

Let allowed atoms be C, H, O, N, AR.

Let additional species be N2.

Let temperature exponent be n\_k.

Let order of reaction be n.

Let units for A be [ cm<sup>3(n-1)</sup> / ( s \* mole<sup>(n-1)</sup> \* K<sup>n\_k</sup> ) ].

Let units for E be [ kJ / mole ].

Let symbol for soot be SOOT.

# --- H reactions --- #

5: 2 H + M1 -> H2 + M1 { a = 1.780e+18 n = -1.000 E = 0.000 }

# --- Excited species reactions --- #

32: N2O + H -> OH\* + N2 { a = 1.600e+14 n = 0.000 E = 210.455 }  
 # R119: H + O + M -> OH\* + M { a = 6.000e+14 n = 0.000 E = 29.037 }  
 # R120: OH\* + AR -> OH + AR { a = 2.170e+10 n = 0.500 E = 8.619 }  
 # R121: OH\* + H2O -> OH + H2O { a = 5.920e+12 n = 0.500 E = -3.602 }  
 # R122: OH\* + H -> OH + H { a = 1.500e+12 n = 0.500 E = 0.000 }  
 # R123: OH\* + H2 -> OH + H2 { a = 2.950e+12 n = 0.500 E = -1.857 }  
 # R124: OH\* + O2 -> OH + O2 { a = 2.100e+12 n = 0.500 E = -2.017 }  
 # R125: OH\* + O -> OH + O { a = 1.500e+12 n = 0.500 E = 0.000 }  
 # R126: OH\* + OH -> OH + OH { a = 1.500e+12 n = 0.000 E = 0.000 }  
 # R127: OH\* -> OH { a = 1.400e+06 n = 0.000 E = 0.000 }  
 # R128: CH + O2 -> OH\* + CO { a = 3.240e+14 n = -0.400 E = 17.363 }  
 # R129: OH\* + CO2 -> OH + CO2 { a = 2.750e+12 n = 0.500 E = -4.050 }  
 # R130: OH\* + CO -> OH + CO { a = 3.230e+12 n = 0.500 E = -3.293 }  
 # R131: OH\* + CH4 -> OH + CH4 { a = 3.360e+12 n = 0.500 E = -2.657 }  
 # R132: C2 + OH -> CO + CH\* { a = 1.110e+13 n = 0.000 E = 0.000 }  
 # R133: C2H + O -> CO + CH\* { a = 6.200e+12 n = 0.000 E = 0.000 }  
 # R134: C2H + O2 -> CO2 + CH\* { a = 2.170e+10 n = 0.000 E = 0.000 }  
 # R135: C + H + M -> CH\* + M { a = 3.630e+13 n = 0.000 E = 0.000 }  
 # R136: CH\* -> CH { a = 1.860e+06 n = 0.000 E = 0.000 }  
 # R137: CH\* + AR -> CH + AR { a = 4.000e+10 n = 0.500 E = 0.000 }  
 # R138: CH\* + O2 -> CH + O2 { a = 2.480e+06 n = 2.140 E = -7.196 }  
 # R139: CH\* + H2O -> CH + H2O { a = 5.6300e+13 n = 0.000 E = 0.000 }  
 # R140: CH\* + H2 -> CH + H2 { a = 1.470e+14 n = 0.000 E = 5.690 }  
 # R141: CH\* + CO2 -> CH + CO2 { a = 2.410e-01 n = 4.300 E = -7.087 }  
 # R142: CH\* + CO -> CH + CO { a = 2.440e+12 n = 0.500 E = 0.000 }  
 # R143: CH\* + CH4 -> CH + CH4 { a = 1.730e+13 n = 0.000 E = 0.698 }

# --- O reactions --- #

10: H + O + M3 -> OH + M3 { a = 9.430e+18 n = -1.000 E = 0.000 }

2f: O + H2 -> H + OH { a = 4.590e+04 n = 2.700 E = 26.190 }

# --- OH reactions --- #

14f:  $2 \text{ OH} + \text{M6} \rightarrow \text{H}_2\text{O}_2 + \text{M6}$  { a = 2.010e+17 n = -0.580 E = -9.590  
     ai = 1.110e+14 ni = -0.370 Ei = 0.000  
     fca = 2.654e-01 fcta = 9.400e+01 fcb = 7.346e-01 fctb = 1.756e+03 fcc = 1.000e+00 fctc =  
     5.182e+03 }

9f:  $\text{H} + \text{OH} + \text{M2} \rightarrow \text{H}_2\text{O} + \text{M2}$  { a = 4.400e+22 n = -2.000 E = 0.000 }

3f:  $\text{OH} + \text{H}_2 \rightarrow \text{H} + \text{H}_2\text{O}$  { a = 1.730e+08 n = 1.510 E = 14.350 }

4f:  $2 \text{ OH} \rightarrow \text{O} + \text{H}_2\text{O}$  { a = 3.970e+04 n = 2.400 E = -8.830 }

# --- H2O reactions --- #

7:  $2 \text{ H} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{H}_2\text{O}$  { a = 5.620e+19 n = -1.250 E = 0.000 }

# --- O2 reactions --- #

13f:  $\text{H}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{H}$  { a = 5.920e+05 n = 2.430 E = 223.850 }

1f:  $\text{H} + \text{O}_2 \rightarrow \text{O} + \text{OH}$  { a = 2.640e+16 n = -0.670 E = 71.300 }

12f:  $\text{H} + \text{O}_2 + \text{M5} \rightarrow \text{HO}_2 + \text{M5}$  { a = 6.330e+19 n = -1.400 E = 0.000  
     ai = 5.120e+12 ni = 0.440 Ei = 0.000  
     fca = 5.000e-01 fcta = 1.000e-10 fcb = 5.000e-01 fctb = 1.000e+10 fcc = 0.000e+00 fctc =  
     0.000e+00 }

# --- HO2 reactions --- #

18f:  $\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$  { a = 2.890e+13 n = 0.000 E = -2.100 }

15:  $\text{HO}_2 + \text{H} \rightarrow \text{O} + \text{H}_2\text{O}$  { a = 3.970e+12 n = 0.000 E = 2.810 }

21f:  $2 \text{ HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}_2$  { a = 3.660e+14 n = 0.000 E = 50.210 }

17f:  $\text{HO}_2 + \text{O} \rightarrow \text{OH} + \text{O}_2$  { a = 4.000e+13 n = 0.000 E = 0.000 }

16f:  $\text{HO}_2 + \text{H} \rightarrow 2 \text{ OH}$  { a = 7.490e+13 n = 0.000 E = 1.230 }

20f:  $2 \text{ HO}_2 \rightarrow \text{O}_2 + \text{H}_2\text{O}_2$  { a = 1.300e+11 n = 0.000 E = -6.820 }

# --- H2O2 reactions --- #

22f:  $\text{H}_2\text{O}_2 + \text{H} \rightarrow \text{HO}_2 + \text{H}_2$  { a = 6.050e+06 n = 2.000 E = 21.760 }

24:  $\text{H}_2\text{O}_2 + \text{O} \rightarrow \text{HO}_2 + \text{OH}$  { a = 9.630e+06 n = 2.000 E = 16.610 }

23:  $\text{H}_2\text{O}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{OH}$  { a = 2.410e+13 n = 0.000 E = 16.610 }

25f:  $\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{H}_2\text{O}$  { a = 1.740e+12 n = 0.000 E = 1.330 }

26f:  $\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{H}_2\text{O}$  { a = 7.590e+13 n = 0.000 E = 29.770 }

# --- CH reactions --- #

G04:  $\text{CH} + \text{O} \rightarrow \text{CO} + \text{H}$  { a = 5.700e+13 n = 0.000 E = 0.000 }

G09:  $\text{CH} + \text{O}_2 \rightarrow \text{HCO} + \text{O}$  { a = 6.710e+13 n = 0.000 E = 0.000 }

G06f:  $\text{CH} + \text{H}_2 \rightarrow \text{T-CH}_2 + \text{H}$  { a = 1.080e+14 n = 0.000 E = 13.010 }

G08:  $\text{CH} + \text{H}_2\text{O} \rightarrow \text{CH}_2\text{O} + \text{H}$  { a = 5.710e+12 n = 0.000 E = -3.160 }

G05:  $\text{CH} + \text{OH} \rightarrow \text{HCO} + \text{H}$  { a = 3.000e+13 n = 0.000 E = 0.000 }

G07:  $\text{CH} + \text{H}_2 + \text{M9} \rightarrow \text{CH}_3 + \text{M9}$  { a = 4.820e+25 n = -2.800 E = 2.470  
     ai = 1.970e+12 ni = 0.430 Ei = -1.550  
     fca = 4.220e-01 fcta = 1.220e+02 fcb = 5.780e-01 fctb = 2.535e+03 fcc = 1.000e+00 fctc =

9.365e+03 }

# --- T-CH2 reactions --- #

G16: T-CH2 + OH -> CH2O + H { a = 2.000e+13 n = 0.000 E = 0.000 }  
 G26: 2 T-CH2 -> C2H2 + H2 { a = 1.600e+15 n = 0.000 E = 49.970 }  
 G20: T-CH2 + O2 -> HCO + OH { a = 1.060e+13 n = 0.000 E = 6.280 }  
 G14: T-CH2 + H + M9 -> CH3 + M9 { a = 1.040e+26 n = -2.760 E = 6.690  
       ai = 6.000e+14 ni = 0.000 Ei = 0.000  
       fca = 4.380e-01 fcta = 9.100e+01 fcb = 5.620e-01 fctb = 5.836e+03 fcc = 1.000e+00 fctc =  
       8.552e+03 }  
 G22: T-CH2 + HO2 -> CH2O + OH { a = 2.000e+13 n = 0.000 E = 0.000 }  
 G15: T-CH2 + O -> HCO + H { a = 8.000e+13 n = 0.000 E = 0.000 }  
 G17f: T-CH2 + OH -> CH + H2O { a = 1.130e+07 n = 2.000 E = 12.550 }  
 G18f: T-CH2 + H2 -> H + CH3 { a = 5.000e+05 n = 2.000 E = 30.250 }  
 G19: T-CH2 + O2 -> CO2 + 2 H { a = 2.640e+12 n = 0.000 E = 6.280 }  
 G25: T-CH2 + CH -> C2H2 + H { a = 4.000e+13 n = 0.000 E = 0.000 }  
 G27: 2 T-CH2 -> C2H2 + 2 H { a = 2.000e+14 n = 0.000 E = 45.980 }

# --- S-CH2 reactions --- #

G32: S-CH2 + O -> HCO + H { a = 1.500e+13 n = 0.000 E = 0.000 }  
 G35: S-CH2 + O2 -> H + OH + CO { a = 2.800e+13 n = 0.000 E = 0.000 }  
 G39: S-CH2 + H2O -> H2 + CH2O { a = 6.820e+10 n = 0.250 E = -3.910 }  
 G31: S-CH2 + O -> CO + H2 { a = 1.500e+13 n = 0.000 E = 0.000 }  
 G38f: S-CH2 + H2O -> T-CH2 + H2O { a = 3.000e+13 n = 0.000 E = 0.000 }  
 G34f: S-CH2 + H2 -> CH3 + H { a = 7.000e+13 n = 0.000 E = 0.000 }  
 G36: S-CH2 + O2 -> CO + H2O { a = 1.200e+13 n = 0.000 E = 0.000 }  
 G33: S-CH2 + OH -> CH2O + H { a = 3.000e+13 n = 0.000 E = 0.000 }  
 G30f: S-CH2 + H -> CH + H2 { a = 3.000e+13 n = 0.000 E = 0.000 }

# --- CH3 reactions --- #

G69: CH3 + CH -> C2H3 + H { a = 3.000e+13 n = 0.000 E = 0.000 }  
 G72: CH3 + T-CH2 -> C2H4 + H { a = 1.000e+14 n = 0.000 E = 0.000 }  
 G67f: CH3 + H2O2 -> CH4 + HO2 { a = 2.450e+04 n = 2.470 E = 21.670 }  
 G74f: 2 CH3 -> C2H5 + H { a = 6.840e+12 n = 0.100 E = 44.350 }  
 G52: CH3 + O -> CH2O + H { a = 5.540e+13 n = 0.050 E = -0.570 }  
 G66f: CH3 + HO2 -> CH4 + O2 { a = 3.610e+12 n = 0.000 E = 0.000 }  
 G51f: CH3 + H + M9 -> CH4 + M9 { a = 3.470e+38 n = -6.300 E = 21.230  
       ai = 6.920e+13 ni = 0.180 Ei = 0.000  
       fca = 2.170e-01 fcta = 7.400e+01 fcb = 7.830e-01 fctb = 2.941e+03 fcc = 1.000e+00 fctc =  
       6.964e+03 }  
 G57f: CH3 + OH -> S-CH2 + H2O { a = 6.440e+17 n = -1.340 E = 5.930 }  
 G56: CH3 + OH -> H2 + CH2O { a = 8.000e+09 n = 0.000 E = -7.340 }  
 G65: CH3 + HO2 -> CH3O + OH { a = 1.000e+13 n = 0.000 E = 0.000 }  
 G55f: CH3 + OH -> T-CH2 + H2O { a = 5.600e+07 n = 1.600 E = 22.680 }  
 G59: CH3 + O2 -> CH2O + OH { a = 5.870e+11 n = 0.000 E = 57.910 }  
 G73: CH3 + S-CH2 -> C2H4 + H { a = 1.200e+13 n = 0.000 E = -2.390 }  
 G60f: CH3 + O2 + M0 -> CH3O2 + M0 { a = 3.820e+31 n = -4.890 E = 14.360  
       ai = 1.010e+08 ni = 1.630 Ei = 0.000

fca = 9.550e-01 fcta = 8.801e+02 fcb = 4.500e-02 fctb = 2.500e+09 fcc = 1.000e+00 fctc = 1.786e+09 }

G58f: CH3 + O2 -> CH3O + O { a = 1.380e+13 n = 0.000 E = 127.700 }

# --- CH4 reactions --- #

G90f: CH4 + H -> CH3 + H2 { a = 6.600e+08 n = 1.620 E = 45.360 }

G94f: CH4 + T-CH2 -> 2 CH3 { a = 2.460e+06 n = 2.000 E = 34.600 }

G91f: CH4 + O -> CH3 + OH { a = 1.020e+09 n = 1.500 E = 35.980 }

G93: CH4 + CH -> C2H4 + H { a = 6.000e+13 n = 0.000 E = 0.000 }

G92f: CH4 + OH -> CH3 + H2O { a = 1.000e+08 n = 1.600 E = 13.050 }

G95f: CH4 + S-CH2 -> 2 CH3 { a = 1.600e+13 n = 0.000 E = -2.390 }

# --- CO reactions --- #

31: CO + HO2 -> CO2 + OH { a = 3.010e+13 n = 0.000 E = 96.230 }

29f: CO + OH -> CO2 + H { a = 8.780e+10 n = 0.030 E = -0.070 }

G40f: S-CH2 + CO -> T-CH2 + CO { a = 9.000e+12 n = 0.000 E = 0.000 }

G10f: CH + CO + M9 -> HCCO + M9 { a = 2.690e+28 n = -3.740 E = 8.100 }

ai = 5.000e+13 ni = 0.000 Ei = 0.000

fca = 4.243e-01 fcta = 2.370e+02 fcb = 5.757e-01 fctb = 1.652e+03 fcc = 1.000e+00 fctc = 5.069e+03 }

G24f: T-CH2 + CO + M9 -> CH2CO + M9 { a = 2.690e+33 n = -5.110 E = 29.690 }

ai = 8.100e+11 ni = 0.500 Ei = 18.870

fca = 4.093e-01 fcta = 2.750e+02 fcb = 5.907e-01 fctb = 1.226e+03 fcc = 1.000e+00 fctc = 5.185e+03 }

28f: CO + OH -> CO2 + H { a = 8.000e+11 n = 0.140 E = 30.760 }

27: CO + O + M7 -> CO2 + M7 { a = 1.170e+24 n = -2.790 E = 17.540 }

ai = 1.360e+10 ni = 0.000 Ei = 9.970

fca = 0.000e+00 fcta = 0.000e+00 fcb = 0.000e+00 fctb = 0.000e+00 fcc = 1.000e+00 fctc = 0.000e+00 }

30: CO + O2 -> CO2 + O { a = 1.120e+12 n = 0.000 E = 199.580 }

# --- HCO reactions --- #

37f: HCO + H2O -> CO + H + H2O { a = 2.240e+18 n = -1.000 E = 71.130 }

35: HCO + OH -> CO + H2O { a = 3.020e+13 n = 0.000 E = 0.000 }

32f: HCO + H -> CO + H2 { a = 1.200e+14 n = 0.000 E = 0.000 }

33: HCO + O -> CO + OH { a = 3.000e+13 n = 0.000 E = 0.000 }

38f: HCO + O2 -> CO + HO2 { a = 5.310e+10 n = 0.690 E = -0.520 }

G145f: CH3 + HCO -> CH3CHO { a = 5.000e+13 n = 0.000 E = 0.000 }

36f: HCO + M8 -> CO + H + M8 { a = 1.870e+17 n = -1.000 E = 71.130 }

34: HCO + O -> CO2 + H { a = 3.000e+13 n = 0.000 E = 0.000 }

G70: CH3 + HCO -> CH4 + CO { a = 2.650e+13 n = 0.000 E = 0.000 }

# --- CH2O reactions --- #

G48f: CH2O + O2 -> HCO + HO2 { a = 1.000e+14 n = 0.000 E = 167.360 }

G13: CH2O + M9 -> H + HCO + M9 { a = 6.813e+25 n = -2.477 E = 369.290 }

ai = 3.007e+13 ni = 0.573 Ei = 366.420

$fca = 2.176e-01$   $fcta = 2.710e+02$   $fc_b = 7.824e-01$   $fctb = 2.755e+03$   $fcc = 1.000e+00$   $fctc = 6.570e+03$  }

G12: CH<sub>2</sub>O + M<sub>9</sub> → H<sub>2</sub> + CO + M<sub>9</sub> { a = 1.028e+30 n = -3.772 E = 351.866

$ai = 8.717e+09$   $ni = 1.148$   $Ei = 331.996$

$fca = 6.800e-02$   $fcta = 1.970e+02$   $fc_b = 9.320e-01$   $fctb = 1.540e+03$   $fcc = 1.000e+00$   $fctc = 1.030e+04$  }

G45f: CH<sub>2</sub>O + H → HCO + H<sub>2</sub> { a = 5.740e+07 n = 1.900 E = 11.470 }

G49: CH<sub>2</sub>O + HO<sub>2</sub> → HCO + H<sub>2</sub>O<sub>2</sub> { a = 5.600e+06 n = 2.000 E = 50.210 }

G47: CH<sub>2</sub>O + OH → HCO + H<sub>2</sub>O { a = 3.430e+09 n = 1.180 E = -1.870 }

G71: CH<sub>3</sub> + CH<sub>2</sub>O → CH<sub>4</sub> + HCO { a = 3.320e+03 n = 2.810 E = 24.520 }

G43f: CH<sub>2</sub>O + H + M<sub>9</sub> → CH<sub>2</sub>OH + M<sub>9</sub> { a = 1.270e+32 n = -4.820 E = 27.320

$ai = 5.400e+11$   $ni = 0.450$   $Ei = 15.060$

$fca = 2.813e-01$   $fcta = 1.030e+02$   $fc_b = 7.187e-01$   $fctb = 1.291e+03$   $fcc = 1.000e+00$   $fctc = 4.160e+03$  }

G50: CH<sub>2</sub>O + CH → CH<sub>2</sub>CO + H { a = 9.460e+13 n = 0.000 E = -2.160 }

G44f: CH<sub>2</sub>O + H + M<sub>9</sub> → CH<sub>3</sub>O + M<sub>9</sub> { a = 2.200e+30 n = -4.800 E = 23.260

$ai = 5.400e+11$   $ni = 0.450$   $Ei = 10.880$

$fca = 2.420e-01$   $fcta = 9.400e+01$   $fc_b = 7.580e-01$   $fctb = 1.555e+03$   $fcc = 1.000e+00$   $fctc = 4.200e+03$  }

G46: CH<sub>2</sub>O + O → HCO + OH { a = 3.900e+13 n = 0.000 E = 14.810 }

# --- CH<sub>3</sub>O reactions --- #

G79f: CH<sub>3</sub>O + H → S-CH<sub>2</sub> + H<sub>2</sub>O { a = 2.620e+14 n = -0.230 E = 4.480 }

G82: CH<sub>3</sub>O + O<sub>2</sub> → CH<sub>2</sub>O + HO<sub>2</sub> { a = 4.280e-13 n = 7.600 E = -14.770 }

G81: CH<sub>3</sub>O + OH → CH<sub>2</sub>O + H<sub>2</sub>O { a = 5.000e+12 n = 0.000 E = 0.000 }

G78f: CH<sub>3</sub>O + H → CH<sub>3</sub> + OH { a = 1.500e+12 n = 0.500 E = -0.460 }

G77: CH<sub>3</sub>O + H → CH<sub>2</sub>O + H<sub>2</sub> { a = 2.000e+13 n = 0.000 E = 0.000 }

# --- CH<sub>2</sub>OH reactions --- #

G86f: CH<sub>2</sub>OH + H → S-CH<sub>2</sub> + H<sub>2</sub>O { a = 3.280e+13 n = -0.090 E = 2.550 }

G88: CH<sub>2</sub>OH + OH → CH<sub>2</sub>O + H<sub>2</sub>O { a = 5.000e+12 n = 0.000 E = 0.000 }

G84: CH<sub>2</sub>OH + H → CH<sub>2</sub>O + H<sub>2</sub> { a = 2.000e+13 n = 0.000 E = 0.000 }

G87: CH<sub>2</sub>OH + O → CH<sub>2</sub>O + OH { a = 1.000e+13 n = 0.000 E = 0.000 }

G89f: CH<sub>2</sub>OH + O<sub>2</sub> → CH<sub>2</sub>O + HO<sub>2</sub> { a = 1.800e+13 n = 0.000 E = 3.770 }

G85f: CH<sub>2</sub>OH + H → CH<sub>3</sub> + OH { a = 1.650e+11 n = 0.650 E = -1.190 }

# --- CO<sub>2</sub> reactions --- #

G41f: S-CH<sub>2</sub> + CO<sub>2</sub> → T-CH<sub>2</sub> + CO<sub>2</sub> { a = 7.000e+12 n = 0.000 E = 0.000 }

G11: CH + CO<sub>2</sub> → HCO + CO { a = 1.900e+14 n = 0.000 E = 66.070 }

G42: S-CH<sub>2</sub> + CO<sub>2</sub> → CH<sub>2</sub>O + CO { a = 1.400e+13 n = 0.000 E = 0.000 }

# --- CH<sub>3</sub>O<sub>2</sub> reactions --- #

G63: CH<sub>3</sub>O<sub>2</sub> + HO<sub>2</sub> → CH<sub>3</sub>O + OH + O<sub>2</sub> { a = 2.470e+11 n = 0.000 E = -6.570 }

G64: CH<sub>3</sub>O<sub>2</sub> + CH<sub>2</sub>O → CH<sub>3</sub>O + OH + HCO { a = 1.990e+12 n = 0.000 E = 48.830 }

G62: 2 CH<sub>3</sub>O<sub>2</sub> → 2 CH<sub>3</sub>O + O<sub>2</sub> { a = 1.400e+16 n = -1.610 E = 7.780 }

G61: CH<sub>3</sub>O<sub>2</sub> + CH<sub>3</sub> → 2 CH<sub>3</sub>O { a = 1.000e+13 n = 0.000 E = -5.020 }

## # --- C2H2 reactions --- #

R004f: C2H2 + S-CH2 -> C3H3 + H { a = 1.840e+14 n = -0.390 E = 0.000 }  
 G117: C2H2 + O -> T-CH2 + CO { a = 1.250e+07 n = 2.000 E = 7.950 }  
 G121f: C2H2 + OH -> CH2CO + H { a = 7.530e+06 n = 1.550 E = 8.810 }  
 R001f: C2H2 + M9 -> H2C2 + M9 { a = 2.450e+15 n = -0.640 E = 207.940 }  
 G116f: C2H2 + O -> HCCO + H { a = 8.100e+06 n = 2.000 E = 7.950 }  
 G115f: C2H2 + H + M9 -> C2H3 + M9 { a = 6.340e+31 n = -4.660 E = 15.820 }  
     ai = 1.710e+10 ni = 1.270 Ei = 11.330  
     fca = 2.122e-01 fcta = -1.021e+04 fcb = 0.000e+00 fctb = 1.000e+00 fcc = 0.000e+00 fctc =  
     1.000e+00 }  
 G122: C2H2 + OH -> CH3 + CO { a = 1.280e+09 n = 0.730 E = 10.790 }

## # --- H2C2 reactions --- #

R003: H2C2 + O2 -> 2 HCO { a = 1.000e+13 n = 0.000 E = 0.000 }  
 R002: H2C2 + O2 -> T-CH2 + CO2 { a = 3.300e+12 n = 0.000 E = 0.000 }

## # --- C2H3 reactions --- #

R030: HO2 + C2H3 -> O2 + C2H4 { a = 3.087e+11 n = -0.001 E = -0.793 }  
 B04f: 2 C2H3 -> C4H6 { a = 8.430e+13 n = 0.000 E = 0.000 }  
 G131: C2H3 + O -> CH2CHO { a = 1.030e+13 n = 0.210 E = -1.790 }  
 B05f: 2 C2H3 -> I-C4H5 + H { a = 1.200e+22 n = -2.440 E = 57.130 }  
 G130f: C2H3 + H -> C2H2 + H2 { a = 3.000e+13 n = 0.000 E = 0.000 }  
 G134f: C2H3 + O2 -> CH2CHO + O { a = 3.030e+11 n = 0.290 E = 0.050 }  
 R010f: C2H3 + HCO -> C2H3CHO { a = 1.800e+13 n = 0.000 E = 0.000 }  
 R011: C2H3 + CH3 -> C2H2 + CH4 { a = 9.030e+12 n = 0.000 E = -3.200 }  
 G129: C2H3 + H + M9 -> C2H4 + M9 { a = 1.400e+30 n = -3.860 E = 13.890 }  
     ai = 6.080e+12 ni = 0.270 Ei = 1.170  
     fca = 2.180e-01 fcta = 2.075e+02 fcb = 7.820e-01 fctb = 2.663e+03 fcc = 1.000e+00 fctc =  
     6.095e+03 }  
 R009: C2H3 + HCO -> C2H4 + CO { a = 9.000e+13 n = 0.000 E = 0.000 }  
 G135: C2H3 + O2 -> HCO + CH2O { a = 4.580e+16 n = -1.390 E = 4.250 }  
 G132: C2H3 + OH -> C2H2 + H2O { a = 5.000e+12 n = 0.000 E = 0.000 }  
 R013f: C2H3 + CH3 -> A-C3H5 + H { a = 1.930e+18 n = -1.250 E = 32.090 }  
 G133f: C2H3 + O2 -> C2H2 + HO2 { a = 1.340e+06 n = 1.610 E = -1.610 }

## # --- C2H4 reactions --- #

G159: C2H4 + O -> CH3 + HCO { a = 3.890e+08 n = 1.360 E = 3.710 }  
 HP40f: C2H4 + C2H3 -> C4H6 + H { a = 2.150e+12 n = 0.460 E = 62.650 }  
 G154: C2H4 + M9 -> H2C2 + H2 + M9 { a = 5.500e+14 n = 0.000 E = 226.970 }  
 G161f: C2H4 + OH -> C2H5O { a = 3.750e+36 n = -7.800 E = 29.540 }  
 G155f: C2H4 + H + M9 -> C2H5 + M9 { a = 2.030e+39 n = -6.640 E = 24.140 }  
     ai = 1.370e+09 ni = 1.460 Ei = 5.670  
     fca = 1.569e+00 fcta = 2.990e+02 fcb = -5.690e-01 fctb = -9.147e+03 fcc = 1.000e+00 fctc =  
     1.524e+02 }  
 G163f: C2H4 + CH3 + M9 -> N-C3H7 + M9 { a = 3.000e+63 n = -14.600 E = 76.020 }

$a_i = 2.550e+06$   $n_i = 1.600$   $E_i = 23.850$

$f_{ca} = 8.106e-01$   $f_{cta} = 2.770e+02$   $f_{cb} = 1.894e-01$   $f_{ctb} = 8.748e+03$   $f_{cc} = 1.000e+00$   $f_{ctc} = 7.891e+03$  }

G158:  $C_2H_4 + O \rightarrow T-CH_2 + CH_2O$  {  $a = 7.150e+04$   $n = 2.470$   $E = 3.890$  }  
 G156f:  $C_2H_4 + H \rightarrow C_2H_3 + H_2$  {  $a = 1.270e+05$   $n = 2.750$   $E = 48.740$  }  
 B00f:  $H_2C_2 + C_2H_4 \rightarrow C_4H_6$  {  $a = 1.000e+12$   $n = 0.000$   $E = 0.000$  }  
 G157:  $C_2H_4 + O \rightarrow CH_2CHO + H$  {  $a = 7.660e+09$   $n = 0.880$   $E = 4.770$  }  
 G162f:  $C_2H_4 + CH_3 \rightarrow C_2H_3 + CH_4$  {  $a = 2.270e+05$   $n = 2.000$   $E = 38.490$  }  
 R008:  $HO_2 + C_2H_4 \rightarrow H_2O_2 + C_2H_3$  {  $a = 3.972e+10$   $n = 0.227$   $E = 96.633$  }  
 G160f:  $C_2H_4 + OH \rightarrow C_2H_3 + H_2O$  {  $a = 2.230e+04$   $n = 2.750$   $E = 9.270$  }

# --- C2H5 reactions --- #

R035:  $C_2H_5 + HO_2 \rightarrow C_2H_5O + OH$  {  $a = 3.100e+13$   $n = 0.000$   $E = 0.000$  }  
 R032:  $C_2H_5 + HCO \rightarrow C_2H_6 + CO$  {  $a = 1.200e+14$   $n = 0.000$   $E = 0.000$  }  
 G171f:  $C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$  {  $a = 1.920e+07$   $n = 1.020$   $E = -8.510$  }  
 G164:  $C_2H_5 + H + M_9 \rightarrow C_2H_6 + M_9$  {  $a = 1.990e+41$   $n = -7.080$   $E = 27.970$  }

$a_i = 5.210e+17$   $n_i = -0.990$   $E_i = 6.610$

$f_{ca} = 1.578e-01$   $f_{cta} = 1.250e+02$   $f_{cb} = 8.422e-01$   $f_{ctb} = 2.219e+03$   $f_{cc} = 1.000e+00$   $f_{ctc} = 6.882e+03$  }

R034:  $C_2H_5 + HO_2 \rightarrow C_2H_4 + H_2O_2$  {  $a = 3.000e+11$   $n = 0.000$   $E = 0.000$  }  
 G167:  $C_2H_5 + O \rightarrow C_2H_5O$  {  $a = 3.170e+13$   $n = 0.030$   $E = -1.650$  }  
 G166:  $C_2H_5 + CH_3 \rightarrow C_2H_4 + CH_4$  {  $a = 1.180e+04$   $n = 2.450$   $E = 12.220$  }  
 R033:  $C_2H_5 + HO_2 \rightarrow C_2H_6 + O_2$  {  $a = 3.000e+11$   $n = 0.000$   $E = 0.000$  }

# --- C2H6 reactions --- #

G173f:  $C_2H_6 + M_9 \rightarrow 2 CH_3 + M_9$  {  $a = 3.720e+65$   $n = -13.140$   $E = 425.010$  }  
 $a_i = 1.880e+50$   $n_i = -9.720$   $E_i = 449.120$

$f_{ca} = 6.100e-01$   $f_{cta} = 1.000e+02$   $f_{cb} = 3.900e-01$   $f_{ctb} = 1.900e+03$   $f_{cc} = 1.000e+00$   $f_{ctc} = 6.000e+03$  }

G178f:  $C_2H_6 + CH_3 \rightarrow C_2H_5 + CH_4$  {  $a = 8.430e+14$   $n = 0.000$   $E = 93.120$  }  
 G174f:  $C_2H_6 + H \rightarrow C_2H_5 + H_2$  {  $a = 1.700e+05$   $n = 2.700$   $E = 24.020$  }  
 G177:  $C_2H_6 + S-CH_2 \rightarrow C_2H_5 + CH_3$  {  $a = 4.000e+13$   $n = 0.000$   $E = -2.300$  }  
 R036f:  $C_2H_6 + HO_2 \rightarrow C_2H_5 + H_2O_2$  {  $a = 2.610e+02$   $n = 3.370$   $E = 66.580$  }  
 G175:  $C_2H_6 + O \rightarrow C_2H_5 + OH$  {  $a = 3.170e+01$   $n = 3.800$   $E = 13.100$  }  
 G176f:  $C_2H_6 + OH \rightarrow C_2H_5 + H_2O$  {  $a = 1.610e+06$   $n = 2.220$   $E = 3.100$  }

# --- HCCO reactions --- #

G110:  $HCCO + O \rightarrow H + 2 CO$  {  $a = 1.000e+14$   $n = 0.000$   $E = 0.000$  }  
 G112:  $HCCO + CH \rightarrow C_2H_2 + CO$  {  $a = 5.000e+13$   $n = 0.000$   $E = 0.000$  }  
 R020:  $HCCO + CH_3 \rightarrow C_2H_4 + CO$  {  $a = 5.000e+13$   $n = 0.000$   $E = 0.000$  }  
 G111:  $HCCO + O_2 \rightarrow OH + 2 CO$  {  $a = 4.200e+10$   $n = 0.000$   $E = 3.570$  }  
 G109f:  $HCCO + H \rightarrow S-CH_2 + CO$  {  $a = 1.000e+14$   $n = 0.000$   $E = 0.000$  }  
 R022:  $HCCO + OH \rightarrow 2 HCO$  {  $a = 1.000e+13$   $n = 0.000$   $E = 0.000$  }  
 G114:  $2 HCCO \rightarrow C_2H_2 + 2 CO$  {  $a = 1.000e+13$   $n = 0.000$   $E = 0.000$  }  
 R007:  $C_2H_2 + HCCO \rightarrow C_3H_3 + CO$  {  $a = 1.000e+11$   $n = 0.000$   $E = 12.550$  }  
 G113:  $HCCO + T-CH_2 \rightarrow C_2H_3 + CO$  {  $a = 3.000e+13$   $n = 0.000$   $E = 0.000$  }

## # --- CH2CO reactions --- #

R024: CH2CO + T-CH2 -> C2H4 + CO { a = 1.000e+12 n = 0.000 E = 0.000 }  
 G123f: CH2CO + H -> HCCO + H2 { a = 5.000e+13 n = 0.000 E = 33.470 }  
 R027f: CH2CO + CH3 -> HCCO + CH4 { a = 7.500e+12 n = 0.000 E = 54.390 }  
 R026: CH2CO + CH3 -> C2H5 + CO { a = 9.000e+10 n = 0.000 E = 0.000 }  
 G125f: CH2CO + O -> HCCO + OH { a = 1.000e+13 n = 0.000 E = 33.470 }  
 G126: CH2CO + O -> T-CH2 + CO2 { a = 1.750e+12 n = 0.000 E = 5.650 }  
 G127f: CH2CO + OH -> HCCO + H2O { a = 7.500e+12 n = 0.000 E = 8.370 }  
 R025f: CH2CO + T-CH2 -> HCCO + CH3 { a = 3.600e+13 n = 0.000 E = 46.020 }  
 R023: CH2CO + OH -> CH2OH + CO { a = 5.000e+12 n = 0.000 E = 0.000 }  
 G124f: CH2CO + H -> CH3 + CO { a = 1.500e+09 n = 1.380 E = 2.570 }

## # --- CH2CHO reactions --- #

R028: CH2CHO + CH3 -> C2H5 + HCO { a = 4.900e+14 n = -0.500 E = 0.000 }  
 G139: CH2CHO + O2 -> OH + CO + CH2O { a = 1.810e+10 n = 0.000 E = 0.000 }  
 G144: CH2CHO + OH -> HCO + CH2OH { a = 3.010e+13 n = 0.000 E = 0.000 }  
 G141: CH2CHO + H -> CH3 + HCO { a = 2.200e+13 n = 0.000 E = 0.000 }  
 G142: CH2CHO + H -> CH2CO + H2 { a = 1.100e+13 n = 0.000 E = 0.000 }  
 G136f: CH2CHO -> CH2CO + H { a = 1.320e+34 n = -6.570 E = 206.930 }  
 G140: CH2CHO + O2 -> OH + 2 HCO { a = 2.350e+10 n = 0.000 E = 0.000 }  
 G137: CH2CHO -> CH3 + CO { a = 6.510e+34 n = -6.870 E = 197.460 }  
 G138: CH2CHO + O -> CH2O + HCO { a = 3.170e+13 n = 0.030 E = -1.650 }  
 G143: CH2CHO + OH -> H2O + CH2CO { a = 1.200e+13 n = 0.000 E = 0.000 }

## # --- CH3CHO reactions --- #

G150: CH3CHO + O2 -> CH3 + CO + HO2 { a = 3.010e+13 n = 0.000 E = 163.800 }  
 G151: CH3CHO + OH -> CH3 + CO + H2O { a = 2.340e+10 n = 0.730 E = -4.660 }  
 G152: CH3CHO + HO2 -> CH3 + CO + H2O2 { a = 3.010e+12 n = 0.000 E = 49.890 }  
 G146: CH3CHO + O -> CH2CHO + OH { a = 2.920e+12 n = 0.000 E = 7.570 }  
 G153: CH3CHO + CH3 -> CH3 + CO + CH4 { a = 2.720e+06 n = 1.770 E = 24.770 }  
 G148: CH3CHO + H -> CH3 + CO + H2 { a = 2.050e+09 n = 1.160 E = 10.060 }  
 G147f: CH3CHO + H -> CH2CHO + H2 { a = 2.050e+09 n = 1.160 E = 10.060 }  
 G149: CH3CHO + O -> CH3 + CO + OH { a = 2.920e+12 n = 0.000 E = 7.570 }

## # --- C2H5O reactions --- #

G169f: C2H5O -> CH3CHO + H { a = 5.450e+15 n = -0.690 E = 93.010 }  
 G168f: C2H5O -> CH3 + CH2O { a = 1.320e+20 n = -2.020 E = 86.820 }

## # --- C3H3 reactions --- #

R064: C3H3 + HO2 -> P-C3H4 + O2 { a = 3.000e+11 n = 0.000 E = 0.000 }  
 R067: C3H3 + HCO -> P-C3H4 + CO { a = 2.500e+13 n = 0.000 E = 0.000 }  
 R057: C3H3 + OH -> C2H4 + CO { a = 1.280e+09 n = 0.730 E = 10.790 }  
 B08f: C3H3 + CH3 + M9 -> C4H6 + M9 { a = 2.600e+57 n = -11.940 E = 40.890 }  
       ai = 1.500e+12 ni = 0.000 Ei = 0.000  
       fca = 8.250e-01 fcta = 1.341e+03 fcb = 1.750e-01 fctb = 6.000e+04 fcc = 1.000e+00 fctc =



9.770e+03 }

R056: C3H3 + OH -> C2H3CHO { a = 7.530e+06 n = 1.550 E = 8.810 }  
 R062: C3H3 + HO2 -> OH + CO + C2H3 { a = 8.000e+11 n = 0.000 E = 0.000 }  
 R061: C3H3 + O2 -> CH2CO + HCO { a = 1.700e+05 n = 1.700 E = 6.280 }  
 R059: C3H3 + OH -> CH2O + C2H2 { a = 1.880e+36 n = -7.800 E = 29.540 }

# --- P-C3H4 reactions --- #

R094: P-C3H4 + OH -> C2H5 + CO { a = 1.280e+09 n = 0.730 E = 10.790 }  
 R080f: P-C3H4 + OH -> C3H3 + H2O { a = 8.050e+05 n = 2.220 E = 3.100 }  
 R079: P-C3H4 + O -> C3H3 + OH { a = 4.490e+07 n = 1.920 E = 23.810 }  
 R093: P-C3H4 + OH -> CH2CO + CH3 { a = 7.530e+06 n = 1.550 E = 8.810 }  
 R081f: P-C3H4 + CH3 -> C3H3 + CH4 { a = 4.220e+14 n = 0.000 E = 93.120 }  
 R088: P-C3H4 + O -> HCCO + CH3 { a = 4.050e+06 n = 2.000 E = 7.950 }  
 R072f: P-C3H4 + H -> C2H2 + CH3 { a = 6.360e+13 n = 0.000 E = 18.850 }  
 R054f: P-C3H4 + M0 -> C3H3 + H + M0 { a = 2.150e+43 n = -6.810 E = 420.610 }  
 R082: P-C3H4 + HO2 -> C3H3 + H2O2 { a = 1.300e+02 n = 3.370 E = 66.580 }  
 R078f: P-C3H4 + H -> C3H3 + H2 { a = 8.500e+04 n = 2.700 E = 24.020 }  
 R065: P-C3H4 + O2 -> CH3 + HCO + CO { a = 4.000e+14 n = 0.000 E = 175.430 }  
 R089: P-C3H4 + O -> C2H4 + CO { a = 6.250e+06 n = 2.000 E = 7.950 }

# --- A-C3H5 reactions --- #

R115: A-C3H5 + HCO -> C3H6 + CO { a = 6.000e+13 n = 0.000 E = 0.000 }  
 R110: A-C3H5 + O2 -> C2H3CHO + OH { a = 3.360e+05 n = 1.810 E = 80.290 }  
 R014f: A-C3H5 + H -> C3H6 { a = 5.930e+54 n = -11.760 E = 98.530 }  
 R117: A-C3H5 + HO2 -> C3H5O + OH { a = 1.190e+09 n = 1.030 E = -9.410 }  
 R114: A-C3H5 + OH -> C2H3CHO + 2 H { a = 4.200e+32 n = -5.160 E = 126.050 }  
 R111: A-C3H5 + O2 -> C2H2 + CH2O + OH { a = 9.710e+20 n = -2.700 E = 104.520 }  
 R112: A-C3H5 + O2 -> CH2CHO + CH2O { a = 3.080e+09 n = 0.370 E = 70.750 }  
 R113: A-C3H5 + O -> C2H3CHO + H { a = 2.000e+14 n = 0.000 E = 0.000 }  
 R116f: A-C3H5 + HO2 -> C3H6 + O2 { a = 2.660e+12 n = 0.000 E = 0.000 }

# --- C3H6 reactions --- #

R144f: C3H6 + HO2 -> A-C3H5 + H2O2 { a = 2.380e+04 n = 2.550 E = 69.000 }  
 R145: C3H6 + CH3 -> A-C3H5 + CH4 { a = 4.570e-01 n = 3.650 E = 29.930 }  
 B09f: C3H6 + C2H3 -> C4H6 + CH3 { a = 7.230e+11 n = 0.000 E = 20.920 }  
 R139f: C3H6 + H -> A-C3H5 + H2 { a = 6.400e+13 n = 0.000 E = 34.650 }  
 R142: C3H6 + O -> C2H3CHO + 2 H { a = 3.830e+09 n = 0.880 E = 4.770 }  
 R138f: C3H6 + H -> C2H4 + CH3 { a = 4.800e+13 n = 0.000 E = 17.300 }  
 G195f: C3H6 + H + M9 -> N-C3H7 + M9 { a = 6.260e+38 n = -6.660 E = 29.290  
     ai = 2.500e+11 ni = 0.510 Ei = 10.960  
     fca = 0.000e+00 fcta = 1.000e+03 fcb = 1.000e+00 fctb = 1.310e+03 fcc = 1.000e+00 fctc =  
     4.810e+04 }

R140: C3H6 + O -> CH2CHO + CH3 { a = 5.090e+07 n = 1.660 E = 2.750 }  
 R143: C3H6 + O -> A-C3H5 + OH { a = 9.950e+04 n = 2.680 E = 15.550 }  
 R150f: C3H6 + OH -> A-C3H5 + H2O { a = 1.890e+05 n = 2.500 E = 2.800 }  
 R012f: C3H6 -> C2H3 + CH3 { a = 4.040e+42 n = -7.670 E = 467.900 }  
 R141: C3H6 + O -> C2H5 + HCO { a = 1.950e+08 n = 1.360 E = 3.710 }

## # --- N-C3H7 reactions --- #

G185: N-C3H7 + O -> C2H5 + CH2O { a = 9.600e+13 n = 0.000 E = 0.000 }  
 G187: N-C3H7 + OH -> C3H6 + H2O { a = 2.410e+13 n = 0.000 E = 0.000 }  
 G193: N-C3H7 + CH3 -> C3H6 + CH4 { a = 3.310e+12 n = 0.000 E = -3.220 }  
 G189f: N-C3H7 + O2 -> C3H6 + HO2 { a = 3.700e+16 n = -1.630 E = 14.300 }  
 G181: N-C3H7 + H -> C2H5 + CH3 { a = 3.700e+24 n = -2.920 E = 52.320 }

## # --- C2H3CHO reactions --- #

R095: C2H3CHO + H -> C2H3 + CO + H2 { a = 4.090e+09 n = 1.160 E = 10.060 }  
 R096: C2H3CHO + O -> C2H3 + CO + OH { a = 5.840e+12 n = 0.000 E = 7.570 }  
 R099: C2H3CHO + CH3 -> C2H3 + CO + CH4 { a = 3.490e-08 n = 6.210 E = 6.820 }  
 R097: C2H3CHO + OH -> C2H3 + CO + H2O { a = 2.890e+08 n = 1.350 E = -6.580 }  
 R098: C2H3CHO + HO2 -> C2H3 + CO + H2O2 { a = 4.090e+04 n = 2.500 E = 42.690 }

## # --- C3H5O reactions --- #

R135: C3H5O + O2 -> C2H3CHO + HO2 { a = 1.000e+12 n = 0.000 E = 25.100 }  
 R137f: C3H5O -> C2H3 + CH2O { a = 2.030e+12 n = 0.090 E = 98.580 }  
 R136: C3H5O -> C2H3CHO + H { a = 1.000e+14 n = 0.000 E = 121.750 }

## # --- I-C4H5 reactions --- #

B49f: I-C4H5 + H2O2 -> C4H6 + HO2 { a = 1.210e+10 n = 0.000 E = -2.490 }  
 B48: I-C4H5 + HO2 -> C4H6 + O2 { a = 6.000e+11 n = 0.000 E = 0.000 }  
 B47: I-C4H5 + HCO -> C4H6 + CO { a = 5.000e+12 n = 0.000 E = 0.000 }  
 B50: I-C4H5 + O2 -> CH2CO + CH2CHO { a = 2.160e+10 n = 0.000 E = 10.460 }  
 B51: I-C4H5 + O -> C3H3 + CH2O { a = 3.170e+13 n = 0.030 E = -1.650 }  
 B45: I-C4H5 + H -> C3H3 + CH3 { a = 2.000e+13 n = 0.000 E = 8.370 }  
 B10: H + I-C4H5 -> C4H6 { a = 3.987e+33 n = -5.924 E = 44.841 }

## # --- C4H6 reactions --- #

B17f: C4H6 + H -> I-C4H5 + H2 { a = 6.650e+05 n = 2.530 E = 38.660 }  
 B23f: C4H6 + CH3 -> I-C4H5 + CH4 { a = 1.000e+14 n = 0.000 E = 82.840 }  
 B21f: C4H6 + OH -> I-C4H5 + H2O { a = 3.100e+06 n = 2.000 E = 1.800 }  
 B19: C4H6 + O -> I-C4H5 + OH { a = 7.500e+06 n = 1.900 E = 15.650 }  
 B28: C4H6 + O -> A-C3H5 + CO + H { a = 7.660e+09 n = 0.880 E = 4.770 }  
 B25f: C4H6 + C2H3 -> I-C4H5 + C2H4 { a = 2.500e+13 n = 0.000 E = 82.840 }  
 B29: C4H6 + O -> P-C3H4 + CH2O { a = 7.150e+04 n = 2.470 E = 3.890 }  
 B14: H + C4H6 -> CH3 + P-C3H4 { a = 9.655e+16 n = -1.020 E = 61.547 }  
 B31: C4H6 + OH -> A-C3H5 + CH2O { a = 3.750e+36 n = -7.800 E = 29.540 }  
 B30: C4H6 + O -> A-C3H5 + HCO { a = 3.890e+08 n = 1.360 E = 3.710 }

## # --- C4H7 reactions --- #

HP44: C4H7 + C2H5 -> C4H6 + C2H6 { a = 3.980e+12 n = 0.000 E = 0.000 }

HP39: C4H7 -> C2H4 + C2H3 { a = 1.000e+11 n = 0.000 E = 154.810 }  
HP46: C4H7 + HO2 -> A-C3H5 + CH2O + OH { a = 7.000e+12 n = 0.000 E = -4.180 }  
HP45: C4H7 + A-C3H5 -> C4H6 + C3H6 { a = 6.310e+12 n = 0.000 E = 0.000 }  
HP47: C4H7 + CH3O2 -> A-C3H5 + CH2O + CH3O { a = 7.000e+12 n = 0.000 E = -4.180 }  
HP43: C4H7 + CH3 -> C4H6 + CH4 { a = 8.000e+12 n = 0.000 E = 0.000 }  
HP41: C4H7 + H -> C4H6 + H2 { a = 3.160e+13 n = 0.000 E = 0.000 }  
HP38: C4H7 -> C4H6 + H { a = 1.200e+14 n = 0.000 E = 206.270 }  
HP42: C4H7 + O2 -> C4H6 + HO2 { a = 1.000e+09 n = 0.000 E = 0.000 }

# --- P-C4H8 reactions --- #

HP35: P-C4H8 -> A-C3H5 + CH3 { a = 5.000e+15 n = 0.000 E = 297.060 }  
HP37: P-C4H8 + OH -> C4H7 + H2O { a = 2.250e+13 n = 0.000 E = 9.280 }  
HP36: P-C4H8 + H -> C4H7 + H2 { a = 5.000e+13 n = 0.000 E = 16.320 }

# --- C5H9 reactions --- #

HP31: C5H9 -> A-C3H5 + C2H4 { a = 2.500e+13 n = 0.000 E = 188.280 }  
HP32: C5H9 -> C4H6 + CH3 { a = 1.340e+15 n = -0.520 E = 160.330 }

# --- C5H10 reactions --- #

HP30: C5H10 + OH -> C5H9 + H2O { a = 3.000e+13 n = 0.000 E = 5.150 }  
HP28: C5H10 -> C2H5 + A-C3H5 { a = 9.170e+20 n = -1.630 E = 309.570 }  
HP29: C5H10 + H -> C5H9 + H2 { a = 3.700e+13 n = 0.000 E = 16.320 }

# --- C5H11 reactions --- #

HP26: C5H11 -> C2H4 + N-C3H7 { a = 7.850e+12 n = 0.240 E = 129.490 }  
HP27: C5H11 -> H + C5H10 { a = 8.460e+14 n = -0.470 E = 157.390 }

# --- C7H13 reactions --- #

HP25: C7H13 -> C4H7 + C3H6 { a = 2.500e+13 n = 0.000 E = 188.280 }  
HP24: C7H13 -> A-C3H5 + P-C4H8 { a = 2.500e+13 n = 0.000 E = 188.280 }

# --- C7H14 reactions --- #

HP20: C7H14 + H -> C7H13 + H2 { a = 3.700e+13 n = 0.000 E = 16.320 }  
HP22: C7H14 + OH -> C5H11 + CH3CHO { a = 9.870e+22 n = -3.620 E = 12.150 }  
HP21: C7H14 + OH -> C7H13 + H2O { a = 3.000e+13 n = 0.000 E = 5.150 }  
HP19: C7H14 -> C4H7 + N-C3H7 { a = 1.190e+22 n = -1.870 E = 308.010 }

# --- C7H15 reactions --- #

HP13: C7H15 + HO2 -> C7H15O + OH { a = 7.000e+12 n = 0.000 E = -4.180 }  
HP08: C7H15 -> C5H11 + C2H4 { a = 2.850e+13 n = -0.210 E = 124.570 }

HP11: C7H15 -> C2H5 + C5H10 { a = 6.940e+12 n = 0.140 E = 125.200 }  
HP14: C7H15 + CH3O2 -> C7H15O + CH3O { a = 7.000e+12 n = 0.000 E = -4.180 }  
HP12: C7H15 -> C7H14 + H { a = 1.410e+15 n = -0.530 E = 156.520 }  
HP80: C7H15 + O2 -> C7H15O2 { a = 1.680e+13 n = -0.110 E = 1.010 }  
HP10: C7H15 -> N-C3H7 + P-C4H8 { a = 1.230e+12 n = 0.090 E = 127.660 }

# --- N-C7H16 reactions --- #

HP03: N-C7H16 + H -> C7H15 + H2 { a = 1.750e+06 n = 2.600 E = 18.250 }  
HP06: N-C7H16 + O2 -> C7H15 + HO2 { a = 2.890e+13 n = 0.200 E = 209.660 }  
HP07: N-C7H16 + HO2 -> C7H15 + H2O2 { a = 7.570e+12 n = 0.210 E = 73.780 }  
HP05: N-C7H16 + OH -> C7H15 + H2O { a = 7.400e+08 n = 1.500 E = 1.080 }  
HP04: N-C7H16 + O -> C7H15 + OH { a = 1.720e+05 n = 2.810 E = 9.460 }  
HP01: N-C7H16 -> C5H11 + C2H5 { a = 8.100e+77 n = -17.620 E = 503.750 }

# --- C7H14O reactions --- #

HP90: C7H14O + OH -> C5H11 + CH2CO + H2O { a = 3.680e+12 n = 0.000 E = 0.000 }

# --- C7H15O reactions --- #

HP15: C7H15O -> C5H11 + CH3CHO { a = 8.920e+19 n = -2.030 E = 87.880 }  
HP16: C7H15O -> 2 N-C3H7 + HCO { a = 6.180e+16 n = -1.360 E = 77.480 }

# --- C7H15O2 reactions --- #

HP82: C7H15O2 -> C7H14OOH { a = 1.880e+05 n = 1.680 E = 79.510 }  
HP81: C7H15O2 -> C7H15 + O2 { a = 1.920e+22 n = -2.110 E = 156.080 }

# --- C7H14OOH reactions --- #

HP84: C7H14OOH -> C7H14 + HO2 { a = 5.850e+03 n = 2.400 E = 64.080 }  
HP83: C7H14OOH -> C7H15O2 { a = 7.640e+05 n = 0.910 E = 25.450 }  
HP86: C7H14OOH + O2 -> C7H15O4 { a = 1.510e+13 n = -0.090 E = 0.530 }  
HP85: C7H14OOH -> C7H14O + OH { a = 3.970e-10 n = 5.690 E = 1.570 }

# --- OC7H13OOH reactions --- #

HP89: OC7H13OOH -> N-C3H7 + CH3CHO + CH2CO + OH { a = 3.260e+09 n = 1.930 E = 161.110 }

# --- C7H15O4 reactions --- #

HP88: C7H15O4 -> OC7H13OOH + OH { a = 4.250e+10 n = -0.110 E = 81.480 }  
HP87: C7H15O4 -> C7H14OOH + O2 { a = 1.710e+22 n = -2.130 E = 155.320 }

# --- N2 reactions --- #

G28f: S-CH2 + N2 -> T-CH2 + N2 { a = 1.500e+13 n = 0.000 E = 2.510 }

Let M1 = + 0 [H2O] + 0 [H2] + 0 [CO2] + 1.0 [OTHER].

Let M3 = + 12 [H2O] + 2 [H2] + 3.6 [CO2] + 1.75 [CO] + 1.0 [OTHER].

Let M6 = + 6 [H2O] + 2 [H2] + 3.6 [CO2] + 1.75 [CO] + 1.0 [OTHER].

Let M2 = + 6.3 [H2O] + 2 [H2] + 3.6 [CO2] + 1.75 [CO] + 1.0 [OTHER].

Let M5 = + 11.89 [H2O] + 0.75 [H2] + 2.18 [CO2] + 1.09 [CO] + 0.85 [O2] + 1.0 [OTHER].

Let M9 = + 6 [H2O] + 2 [H2] + 2 [CH4] + 2 [CO2] + 1.5 [CO] + 3 [C2H6] + 1.0 [OTHER].

Let M0 = + 1.0 [OTHER].

Let M7 = + 12 [H2O] + 2 [H2] + 3.6 [CO2] + 1.75 [CO] + 1.0 [OTHER].

Let M8 = + 2 [H2] + 3.6 [CO2] + 1.75 [CO] + 0 [H2O] + 1.0 [OTHER].