Supplementary Material

The following contains supplementary materials in support of the manuscript entitled “*Ignition Process and Flame Lift-off Characteristics of Dimethyl Ether (DME) Spray*” by K. Cung, A. Moiz, X. Zhu, and S-Y. Lee. This manuscript is being submitted to Frontier of Mechanical Engineering Special Issue: Advancement of Low Temperature Engine Combustion Strategies. For questions or comments, please contact Khanh Cung at khanh.cung@swri.org.

# Supplementary Data

DME reduced mechanism (45 species, 249 reactions)

! Reduced DME mechanism (45 species, 249 reactions)

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! Citation: Cung, K., Zhu, X., Moiz, A.A., Lee, S.-Y., and De Ojeda, W. (2016b).

! Characteristics of Formaldehyde (CH2O) Formation in Dimethyl Ether (DME) Spray

! Combustion Using PLIF Imaging.

! SAE Int. J. Fuels Lubr. 9(1), 138-148. doi: 10.4271/2016-01-0864.

ELEMENTS

H O C N AR

END

SPECIES

H H2 O O2 OH

H2O N2 CO HCO CO2

CH3 CH4 HO2 H2O2 CH2O

CH3O C2H6 CH2 CH CH3OH

CH2OH CH3O2 CH3O2H HCO2 CH3OCH3

CH3OCH2 CH3OCH2O2 CH2OCH2O2H CH3OCH2O O2CH2OCH2O2H

HO2CH2OCHO OCH2OCHO HOCH2OCO HOCH2O HCO2H

CH3OCHO CH3OCO AR HCH N

NNH NO NO2 N2O HCN

END

REACTIONS

!MOLES CAL/MOLE

!Added from DME original

CH3+H(+M)=CH4(+M) 2.14E15 -0.4 0.0E0

 H2/2.0/

 H2O/5.0/

 CO/2.0/

 CO2/3.0/

 LOW/3.31E30 -4.0E0 2.108E3/

 TROE/0.0E0 1.0E-15 1.0E-15 4.0E1/

CH4+H=CH3+H2 1.727E4 3.0 8.224E3

 REV/6.61E2 3.0E0 7.744E3/

CH4+OH=CH3+H2O 1.93E5 2.4 2.106E3

 REV/4.82E2 2.9E0 1.486E4/

CH4+O=CH3+OH 2.13E6 2.21 6.48E3

 REV/3.557E4 2.21E0 3.92E3/

HCO+OH=CO+H2O 1.02E14 0.0 0.0E0

 REV/2.896E15 0.0E0 1.052E5/

CO+OH=CO2+H 1.4E5 1.95 -1.347E3

 REV/1.568E7 1.95E0 2.099E4/

H+O2=O+OH 1.97E14 0.0 1.654E4

 REV/1.555E13 0.0E0 4.25E2/

O+H2=H+OH 5.08E4 2.67 6.292E3

 REV/2.231E4 2.67E0 4.197E3/

O+H2O=2OH 2.97E6 2.02 1.34E4

 REV/3.013E5 2.02E0 -3.85E3/

OH+H2=H+H2O 2.16E8 1.51 3.43E3

 REV/9.352E8 1.51E0 1.858E4/

HCO+M=H+CO+M 1.86E17 -1.0 1.7E4

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 REV/6.467E13 0.0E0 -4.42E2/

H2O2+OH=H2O+HO2 1.0E12 0.0 0.0E0

 REV/1.685E11 3.3E-1 3.146E4/

 DUP

CH3OH(+M)=CH3+OH(+M) 1.9E16 0.0 9.173E4

 H2/2.0/

 H2O/16.0/

 CO/2.0/

 CO2/3.0/

 LOW/2.95E44 -7.35E0 9.546E4/

 TROE/4.14E-1 2.79E2 5.459E3/

CH3OH+HO2=CH2OH+H2O2 3.98E13 0.0 1.94E4

 REV/3.13E15 -9.0E-1 1.075E4/

CH3+HO2=CH3O+OH 1.1E13 0.0 0.0E0

 REV/4.78E14 -3.5E-1 2.455E4/

CO+HO2=CO2+OH 3.01E13 0.0 2.3E4

 REV/6.435E15 -3.3E-1 8.461E4/

2CH3(+M)=C2H6(+M) 9.214E16 -1.17 6.358E2

 H2/2.0/

 H2O/5.0/

 CO/2.0/

 CO2/3.0/

 LOW/1.135E36 -5.246E0 1.705E3/

 TROE/4.05E-1 1.12E3 6.96E1 1.0E15/

H2O+M=H+OH+M 1.837E27 -3.0 1.226E5

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 REV/2.25E22 -2.0E0 0.0E0/

H+O2(+M)=HO2(+M) 1.475E12 0.6 0.0E0

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 LOW/3.5E16 -4.1E-1 -1.116E3/

 TROE/5.0E-1 1.0E-30 1.0E30/

CO+O(+M)=CO2(+M) 1.8E10 0.0 2.384E3

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 LOW/1.35E24 -2.788E0 4.191E3/

CO+O2=CO2+O 1.068E-15 7.13 1.332E4

 REV/9.444E-15 7.13E0 1.954E4/

HCO+H=CO+H2 7.34E13 0.0 0.0E0

 REV/4.813E14 0.0E0 9.0E4/

HCO+O=CO+OH 3.02E13 0.0 0.0E0

 REV/8.697E13 0.0E0 8.79E4/

CH2O+M=HCO+H+M 6.283E29 -3.57 9.32E4

 REV/2.66E24 -2.57E0 4.27E2/

CH2O+OH=HCO+H2O 3.43E9 1.18 -4.47E2

 REV/1.186E9 1.18E0 2.938E4/

CH2O+H=HCO+H2 9.334E8 1.5 2.976E3

 REV/7.453E7 1.5E0 1.765E4/

CH2O+O=HCO+OH 6.26E9 1.15 2.26E3

 REV/2.195E8 1.15E0 1.484E4/

CH3+OH=CH2O+H2 2.25E13 0.0 4.3E3

 REV/6.756E14 0.0E0 7.603E4/

CH3+O=CH2O+H 8.0E13 0.0 0.0E0

 REV/1.055E15 0.0E0 6.963E4/

CH3+O2=CH3O+O 1.995E18 -1.57 2.923E4

 REV/3.585E18 -1.59E0 -1.61E3/

CH2O+CH3=HCO+CH4 3.636E-6 5.42 9.98E2

 REV/7.584E-6 5.42E0 1.615E4/

HCO+CH3=CH4+CO 1.21E14 0.0 0.0E0

 REV/2.073E16 0.0E0 9.048E4/

CH3O(+M)=CH2O+H(+M) 5.45E13 0.0 1.35E4

 LOW/2.344E25 -2.7E0 3.06E4/

HO2+O=OH+O2 3.25E13 0.0 0.0E0

 REV/7.857E14 -3.3E-1 5.539E4/

HCO+HO2=CH2O+O2 2.974E10 0.33 -3.861E3

 REV/2.05E13 0.0E0 3.895E4/

CH3O+O2=CH2O+HO2 5.5E10 0.0 2.424E3

 REV/1.318E9 3.5E-1 3.139E4/

CH3+HO2=CH4+O2 3.0E12 0.0 0.0E0

 REV/4.314E15 -3.3E-1 5.796E4/

HCO+O2=CO+HO2 7.58E12 0.0 4.1E2

 REV/9.029E11 3.3E-1 3.293E4/

HO2+H=2OH 7.08E13 0.0 3.0E2

 REV/1.352E14 -3.3E-1 3.957E4/

HO2+H=H2+O2 1.66E13 0.0 8.2E2

 REV/9.138E14 -3.3E-1 5.83E4/

HO2+OH=H2O+O2 2.89E13 0.0 -5.0E2

 REV/6.888E15 -3.3E-1 7.214E4/

H2O2+O2=2HO2 5.942E17 -0.66 5.315E4

 REV/4.2E14 0.0E0 1.198E4/

 DUP

2OH(+M)=H2O2(+M) 1.236E14 -0.37 0.0E0

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 LOW/3.041E30 -4.63E0 2.049E3/

 TROE/4.7E-1 1.0E2 2.0E3 1.0E15/

H2O2+H=H2O+OH 2.41E13 0.0 3.97E3

 REV/7.75E12 0.0E0 7.471E4/

CH4+HO2=CH3+H2O2 3.42E11 0.0 1.929E4

 REV/3.365E11 -3.3E-1 2.502E3/

CH2O+HO2=HCO+H2O2 5.82E-3 4.53 6.557E3

 REV/1.194E-2 4.2E0 4.921E3/

OH+M=O+H+M 3.909E22 -2.0 1.053E5

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 REV/4.72E18 -1.0E0 0.0E0/

O2+M=2O+M 6.473E20 -1.5 1.215E5

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 REV/6.17E15 -5.0E-1 0.0E0/

H2+M=2H+M 4.57E19 -1.4 1.044E5

 H2/2.5/

 H2O/12.0/

 CO/1.9/

 CO2/3.8/

 REV/2.423E15 -4.0E-1 -3.04E3/

CH2+O2=CO+H2O 7.28E19 -2.54 1.809E3

 REV/8.508E20 -2.54E0 1.798E5/

CH2+O2=HCO+OH 1.29E20 -3.3 2.84E2

 REV/5.31E19 -3.3E0 7.317E4/

CH2+O=>CO+2H 5.0E13 0.0 0.0E0

CH2+H=CH+H2 1.0E18 -1.56 0.0E0

 REV/7.026E17 -1.56E0 2.99E3/

CH2+OH=CH+H2O 1.13E7 2.0 3.0E3

 REV/3.437E7 2.0E0 2.115E4/

CH2+O2=>CO2+2H 3.29E21 -3.3 2.868E3

CH+O2=HCO+O 3.3E13 0.0 0.0E0

 REV/4.402E13 0.0E0 7.199E4/

CH3OH+OH=CH2OH+H2O 7.1E6 1.8 -5.96E2

 REV/3.293E1 3.46E0 2.272E4/

CH3OH+H=CH3O+H2 3.6E12 0.0 6.095E3

 REV/7.467E12 -2.0E-2 7.825E3/

CH3OH+H=CH2OH+H2 1.44E13 0.0 6.095E3

 REV/1.543E7 1.66E0 1.425E4/

CH3OH+CH3=CH2OH+CH4 3.19E1 3.17 7.172E3

 REV/8.927E-4 4.83E0 1.581E4/

CH3OH+O=CH2OH+OH 3.88E5 2.5 3.08E3

 REV/4.96E3 2.5E0 8.781E3/

CH2OH+O2=CH2O+HO2 3.81E6 2.0 1.641E3

 REV/1.768E11 6.7E-1 2.418E4/

CH2OH(+M)=CH2O+H(+M) 2.8E14 -0.73 3.282E4

 LOW/6.01E33 -5.39E0 3.62E4/

 TROE/9.6E-1 6.76E1 1.855E3 7.543E3/

H2O2+O=OH+HO2 9.55E6 2.0 3.97E3

 REV/2.541E7 1.68E0 1.985E4/

CH2+O2=CH2O+O 3.29E21 -3.3 2.868E3

 REV/3.862E22 -3.3E0 6.318E4/

CH2+O2=CO2+H2 1.01E21 -3.3 1.508E3

 REV/3.054E23 -3.3E0 1.867E5/

CH3OH+CH2O=2CH3O 3.835E13 0.05 8.472E4

 REV/6.03E13 0.0E0 0.0E0/

CH2O+CH3O=CH3OH+HCO 1.15E11 0.0 1.28E3

 REV/3.02E11 0.0E0 1.816E4/

CH4+CH3O=CH3+CH3OH 1.57E11 0.0 8.842E3

 REV/1.046E9 0.0E0 5.0E4/

CH3O+CH3OH=CH2OH+CH3OH 3.0E11 0.0 4.074E3

 REV/1.549E5 1.68E0 1.05E4/

CH3OH+OH=CH3O+H2O 1.0E6 2.1 4.967E2

 REV/8.981E6 2.08E0 1.738E4/

CH2O+M=CO+H2+M 1.826E32 -4.42 8.712E4

 REV/5.07E27 -3.42E0 8.435E4/

H2O2+H=H2+HO2 4.82E13 0.0 7.95E3

 REV/1.875E12 3.3E-1 2.426E4/

HCO+O=CO2+H 3.0E13 0.0 0.0E0

 REV/9.677E15 0.0E0 1.102E5/

CH3+M=CH2+H+M 1.968E16 0.0 9.252E4

 REV/2.107E11 1.0E0 -1.962E4/

CH3+H=CH2+H2 9.0E13 0.0 1.51E4

 REV/1.818E13 0.0E0 1.04E4/

CH3+OH=CH2+H2O 3.0E6 2.0 2.5E3

 REV/2.623E6 2.0E0 1.296E4/

CH3OH(+M)=CH2OH+H(+M) 2.69E16 -0.08 9.894E4

 LOW/2.34E40 -6.33E0 1.031E5/

 TROE/7.73E-1 6.93E2 5.333E3/

CH2OH+CH2O=CH3OH+HCO 1.292E-1 4.56 6.596E3

 REV/9.63E3 2.9E0 1.311E4/

H2O2+O2=2HO2 1.839E14 -0.66 3.955E4

 REV/1.3E11 0.0E0 -1.629E3/

 DUP

H2O2+OH=H2O+HO2 5.8E14 0.0 9.56E3

 REV/9.771E13 3.3E-1 4.102E4/

 DUP

CH3O2+M=CH3+O2+M 4.343E27 -3.42 3.047E4

 REV/5.44E25 -3.3E0 0.0E0/

CH3O2H=CH3O+OH 6.31E14 0.0 4.23E4

 REV/1.166E11 6.0E-1 -1.771E3/

CH3O2+CH2O=CH3O2H+HCO 1.99E12 0.0 1.167E4

 REV/8.504E12 -5.0E-1 7.009E3/

CH4+CH3O2=CH3+CH3O2H 1.81E11 0.0 1.848E4

 REV/3.708E11 -5.0E-1 -1.327E3/

CH3OH+CH3O2=CH2OH+CH3O2H 1.81E12 0.0 1.371E4

 REV/1.038E8 1.16E0 2.542E3/

CH3O2+CH3=2CH3O 7.0E12 0.0 -1.0E3

 REV/2.971E16 -9.3E-1 2.831E4/

CH3O2+HO2=CH3O2H+O2 1.75E10 0.0 -3.275E3

 REV/5.156E13 -8.3E-1 3.488E4/

CH3OH+O2=CH2OH+HO2 2.05E13 0.0 4.49E4

 REV/3.989E5 1.99E0 -4.424E3/

2CH3O2=>CH2O+CH3OH+O2 3.11E14 -1.61 -1.051E3

2CH3O2=>O2+2CH3O 1.4E16 -1.61 1.86E3

HCO2+M=H+CO2+M 2.443E15 -0.5 2.65E4

 REV/7.5E13 0.0E0 2.9E4/

CH3+O2=CH2O+OH 7.47E11 0.0 1.425E4

 REV/7.778E11 0.0E0 6.777E4/

CH3OCH3=CH3+CH3O 4.86E55 -11.56 1.021E5

 REV/1.173E54 -1.188E1 2.31E4/

CH3OCH3+OH=CH3OCH2+H2O 9.35E5 2.29 -7.8E2

 REV/1.03E6 1.99E0 2.329E4/

CH3OCH3+H=CH3OCH2+H2 7.721E6 2.09 3.384E3

 REV/1.964E6 1.79E0 1.23E4/

CH3OCH3+O=CH3OCH2+OH 1.855E-3 5.29 -1.09E2

 REV/2.073E-4 5.0E0 6.708E3/

CH3OCH3+HO2=CH3OCH2+H2O2 1.68E13 0.0 1.769E4

 REV/1.098E14 -6.2E-1 1.029E4/

CH3OCH3+CH3O2=CH3OCH2+CH3O2H 1.68E13 0.0 1.769E4

 REV/2.287E14 -8.0E-1 7.27E3/

CH3OCH3+CH3=CH3OCH2+CH4 1.445E-6 5.73 5.699E3

 REV/9.603E-6 5.43E0 1.509E4/

CH3OCH3+O2=CH3OCH2+HO2 4.1E13 0.0 4.491E4

 REV/1.895E11 3.0E-2 -3.659E3/

CH3OCH3+CH3O=CH3OCH2+CH3OH 6.02E11 0.0 4.074E3

 REV/7.383E10 -2.7E-1 1.026E4/

CH3OCH2=CH2O+CH3 1.6E13 0.0 2.55E4

 REV/2.002E12 0.0E0 2.4E4/

CH3OCH2+CH3O=CH3OCH3+CH2O 2.41E13 0.0 0.0E0

 REV/1.25E14 3.2E-1 7.854E4/

CH3OCH2+CH2O=CH3OCH3+HCO 5.49E3 2.8 5.862E3

 REV/1.723E3 3.1E0 1.162E4/

CH3OCH2+HO2=CH3OCH2O+OH 9.0E12 0.0 0.0E0

 REV/2.535E15 -4.8E-1 3.051E4/

CH3OCH2O2=CH3OCH2+O2 4.439E19 -1.59 3.624E4

 REV/2.0E12 0.0E0 0.0E0/

CH3OCH2O=CH3O+CH2O 5.18E12 -0.13 1.937E4

 REV/1.0E11 0.0E0 1.19E4/

CH3OCH2O2=CH2OCH2O2H 6.0E10 0.0 2.158E4

 REV/1.248E12 -7.7E-1 1.122E4/

CH2OCH2O2H=>OH+2CH2O 1.5E13 0.0 2.076E4

O2CH2OCH2O2H=CH2OCH2O2H+O2 1.924E19 -1.62 3.627E4

 REV/7.0E11 0.0E0 0.0E0/

O2CH2OCH2O2H=HO2CH2OCHO+OH 4.0E10 0.0 1.858E4

 REV/7.814E3 1.49E0 5.881E4/

HO2CH2OCHO=OCH2OCHO+OH 2.0E16 0.0 4.05E4

 REV/1.761E9 1.49E0 -3.185E3/

OCH2OCHO=CH2O+HCO2 5.964E16 -1.5 1.962E4

 REV/1.25E11 0.0E0 1.19E4/

CH3O+CH3=CH2O+CH4 2.4E13 0.0 0.0E0

 REV/8.27E14 2.0E-2 8.693E4/

OCH2OCHO=HOCH2OCO 1.0E11 0.0 1.4E4

 REV/2.746E8 -7.9E-1 2.008E4/

HOCH2OCO=HOCH2O+CO 2.177E16 -2.69 1.72E4

 REV/1.5E11 0.0E0 4.8E3/

HOCH2OCO=CH2OH+CO2 8.672E17 -3.45 1.908E4

 REV/1.5E11 0.0E0 3.52E4/

CH2OH+HO2=HOCH2O+OH 1.0E13 0.0 0.0E0

 REV/8.515E16 -1.09E0 3.309E4/

HOCH2O=CH2O+OH 1.482E17 -1.21 2.124E4

 REV/4.5E15 -1.1E0 0.0E0/

HOCH2O=HCO2H+H 1.0E14 0.0 1.49E4

 REV/5.904E11 6.4E-1 9.214E3/

HCO2H+M=CO+H2O+M 2.3E13 0.0 5.0E4

 REV/1.422E10 4.6E-1 4.684E4/

HCO2H+M=CO2+H2+M 1.5E16 0.0 5.7E4

 REV/2.399E14 4.6E-1 6.102E4/

2CH3OCH2O2=>O2+2CH3OCH2O 1.547E23 -4.5 0.0E0

CH3OCH2O=CH3OCHO+H 1.745E16 -0.66 1.172E4

 REV/1.0E13 0.0E0 7.838E3/

CH3OCHO=CH3+HCO2 1.392E18 -0.99 7.914E4

 REV/1.0E13 0.0E0 0.0E0/

CH3OCHO+O2=CH3OCO+HO2 1.0E13 0.0 4.97E4

 REV/8.437E9 -9.6E-1 8.0E0/

CH3OCHO+OH=CH3OCO+H2O 2.34E7 1.61 -3.5E1

 REV/4.706E6 3.2E-1 2.291E4/

CH3OCHO+HO2=CH3OCO+H2O2 1.22E12 0.0 1.7E4

 REV/1.456E12 -1.61E0 8.482E3/

CH3OCHO+O=CH3OCO+OH 2.35E5 2.5 2.23E3

 REV/4.794E3 1.21E0 7.925E3/

CH3OCHO+H=CH3OCO+H2 4.55E6 2.0 5.0E3

 REV/2.113E5 7.1E-1 1.279E4/

CH3OCHO+CH3=CH3OCO+CH4 7.55E-1 3.46 5.481E3

 REV/9.161E-1 2.17E0 1.375E4/

CH3OCHO+CH3O=CH3OCO+CH3OH 5.48E11 0.0 5.0E3

 REV/1.227E10 -1.26E0 1.106E4/

CH3OCHO+CH3O2=CH3OCO+CH3O2H 1.22E12 0.0 1.7E4

 REV/3.033E12 -1.79E0 5.462E3/

CH3OCO=CH3O+CO 7.451E12 -1.76 1.715E4

 REV/1.5E11 0.0E0 3.0E3/

CH3OCO=CH3+CO2 1.514E12 -1.78 1.382E4

 REV/1.5E11 0.0E0 3.673E4/

CH3OCH3+HCO2=CH3OCH2+HCO2H 1.0E13 0.0 1.769E4

 REV/4.884E12 -2.6E-1 2.508E4/

HCO2H=HCO+OH 4.593E18 -0.46 1.083E5

 REV/1.0E14 0.0E0 0.0E0/

CH2O+HCO2=HCO+HCO2H 5.6E12 0.0 1.36E4

 REV/8.584E11 4.0E-2 2.675E4/

HCO2+HO2=HCO2H+O2 3.5E10 0.0 -3.275E3

 REV/3.699E12 -2.9E-1 5.269E4/

HCO2+H2O2=HCO2H+HO2 2.4E12 0.0 1.0E4

 REV/1.793E11 3.6E-1 2.479E4/

HCO2H+OH=>H2O+CO2+H 2.62E6 2.06 9.16E2

HCO2H+OH=>H2O+CO+OH 1.85E7 1.51 -9.62E2

HCO2H+H=>H2+CO2+H 4.24E6 2.1 4.868E3

HCO2H+H=>H2+CO+OH 6.03E13 -0.35 2.988E3

HCO2H+CH3=>CH4+CO+OH 3.9E-7 5.8 2.2E3

HCO2H+HO2=>H2O2+CO+OH 1.0E12 0.0 1.192E4

HCO2H+O=>CO+2OH 1.77E18 -1.9 2.975E3

!

! CH4 Methane reactions

!

!CH4+O2=CH3+HO2 7.94E13 0.0 56000.0 !b24

! CH4+H=CH3+H2 5.47E07 1.97 11210.0 !a;rmHR

! CH4+H=CH3+H2 1.33E04 3.0 8040. !Baulch'92;addHR

!CH4+H=CH3+H2 1.48E14 0.0 13585. ![knyazev 1996a]

! CH4+OH=CH3+H2O 5.72E06 1.96 2639.0 !a;remHR

!CH4+OH=CH3+H2O 1.57E07 1.83 2780.0 !Baulch'92;addHR

!!! CH4+O=CH3+OH 6.93E08 1.56 8484.0 !a CST-rem

!CH4+HO2=CH3+H2O2 1.81E11 0.0 18580.0 !a

!

! CH3OH methanol reactions

!

!!! CH3OH+M=CH3+OH+M 8.86E46 -7.93 102641.0 !d156

!CH3OH+M=CH3+OH+M 3.50E16 0.0 66444.0 !!! CST

!!! CH3OH+M=CH2OH+H+M 7.20E46 -7.93 107705.0 !d157

!CH3OH+M=CH2OH+H+M 1.75E15 0.0 66444.0 !!! CST

!!! CST-new

CH3OH+M=CH2+H2O+M 7.0E15 0.0 6.6444E4

!CH3OH+CH3=CH2OH+CH4 3.19E01 3.17 7172.0 !d165

!CH3OH+CH3=CH3O+CH4 1.45E01 3.10 6935.0 !d166

!CH3OH+HO2=H2O2+CH2OH 9.64E10 0.0 12579.0 !Corrected, ras

!CH3OH+O=OH+CH2OH 3.80E05 2.5 3080.0 !d160

!84WAR(.3-1.0)

CH3OH+O=OH+CH3O 1.0E13 0.0 4.684E3

!CH3OH+O2=CH2OH+HO2 2.05E13 0.0 44717.0 !d163

!!! CH3OH+OH=H2O+CH2OH 1.50E13 0.0 5960.0 !d161

!CH3OH+OH=H2O+CH2OH 1.00E13 0.0 1697.0 !!! CST

!!! CH3OH+OH=H2O+CH3O 1.50E13 0.0 5960.0 !d162

!CH3OH+OH=H2O+CH3O 1.00E13 0.0 1697.0 !!! CST

!CH3OH+CH2OH=CH3OH+CH3O 7.83E09 0.0 12062.0 !87TSA

!!! CH3OH+H=CH2OH+H2 3.20E13 0.0 6095.0 !d158

!CH3OH+H=CH2OH+H2 3.98E13 0.0 6095.0 !!! CST

!!! CH3OH+H=CH3O+H2 8.06E12 0.0 6095.0 !d159

!CH3OH+H=CH3O+H2 3.98E13 0.0 6095.0 !!! CST

!!! CST-new

CH3OH+HCH=CH2OH+CH3 1.58E12 0.0 5.736E3

!

! CH3O methoxy radical reactions[CH3O C2H5O-) alkoxy radicals]

!

!CH3O+M=CH2O+H+M 9.37E24 -2.7 30590.0 !a

!b38

CH3O+H=CH2O+H2 2.0E13 0.0 0.0E0

!b40

CH3O+OH=CH2O+H2O 1.0E13 0.0 0.0E0

!b42

CH3O+O=CH2O+OH 1.0E13 0.0 0.0E0

!CH3O+O2=CH2O+HO2 6.30E10 0.0 2600.0 !b44\_a

!d48

CH3O+HO2=CH2O+H2O2 3.01E11 0.0 0.0E0

!!! CH3O+CO=CH3+CO2 1.75E13 0.0 11797.0 !d49

!d49 Correct typo

CH3O+CO=CH3+CO2 1.57E13 0.0 1.1797E4

!

! CH2OH hydroxymethyl Rxns [CH2OH CH3CHOH-)hydroxyalkyl radicals]

!

!CH2OH+M=CH2O+H+M 1.67E24 -2.5 34190.0 !a

!b43

CH2OH+O=CH2O+OH 1.0E13 0.0 0.0E0

!CH2OH+O2=CH2O+HO2 2.41E14 0.0 5000.0 !a

!b41

CH2OH+OH=CH2O+H2O 1.0E13 0.0 0.0E0

!b39

CH2OH+H=CH2O+H2 2.0E13 0.0 0.0E0

!d170

CH2OH+HO2=CH2O+H2O2 1.2E13 0.0 0.0E0

!d171

CH2OH+HCO=CH3OH+CO 1.2E14 0.0 0.0E0

!CH2OH+CH2O=CH3OH+HCO 5.54E03 2.81 5682.0 !d173

!!! 2CH2OH=CH3OH+CH2O 1.20E13 0.0 0.0 !d174

!!! CST

2CH2OH=CH3OH+CH2O 4.82E12 0.0 0.0E0

!87TSA

CH2OH+HCO=2CH2O 1.81E14 0.0 0.0E0

!

! CH3 methyl reactions

!

!92BAU/COBrmHR

CH3+M=CH+H2+M 6.9E14 0.0 8.25E4

!Su\_Te.'94,add.HR

CH3=CH2+H 1.14E16 0.09 1.0967E5

!!! CH3+H+M=CH4+M 8.00E26 -3.0 0.0 !b23

!!! H2/2.0/ CO/2.0/ CO2/3.0/ H2O/5.0/

! CH3+H(+M)=CH4(+M) 1.00E17 -0.8 315.0 !!! CSTremHR

! LOW /7.00E33 -4.88 9.310/

! TROE /0.7086 134.0 1784.0 5740.0/

! H2/2.0/ CO/1.5/ CO2/2.0/ H2O/6.0/ CH4/2.0/ C2H6/3.0/

!Baulch'92, addedHR

CH3+H=CH4 2.11E14 0.0 3.974E4

!CH3+HO2=CH3O+OH 2.00E13 0.0 1076.0 !a

!CH3+O=CH2O+H 6.03E13 0.0 0.0 !71DEA/KIS

!87DEA/WES

CH3+O=CH3O 1.78E14 -2.14 6.03E2

!CH3+O2=CH3O+O 7.26E11 0.39 27363.0 !87DEA/WES

!92GLA

CH3+O2=CH2OH+O 1.29E13 0.0 2.69E4

!87DEA/WES

CH3+OH=CH3OH 1.24E43 -9.49 1.0471E4

!!! CST-new

CH3+OH=CH2OH+H 1.09E11 0.4 -7.08E2

!87DEA/WES

CH3+OH=CH3O+H 8.93E11 -0.02 1.3073E4

!!! CST-new

CH3+OH=HCH+H2O 7.5E6 2.0 5.0E3

!CH3+OH=CH2O+H2 3.98E10 -0.02 8765.0 !87DEA/WES

!92GLA

CH3+HO2=CH2OH+OH 2.0E13 0.0 0.0E0

!CH3+HCO=CH4+CO 1.20E14 0.0 0.0 !a

!87TSA

CH3+CH2OH=CH4+CH2O 2.41E12 0.0 0.0E0

!CH3+CH3O=CH4+CH2O 2.41E13 0.0 0.0 !86TSA/HAM

!CH3+CH2O=CH4+HCO 5.54E03 2.81 5863.0 !a

! CH3+CH3=C2H5+H 3.01E13 0.0 13510. !Baulch'92, added HR

!CH3+CH3=C2H5+H 3.69E13 -0.449 13260. !QRRK, HR, 1atm

!CH3+CH3=C2H4+H2 1.00E16 0.0 32030. !War/Gard'84, added HR

! ! CH3+CH3=C2H4+H2 2.35E21 -2.289 7260. !QRRK, HR, 1 atm

!QRRK, HR, 1 atm

2CH3=C2H6 5.24E53 -12.344 1.772E4

! CH3+CH3=C2H6 1.02E13 0.0 0. !Glaenzer+al.'76,addHR

!

! Triplet Methylene reactions

!

!92GLA

HCH+H+M=CH3+M 2.4E31 -4.38 0.0E0

!b46

HCH+H=CH+H2 1.0E18 -1.56 0.0E0

!b66

HCH+O=CO+2H 5.0E13 0.0 0.0E0

!b67

HCH+O=CO+H2 3.0E13 0.0 0.0E0

!b68

HCH+O2=CO2+2H 1.6E12 0.0 1.0E3

!b69

HCH+O2=CH2O+O 5.0E13 0.0 9.0E3

!b70

HCH+O2=CO2+H2 6.9E11 0.0 5.0E2

!b71

HCH+O2=CO+H2O 1.9E10 0.0 -1.0E3

!b72

HCH+O2=CO+OH+H 8.6E10 0.0 -5.0E2

!b73

HCH+O2=HCO+OH 4.3E10 0.0 -5.0E2

!b47

HCH+OH=CH+H2O 1.13E7 2.0 3.0E3

!b48

HCH+OH=CH2O+H 2.5E13 0.0 0.0E0

!b65

HCH+CO2=CH2O+CO 1.1E11 0.0 1.0E3

!b136

CH2+M=HCH+M 1.0E13 0.0 0.0E0

 H/0.0/

 H2O/0.0/

!!! CST-new

HCH+HCO=CH3+CO 1.81E13 0.0 0.0E0

!!! CST-new

HCH+CH3O=CH3+CH2O 1.81E13 0.0 0.0E0

!

! Singlet Methylene reactions

!

!b137

CH2+CH4=2CH3 4.0E13 0.0 0.0E0

!CH2+H2=CH3+H 7.00E13 0.0 0.0 !140;rmHR

! CH3+H=CH2+H2 6.03E13 0.0 15100. !Baulch'92;addHR

!b142

CH2+H2O=HCH+H2O 3.0E13 0.0 0.0E0

!b145

CH2+H=HCH+H 2.0E14 0.0 0.0E0

!CH2+O=H+H+CO 3.00E13 0.0 0.0 !b146

!!! CH2+O=H2+CO 1.51E13 0.0 0.0 !d

!!! CST

CH2+O=H2+CO 7.83E12 0.0 0.0E0

!!! CH2+O2=CO2+2H 1.59E12 0.0 1000.0 !d

!CH2+O2=CO2+2H 7.83E12 0.0 0.0 !!! CST

!!! CH2+O2=O+CH2O 2.00E13 0.0 9000.0 !d

!CH2+O2=O+CH2O 7.83E12 0.0 0.0 !!! CST

!!! CH2+O2=H2+CO2 6.90E11 0.0 500.0 !d

!CH2+O2=H2+CO2 7.83E12 0.0 0.0 !!! CST

!!! CH2+O2=H+CO+OH 1.30E13 0.0 1505.7 !87FRE/WAR

!!! CST

CH2+O2=H+CO+OH 7.83E12 0.0 0.0E0

!!! CH2+OH=CH+H2O 4.50E13 0.0 3000.0 !d CST-rem

!b147

CH2+OH=CH2O+H 3.01E13 0.0 0.0E0

!CH2+H=CH+H2 3.01E13 0.0 0.0 !b148

!b149

CH2+CO2=CH2O+CO 3.0E12 0.0 0.0E0

!d

CH2+HO2=CH2O+OH 3.01E13 0.0 0.0E0

!d

CH2+H2O2=CH3O+OH 3.01E13 0.0 0.0E0

!d

CH2+HCO=CO+CH3 1.81E13 0.0 0.0E0

!d

CH2+CH2O=HCO+CH3 1.2E12 0.0 0.0E0

!84FAR/JUS(.9-2.3K)

CH2+O=CH+OH 3.0E14 0.0 1.1923E4

!b50

CH+O=CO+H 5.7E13 0.0 0.0E0

!92BAU/COB

CH+O2=CO+OH 3.3E13 0.0 0.0E0

! CH+O2=HCO+O 3.30E13 0.0 0.0 !b49

!b51

CH+OH=HCO+H 3.0E13 0.0 0.0E0

!b53

CH+CO2=HCO+CO 3.4E12 0.0 6.9E2

!b55

CH+H2O=CH2O+H 1.17E15 -0.75 0.0E0

!88ZAB/FLE3

CH+H2O=CH2OH 5.71E12 0.0 -7.55E2

!

! HCO aldehyde reactions

!

! HCO+O=CO2+H 3.00E13 0.0 0.0 !b82

!92BAU/COB

HCO+O2=CO2+OH 3.31E12 -0.4 0.0E0

!d

HCO+HO2=CO2+OH+H 3.0E13 0.0 0.0E0

!86TSA/HAM

HCO+CH3O=CH3OH+CO 9.04E13 0.0 0.0E0

!g

2HCO=CH2O+CO 4.5E13 0.0 0.0E0

!HCO+O2=CO+HO2 3.3E13 -0.4 0.0 !b83

!HCO+OH=CO+H2O 3.02E13 0.0 0.0 !a

!HCO+M=H+CO+M 2.50E14 0.0 16802.0 !b79

!HCO+H=CO+H2 2.00E14 0.0 0.0 !e

!HCO+O=CO+OH 3.00E13 0.0 0.0 !b81

!!! CST-new

2HCO=2CO+H2 3.01E12 0.0 0.0E0

!

! CO \_ CO2 reactions

!

!CO+O+M=CO2+M 2.51E13 0.0 -4540.0 !a, for N2

! H2/2.500/ H2O/12.0/ CO2/3.800/ CO/1.900/ !! for N2, HR

! !CO+O+M=CO2+M 2.19E13 0.0 -4540.0 !! rev for Ar, ras

! H2/3.333/ H2O/16.0/ CO2/5.067/ CO/2.533/ !! rev for Ar, ras

!CO+OH=CO2+H 3.09E11 0.0 735.0 !72DFX

!CO+O2=CO2+O 2.51E12 0.0 47690.0 !a

!CO+HO2=CO2+OH 6.03E13 0.0 22950.0 !a

!

! H2O2 reactions

!

! H2O2+M=OH+OH+M 1.20E17 0.0 45500.0 !a

! H2/2.500/ H2O/12.0/ CO2/3.800/ CO/1.900/ !! for N2, HR

! H2O2+M=OH+OH+M 8.51E16 0.0 45500.0 !! rev for Ar, ras

! H2/3.333/ H2O/16.0/ CO2/5.067/ CO/2.533/ !! rev for Ar, ras

! H2O2+H=HO2+H2 4.79E13 0.0 7950.0 !a

! H2O2+H=OH+H2O 1.00E13 0.0 3590.0 !a

!H2O2+O=OH+HO2 9.55E6 2.0 3970.0 !a

!d

H2O2+O=O2+H2O 9.55E6 2.0 3.97E3

!

! HO2 peroxyl reactions

!

!92BAU/COB

HO2+H=H2O+O 3.0E13 0.0 1.07E3

!HO2+H=H2+O2 6.61E13 0.0 2130.0 !a

!HO2+H=OH+OH 1.40E14 0.0 1073.0 !b07

!HO2+OH=H2O+O2 7.50E12 0.0 0.0 !b06

!HO2+HO2=H2O2+O2 2.00E12 0.0 0.0 !b18

!

! H2 \_ H \_ OH \_ O reactions

!

! H2+OH=H2O+H 2.14E8 1.51 3430.0 !a

!b01

H2+O2=2OH 1.7E13 0.0 4.778E4

!H+O2=OH+O 1.91E14 0.0 16440.0 !a

!H+O2+M=HO2+M 3.61E17 -0.72 0.0 !b05

! H2O/18.6/ CO2/4.2/ H2/2.9/ CO/2.1/

!2H+M=H2+M 1.00E18 -1.0 0.0 !b10

!b11

2H+H2=2H2 9.2E16 -0.6 0.0E0

!b12

2H+H2O=H2+H2O 6.0E19 -1.25 0.0E0

!b13

2H+CO2=H2+CO2 5.49E20 -2.0 0.0E0

! 01

CH3+NO2=CH3O+NO 1.3E13 0.0 0.0E0

! 13147 ! 12

2NO2=2NO+O2 1.63E12 0.0 2.6294E4

! 14750 ! 02

CO+NO2=NO+CO2 1.9E12 0.0 2.95E4

!)N2O3=NO+NO2 4.58E16 0.00 4912. ! 2456 ! 14

! \*\*\*\*\*\*\* Reactions from Grimech-3 \*\*\*\*\*\*\*\*\*\*\*\*

N+NO=N2+O 2.7E13 0.0 3.55E2

N+O2=NO+O 9.0E9 1.0 6.5E3

N+OH=NO+H 3.36E13 0.0 3.85E2

N2O+O=N2+O2 1.4E12 0.0 1.081E4

N2O+O=2NO 2.9E13 0.0 2.315E4

N2O+H=N2+OH 3.87E14 0.0 1.888E4

N2O+OH=N2+HO2 2.0E12 0.0 2.106E4

N2O(+M)=N2+O(+M) 7.91E10 0.0 5.602E4

 H2/2.0/

 H2O/6.0/

 CH4/2.0/

 CO/1.5/

 CO2/2.0/

 C2H6/3.0/

 AR/0.625/

 LOW/6.37E14 0.0E0 5.664E4/

HO2+NO=NO2+OH 2.11E12 0.0 -4.8E2

NO+O+M=NO2+M 1.06E20 -1.41 0.0E0

 H2/2.0/

 H2O/6.0/

 CH4/2.0/

 CO/1.5/

 CO2/2.0/

 C2H6/3.0/

 AR/0.7/

NO2+O=NO+O2 3.9E12 0.0 -2.4E2

NO2+H=NO+OH 1.32E14 0.0 3.6E2

NNH=N2+H 3.3E8 0.0 0.0E0

NNH+M=N2+H+M 1.3E14 -0.11 4.98E3

 H2/2.0/

 H2O/6.0/

 CH4/2.0/

 CO/1.5/

 CO2/2.0/

 C2H6/3.0/

 AR/0.7/

NNH+O2=HO2+N2 5.0E12 0.0 0.0E0

NNH+O=OH+N2 2.5E13 0.0 0.0E0

NNH+H=H2+N2 5.0E13 0.0 0.0E0

NNH+OH=H2O+N2 2.0E13 0.0 0.0E0

NNH+CH3=CH4+N2 2.5E13 0.0 0.0E0

CH+N2=HCN+N 3.12E9 0.88 2.013E4

CH+NO=HCN+O 4.1E13 0.0 0.0E0

CH+NO=N+HCO 2.46E13 0.0 0.0E0

CH2+NO=OH+HCN 2.9E14 -0.69 7.6E2

CH3+NO=HCN+H2O 9.6E13 0.0 2.88E4

CH3+N=HCN+H2 3.7E12 0.15 -9.0E1

N+CO2=NO+CO 3.0E12 0.0 1.13E4

END

THERMO

!ALL

 300.000 1000.000 5000.000

H 120186H 1 G 300.0 5000.0 1000.0 1

 2.5E0 0.0E0 0.0E0 0.0E0 0.0E0 2

 2.547163E4 -4.601176E-1 2.5E0 0.0E0 0.0E0 3

 0.0E0 0.0E0 2.547163E4 -4.601176E-1 4

H2 121286H 2 G 300.0 5000.0 1000.0 1

 2.991423E0 7.000644E-4 -5.633829E-8 -9.231578E-12 1.582752E-15 2

 -8.35034E2 -1.35511E0 3.298124E0 8.249442E-4 -8.143015E-7 3

 -9.475434E-11 4.134872E-13 -1.012521E3 -3.294094E0 4

O 120186O 1 G 300.0 5000.0 1000.0 1

 2.54206E0 -2.755062E-5 -3.102803E-9 4.551067E-12 -4.368052E-16 2

 2.92308E4 4.920308E0 2.946429E0 -1.638166E-3 2.421032E-6 3

 -1.602843E-9 3.890696E-13 2.914764E4 2.963995E0 4

O2 121386O 2 G 300.0 5000.0 1000.0 1

 3.697578E0 6.135197E-4 -1.258842E-7 1.775281E-11 -1.136435E-15 2

 -1.23393E3 3.189166E0 3.212936E0 1.127486E-3 -5.75615E-7 3

 1.313877E-9 -8.768554E-13 -1.005249E3 6.034738E0 4

OH -THERMH 1O 1 G 300.0 5000.0 1357.0 1

 2.62599754E0 1.31992406E-3 -3.5972467E-7 4.256308E-11-1.82048016E-15 2

 4.12085374E3 7.10667307E0 3.43586219E0 2.02235804E-4 -1.13546412E-7 3

 2.42445149E-10-7.43651031E-14 3.74321252E3 2.45014127E0 4

H2O -20387H 2O 1 G 300.0 5000.0 1000.0 1

 2.672146E0 3.056293E-3 -8.73026E-7 1.200996E-10 -6.391618E-15 2

 -2.989921E4 6.862817E0 3.386842E0 3.474982E-3 -6.354696E-6 3

 6.968581E-9 -2.506588E-12 -3.020811E4 2.590233E0 4

N2 121286N 2 G 300.0 5000.0 1000.0 1

 2.92664E0 1.487977E-3 -5.684761E-7 1.009704E-10 -6.753351E-15 2

 -9.227977E2 5.980528E0 3.298677E0 1.40824E-3 -3.963222E-6 3

 5.641515E-9 -2.444855E-12 -1.0209E3 3.950372E0 4

CO 121286O 1C 1 G 300.0 5000.0 1000.0 1

 3.025078E0 1.442689E-3 -5.630828E-7 1.018581E-10 -6.910952E-15 2

 -1.426835E4 6.108218E0 3.262452E0 1.511941E-3 -3.881755E-6 3

 5.581944E-9 -2.474951E-12 -1.431054E4 4.848897E0 4

HCO 121286H 1O 1C 1 G 300.0 5000.0 1000.0 1

 3.557271E0 3.345573E-3 -1.335006E-6 2.470573E-10 -1.713851E-14 2

 3.916324E3 5.552299E0 2.89833E0 6.199147E-3 -9.623084E-6 3

 1.089825E-8 -4.574885E-12 4.159922E3 8.983614E0 4

CO2 121286O 2C 1 G 300.0 5000.0 1000.0 1

 4.453623E0 3.140169E-3 -1.278411E-6 2.393997E-10 -1.669033E-14 2

 -4.896696E4 -9.553959E-1 2.275725E0 9.922072E-3 -1.040911E-5 3

 6.866687E-9 -2.11728E-12 -4.837314E4 1.018849E1 4

CH3 121286H 3C 1 G 300.0 5000.0 1000.0 1

 2.844052E0 6.137974E-3 -2.230345E-6 3.785161E-10 -2.452159E-14 2

 1.643781E4 5.452697E0 2.430443E0 1.11241E-2 -1.68022E-5 3

 1.621829E-8 -5.864953E-12 1.642378E4 6.789794E0 4

CH4 121286H 4C 1 G 300.0 5000.0 1000.0 1

 1.683479E0 1.023724E-2 -3.875129E-6 6.785585E-10 -4.503423E-14 2

 -1.008079E4 9.623395E0 7.787415E-1 1.747668E-2 -2.783409E-5 3

 3.049708E-8 -1.223931E-11 -9.825229E3 1.372219E1 4

HO2 -THERMH 1O 2 G 300.0 5000.0 1390.0 1

 4.10547423E0 2.38452835E-3 -8.06347989E-7 1.24191723E-10-7.16400108E-15 2

 3.98127689E2 3.12515836E0 3.18310656E0 3.6676795E-3 -9.32385122E-7 3

-3.25852919E-10 1.51139912E-13 8.09181013E2 8.39371099E0 4

H2O2 120186H 2O 2 G 300.0 5000.0 1000.0 1

 4.573167E0 4.336136E-3 -1.474689E-6 2.348904E-10 -1.431654E-14 2

 -1.800696E4 5.01137E-1 3.388754E0 6.569226E-3 -1.485013E-7 3

 -4.625806E-9 2.471515E-12 -1.766315E4 6.785363E0 4

CH2O 121286H 2O 1C 1 G 300.0 5000.0 1000.0 1

 2.995606E0 6.681321E-3 -2.628955E-6 4.737153E-10 -3.212517E-14 2

 -1.532037E4 6.912572E0 1.652731E0 1.263144E-2 -1.888168E-5 3

 2.050031E-8 -8.413237E-12 -1.48654E4 1.378482E1 4

CH3O 121686H 3O 1C 1 G 300.0 3000.0 1000.0 1

 3.7708E0 7.871497E-3 -2.656384E-6 3.944431E-10 -2.112616E-14 2

 1.278325E2 2.929575E0 2.106204E0 7.216595E-3 5.338472E-6 3

 -7.377636E-9 2.075611E-12 9.786011E2 1.315218E1 4

C2H6 121686H 6C 2 G 300.0 4000.0 1000.0 1

 4.825938E0 1.384043E-2 -4.557259E-6 6.724967E-10 -3.598161E-14 2

 -1.271779E4 -5.239507E0 1.462539E0 1.549467E-2 5.780507E-6 3

 -1.257832E-8 4.586267E-12 -1.123918E4 1.443229E1 4

CH2 120186H 2C 1 G 250.0 4000.0 1000.0 1

 3.636408E0 1.933057E-3 -1.687016E-7 -1.009899E-10 1.808256E-14 2

 4.534134E4 2.156561E0 3.762237E0 1.159819E-3 2.489585E-7 3

 8.800836E-10 -7.332435E-13 4.536791E4 1.712578E0 4

CH 121286H 1C 1 G 300.0 5000.0 1000.0 1

 2.196223E0 2.340381E-3 -7.058201E-7 9.007582E-11 -3.85504E-15 2

 7.086723E4 9.178373E0 3.200202E0 2.072876E-3 -5.134431E-6 3

 5.73389E-9 -1.955533E-12 7.045259E4 3.331588E0 4

CH3OH 121686H 4O 1C 1 G 300.0 5000.0 1000.0 1

 4.029061E0 9.376593E-3 -3.050254E-6 4.358793E-10 -2.224723E-14 2

 -2.615791E4 2.378196E0 2.660115E0 7.341508E-3 7.170051E-6 3

 -8.793194E-9 2.39057E-12 -2.535348E4 1.123263E1 4

CH2OH 120186H 3O 1C 1 G 250.0 4000.0 1000.0 1

 6.32752E0 3.608271E-3 -3.201547E-7 -1.93875E-10 3.509705E-14 2

 -4.474509E3 -8.329366E0 2.862628E0 1.001527E-2 -5.285436E-7 3

 -5.13854E-9 2.246041E-12 -3.349679E3 1.039794E1 4

CH3O2 -THERMH 3O 2C 1 G 300.0 5000.0 1385.0 1

 5.95787891E0 7.90728626E-3 -2.68246234E-6 4.13891337E-10 -2.3900733E-14 2

 -1.53574838E3 -4.71963886E0 4.26146906E0 1.00873599E-2 -3.21506184E-6 3

 2.09409267E-10 4.18339103E-14 -6.84394259E2 5.1633032E0 4

CH3O2H -THERMH 4O 2C 1 G 300.0 5000.0 1390.0 1

 8.43117091E0 8.06817909E-3 -2.77094921E-6 4.31332243E-10-2.50692146E-14 2

 -1.96678771E4 -1.91170629E1 3.23442817E0 1.90129767E-2 -1.13386287E-5 3

 3.40306653E-9-4.11830222E-13 -1.77197926E4 9.25623949E0 4

HCO2 -THERMH 1O 2C 1 G 300.0 5000.0 1690.0 1

 6.12628782E0 3.75602932E-3 -1.42010352E-6 2.364292E-10-1.44167651E-14 2

 -2.17698466E4 -8.01574694E0 1.35213452E0 1.50082004E-2 -1.09896141E-5 3

 3.7367984E-9-4.81014498E-13 -2.02253647E4 1.74373147E1 4

CH3OCH3 -THERMH 6O 1C 2 G 300.0 5000.0 1368.0 1

 8.27745836E0 1.32135539E-2 -4.53264362E-6 7.05316507E-10-4.09933283E-14 2

 -2.619827E4 -2.15190894E1 1.5076345E0 2.39914228E-2 -8.689105E-6 3

-9.66835762E-11 4.89319361E-13 -2.32810894E4 1.67317297E1 4

CH3OCH2 -THERMH 5O 1C 2 G 300.0 5000.0 1376.0 1

 8.17137842E0 1.10086181E-2 -3.82352277E-6 5.99637202E-10-3.50317513E-14 2

 -3.41941605E3 -1.78650856E1 2.91327415E0 2.03364659E-2 -9.59712342E-6 3

 2.07478525E-9-1.71343362E-13 -1.1884424E3 1.16066817E1 4

CH3OCH2O2 -THERMH 5O 3C 2 G 300.0 5000.0 1389.0 1

 1.24249729E1 1.18705986E-2 -4.07906532E-6 6.35310809E-10-3.69427867E-14 2

 -2.29679238E4 -3.53740145E1 2.21029612E0 3.68877454E-2 -2.82561555E-5 3

 1.15730533E-8 -1.9713047E-12 -1.9494094E4 1.91463601E1 4

CH2OCH2O2H -THERMH 5O 3C 2 G 300.0 5000.0 1393.0 1

 1.51191783E1 9.23718883E-3 -3.19127505E-6 4.99114678E-10-2.91162488E-14 2

 -1.84114867E4 -4.85706618E1 2.52895507E0 4.2412829E-2 -3.73406386E-5 3

 1.66639333E-8-2.96443312E-12 -1.44293306E4 1.76899251E1 4

CH3OCH2O -THERMH 5O 2C 2 G 300.0 5000.0 2012.0 1

 8.60261845E0 1.35772195E-2 -4.84661602E-6 7.77766193E-10-4.62633624E-14 2

 -2.13762444E4 -1.75775023E1 3.25889339E0 2.22146359E-2 -7.7855634E-6 3

-2.41484158E-10 4.51914496E-13 -1.92377212E4 1.23680069E1 4

O2CH2OCH2O2H 98-TRMH 5O 5C 2 G 300.0 5000.0 1402.0 1

 1.92038046E1 1.04394841E-2 -3.60582939E-6 5.63792843E-10-3.28807214E-14 2

 -3.79207055E4 -6.51847273E1 1.99640551E0 5.83226232E-2 -5.53259778E-5 3

 2.5981054E-8-4.77141005E-12 -3.27628742E4 2.44215005E1 4

HO2CH2OCHO -THERMH 4O 4C 2 G 300.0 5000.0 1387.0 1

 1.64584298E1 8.52683511E-3 -3.041135E-6 4.85596908E-10-2.87316334E-14 2

 -6.23959608E4 -5.38924139E1 3.47935703E0 4.02952392E-2 -3.30109296E-5 3

 1.34360117E-8 -2.1860158E-12 -5.80629934E4 1.52521392E1 4

OCH2OCHO -THERMH 3O 3C 2 G 300.0 5000.0 1475.0 1

 1.20233916E1 8.11262659E-3 -2.91356462E-6 4.67340384E-10-2.77375525E-14 2

 -4.33647231E4 -3.33691809E1 5.19690837E0 1.58839723E-2 3.53540547E-7 3

 -6.10456923E-9 1.94661801E-12 -4.02242792E4 6.11645828E0 4

HOCH2OCO -THERMH 3O 3C 2 G 300.0 5000.0 1439.0 1

 1.46703686E1 5.35812603E-3 -1.94490233E-6 3.1417919E-10-1.87391432E-14 2

 -4.69661949E4 -3.69483137E1 5.75763608E0 2.29536196E-2 -1.29175655E-5 3

 2.07080009E-9 2.3308824E-13 -4.36536058E4 1.18884577E1 4

HOCH2O -THERMH 3O 2C 1 G 300.0 5000.0 1452.0 1

 6.39521515E0 7.43673043E-3 -2.50422354E-6 3.84879712E-10-2.21778689E-14 2

 -2.47500385E4 -7.29290847E0 4.11183145E0 7.53850697E-3 3.7733737E-6 3

 -5.38746005E-9 1.45615887E-12 -2.34414546E4 6.81381989E0 4

HCO2H -THERMH 2O 2C 1 G 300.0 5000.0 1376.0 1

 6.68733013E0 5.14289368E-3 -1.82238513E-6 2.89719163E-10-1.70892199E-14 2

 -4.839954E4 -1.13104798E1 1.43548185E0 1.63363016E-2 -1.06257421E-5 3

 3.32132977E-9-4.02176103E-13 -4.64616504E4 1.72885798E1 4

CH3OCHO -THERMH 4O 2C 2 G 300.0 5000.0 1686.0 1

 8.69123518E0 1.15503122E-2 -4.27782486E-6 7.02533059E-10-4.24333552E-14 2

 -4.64364769E4 -1.89301478E1 3.08839783E0 2.03760048E-2 -6.8477704E-6 3

-7.28186203E-10 5.62130216E-13 -4.41855167E4 1.25364719E1 4

CH3OCO -THERMH 3O 2C 2 G 300.0 5000.0 1362.0 1

 1.308776E1 4.5354495E-3 -1.65096364E-6 2.67197277E-10-1.59576863E-14 2

 -2.466164E4 -3.27914051E1 3.94199159E0 2.43434884E-2 -1.6559556E-5 3

 4.58537411E-9-3.31795708E-13 -2.14404829E4 1.66954362E1 4

!! Thermo from DME original

AR 120186AR 1 G 300.0 5000.0 1000.0 1

 2.5E0 0.0E0 0.0E0 0.0E0 0.0E0 2

 -7.45375E2 4.366001E0 2.5E0 0.0E0 0.0E0 3

 0.0E0 0.0E0 -7.45375E2 4.366001E0 4

HCH BURCATH 2C 1 G 300.0 5000.0 1368.0 1

 2.49583264E0 3.52943326E-3 -9.63343036E-7 1.18888184E-10-5.56170848E-15 2

 4.62249453E4 8.50808173E0 3.59749026E0 1.12033951E-3 1.01034198E-6 3

-6.06023665E-10 9.61560175E-14 4.5825048E4 2.53129363E0 4

N L-6-88N 1 G 200.0 6000.0 1000.0 1

 2.4159429E0 1.7489065E-4 -1.1902369E-7 3.0226245E-11 -2.0360982E-15 2

 5.6133773E4 4.6496096E0 2.5E0 0.0E0 0.0E0 3

 0.0E0 0.0E0 5.6104637E4 4.1939087E0 4

NNH T07-93H 1N 2 G 200.0 6000.0 1000.0 1

 3.7667544E0 2.8915082E-3 -1.041662E-6 1.6842594E-10 -1.0091896E-14 2

 2.8650697E4 4.4705067E0 4.3446927E0 -4.8497072E-3 2.0059459E-5 3

 -2.1726464E-8 7.9469539E-12 2.8791973E4 2.977941E0 4

NO RUS-78O 1N 1 G 200.0 6000.0 1000.0 1

 3.2606056E0 1.1911043E-3 -4.2917048E-7 6.9457669E-11 -4.0336099E-15 2

 9.9209746E3 6.3693027E0 4.2184763E0 -4.638976E-3 1.1041022E-5 3

 -9.3361354E-9 2.803577E-12 9.844623E3 2.2808464E0 4

NO2 L-7-88O 2N 1 G 200.0 6000.0 1000.0 1

 4.8847542E0 2.1723956E-3 -8.2806906E-7 1.574751E-10 -1.0510895E-14 2

 2.3164983E3 -1.1741695E-1 3.9440312E0 -1.585429E-3 1.6657812E-5 3

 -2.0475426E-8 7.8350564E-12 2.8966179E3 6.3119917E0 4

N2O L-7-88O 1N 2 G 200.0 6000.0 1000.0 1

 4.8230729E0 2.6270251E-3 -9.5850874E-7 1.6000712E-10 -9.7752303E-15 2

 8.0734048E3 -2.2017207E0 2.2571502E0 1.1304728E-2 -1.3671319E-5 3

 9.6819806E-9 -2.9307182E-12 8.7417744E3 1.0757992E1 4

HCN GRI-98H 1C 1N 1 G 200.0 6000.0 1000.0 1

 3.8022392E0 3.1464228E-3 -1.0632185E-6 1.6619757E-10 -9.799757E-15 2

 1.4407292E4 1.5754601E0 2.2589886E0 1.005117E-2 -1.3351763E-5 3

 1.0092349E-8 -3.0089028E-12 1.4712633E4 8.9164419E0 4

END

!!Added from DME

AR 0 136.500 3.330 0.000 0.000 0.000

AS 0 1045.500 4.580 0.000 0.000 0.000 ! MEC

ASH 1 199.300 4.215 0.000 0.000 1.000 ! MEC

ASH2 2 229.600 4.180 0.000 0.000 1.000 ! MEC

C 0 71.400 3.298 0.000 0.000 0.000 ! \*

C2 1 97.530 3.621 0.000 1.760 4.000

C2O 1 232.400 3.828 0.000 0.000 1.000 ! \*

CN2 1 232.400 3.828 0.000 0.000 1.000 ! OIS

C2H 1 265.300 3.721 0.000 0.000 2.500 ! NMM

C2H2 1 265.300 3.721 0.000 0.000 2.500 ! NMM

C2H2OH 2 224.700 4.162 0.000 0.000 1.000 ! \*

C2H3 2 265.300 3.721 0.000 0.000 1.000 ! NMM

C2H4 2 238.400 3.496 0.000 0.000 1.500 ! NMM

C2H5 2 247.500 4.350 0.000 0.000 1.500 ! NMM

C2H5OH 2 470.600 4.410 0.000 0.000 1.500 ! NMM

C2H5O2H 2 470.600 4.410 0.000 0.000 1.500 ! C2H5OH

C2H4OH 2 470.600 4.410 0.000 0.000 1.500 ! C2H5OH

C2H4O2H 2 470.600 4.410 0.000 0.000 1.500 ! C2H5OH

HOC2H4OH 2 510.5 4.762 2.2 0.0 1.5 ! WJP

O2C2H4OH 2 510.5 4.762 2.2 0.0 1.5 ! HOC2H4OH

O2C2H4O2H 2 510.5 4.762 2.2 0.0 1.5 ! HOC2H4OH

C2H5O 2 470.600 4.410 0.000 0.000 1.500 ! NMM

C2H5O2 2 470.600 4.410 0.000 0.000 1.500 ! C2H5O

PC2H4OH 2 470.600 4.410 0.000 0.000 1.500 ! NMM

SC2H4OH 2 470.600 4.410 0.000 0.000 1.500 ! NMM

C2H6 2 247.500 4.350 0.000 0.000 1.500 ! NMM

C2N 1 232.400 3.828 0.000 0.000 1.000 ! OIS

C2N2 1 349.000 4.361 0.000 0.000 1.000 ! OIS

C3H2 2 209.000 4.100 0.000 0.000 1.000 ! \*

C3H2(S) 2 209.000 4.100 0.000 0.000 1.000 ! \*

C3H3 1 324.800 4.290 0.000 0.000 1.000 ! NMM

C4H3 1 357.000 4.720 0.000 0.000 1.000 ! NMM

C3H4O 2 443.200 4.120 0.000 0.000 1.000 ! NMM

CHCHCHO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

HCCCHO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

HCCCO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

H2CCHCO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

CH3CCO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

CH3CHCO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

CH2CHCO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

C2H3CO 2 443.200 4.120 0.000 0.000 1.000 ! NMM

CH2CH2CHO 2 424.600 4.820 0.000 0.000 1.000 ! NMM

C2H5CO 2 424.600 4.820 0.000 0.000 1.000 ! NMM

CH3OCH3 2 395.0 4.037 1.3 0.0 1.0 ! SVE,RPD

CH3OCH2 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3OCH2O2 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH2OCH2O2H 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3OCH2O2H 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3OCH2OH 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3OCH2O 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3OCHO 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3OCO 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH2OCHO 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

O2CH2OCH2O2H 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

HO2CH2OCHO 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

OCH2OCHO 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

HOCH2OCO 2 395.0 4.037 1.3 0.0 1.0 ! CH3OCH3

CH3COCH3 2 435.500 4.860 2.9 0.000 1.000 ! NMM,WJP

CH3COCH2 2 435.500 4.860 2.9 0.000 1.000 ! CH3COCH3

CH3COCH2O2 2 435.500 4.860 2.9 0.000 1.000 ! CH3COCH3

CH3COCH2O2H 2 435.500 4.860 2.9 0.000 1.000 ! CH3COCH3

CH3COCH2O 2 435.500 4.860 2.9 0.000 1.000 ! CH3COCH3

CH2CH2COCH3 2 435.500 4.860 2.9 0.000 1.000 ! CH3COCH3

C2H5COCH3 2 454.0 5.413 3.3 0.000 1.000 ! WJP,RPD

C2H5COCH2 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

C2H3COCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH2CH2COCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH3CHCOCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH3CHOOHCOCH2 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH2CHOOHCOCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH3CHOOHCOCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH3CHOOHCOCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

CH3CHOOCOCH3 2 454.0 5.413 3.3 0.000 1.000 ! C2H5COCH3

C3H4 1 324.800 4.290 0.000 0.000 1.000 ! NMM

C3H4-A 1 324.800 4.290 0.000 0.000 1.000 ! NMM

C3H4-P 1 324.800 4.290 0.000 0.000 1.000 ! NMM

C3H4C 2 324.800 4.290 0.000 0.000 1.000 ! NMM

C3H6 2 307.800 4.140 0.000 0.000 1.000 ! NMM

C3H6OH 2 487.900 4.820 0.000 0.000 1.000 ! NMM

HOC3H6O2 2 487.900 4.820 0.000 0.000 1.000 ! NMM

C3H5O 2 411.000 4.820 0.000 0.000 1.000 ! NMM

C3H7 2 303.400 4.810 0.000 0.000 1.000 ! NMM

C4H6 2 357.000 4.720 0.000 0.000 1.000 ! NMM

IC3H7 2 303.400 4.810 0.000 0.000 1.000 ! NMM

NC3H7 2 303.400 4.810 0.000 0.000 1.000 ! NMM

C3H8 2 303.400 4.810 0.000 0.000 1.000 ! NMM

C4H 1 357.000 4.720 0.000 0.000 1.000 ! NMM

C4H2 1 357.000 4.720 0.000 0.000 1.000 ! NMM

C4H2OH 2 224.700 4.162 0.000 0.000 1.000 ! \*

CH3CHCCH 2 355.000 4.650 0.000 0.000 1.000 ! NMM

IC4H7 2 355.000 4.650 0.000 0.000 1.000 ! NMM

C4H7 2 355.000 4.650 0.000 0.000 1.000 ! NMM

C4H8 2 355.000 4.650 0.000 0.000 1.000 ! NMM

C4H8-1 2 355.000 4.650 0.000 0.000 1.000 ! NMM

C4H8-2 2 355.000 4.650 0.000 0.000 1.000 ! NMM

PC4H9 2 352.000 5.240 0.000 0.000 1.000 ! NMM

C4H9 2 352.000 5.240 0.000 0.000 1.000 ! NMM

SC4H9 2 352.000 5.240 0.000 0.000 1.000 ! NMM

TC4H9 2 352.000 5.240 0.000 0.000 1.000 ! NMM

IC4H9 2 352.000 5.240 0.000 0.000 1.000 ! NMM

PC4H9O 2 496.000 5.200 0.000 0.000 1.000 ! NMM

TC4H9O 2 496.000 5.200 0.000 0.000 1.000 ! NMM

C4H8OH-1 2 496.000 5.200 0.000 0.000 1.000 ! NMM

SC4H9O 2 496.000 5.200 0.000 0.000 1.000 ! NMM

IC4H9O 2 496.000 5.200 0.000 0.000 1.000 ! NMM

C4H8OH-2 2 496.000 5.200 0.000 0.000 1.000 ! NMM

IC4H8OH 2 496.000 5.200 0.000 0.000 1.000 ! NMM

O2C4H8OH-1 2 496.000 5.200 0.000 0.000 1.000 ! \*

O2C4H8OH-2 2 496.000 5.200 0.000 0.000 1.000 ! \*

IO2C4H8OH 2 496.000 5.200 0.000 0.000 1.000 ! \*

C4H7O 2 496.000 5.200 0.000 0.000 1.000 ! NMM

IC4H7O 2 496.000 5.200 0.000 0.000 1.000 ! NMM

C5H2 1 408.000 5.200 0.000 0.000 1.000 ! NMM

C5H3 1 408.000 5.200 0.000 0.000 1.000 ! NMM

C5H5 1 408.000 5.200 0.000 0.000 1.000 ! NMM

C5H6 1 408.000 5.200 0.000 0.000 1.000 ! NMM

C5H7 2 408.000 5.200 0.000 0.000 1.000 ! NMM

CYC5H7 2 408.000 5.200 0.000 0.000 1.000 !

C5H8 2 408.000 5.200 0.000 0.000 1.000 ! NMM

C6H2 1 408.000 5.200 0.000 0.000 1.000 ! NMM

C6H4 2 412.300 5.349 0.000 0.000 1.000 ! JAM

C6H5 2 412.300 5.349 0.000 0.000 1.000 ! JAM

C6H5(L) 2 412.300 5.349 0.000 0.000 1.000 ! JAM

C6H5OH 2 450.000 5.500 0.000 0.000 1.000 ! NMM

C6H5O 2 450.000 5.500 0.000 0.000 1.000 ! JAM

OKETPHNL 2 450.000 5.500 0.000 0.000 1.000 !

C6H4O2 2 450.000 5.500 0.000 0.000 1.000

C5H4O 2 450.000 5.500 0.000 0.000 1.000 ! NMM

C5H4OH 2 450.000 5.500 0.000 0.000 1.000 ! NMM

C5H5O 2 450.000 5.500 0.000 0.000 1.000 ! NMM

C5H5OH 2 450.000 5.500 0.000 0.000 1.000 ! NMM

C6H5C2H 2 468.500 5.230 0.000 0.000 1.000 ! NMM

LC6H5 2 426.300 5.510 0.000 0.000 1.000

LC3H3C3H2 2 426.300 5.510 0.000 0.000 1.000

LC3H4C3H2 2 426.300 5.510 0.000 0.000 1.000

LC3H3C3H3 2 426.300 5.510 0.000 0.000 1.000

C6H6 2 468.500 5.230 0.000 10.30 1.000 ! NMM

C6H7 2 468.500 5.230 0.000 0.000 1.000 ! NMM

CYC6H7 2 468.500 5.230 0.000 0.000 1.000 ! NMM

CYC6H8 2 468.500 5.230 0.000 0.000 1.000 ! NMM

C6H5CH2 2 495.300 5.680 0.000 0.000 1.000 ! NMM

C6H5CH3 2 495.300 5.680 0.430 12.30 1.000 ! NMM

C6H4CH3 2 495.300 5.680 0.000 0.000 1.000 ! NMM

CH3C6H4 2 495.300 5.680 0.000 0.000 1.000 ! NMM

C6H5CO 2 622.400 5.530 0.000 0.000 1.000 ! NMM

C6H5CHO 2 622.400 5.530 0.000 0.000 1.000 ! NMM

C6H5CH2OH 2 622.400 5.530 0.000 0.000 1.000 ! NMM

OC6H4CH3 2 621.100 5.640 0.000 0.000 1.000 ! NMM

HOC6H4CH3 2 621.100 5.640 0.000 0.000 1.000 ! NMM

XYLYLENE 2 523.600 6.182 0.000 0.000 1.000

XYLYLRAD 2 523.600 6.182 0.000 0.000 1.000

C6H5C2H5 2 523.600 5.960 0.000 0.000 1.000 ! NMM

ACH3C2H3 2 523.600 5.960 0.000 0.000 1.000

ACH3C2H5 2 523.600 5.960 0.000 0.000 1.000

ACH2RC2H3 2 523.600 5.960 0.000 0.000 1.000

ACH3CH3 2 523.600 5.960 0.000 0.000 1.000 !

ACH3RCH2 2 523.600 5.960 0.000 0.000 1.000

C6H9 2 426.300 5.510 0.000 0.000 1.000 ! NMM

C6H10 2 426.300 5.510 0.000 0.000 1.000 ! NMM

C8H14 2 494.000 6.170 0.000 0.000 1.000 ! NMM

IC8H14 2 494.000 6.170 0.000 0.000 1.000 ! NMM

C6H5C2H3 2 546.200 6.000 0.130 15.00 1.000 ! NMM

C6H5CHCH 2 546.200 6.000 0.000 0.000 1.000 ! NMM

C6H5CCH2 2 546.200 6.000 0.000 0.000 1.000

C6H5C2H 2 534.300 5.710 0.770 0.000 1.000 ! NMM

C6H5C2 2 534.300 5.710 0.000 0.000 1.000 ! NMM

C6H4C2H3 2 546.200 6.000 0.000 0.000 1.000 ! NMM

C6H4C2H 2 534.300 5.710 0.000 0.000 1.000 ! NMM

AAC2H5 2 695.000 6.530 0.000 0.000 1.000

AAC2H3 2 689.800 6.500 0.000 0.000 1.000

AARCCH2 2 689.800 6.500 0.000 0.000 1.000

AACCH 2 689.800 6.500 0.000 0.000 1.000

ARACCH 2 689.800 6.500 0.000 0.000 1.000

ARAC2H3 2 687.200 6.490 0.000 0.000 1.000

C6H5CCO 2 588.200 5.940 0.000 0.000 1.0001

C10H7 2 630.400 6.180 0.000 0.000 1.000 ! NMM

C10H7O 2 630.400 6.180 0.000 0.000 1.000 ! NMM

AC2H3C2H5 2 630.400 6.180 0.000 0.000 1.000

AC2H3C2H3 2 630.400 6.180 0.000 0.000 1.000

C10H8 2 630.400 6.180 0.000 16.50 1.000 ! NMM

C10H9 2 630.400 6.180 0.000 0.000 1.000 ! NMM

C10H10 2 630.400 6.180 0.000 0.000 1.000 ! NMM

C10H7CH2 2 660.00 6.350 0.000 0.000 1.000 ! NMM

AACH3CH2 2 660.0 6.350 0.000 0.000 1.000

C10H7OH 2 663.45 6.362 0.000 0.000 1.000

C10H7CH3 2 660.0 6.350 0.000 0.000 1.000 ! NMM

FLRNTHN 2 812.3 7.170 0.000 0.000 1.000 ! NMM

ACEPHEN 2 812.3 7.170 0.000 0.000 1.000

ANTHRACN 2 772.0 6.960 0.000 25.40 1.000

CH3INDENE 2 625.0 6.150 0.000 0.000 1.000

CH3INDENYL 2 625.0 6.150 0.000 0.000 1.000

AAACH3 2 783.9 6.995 0.000 0.000 1.000

P1HENANOL 2 783.9 6.995 0.000 0.000 1.000

P5HENANOL 2 783.9 6.995 0.000 0.000 1.000

P1HANOXY 2 783.9 6.995 0.000 0.000 1.000

P5HANOXY 2 783.9 6.995 0.000 0.000 1.000

AAARCH2 2 783.9 6.995 0.000 0.000 1.000

AAAC2H5 2 816.6 7.160 0.000 0.000 1.000

AAAC2H3 2 812.0 7.137 0.000 0.000 1.000

PHNTHRN 2 772.0 6.960 0.000 38.80 1.000

PENTANAPH 2 772.0 6.960 0.000 0.000 1.000

PENAPRAD 2 772.0 6.960 0.000 0.000 1.000

P1HNTHRNYL 2 772.0 6.960 0.000 38.80 1.000 ! NMM

P5HNTHRNYL 2 772.0 6.960 0.000 38.80 1.000

PYRENE 2 834.9 7.240 0.000 0.000 1.000 ! NMM

CY5PYREN 2 862.0 7.382 0.000 0.000 1.000

H4PENTDEF 2 834.9 7.240 0.000 0.000 1.000

H4PDFRAD 2 834.9 7.240 0.000 0.000 1.000

PYRENYL 2 834.9 7.240 0.000 0.000 1.000 ! NMM

DHPYRENE 2 834.9 7.240 0.000 0.000 1.000

BENZOAP 2 832.5 7.550 1.400 0.000 1.000 ! NMM

SMILEY 2 832.5 7.550 0.000 0.000 1.000

BENZOGHI 2 832.5 7.550 0.000 0.000 1.000

CPENTACD 2 832.5 7.550 0.000 0.000 1.000

ACEC10H8 2 695.4 6.760 0.000 0.000 1.000 ! NMM

ACEC10H7 2 695.4 6.760 0.000 0.000 1.000

INDENE 2 588.6 5.960 0.650 0.000 1.000 ! NMM

INDENYL 2 588.6 5.960 0.000 0.000 1.000 ! NMM

CH3NDENE 2 588.6 5.960 0.000 0.000 1.000 ! NMM

CH3NDNYL 2 588.6 5.960 0.000 0.000 1.000 ! NMM

CH3FLRNE 2 712.6 6.890 0.000 0.000 1.000

CH3FLRNL 2 712.6 6.890 0.000 0.000 1.000

FLRENE 2 712.6 6.890 0.000 0.000 1.000

FLRNYLP 2 712.6 6.890 0.000 0.000 1.000

FLRNYLA 2 712.6 6.890 0.000 0.000 1.000

CH2FLRNE 2 712.6 6.890 0.000 0.000 1.000

C6H5C5H5 2 783.800 6.640 0.000 0.000 1.000

C6H5C5H4 2 783.800 6.640 0.000 0.000 1.000

BIBENZYL 2 783.800 6.640 0.000 0.000 1.000 ! NMM

STILBENE 2 772.0 6.960 0.000 0.000 1.000 ! NMM

STILBNRD 2 772.0 6.960 0.000 0.000 1.000 ! NMM

ANTHRACN 2 772.0 6.960 0.000 0.000 1.000 ! NMM

DHANTHRN 2 772.0 6.960 0.000 0.000 1.000

OBZYLTOL 2 772.0 6.960 0.000 0.000 1.000

OBZYLTLR 2 772.0 6.960 0.000 0.000 1.000

DMDP 2 712.6 6.890 0.000 0.000 1.000

DMDPRD 2 712.6 6.890 0.000 0.000 1.000

CH 1 80.000 2.750 0.000 0.000 0.000

CH2 1 144.000 3.800 0.000 0.000 0.000

SCH2 1 144.000 3.800 0.000 0.000 0.000

CH2(S) 1 144.000 3.800 0.000 0.000 0.000

CH2CHCCH 2 373.700 4.790 0.000 0.000 1.000 ! NMM

CH2CHCCH2 2 373.700 4.790 0.000 0.000 1.000 ! NMM

CH3CCCH2 2 357.100 4.720 0.000 0.000 1.000

CH3CHCCH2 2 357.100 4.720 0.000 0.000 1.000

CH2CH2CCH 2 373.700 4.790 0.000 0.000 1.000 ! NMM

CH2CHCH2 2 316.000 4.220 0.000 0.000 1.000 ! NMM

C3H5-A 2 316.000 4.220 0.000 0.000 1.000

C3H5 2 316.000 4.220 0.000 0.000 1.000

CH2CHCHCH 2 357.100 4.720 0.000 0.000 1.000 ! NMM

CHCHCHCH 2 357.100 4.720 0.000 0.000 1.000 ! NMM

CH2CHCHCH2 2 357.100 4.720 0.000 0.000 1.000 ! NMM

CH2CO 2 436.000 3.970 0.000 0.000 2.000

CH2O 2 498.000 3.590 0.000 0.000 2.000

HCOH 2 498.000 3.590 0.000 0.000 1.000

H2CO 2 498.000 3.590 0.000 0.000 2.000

CH2OH 2 417.000 3.690 1.700 0.000 2.000

CH2CHO 2 436.000 3.970 0.000 0.000 2.000

CHOCHO 1 440.200 4.010 0.000 0.000 2.000 ! NMM

CHOCO 1 440.200 4.010 0.000 0.000 2.000 ! NMM

CH3 1 144.000 3.800 0.000 0.000 0.000

CH3CC 2 252.000 4.760 0.000 0.000 1.000 ! JAM

CH3CHCCH 2 373.700 4.790 0.000 0.000 1.000 ! NMM

CH3CCCH2 2 357.100 4.720 0.000 0.000 1.000 ! NMM

CH3CCCH3 2 357.100 4.720 0.000 0.000 1.000 ! NMM

CH3CCH2 2 316.000 4.220 0.000 0.000 1.000 ! NMM

C3H5-T 2 316.000 4.220 0.000 0.000 1.000

CH3CHCH 2 316.000 4.220 0.000 0.000 1.000 ! NMM

C3H5-S 2 316.000 4.220 0.000 0.000 1.000

CH3CH2CCH 2 357.100 4.720 0.000 0.000 1.000 ! NMM

CH3CHO 2 436.000 3.970 2.5 0.000 2.000 ! RPD

CH3CO 2 436.000 3.970 2.5 0.000 2.000 ! CH3CHO

CH2O2HCHO 2 436.000 3.970 2.5 0.000 2.000 ! CH3CHO

CH3O 2 417.000 3.690 1.700 0.000 2.000

CH3OO 2 417.000 3.690 1.700 0.000 2.000 ! CH3O

CH3OH 2 481.800 3.626 1.7 0.000 1.000 ! SVE,RPD

CH3O2H 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

CH3O2 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

CH2O2 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HOCH2O 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HOCH2O2H 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

OCH2O2H 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HOCH2O2 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HOCO2 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HCO3H 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HCO3 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HCO2 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

HCO2H 2 481.800 3.626 1.7 0.000 1.000 ! CH3OH

CH4 2 141.400 3.746 0.000 2.600 13.000

CH4O 2 417.000 3.690 1.700 0.000 2.000

CN 1 75.000 3.856 0.000 0.000 1.000 ! OIS

CNC 1 232.400 3.828 0.000 0.000 1.000 ! OIS

CNN 1 232.400 3.828 0.000 0.000 1.000 ! OIS

CO 1 98.100 3.650 0.000 1.950 1.800

CO2 1 244.000 3.763 0.000 2.650 2.100

F 0 80.000 2.750 0.000 0.000 0.000

F2 1 125.700 3.301 0.000 1.600 3.800

H 0 145.000 2.050 0.000 0.000 0.000

GAH 1 335.500 4.240 0.000 0.000 1.000 ! MEC

H2C4O 2 357.000 5.180 0.000 0.000 1.000 ! JAM

H2 1 38.000 2.920 0.000 0.790 280.000

H2CCC 2 265.300 3.721 0.000 0.000 1.000 ! \*

H2CCC(S) 2 265.300 3.721 0.000 0.000 1.000 ! \*

H2CCCH 2 252.000 4.760 0.000 0.000 1.000 ! JAM

H2CCCCH 2 357.100 4.720 0.000 0.000 1.000 ! NMM

H2CCCCH2 2 357.100 4.720 0.000 0.000 1.000 ! NMM

H2CCCCCH 1 408.000 5.200 0.000 0.000 1.000 ! NMM

H2CN 1 569.000 3.630 0.000 0.000 1.000 ! OS/JM

H2NO 2 116.700 3.492 0.000 0.000 1.000 ! JAM

H2O 2 572.400 2.605 1.844 0.000 4.000

H2O2 2 107.400 3.458 0.000 0.000 3.800

H2S 2 301.000 3.600 0.000 0.000 1.000 ! OIS

HC2N2 1 349.000 4.361 0.000 0.000 1.000 ! OIS

HCCHCCH 2 357.100 4.720 0.000 0.000 1.000 ! NMM

HCCO 2 150.000 2.500 0.000 0.000 1.000 ! \*

HCCOH 2 436.000 3.970 0.000 0.000 2.000

HCCCHCCH 1 408.000 5.200 0.000 0.000 1.000 ! NMM

HCN 1 569.000 3.630 0.000 0.000 1.000 ! OIS

HCO 2 498.000 3.590 0.000 0.000 0.000

HCO+ 1 498.000 3.590 0.000 0.000 0.000

HE 0 10.200 2.576 0.000 0.000 0.000 ! \*

HF 1 330.000 3.148 1.920 2.460 1.000 ! SV/MEC

HF0 1 352.000 2.490 1.730 0.000 5.000

HF1 1 352.000 2.490 1.730 0.000 5.000

HF2 1 352.000 2.490 1.730 0.000 5.000

HF3 1 352.000 2.490 1.730 0.000 5.000

HF4 1 352.000 2.490 1.730 0.000 5.000

HF5 1 352.000 2.490 1.730 0.000 5.000

HF6 1 352.000 2.490 1.730 0.000 5.000

HF7 1 352.000 2.490 1.730 0.000 5.000

HF8 1 352.000 2.490 1.730 0.000 5.000

HCNO 2 232.400 3.828 0.000 0.000 1.000 ! JAM

HOCN 2 232.400 3.828 0.000 0.000 1.000 ! JAM

HNCO 2 232.400 3.828 0.000 0.000 1.000 ! OIS

HNNO 2 232.400 3.828 0.000 0.000 1.000 ! \*

HNO 2 116.700 3.492 0.000 0.000 1.000 ! \*

HNOH 2 116.700 3.492 0.000 0.000 1.000 ! JAM

HO2 2 107.400 3.458 0.000 0.000 1.000 ! \*

HSO2 2 252.000 4.290 0.000 0.000 1.000 ! OIS

N 0 71.400 3.298 0.000 0.000 0.000 ! \*

N2 1 97.530 3.621 0.000 1.760 4.000

N2H2 2 71.400 3.798 0.000 0.000 1.000 ! \*

N2H3 2 200.000 3.900 0.000 0.000 1.000 ! \*

N2H4 2 205.000 4.230 0.000 4.260 1.500

N2O 1 232.400 3.828 0.000 0.000 1.000 ! \*

NCN 1 232.400 3.828 0.000 0.000 1.000 ! OIS

NCO 1 232.400 3.828 0.000 0.000 1.000 ! OIS

NH 1 80.000 2.650 0.000 0.000 4.000

NH2 2 80.000 2.650 0.000 2.260 4.000

NH3 2 481.000 2.920 1.470 0.000 10.000

NNH 2 71.400 3.798 0.000 0.000 1.000 ! \*

NO 1 97.530 3.621 0.000 1.760 4.000

NCNO 2 232.400 3.828 0.000 0.000 1.000 ! OIS

NO2 2 200.000 3.500 0.000 0.000 1.000 ! \*

O 0 80.000 2.750 0.000 0.000 0.000

O2 1 107.400 3.458 0.000 1.600 3.800

O3 2 180.000 4.100 0.000 0.000 2.000

OH 1 80.000 2.750 0.000 0.000 0.000

S 0 847.000 3.839 0.000 0.000 0.000 ! OIS

S2 1 847.000 3.900 0.000 0.000 1.000 ! OIS

SH 1 847.000 3.900 0.000 0.000 1.000 ! OIS

SO 1 301.000 3.993 0.000 0.000 1.000 ! OIS

SO2 2 252.000 4.290 0.000 0.000 1.000 ! OIS

SO3 2 378.400 4.175 0.000 0.000 1.000 ! OIS

SIH4 2 207.6 4.084 0.000 0.000 1.000 ! MEC

SIH3 2 170.3 3.943 0.000 0.000 1.000 ! MEC

SIH2 2 133.1 3.803 0.000 0.000 1.000 ! MEC

SIH 1 95.8 3.662 0.000 0.000 1.000 ! MEC

SI 0 3036. 2.910 0.000 0.000 0.000 ! MEC

SI2H6 2 301.3 4.828 0.000 0.000 1.000 ! MEC

SI2H5 2 306.9 4.717 0.000 0.000 1.000 ! MEC

SI2H4 2 312.6 4.601 0.000 0.000 1.000 ! MEC

SI2H3 2 318.2 4.494 0.000 0.000 1.000 ! MEC

SI2H2 2 323.8 4.383 0.000 0.000 1.000 ! MEC

SI2 1 3036. 3.280 0.000 0.000 1.000 ! MEC

SI3 2 3036. 3.550 0.000 0.000 1.000 ! MEC

SIF3 2 309.6 4.359 0.000 0.000 1.000 ! MEC

SIF3NH2 2 231.0 4.975 0.000 0.000 1.000 ! MEC

SIF4 2 171.9 4.880 0.000 0.000 1.000 ! SVE

SIHF3 2 180.8 4.681 0.000 0.000 1.000 ! MEC

H2SISIH2 2 312.6 4.601 0.000 0.000 1.000 ! MEC

H3SISIH 2 312.6 4.601 0.000 0.000 1.000 ! MEC

SI3H8 2 331.2 5.562 0.000 0.000 1.000 ! MEC

ASH3 2 259.8 4.145 0.000 0.000 1.000 ! MEC

AS2 1 1045.5 5.510 0.000 0.000 1.000 ! MEC

GAME3 2 378.2 5.52 0.000 0.000 1.000 ! MEC

GAME2 2 675.8 5.22 0.000 0.000 1.000 ! MEC

GAME 2 972.7 4.92 0.000 0.000 1.000 ! MEC

GA 0 2961.8 4.62 0.000 0.000 0.000 ! MEC

K 0 850. 4.25 0.000 0.000 1.000 ! SINGH

KOH 2 1213. 4.52 0.000 0.000 1.000 ! SINGH

KO2 2 1213. 4.69 0.000 0.000 1.000 ! SINGH

KH 1 93.3 3.542 0.000 0.000 1.000 ! SINGH

K+ 0 850. 4.25 0.000 0.000 1.000 ! SINGH

E 0 850. 425. 0.000 0.000 1.000 ! SINGH

KCL 1 1989. 4.186 0.000 0.000 1.000 ! SINGH

CL 0 130.8 3.613 0.000 0.000 1.000 ! SINGH

CL- 0 130.8 3.613 0.000 0.000 1.000 ! SINGH

HCL 1 344.7 3.339 1.084 0.000 1.000 ! SINGH

KO 1 383.0 3.812 0.000 0.000 1.000 ! SINGH

NC10H22 2 540.0 7.085 0.0 0.0 1.0 ! WJP

C10H22-335 2 522.0 6.873 0.0 0.0 1.0 ! WJP

C10H22-2255 2 497.3 6.899 0.0 0.0 1.0 ! WJP

IC8H18 2 458.5 6.414 0.0 0.0 1.0 ! WJP

AC8H17 2 458.5 6.414 0.0 0.0 1.0 ! WJP

BC8H17 2 458.5 6.414 0.0 0.0 1.0 ! WJP

CC8H17 2 458.5 6.414 0.0 0.0 1.0 ! WJP

DC8H17 2 458.5 6.414 0.0 0.0 1.0 ! WJP

C8H17OH-1 2 581.3 6.506 2.0 0.0 1.0 ! WJP

AC8H17O 2 581.3 6.506 2.0 0.0 1.0 ! WJP

BC8H17O 2 581.3 6.506 2.0 0.0 1.0 ! WJP

CC8H17O 2 581.3 6.506 2.0 0.0 1.0 ! WJP

DC8H17O 2 581.3 6.506 2.0 0.0 1.0 ! WJP

C8H16-1 2 485.6 6.440 0.3 0.0 1.0 ! WJP

IC8H16 2 485.6 6.440 0.3 0.0 1.0 ! WJP

JC8H16 2 485.6 6.440 0.3 0.0 1.0 ! WJP

IC8H15 2 485.6 6.440 0.3 0.0 1.0 ! WJP

IC8H14 2 485.6 6.440 0.3 0.0 1.0 ! WJP

NC7H16 2 459.6 6.253 0.0 0.0 1.0 ! WJP

NEOC7H16 2 437.3 6.168 0.0 0.0 1.0 ! WJP

C7H162-4 2 437.3 6.168 0.0 0.0 1.0 ! WJP

QC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

PC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

OC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

NC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

XC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

YC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

ZC7H15 2 437.3 6.168 0.0 0.0 1.0 ! WJP

C7H15OH-1 2 561.0 6.317 1.7 0.0 1.0 ! WJP

QC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

PC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

OC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

NC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

XC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

YC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

ZC7H15O 2 561.0 6.317 1.7 0.0 1.0 ! WJP

C7H14-1 2 457.8 6.173 0.3 0.0 1.0 ! WJP

IBC7H14 2 439.2 6.151 0.0 0.0 1.0 ! WJP

OC7H14 2 439.2 6.151 0.0 0.0 1.0 ! WJP

PC7H14 2 439.2 6.151 0.0 0.0 1.0 ! WJP

XC7H14 2 439.2 6.151 0.0 0.0 1.0 ! WJP

YC7H14 2 439.2 6.151 0.0 0.0 1.0 ! WJP

PC7H13 2 439.2 6.151 0.0 0.0 1.0 ! WJP

XC7H13 2 439.2 6.151 0.0 0.0 1.0 ! WJP

NC6H14 2 427.4 5.946 0.0 0.0 1.0 ! WJP

NEOC6H14 2 406.1 5.842 0.0 0.0 1.0 ! WJP

XC6H14 2 416.7 5.852 0.0 0.0 1.0 ! WJP

C6H14-3 2 422.5 5.870 0.0 0.0 1.0 ! WJP

IC6H14 2 422.5 5.870 0.0 0.0 1.0 ! WJP

FC6H13 2 406.1 5.842 0.0 0.0 1.0 ! WJP

GC6H13 2 406.1 5.842 0.0 0.0 1.0 ! WJP

HC6H13 2 406.1 5.842 0.0 0.0 1.0 ! WJP

AC6H13 2 422.5 5.870 0.0 0.0 1.0 ! WJP

BC6H13 2 422.5 5.870 0.0 0.0 1.0 ! WJP

CC6H13 2 422.5 5.870 0.0 0.0 1.0 ! WJP

DC6H13 2 422.5 5.870 0.0 0.0 1.0 ! WJP

EC6H13 2 422.5 5.870 0.0 0.0 1.0 ! WJP

C6H13OH-1 2 541.5 5.674 1.8 0.0 1.0 ! WJP

FC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

GC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

HC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

AC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

BC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

CC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

DC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

EC6H13O 2 541.5 5.674 1.8 0.0 1.0 ! WJP

NEOC6H12 2 397.9 5.767 0.0 0.0 1.0 ! WJP

KC6H12 2 435.9 5.807 0.0 0.0 1.0 ! WJP

JC6H12 2 415.3 5.794 0.0 0.0 1.0 ! WJP

CC6H12 2 414.4 5.872 0.0 0.0 1.0 ! WJP

C-C6H12-C 2 411.9 5.860 0.0 0.0 1.0 ! WJP

H-C6H12 2 430.6 5.843 0.0 0.0 1.0 ! WJP

H-C6H12-C 2 433.6 5.825 0.0 0.0 1.0 ! WJP

BC6H12 2 430.1 5.833 0.0 0.0 1.0 ! WJP

C6H12-3 2 431.5 5.859 0.0 0.0 1.0 ! WJP

C6H12-C-3 2 428.9 5.830 0.3 0.0 1.0 ! WJP

C6H12-2 2 429.6 5.829 0.0 0.0 1.0 ! WJP

C6H12-C-2 2 432.4 5.827 0.0 0.0 1.0 ! WJP

C6H12-1 2 423.2 5.834 0.4 0.0 1.0 ! WJP

AC6H12 2 430.1 5.833 0.0 0.0 1.0 ! WJP

DC6H12 2 414.4 5.872 0.0 0.0 1.0 ! WJP

NEOC6H11 2 397.9 5.767 0.0 0.0 1.0 ! WJP

IC6H11 2 430.1 5.833 0.0 0.0 1.0 ! WJP

IC6H12 2 430.1 5.833 0.0 0.0 1.0 ! WJP

NC5H12 2 391.7 5.591 0.0 0.0 1.0 ! WJP

NEOC5H12 2 357.8 5.550 0.0 0.0 1.0 ! WJP

NEOC5H11 2 357.8 5.550 0.0 0.0 1.0 ! WJP

IC5H12 2 382.1 5.548 0.0 0.0 1.0 ! WJP

NC5H12 2 391.7 5.591 0.0 0.0 1.0 ! WJP

NC5H12 2 391.7 5.591 0.0 0.0 1.0 ! WJP

NC5H12 2 391.7 5.591 0.0 0.0 1.0 ! WJP

IC5H12 2 382.1 5.548 0.0 0.0 1.0 ! WJP

IC5H12 2 382.1 5.548 0.0 0.0 1.0 ! WJP

IC5H12 2 382.1 5.548 0.0 0.0 1.0 ! WJP

IC5H12 2 382.1 5.548 0.0 0.0 1.0 ! WJP

AC5H11 2 523.2 5.664 1.7 0.0 1.0 ! WJP

BC5H11 2 523.2 5.664 1.7 0.0 1.0 ! WJP

CC5H11 2 523.2 5.664 1.7 0.0 1.0 ! WJP

DC5H11 2 523.2 5.664 1.7 0.0 1.0 ! WJP

CC5H10 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C5H11-1 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C5H11-2 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C5H11-3 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C5H11OH-1 2 523.2 5.664 1.7 0.0 1.0 ! WJP

IC5H11OH-1 2 451.9 6.041 0.0 0.0 1.0 ! WJP

IC5H11OH-2 2 431.4 5.624 1.9 0.0 1.0 ! WJP

C5H11O-1 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C5H11O-2 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C5H11O-3 2 523.2 5.664 1.7 0.0 1.0 ! WJP

AC5H11O 2 523.2 5.664 1.7 0.0 1.0 ! WJP

BC5H11O 2 523.2 5.664 1.7 0.0 1.0 ! WJP

CC5H11O 2 523.2 5.664 1.7 0.0 1.0 ! WJP

DC5H11O 2 523.2 5.664 1.7 0.0 1.0 ! WJP

NEOC5H11O 2 523.2 5.664 1.7 0.0 1.0 ! WJP

C2H5COC2H5 2 476.7 5.714 2.7 0.0 1.0 ! WJP

IC3H7COCH3 2 469.0 5.632 2.8 0.0 1.0 ! WJP

NC3H7COCH3 2 477.0 5.735 2.5 0.0 1.0 ! WJP

C-C5H10 2 372.1 5.446 0.0 0.0 1.0 ! WJP

BC5H10 2 391.4 5.550 0.0 0.0 1.0 ! WJP

AC5H10 2 386.6 5.532 0.5 0.0 1.0 ! WJP

C5H10-2 2 396.8 5.458 0.0 0.0 1.0 ! WJP

C5H10-1 2 386.2 5.489 0.4 0.0 1.0 ! WJP

C5H9 2 396.8 5.458 0.0 0.0 1.0 ! WJP

IC5H9 2 386.6 5.532 0.5 0.0 1.0 ! WJP

C4H10 2 350.9 5.206 0.0 0.0 1.0 ! WJP

NC4H10 2 350.9 5.206 0.0 0.0 1.0 ! WJP

IC4H10 2 335.7 5.208 0.1 0.0 1.0 ! WJP

NC4H9OH 2 502.2 5.356 1.8 0.0 1.0 ! WJP

IC4H7OH 2 502.2 5.356 1.8 0.0 1.0 ! WJP

IC4H6OH 2 502.2 5.356 1.8 0.0 1.0 ! WJP

IC3H7CHO 2 436.4 5.352 0.0 0.0 1.0 ! WJP:TCPC

NC3H7CHO 2 464.2 5.009 2.6 0.0 1.0 ! WJP

IC3H7CO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

NC3H7CO 2 464.2 5.009 2.6 0.0 1.0 ! WJP

IC3H6CHO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

TC3H6CHO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

TC3H6OCHO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

IC3H6CO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

IC3H5CHO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

IC3H5CO 2 436.4 5.352 0.0 0.0 1.0 ! WJP

IC4H8 2 344.5 5.089 0.5 0.0 1.0 ! WJP

C4H8-2 2 354.1 5.135 0.0 0.0 1.0 ! WJP

C4H8-S-2 2 359.7 5.076 0.3 0.0 1.0 ! WJP

C4H8-1 2 345.7 5.088 0.3 0.0 1.0 ! WJP

C4H6-1,3 2 350.4 4.984 0.0 0.0 1.0 ! WJP

C4H6-1,2 2 370.3 4.984 0.4 0.0 1.0 ! WJP

C3H6O 2 403.6 4.968 2.0 0.0 1.0 ! WJP

C2H5CHO 2 435.2 4.662 2.7 0.0 1.0 ! WJP

NC3H7OH 2 481.5 4.997 1.7 0.0 1.0 ! WJP

IC3H7OH 2 459.5 5.036 1.7 0.0 1.0 ! WJP: FROM TCPC

CH3OC2H5 2 364.6 4.998 1.2 0.0 1.0 ! WJP

IC3H5OH 2 459.5 5.036 1.7 0.0 1.0 ! WJP: IC3H7OH

TC3H6OH 2 459.5 5.036 1.7 0.0 1.0 ! WJP: IC3H7OH

NC3H7O 2 481.5 4.997 1.7 0.0 1.0 ! WJP

IC3H7O 2 459.5 5.036 1.7 0.0 1.0 ! WJP: IC3H7OH

C3H5OH 2 481.5 4.997 1.7 0.0 1.0 ! WJP

C2H3CHO 2 428.8 4.958 2.9 0.0 1.0 ! WJP

CH3CO2H 2 514.0 5.007 1.3 0.0 1.0 ! WJP

CH3CO2 2 514.0 5.007 1.3 0.0 1.0 ! CH3CO2H

CH3CO3 2 514.0 5.007 1.3 0.0 1.0 ! CH3CO2H

CH3CO3H 2 514.0 5.007 1.3 0.0 1.0 ! CH3CO2H

C2H3O1-2 2 387.3 4.349 1.9 0.0 1.0 ! C2H4O

C2H4O 2 387.3 4.349 1.9 0.0 1.0 ! WJP

C2H4O1-2 2 387.3 4.349 1.9 0.0 1.0 ! WJP

CH2CCH2OH 2 481.5 4.997 1.7 0.0 1.0 ! WJP