0.0	-332.0
	Low pressure limit: 0.27000E+28 -0.35000E+01 0.00000E+00			
781.	CH3NO2=CH3ONO	2.90E+14	0.0	67000.0
782.	C2H5+NO2=C2H5O+NO	1.00E+13	0.0	0.0
783.	C2H5O+NO2=CH3HCO+HONO	4.00E+11	0.0	0.0
784.	C2H5O+NO=CH3HCO+HNO	1.30E+14	-0.7	0.0
785.	C2H5O2+NO=C2H5O+NO2	3.00E+12	0.0	-358.0
786.	HO2+NO+M=HONO2+M	2.23E-12	-3.5	2200.0
787.	NO2+OH(+M)=HONO2(+M)	3.61E+13	0.0	0.0
	Low pressure limit: 0.14400E+26 -0.29000E+01 0.00000E+00			
788.	HONO2+OH=H2O+NO3	1.03E+10	0.0	-1240.0
789.	NO3+OH=HO2+NO2	1.38E+13	0.0	0.0
790.	NO3+O=O2+NO2	1.02E+13	0.0	0.0
791.	NO3+H=NO2+OH	6.00E+13	0.0	0.0
792.	NO3+HO2=O2+HONO2	5.60E+11	0.0	0.0
793.	NO3+HO2=O2+OH+NO2	2.00E+12	0.0	0.0
794.	NO3+NO3=O2+NO2+NO2	5.12E+11	0.0	4840.0
795.	NO3+M=O2+NO+M	2.05E+08	1.0	12122.0
796.	NO3+NO2=NO2+NO+O2	2.35E+10	0.0	2960.0
797.	NO3+NO=NO2+NO2	1.08E+13	0.0	-219.0
798.	NO2+O(+M)=NO3(+M)	1.20E+13	0.0	0.0
	Low pressure limit: 0.29400E+22 -0.20000E+01 0.00000E+00			
799.	NO2+O3=NO3+O2	7.23E+10	0.0	4870.0
800.	O+O2+M=O3+M	1.88E+21	-2.8	0.0
801.	O+O3=O2+O2	4.80E+12	0.0	4090.0
802.	H+O3=OH+O2	8.43E+13	0.0	950.0
803.	OH+O3=HO2+O2	1.14E+12	0.0	2000.0
804.	NO+O3=NO2+O2	1.08E+12	0.0	2720.0
805.	HO2+O3=OH+O2+O2	8.43E+09	0.0	1200.0
806.	CH3+O3=CH3O+O2	1.57E+12	0.0	0.0
807.	CH3+HONO=CH4+NO2	8.10E+05	1.9	5504.0
808.	C2H5+HONO=C2H6+NO2	8.10E+05	1.9	5504.0
809.	C2H3+HONO=C2H4+NO2	8.10E+05	1.9	5504.0
810.	CH3O+HONO=CH3OH+NO2	8.10E+05	1.9	5504.0
811.	CH3O2H+H=CH3O2+H2	8.80E+10	0.0	1860.0
812.	CH3O2H+H=CH3O+H2O	8.20E+10	0.0	1860.0
813.	CH3O2H+O=CH3O2+OH	1.00E+12	0.0	3000.0

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814. CH3O2H+OH=CH3O2+H2O                    1.80E+12    0.0     -378.0
815. C2H4+OH=C2H4OH                         1.29E+12    0.0     -817.0
816. C2H4OH+O2=HOC2H4O2                     1.00E+12    0.0    -1100.0
817. HOC2H4O2=CH2O+CH2O+OH                  6.00E+10    0.0    24500.0
818. HOC2H4O2+NO=CH2OH+CH2O+NO2             2.53E+12    0.0     -358.0
```

III. Ab-initio calculations for estimating the $\Delta H_f^0{}_{298K}$ for CH_3NO_2

Ab-initio electronic structure calculations were performed using the Gaussian 03[1] suite of programs. Input structures were generated using CHEM3D, a part of the CHEMOFFICE[2] suite of programs. MOLEKEL[3] and gOPENMOL[4] were used to visualize the minima. $\Delta H_f^0{}_{298K}$ was computed using energetics at G3[5] and G3B3[6] levels of theory. We have adopted the use of atomization as well as a balanced isodesmic reactions (Reaction R1) using CH_3NO, NO, NO_2, N_2O and N_2 as reference species to account for the incomplete cancellation of electron correlation energy when estimating heats of reaction (ΔH_r) and subsequently the heats of formation (ΔH_f^0).

$$CH_3NO_2 + 2NO + N_2O = CH_3NO + 2NO_2 + N_2 \qquad (R1)$$

Such isodesmic schemes[7] are known to obtain accurate ΔH_f^0 as long as the reference species have well characterized ΔH_f^0. ΔH_f^0 for the reference species in R1 were taken from the Burcat and Ruscic compilations[8]. Heats of formation were calculated using the procedure outlined by Notario et al.[9]. The lowest frequency mode (23 cm^{-1} at B3LYP/6-31G(d) and 20 cm^{-1} at HF/6-31G(d) levels of theory) in CH_3NO_2 was treated as a free rotor when calculating the contributions to the integrated heat capacity H(T)-H(0).

Table 1: Heats of formation from ab-initio calculations

Level of Theory	CH_3NO_2 $\Delta H_f^0{}_{298K}$ (kcal/mol)	CH_3NO_2 $\Delta H_f^0{}_{0K}$ (kcal/mol)
G3-Atomization	-18.076	-14.751
G3-Isodesmic R1	-19.117	-15.791
G3B3-Atomization	-18.766	-15.478
G3B3-Isodesmic R1	-18.623	-15.335

Molecular properties for CH_3NO_2

Optimized geometry (B3LYP/6-31G(d))

C	0.435985	0.857575	0.104389
N	-0.207145	-0.433975	-0.303552
O	0.432362	-1.466956	-0.135613
O	-1.334607	-0.354634	-0.780998
H	-0.225485	1.333593	0.829522
H	0.506444	1.479184	-0.789492
H	1.414357	0.637900	0.525647

Vibrational frequencies (Unscaled B3LYP/6-31G(d))
23.6, 477.5, 616.3, 657.3, 928.7, 1119.0, 1144.2, 1419.2, 1445.1, 1491.4, 1501.4, 1681.2, 3103.2, 3192.8, 3226.9

Moments of inertia I_a, I_b, I_c (gm-cm^2) $*$ 1$*10^{-39}$ (Obtained using B3LYP/6-31G(d) geometry)
6.8819, 7.9977, 14.3477

Reduced moment of inertia for CH_3 internal rotation I_r (gm-cm^2) $*$ 1$*10^{-39}$
0.49899

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