Supporting Information

Study on a novel methodology for developing skeletal mechanism of RP-3 aviation kerosene

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S1. The skeletal mechanism for surrogate fuel

ELEMENTS
C H N O AR HE
END
SPECIES
N2
AR
H2
H
O2
O
H2O
OHS2
H2O2
HO2
CO
CO2
CH4
CH3
CH2
CH3O2H
CH3O2
CH3OH
CH3O
CH2OH
CH2O
HCO
HO2CHO
O2CHO
C2H6
C2H5
C2H5O2H
C2H5O2
C2H4
C2H3
C2H3OO
C2H2
C2H
C2H5O
CH3CHO
CH3CO
CH2CHO
CH2CO
HCCO
C3H8

IC3H7
IC3H7O2
IC3H7O
C3H6
C3H5-A
C3H5-S
C3H5-T
C3H5O
AC3H5OOH
C3H4-P
C3H4-A
C3H3
C3H3O
C2H3CHO
C2H3CO
CH3COCH2
IC4H9
TC4H9
IC3H5CO
IC4H9O2
TC4H9O2
IC4H8O2H-I
IC4H8O2H-T
IC4H8
IC4H7
IC4H7-I1
IC4H7O
C4H8-1
C4H6
C6H101-5
C6H9-A
C8H18-25
C8H17
C8H17-OO
C8-QOOH
C8-OOQOOH
C8-KET
C6H13CO
NC3H7
NC3H7O2
NC3H7O
C3H6OOH1-2
C3H6O1-2
CH3CHCHO
CH3CHCO
PC4H9

C4H72-1OOH
C4H71-3OOH
C4H71-1
C4H71-3
C4H71-1O2
C3H6CHO-3
NC12H26
C12H25
C12H25-OO
C12-QOOH
C12-OOQOOH
C12-KET
C12H24
C12H23
HE
OHV
CH2(S)
CH
CHV
HCOH
HOCH2O
HOCHO
OCHO
CHCHO
C8H9
C8H9O
C8H9OO
C9H12
C8H9CH2
C7H9
C8H9CH2O
C8H9CHO
C8H9CO
C7H9O
C6H9
C8H10
PC2H4OH
O2C2H4OH
C4H5-N
C6H6
C5H4O
Decalin
RDecalin
RDec-OO
Dec-QOOH
Dec-OOQOOH

Dec-KET
CYC6H10
CYC6H9-3
C4H7
DCYC10H16
DCLD1-3R
C8H12
X135C6H7-3R
LC5H7
CYC5H5
CYC5H6
CYC6H8-13
C6H9-13-6
N
NH
NNH
NO
NO2
N2O
HNO
HCN
END
REACTIONS MOLES CAL/MOLE
!
!\KINETICS_MODULE: \H2_O2
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
!
!\SUBMECH: \H2
!\REACTIONCLASS: \UNIMOL \A \N \EA
!\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
!3RD BODY COLLIDER EFFICIENCIES
H2+M=2H+M 4.577E19 -1.4 1.044E5
H2/2.5/
H2O/12.0/
CO/1.9/
CO2/3.8/
CH4/2.0/
C2H6/3.0/
!\REACTIONCLASS: \ABSTRACTION \A \N \EA
!!
!\SITE: \UNDEF

```
!\AUTHOR: AK !\REF:SUTHERLAND ET AL., 21ST SYMPOSIUM, P. 929 (1986) !\COMMENT:
H2+O=H+OH       5.08E4 2.67 6.292E3
!\AUTHOR: AK !\REF:LAM ET AL. SUBMITTED IJCK !\COMMENT
H2+OH=H+H2O       4.38E13 0.0 6.99E3
!\SUBMECH: \O2
!\MECHCOMMENTS:
!\MECHWARNINGS:
!\REACTIONCLASS:   \UNIMOL                                   \A                  \N
\EA
!!
!\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
!3RD BODY COLLIDER EFFICIENCIES
2O+M=O2+M       6.165E15 -0.5 0.0E0
      H2/2.5/
      H2O/12.0/
      CO/1.9/
      CO2/3.8/
      CH4/2.0/
      C2H6/3.0/
!!
!\REACTIONCLASS:   \RADICAL_ADDITION\H                       \A                  \N
\EA
!!
!\AUTHOR: AK !\REF: HONG ET AL. PROC. OF THE COMB. INST. 33 (2011) 309?16 !\COMMENT: 2
PARAMETER FIT
O2+H=O+OH       1.04E14 0.0 1.5286E4
!\ENDSUBMECH: \O2
!\SUBMECH: \H2O
!\MECHCOMMENTS:
!\MECHWARNINGS:
!\REACTIONCLASS:   \UNIMOL                                   \A                  \N
\EA
!!
!\AUTHOR: AK !\REF: LI IJCK 36: 566?75, 2004 !\COMMENT:OPTIMISED TO FIT H2 AND CH4
FLAMES DATA
!3RD BODY COLLIDER EFFICIENCIES
H+OH+M=H2O+M       3.5E22 -2.0 0.0E0
      H2/0.73/
      H2O/3.65/
      CH4/2.0/
      C2H6/3.0/
!!
!\REACTIONCLASS:   \ABSTRACTION                              \A                  \N
\EA
!!
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!\AUTHOR: AK !\REF: SUTHERLAND ET AL., 23RD SYMPOSIUM, P. 51 (1990) !\COMMENT:
O+H2O=2OH 6.7E7 1.704 1.49868E4
!!
!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N
\EA
!!
!\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
!3RD BODY COLLIDER EFFICIENCIES
O+H+M=OH+M 4.714E18 -1.0 0.0E0
H2/2.5/
H2O/12.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
!\SUBMECH: \H2O2
!\MECHCOMMENTS:
!\MECHWARNINGS:
!\REACTIONCLASS: \UNIMOL \A \N
\EA
!!
!H2O2(+H2O)(=)OH+OH(+H2O) 2.000E+012 0.900 48749.0 !\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601 (2011)!\COMMENT: RATE CONSTANT IS FOR N2
!LOW/ 1.865E+025 -2.300 48749.0/
!TROE/ 5.100E-001 1.000E-030 1.000E+030/
!\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601 (2011)!\COMMENT: RATE CONSTANT IS FOR N2, !\COMMENT: EFFICIENCIS OF H2O FROM THE SAME REF,
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
H2O2(+M)=2OH(+M) 2.0E12 0.9 4.8749E4
H2O/7.65/
CO2/1.6/
N2/1.5/
O2/1.2/
H2O2/7.7/
H2/3.7/
CO/2.8/
LOW/2.49E24 -2.3E0 4.8749E4/
TROE/4.3E-1 1.0E-30 1.0E30/
!!
H2O2+H=H2O+OH 2.41E13 0.0 3.97E3
!\AUTHOR: AK !\REF: ELLINGSON J. PHYS. CHEM. (2007) 111, (51), 13554-13566 !\COMMENT:
H2O2+H=H2+HO2 2.15E10 1.0 6.0E3

!\AUTHOR: AK !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
H2O2+O=OH+HO2 9.55E6 2.0 3.97E3
!\AUTHOR: AK !\REF: HONG ET AL. J. PHYS. CHEM. A 114 (2010) 5718-5727 !\COMMENT:
H2O2+OH=H2O+HO2 1.74E12 0.0 3.18E2
DUP
!\AUTHOR: !\REF: !\COMMENT:
H2O2+OH=H2O+HO2 7.59E13 0.0 7.269E3
DUP
!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: KPS !\REF: NOT A CLUE WHAT REFERENCE IS HERE AS MECHANISM IS A MESS !\COMMENT: WARNING
HO2+H=2OH 7.079E13 0.0 2.95E2
!\AUTHOR: AK !\REF:MICHAEL SUTHERLAND 2000 !\COMMENT:
HO2+H=H2+O2 1.1402E10 1.0827 5.5378E2
!\AUTHOR: AK !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)
HO2+O=OH+O2 3.25E13 0.0 0.0E0
!\AUTHOR: ?? !\REF: hong pci 2013 1015C !\COMMENT: WARNING
OH+HO2=H2O+O2 7.0E12 0.0 -1.09296E3
DUP
!\AUTHOR: !\REF: !\COMMENT:
OH+HO2=H2O+O2 4.5E14 0.0 1.09296E4
DUP
!\AUTHOR: AK !\REF: hong pci 2013, kapel 2002 !\COMMENT: WARNING
2HO2=H2O2+O2 1.0E14 0.0 1.1040883E4
DUP
!\AUTHOR: !\REF: !\COMMENT:
2HO2=H2O2+O2 1.9E11 0.0 -1.4089248E3
DUP
!!
!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N \EA
!!
!\AUTHOR: AK !\REF:FERNANDES PCCP 2008 !COMMENT: Efficiencis of AR and HE derived from seperated reactions,
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
H+O2(+M)=HO2(+M) 4.65E12 0.44 0.0E0
H2/1.3/
CO/1.9/
CO2/3.8/
H2O/10.0/

```
      CH4/2.0/
      C2H6/3.0/
      LOW/1.737E19 -1.23E0 0.0E0/
      TROE/6.7E-1 1.0E-30 1.0E30 1.0E30/
!H+O2(+AR)(=)HO2(+AR) 4.650E+012 0.440 0.0 !\AUTHOR: AK !\REF: BATES ET AL. PCCP 3 (2001) 2337-2342 !\COMMENT: WARNING: HAS BEEN REMOVED FROM LATEST VERSION OF KZ MECHANISM
!LOW/ 6.810E+018 -1.200 0.0/
!TROE/ 7.000E-001 1.000E-030 1.000E+030 1.000E+030/
!
!H+O2(+HE)(=)HO2(+HE) 4.650E+012 0.440 0.0 !\AUTHOR: AK !\REF: ?? NOT WELL DEFINED IN MECHANISM?! !\COMMENT: WARNING: LPL OF ABOVE RATE CONSTANT OR THIS ONE HAS BEEN MULTIPLIED BY 1.5
!LOW/ 9.192E+018 -1.200 0.0/
!TROE/ 5.900E-001 1.000E-030 1.000E+030 1.000E+030/!
!\END_KINETICS_MODULE: \H2_O2
!
!
CO+O(+M)=CO2(+M)       1.362E10 0.0 2.384E3
      H2/2.0/
      H2O/12.0/
      CO/1.75/
      CO2/3.6/
      LOW/1.173E24 -2.79E0 4.191E3/
!!
CO+OH=CO2+H       7.015E4 2.053 -3.557E2
      DUP
!\AUTHOR: !\REF: !\COMMENT:
CO+OH=CO2+H       5.757E12 -0.664 3.318E2
      DUP
!!
!\REACTIONCLASS:    \RADICAL_ADDITION\HO2                    \A                    \N
\EA
!!
!\AUTHOR: ?? !\REF: YOU ET AL. J. PHYS. CHEM. A 2007, 111, 4031-4042 !\COMMENT:
CO+HO2=CO2+OH       1.57E5 2.18 1.794E4
!!
!\REACTIONCLASS:    \R+O2                    \A                    \N
\EA
!!
!\AUTHOR: ?? !\REF: 86TSA/ HAM * 0.44 !\COMMENT:
CO+O2=CO2+O       1.119E12 0.0 4.77E4
!\SUBMECH: \CH4
!\MECHCOMMENTS:
!\MECHWARNINGS:
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!-------------------------------------------------------------------------------------------------------------------
-
!!
!\REACTIONCLASS:  \UNIMOL                                    \A          \N
\EA
!!
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
CH3+H(+M)=CH4(+M)       1.27E16 -0.63 3.83E2
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      CH4/2.0/
      C2H6/3.0/
      LOW/2.477E33 -4.76E0 2.44E3/
      TROE/7.83E-1 7.4E1 2.941E3 6.964E3/
!!
!\REACTIONCLASS:  \RH_R_ABSTRACTION                          \A          \N
\EA
!!
!\AUTHOR: !\REF: BAULCH, D.L.; ET AL.,J. PHYS. CHEM. REF. DATA (2005) !\COMMENT:
CH4+H=CH3+H2       6.14E5 2.5 9.587E3
!\AUTHOR: !\REF: !REF:GRI 3.0 !\COMMENT: WARNING: WHAT IS REFERENCE FOR GRI
MECHANISM?
CH4+O=CH3+OH       1.02E9 1.5 8.6E3
!\AUTHOR: !\REF: CURRAN ESTIMATE, FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT
ARE REFERENCES TO RATE CONSTANTS IN NIST?
CH4+OH=CH3+H2O       5.83E4 2.6 2.19E3
!\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-
7054. !\COMMENT: 1.695E+001 in AramcoMech1.3 (with Ax1.5)
CH4+HO2=CH3+H2O2       1.13E1 3.74 2.101E4
!\AUTHOR: !\REF: NEW FIT FROM HJC !\COMMENT: WARNING: WHAT IS SOURCE OF THIS
RATE CONSTANT??
CH4+CH3O2=CH3+CH3O2H       9.6E-1 3.77 1.781E4
!\AUTHOR: !\REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279?86 !\COMMENT:
CH3+HO2=CH4+O2       1.16E5 2.23 -3.022E3
!!
!\REACTIONCLASS:  \RADICAL_ADDITION\CH2                      \A          \N
\EA
!!
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH4+CH2=2CH3       2.46E6 2.0 8.27E3
CH2+H(+M)=CH3(+M)       2.5E16 -0.8 0.0E0
      H2/2.0/
```

```
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      CH4/2.0/
      C2H6/3.0/
      LOW/3.2E27 -3.14E0 1.23E3/
      TROE/6.8E-1 7.8E1 1.995E3 5.59E3/
!!
!\REACTIONCLASS: \RADICAL_RECOMBINATIONS \A \N \EA
!!
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT:
CH2+O2=HCO+OH       1.06E13 0.0 1.5E3
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT:
CH2+O2=>CO2+2H      2.64E12 0.0 1.5E3
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT:
CH2+O=>CO+2H        5.0E13 0.0 0.0E0
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
CH3+O2(+M)=CH3O2(+M)        7.812E9 0.9 0.0E0
      LOW/6.85E24 -3.0E0 0.0E0/
      TROE/6.0E-1 1.0E3 7.0E1 1.7E3/
!\AUTHOR: ?? !\REF:N. K. SRINIVASAN ET AL.,J. PHYS. CHEM. A 109, 7902-7914 (2005) !\COMMENT:
CH3+O2=CH3O+O       7.546E12 0.0 2.832E4
!\AUTHOR: ?? !\REF: PERSONAL COMMUNICATION, STEVE KLIPPENSTEIN !\COMMENT: WARNING: HAS THIS BEEN PUBLISHED?
CH3+O2=CH2O+OH      2.641E0 3.283 8.105E3
!!
!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N \EA
!!
!\AUTHOR: !\REF:HARDING AND KLIPPENSTEIN 2B04, 30TH SYMP 2004. !\COMMENT:
CH3+O=CH2O+H        5.54E13 0.05 -1.36E2
!\AUTHOR: ?? !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:
CH3+OH=CH2O+H2      3.502E5 1.441 -3.244E3
      PLOG/1.0E-2 3.502E5 1.441E0 -3.244E3/
      PLOG/1.0E-1 8.854E5 1.327E0 -2.975E3/
      PLOG/1.0E0 1.65E7 9.73E-1 -2.01E3/
      PLOG/1.0E1 5.374E9 2.87E-1 2.8E2/
      PLOG/1.0E2 9.494E18 -2.199E0 9.769E3/
!\AUTHOR: ?? !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT: INCREASED BY FACTOR OF 2
CH3+OH=CH2OH+H      1.621E10 0.965 3.21E3
      PLOG/1.0E-2 1.621E10 9.65E-1 3.214E3/
      PLOG/1.0E-1 1.807E10 9.5E-1 3.247E3/
```

PLOG/1.0E0 4.686E10 8.33E-1 3.566E3/
PLOG/1.0E1 1.525E13 1.34E-1 5.641E3/
PLOG/1.0E2 3.59E14 -1.86E-1 8.601E3/
!\AUTHOR: ?? !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:
CH3+OH=H+CH3O 1.186E9 1.016 1.194E4
PLOG/1.0E-2 1.186E9 1.016E0 1.194E4/
PLOG/1.0E-1 1.188E9 1.016E0 1.194E4/
PLOG/1.0E0 1.23E9 1.011E0 1.195E4/
PLOG/1.0E1 1.798E9 9.65E-1 1.206E4/
PLOG/1.0E2 5.242E10 5.51E-1 1.307E4/
!\AUTHOR: ?? !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:
CH3+OH=CH2+H2O 4.293E4 2.568 3.9978E3
!!
!\REACTIONCLASS: \R+HO2 \A \N \EA
!!
!\AUTHOR: ?? !\REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279?86 !\COMMENT:
CH3+HO2=CH3O+OH 1.0E12 0.269 -6.875E2
CH3O2+O=CH3O+O2 3.6E13 0.0 0.0E0
!\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\COMMENT:
CH3O2+H=CH3O+OH 9.6E13 0.0 0.0E0
!\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\COMMENT:
CH3O2+OH=CH3OH+O2 6.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LIGHTFOOT,P.D. ETAL., ATMOS. ENVIRON. PART A: 26, 1805-1961 (1992) !\COMMENT:
CH3O2+HO2=CH3O2H+O2 2.47E11 0.0 -1.57E3
!\AUTHOR: !\REF:!REF:Tsang, W., J. Phys. Chem. Ref. Data 15, 1087 (1986) !\COMMENT: ADDED 29/07/2015
CH3O2+H2O2=CH3O2H+HO2 2.41E12 0.0 9.936E3
!\AUTHOR: !\REF:KEIFFER, M. ET AL.,J. CHEM. SOC. FARADAY TRANS. 2: 84, 505 (1988) !\COMMENT:
CH3O2+CH3=2CH3O 5.08E12 0.0 -1.411E3
!\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\COMMENT:
2CH3O2=>CH2O+CH3OH+O2 3.11E14 -1.61 -1.051E3
!\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\COMMENT:
2CH3O2=>O2+2CH3O 1.4E16 -1.61 1.86E3
H2+CH3O2=H+CH3O2H 1.5E14 0.0 2.603E4
!!
!\REACTIONCLASS: \KHP_DECOMP \A \N \EA
!!

!\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220. !\COMMENT:
CH3O2H=CH3O+OH 6.31E14 0.0 4.23E4
!\SUBMECH: \CH3OH
!\MECHCOMMENTS: HCOH IS FORMED FROM CH3+OH, IT IS NOT NECESSARY FOR FORMALDEHYDE OXIDATION, AND MINOR FOR CH4/CH3OH
!\MECHWARNINGS:
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
CH3OH(+M)=CH3+OH(+M) 2.084E18 -0.615 9.25406E4
LOW/1.5E43 -6.995E0 9.79922E4/
TROE/-4.748E-1 3.558E4 1.116E3 9.023E3/
!\AUTHOR: !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
CH3OH(+M)=CH2OH+H(+M) 7.896E-3 5.038 8.44674E4
LOW/3.39E42 -7.244E0 1.052303E5/
TROE/-7.391E1 3.705E4 4.15E4 5.22E3/
!!
!\REACTIONCLASS: \RH_R_ABSTRACTIONS \A \N \EA
!!
!\AUTHOR: !\REF:J. CHEM. PHYS. 134, 094302 (2011) !\COMMENT: WARNING INCOMPLETE REFERENCE
CH3OH+H=CH3O+H2 1.99E5 2.56 1.03E4
!\AUTHOR: !\REF:J. CHEM. PHYS. 134, 094302 (2011) !\COMMENT: WARNING INCOMPLETE REFERENCE
CH3OH+H=CH2OH+H2 3.07E5 2.55 5.44E3
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)!\COMMENT: reduced by an order of magnitude from abstraction from the methyl site
CH3OH+O=CH3O+OH 3.88E4 2.5 3.08E3
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH3OH+O=CH2OH+OH 3.88E5 2.5 3.08E3
!\AUTHOR: !\REF:XU ET AL. PROC 31 2007 159-166 !\COMMENT:
CH3OH+OH=CH3O+H2O 1.5E2 3.03 -7.63E2
!\AUTHOR: !\REF:XU ET AL. PROC 31 2007 159-166 !\COMMENT:
CH3OH+OH=CH2OH+H2O 3.08E4 2.65 -8.067E2
!CH3OH+O2(=)CH2OH+HO2 2.050E+013 0.000 44900.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975 !\COMMENT: Ultan removed 21/08/15
!\AUTHOR: !\REF:S. J. Klippenstein, L. B. Harding, M. J. Davis, A. S. Tomlin, R. T. Skodje, PCI, 33 (2011) 351-357
CH3OH+O2=CH3O+HO2 3.58E4 2.27 4.27645E4
!\COMMENT:(above)reduced by an order of magnitude from abstraction from the methyl site due to increased bond strengths, Ultan added 21/08/15

!\AUTHOR: !REF:S. J. Klippenstein, L. B. Harding, M. J. Davis, A. S. Tomlin, R. T. Skodje, PCI, 33 (2011) 351-357 !\COMMENT: Ultan added 21/08/15
CH3OH+O2=CH2OH+HO2 3.58E5 2.27 4.27645E4
!CH3OH+HO2(=)CH2OH+H2O2 1.080E+004 2.550 10530.0 !\AUTHOR: !\REF: CURRAN ESTIMATE !\COMMENT: WARNING: Ultan removed 21/08/15
!\AUTHOR: !\REF: M. Altarawneh, A. H. Al-Muhtaseb, B. Z. Dlugogorski, E. M. Kennedy, J. C. Mackie, J. Comp. Chem. 32 (2011) 1725-1733 !\COMMENT:
CH3OH+HO2=CH3O+H2O2 1.22E12 0.0 2.00707E4
!\AUTHOR: !\REF: M. Altarawneh, A. H. Al-Muhtaseb, B. Z. Dlugogorski, E. M. Kennedy, J. C. Mackie, J. Comp. Chem. 32 (2011) 1725-1733 !\COMMENT:
CH3OH+HO2=CH2OH+H2O2 3.26E13 0.0 1.87822E4
!CH3OH+CH3(=)CH3O+CH4 1.440E+001 3.100 6935.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)!\COMMENT: Ultan removed 21/08/15
!CH3OH+CH3(=)CH2OH+CH4 3.190E+001 3.170 7172.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT: Ultan removed 21/08/15
!\AUTHOR: !\REF:I. M. Alecu, D. G. Truhlar, J. Phys. Chem. A, 115 (2011) 14599-14611 !\COMMENT: Ultan added 21/08/15
CH3OH+CH3=CH2OH+CH4 2.13E-1 3.953 7.0551E3
!\AUTHOR: !\REF:I. M. Alecu, D. G. Truhlar, J. Phys. Chem. A, 115 (2011) 14599-14611 !\COMMENT: Ultan added 21/08/15
CH3OH+CH3=CH3O+CH4 3.22E3 2.425 8.5795E3
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH3OH+HCO=CH2OH+CH2O 9.63E3 2.9 1.311E4
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH3OH+CH3O=CH2OH+CH3OH 3.0E11 0.0 4.074E3
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH3OH+CH3O2=CH2OH+CH3O2H 1.81E12 0.0 1.371E4
CH2OH+O2=CH2O+HO2 1.51E15 -1.0 0.0E0
DUP
!\AUTHOR: !\REF: !\COMMENT:
CH2OH+O2=CH2O+HO2 2.41E14 0.0 5.017E3
DUP
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH2OH+H=CH2O+H2 6.0E12 0.0 0.0E0
!\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991). !\COMMENT:
CH2OH+HO2=CH2O+H2O2 1.2E13 0.0 0.0E0
!\AUTHOR: !\REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998) !\COMMENT: Ultan removed 21/08/15
CH2OH+HCO=2CH2O 1.8E14 0.0 0.0E0
!\AUTHOR: !\REF: !\COMMENT: WARNING, NO REF
CH2OH+HCO=CH3OH+CO 1.0E13 0.0 0.0E0
!\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991). !\COMMENT:
CH2OH+CH3O=CH2O+CH3OH 2.4E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH2OH+OH=H2O+CH2O 2.4E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH2OH+O=OH+CH2O 4.2E13 0.0 0.0E0

!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
2CH2OH=CH2O+CH3OH 3.0E12 0.0 0.0E0
CH3O+O2=CH2O+HO2 4.38E-19 9.5 -5.501E3
!\AUTHOR: !\REF:HOYERMANN ET AL., 18TH SYMPOSIUM !\COMMENT:
CH3O+H=CH2O+H2 2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
CH3O+HO2=CH2O+H2O2 3.01E11 0.0 0.0E0
!\AUTHOR: !\REF: WARNING: NO REFERENCE !\COMMENT: WARNING: NO REFERENCE
CH3O+CH3=CH2O+CH4 1.2E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
2CH3O=CH3OH+CH2O 6.03E13 0.0 0.0E0
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
HCO+H(+M)=CH2O(+M) 1.09E12 0.48 -2.6E2
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/1.35E24 -2.57E0 1.425E3/
TROE/7.824E-1 2.71E2 2.755E3 6.57E3/
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT: WARNING: KPS NOT INDIVIDUALLY REFERENCED IN MECHANISM, ASSUMING IT'S FROM LASKIN ET AL
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
CO+H2(+M)=CH2O(+M) 4.3E7 1.5 7.96E4
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/5.07E27 -3.42E0 8.4348E4/
TROE/9.32E-1 1.97E2 1.54E3 1.03E4/
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF: N. K. SRINIVASAN ET AL.,J. PHYS. CHEM. A 109, 7902-7914 (2005) !\COMMENT:

CH2O+O2=HCO+HO2 8.07E15 0.0 5.342E4
!\AUTHOR: !\REF: CURRAN FIT TO NIST DATABASE !\COMMENT:
CH2O+O=HCO+OH 6.26E9 1.15 2.26E3
!\AUTHOR: !\REF: IRDAM ET AL., IJCK 1993, 25, 285 !\COMMENT:
CH2O+H=HCO+H2 5.74E7 1.9 2.74E3
!\AUTHOR: !\REF: V. VASUDEVAN ET AL. IJCK. 37: 98--109 (2005). !\COMMENT:
CH2O+OH=HCO+H2O 7.82E7 1.63 -1.055E3
!\AUTHOR: !\REF: J. PHYS. CHEM. A 109, 12027-12035, 2005 !\COMMENT:
CH2O+HO2=HCO+H2O2 1.88E4 2.7 1.152E4
!\AUTHOR: !\REF: BAULCH ET AL. JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA, 34, 3, 757-1397 2005 !\COMMENT:
CH2O+CH3=HCO+CH4 3.83E1 3.36 4.312E3
!\AUTHOR: !\REF: ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986 !\COMMENT:
CH2O+O2CHO=HCO+HO2CHO 1.99E12 0.0 1.166E4
!\AUTHOR: !\REF:FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998). !\COMMENT:
CH2O+CH3O=HCO+CH3OH 6.62E11 0.0 2.294E3
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
CH2O+CH3O2=HCO+CH3O2H 1.99E12 0.0 1.166E4
!!
!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N \EA
!!
!\AUTHOR: !\REF: LI ET AL. IJCK 2007 !\COMMENT: X1.2
!3RD BODY COLLIDER EFFICIENCIES
HCO+M=H+CO+M 5.7E11 0.66 1.487E4
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:TIMONEN ET AL., JPC, 92:651 (1988) !\COMMENT:
HCO+O2=CO+HO2 7.58E12 0.0 4.1E2
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
HCO+O=CO+OH 3.02E13 0.0 0.0E0
!\AUTHOR: !\REF:TIMONEN ET AL., JPC, 92:651 (1988) !\COMMENT:
HCO+H=CO+H2 7.34E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
HCO+OH=CO+H2O 3.011E13 0.0 0.0E0

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!\AUTHOR: !\REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987) !\COMMENT:
HCO+CH3=CH4+CO        2.65E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
2HCO=CH2O+CO        1.8E13 0.0 0.0E0
!!
!\REACTIONCLASS: \LUMPED_BIMOLECULAR \A \N
\EA
!!
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
HCO+O=CO2+H        3.0E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
HCO+HO2=>CO2+H+OH        3.0E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
2HCO=>H2+2CO        3.0E12 0.0 0.0E0
!!
!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
\EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
CH2O+H(+M)=CH2OH(+M)        5.4E11 0.454 3.6E3
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      CH4/2.0/
      C2H6/3.0/
      LOW/1.27E32 -4.82E0 6.53E3/
      TROE/7.187E-1 1.03E2 1.291E3 4.16E3/
!\AUTHOR: !\REF:HIPPLER ET AL. PCCP. 3: 3450--2458 (2001).
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
CH3O(+M)=CH2O+H(+M)        6.8E13 0.0 2.617E4
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      CH4/2.0/
      C2H6/3.0/
```

LOW/1.867E25 -3.0E0 2.4307E4/
TROE/9.0E-1 2.5E3 1.3E3 1.0E99/
!!
!\REACTIONCLASS: \R+O2 \A \N
\EA
!!
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
HCO+O2=O2CHO 1.2E11 0.0 -1.1E3
2CH3(+M)=C2H6(+M) 2.277E15 -0.69 1.749E2
H2O/5.0/
CO/2.0/
CO2/3.0/
LOW/8.054E31 -3.75E0 9.816E2/
TROE/0.0E0 5.7E2 1.0E30 1.0E30/
!\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003) !\COMMENT:
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
C2H5+H(+M)=C2H6(+M) 5.21E17 -0.99 1.58E3
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/1.99E41 -7.08E0 6.685E3/
TROE/8.42E-1 1.25E2 2.219E3 6.882E3/
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N
\EA
!!
!\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:
C2H6+O2=C2H5+HO2 6.03E13 0.0 5.187E4
!\AUTHOR: !\REF: MIYOSHI,A. ET AL., CHEM. PHYS. LETT. 204, 241-247 (1993) !\COMMENT:
C2H6+O=C2H5+OH 3.55E6 2.4 5.83E3
!\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003) !\COMMENT:
C2H6+H=C2H5+H2 1.15E8 1.9 7.53E3
!\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT IS ORIGINAL SOURCE OF NIST DATA?
C2H6+OH=C2H5+H2O 1.48E7 1.9 9.5E2
!\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054. !\COMMENT:
C2H6+HO2=C2H5+H2O2 3.46E1 3.61 1.692E4
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:

C2H6+CH3=C2H5+CH4 5.55E-4 4.72 3.231E3
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
C2H6+CH3O=C2H5+CH3OH 2.41E11 0.0 7.09E3
!\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995?003 !\COMMENT:
C2H6+CH3O2=C2H5+CH3O2H 1.94E1 3.64 1.71E4
!\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995?003 !\COMMENT:
C2H6+C2H5O2=C2H5+C2H5O2H 8.6E0 3.76 1.72E4
!!
!\REACTIONCLASS: \RADICAL_BETA_SCISSION \A \N \EA
!!
!\AUTHOR: !\REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202 !\COMMENT: :HP AND LP LIMIT*0.7
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
C2H4+H(+M)=C2H5(+M) 9.569E8 1.463 1.355E3
H2/2.0/
H2O/6.0/
CH4/2.0/
CO/1.5/
CO2/2.0/
C2H6/3.0/
LOW/1.419E39 -6.642E0 5.769E3/
TROE/-5.69E-1 2.99E2 -9.147E3 1.524E2/
!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF: CURRAN: FIT TO PRATT/ WOOD 84 AND PRATT/ VELDMAN 76 !\COMMENT: WHAT IS SOURCE OF ORIGINAL DATA? EXPERIMENT? THEORY?
C2H5+H=C2H4+H2 2.0E12 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
2C2H4=C2H5+C2H3 4.82E14 0.0 7.153E4
!\AUTHOR: !\REF:ZHU, R.S. ET AL.,J. CHEM. PHYS. 120:6566:6573 (2004) !\COMMENT:
C2H5+CH3=CH4+C2H4 1.18E4 2.45 -2.921E3
!!
!\REACTIONCLASS: \RADICAL_ADDITION \A \N \EA
!!
!\AUTHOR: !\REF:GRI 3.0 !\COMMENT:
C2H5+O=CH3CHO+H 1.1E14 0.0 0.0E0
!\AUTHOR: !\REF:CURRAN. BASED ON CH3+HO2(=)PRODUCTS !\COMMENT:
C2H5+HO2=C2H5O+OH 1.1E13 0.0 0.0E0

!\AUTHOR: !\REF:CURRAN. BASED ON CH3+HO2(=)PRODUCTS !\COMMENT:
C2H5+CH3O2=C2H5O+CH3O 8.0E12 0.0 -1.0E3
!!
!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA
!!
!\AUTHOR: !\REF:STEWART ET AL C_F 1989 !\COMMENT:
2CH3=H+C2H5 4.74E12 0.105 1.06643E4
PLOG/1.0E-2 4.74E12 1.05E-1 1.06643E4/
PLOG/1.0E-1 2.57E13 -9.6E-2 1.14061E4/
PLOG/1.0E0 3.1E14 -3.62E-1 1.33725E4/
PLOG/1.0E1 2.15E10 8.85E-1 1.35325E4/
PLOG/1.0E2 1.032E2 3.23E0 1.12361E4/
!!
!\REACTIONCLASS: \R+O2 \A \N
\EA
!!
!\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415?427 !\COMMENT:
C2H5+O2=C2H5O2 3.398E53 -13.9 9.279E3
PLOG/4.0E-2 3.398E53 -1.39E1 9.279E3/
PLOG/1.0E0 9.362E59 -1.528E1 1.424E4/
PLOG/1.0E1 1.262E60 -1.491E1 1.624E4/
!\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415?427 !\COMMENT:
C2H5+O2=C2H4+HO2 2.094E9 0.49 -3.914E2
PLOG/4.0E-2 2.094E9 4.9E-1 -3.914E2/
PLOG/1.0E0 1.843E7 1.13E0 -7.206E2/
PLOG/1.0E1 7.561E14 -1.01E0 4.749E3/
!\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415?427 !\COMMENT:
C2H5+O2=CH3CHO+OH 4.908E-6 4.76 2.543E2
PLOG/4.0E-2 4.908E-6 4.76E0 2.543E2/
PLOG/1.0E0 6.803E-2 3.57E0 2.643E3/
PLOG/1.0E1 8.265E2 2.41E0 5.285E3/
!\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415?427 !\COMMENT:
C2H5O2=CH3CHO+OH 1.237E35 -9.42 3.636E4
PLOG/4.0E-2 1.237E35 -9.42E0 3.636E4/
PLOG/1.0E0 1.687E36 -9.22E0 3.87E4/
PLOG/1.0E1 2.52E41 -1.02E1 4.371E4/
!\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415?427 !\COMMENT:
C2H5O2=C2H4+HO2 1.782E32 -7.1 3.284E4
PLOG/4.0E-2 1.782E32 -7.1E0 3.284E4/
PLOG/1.0E0 2.701E37 -8.47E0 3.584E4/
PLOG/1.0E1 1.98E38 -8.46E0 3.79E4/
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N
\EA
!!

!\AUTHOR: !\REF:TSANG _ HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:
H2+C2H5O2=H+C2H5O2H 1.5E14 0.0 2.603E4
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
C2H5O2+HO2=C2H5O2H+O2 1.75E10 0.0 -3.275E3
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
C2H5O2+CH2O=C2H5O2H+HCO 1.99E12 0.0 1.166E4
!\AUTHOR: !\REF:BASED ON CH4+CH3O2 !\COMMENT: WARNING:
C2H5O2+CH4=C2H5O2H+CH3 1.81E11 0.0 1.848E4
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
C2H5O2+CH3OH=C2H5O2H+CH2OH 1.81E12 0.0 1.371E4
!!
!\REACTIONCLASS: \KHP_DECOMP \A \N \EA
!!
!\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995?003 !\COMMENT:
C2H5O2H=C2H5O+OH 6.31E14 0.0 4.23E4
!!
!\REACTIONCLASS: \UNIMOL \A \N \EA
!!
!\AUTHOR: !\REF:GRI 3.0 !\COMMENT:
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
C2H3+H(+M)=C2H4(+M) 6.08E12 0.27 2.8E2
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/1.4E30 -3.86E0 3.32E3/
TROE/7.82E-1 2.075E2 2.663E3 6.095E3/
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:CHECK EFFECT!\!\!\!\! !\COMMENT: WARNING: SOURCE OF REFERENCE IS CONFUSING
C2H4+O2=C2H3+HO2 4.22E13 0.0 5.76231E4
!\AUTHOR: !\REF:KNYAZEV,V.D. ET AL.,J. PHYS. CHEM. 100, 11346-1135 (1996) !\COMMENT:

C2H4+H=C2H3+H2 5.07E7 1.93 1.295E4
!\AUTHOR: !\REF: FROM STANFORD !\COMMENT: WARNING: SOURCE OF RATE CONSTANT IS UNCLEAR
C2H4+OH=C2H3+H2O 2.23E4 2.745 2.2155E3
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
C2H4+CH3O=C2H3+CH3OH 1.2E11 0.0 6.75E3
!\AUTHOR: !\REF:FROM BILL PITZ'S SUGGESTION !\COMMENT: WKM 22/ 04/ 2010 WARNING: WHAT IS JUSTIFICATION FOR THIS RATE CONSTANT? WHY WAS IT SUGGESTED?
C2H4+CH3O2=C2H3+CH3O2H 8.59E0 3.754 2.7132E4
!\AUTHOR: !\REF:FROM BILL PITZ'S SUGGESTION !\COMMENT: WKM 22/ 04/ 2010 WARNING: WHAT IS JUSTIFICATION FOR THIS RATE CONSTANT? WHY WAS IT SUGGESTED?
C2H4+C2H5O2=C2H3+C2H5O2H 8.59E0 3.754 2.7132E4
!\AUTHOR: !\REF: WARNING REFERENCE UNCLEAR !\COMMENT: WARNING: SOURCE OF RATE CONSTANT UNCLEAR IN MECHANISM
C2H4+CH3=C2H3+CH4 9.76E2 2.947 1.5148E4
DUP
!\AUTHOR: !\REF: !\COMMENT:
C2H4+CH3=C2H3+CH4 8.13E-5 4.417 8.8358E3
DUP
!!
!\REACTIONCLASS: \RADICAL_ADDITION \A \N \EA
!!
!\AUTHOR: !\REF: BAULCH ET AL. JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA: 34, 3, 757-1397 2005 !\COMMENT: MAKING BRANCHING RATIO 55:45 WARNING
C2H4+O=CH3+HCO 7.453E6 1.88 1.83E2
!\AUTHOR: !\REF: BAULCH ET AL. JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA: 34, 3, 757-1397 2005 !\COMMENT: MAKING BRANCHING RATIO 55:45 WARNING
C2H4+O=CH2CHO+H 6.098E6 1.88 1.83E2
!!
!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N \EA
!!
!\AUTHOR: !\REF:SJK, J PHYS CHEM 110 2006 6960-6970 !\COMMENT:
C2H4+OH=CH3+CH2O 5.35E0 2.92 -1.7327E3
PLOG/1.0E-2 5.35E0 2.92E0 -1.7327E3/
PLOG/2.5E-2 3.19E1 2.71E0 -1.1723E3/
PLOG/1.0E-1 5.55E2 2.36E0 -1.808E2/
PLOG/1.0E0 1.78E5 1.68E0 2.0605E3/
PLOG/1.0E1 2.37E9 5.6E-1 6.0067E3/
PLOG/1.0E2 2.76E13 -5.0E-1 1.14551E4/
!\AUTHOR: !\REF:SJK, J PHYS CHEM 110 2006 6960-6970 !\COMMENT:
C2H4+OH=CH3CHO+H 2.37E-7 5.3 -2.0506E3
PLOG/1.0E-2 2.37E-7 5.3E0 -2.0506E3/
PLOG/2.5E-2 8.73E-5 4.57E0 -6.18E2/

PLOG/1.0E-1 4.03E-1 3.54E0 1.8817E3/
PLOG/1.0E0 2.38E-2 3.91E0 1.7227E3/
PLOG/1.0E1 8.25E8 1.01E0 1.05073E4/
PLOG/1.0E2 6.8E9 8.1E-1 1.38673E4/
C2H2+H(+M)=C2H3(+M) 1.71E10 1.266 2.709E3
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/6.346E31 -4.664E0 3.78E3/
TROE/7.88E-1 -1.02E4 1.0E-30/
REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=C2H3OO 4.07E27 -4.67 5.222E3
DUP
PLOG/1.0E-2 1.55E24 -5.45E0 9.662E3/
PLOG/1.0E-1 3.48E56 -1.501E1 1.916E4/
PLOG/3.16E-1 1.25E64 -1.697E1 2.129E4/
PLOG/1.0E0 3.34E61 -1.579E1 2.015E4/
PLOG/3.16E0 7.34E53 -1.311E1 1.73E4/
PLOG/1.0E1 4.16E48 -1.121E1 1.6E4/
PLOG/3.16E1 2.33E43 -9.38E0 1.481E4/
PLOG/1.0E2 3.41E39 -8.04E0 1.436E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=C2H3OO 4.07E27 -4.67 5.222E3
DUP
PLOG/1.0E-2 1.78E-9 4.15E0 -4.707E3/
PLOG/1.0E-1 2.36E22 -4.52E0 2.839E3/
PLOG/3.16E-1 2.0E26 -5.43E0 2.725E3/
PLOG/1.0E0 6.13E28 -5.89E0 3.154E3/
PLOG/3.16E0 2.14E29 -5.8E0 3.52E3/
PLOG/1.0E1 3.48E28 -5.37E0 3.636E3/
PLOG/3.16E1 3.32E27 -4.95E0 3.61E3/
PLOG/1.0E2 1.03E27 -4.72E0 3.68E3/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CH2CHO+O 1.76E12 0.15 4.205E3
DUP
PLOG/1.0E-2 7.88E20 -2.67E0 6.742E3/
PLOG/1.0E-1 7.72E20 -2.67E0 6.713E3/
PLOG/3.16E-1 9.87E20 -2.7E0 6.724E3/
PLOG/1.0E0 7.1E20 -2.65E0 6.489E3/
PLOG/3.16E0 4.5E20 -2.53E0 6.406E3/
PLOG/1.0E1 1.76E23 -3.22E0 8.697E3/

PLOG/3.16E1 3.14E25 -3.77E0 1.153E4/
PLOG/1.0E2 1.02E26 -3.8E0 1.391E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CH2CHO+O 1.76E12 0.15 4.205E3
DUP
PLOG/1.0E-2 1.36E10 6.2E-1 -2.776E2/
PLOG/1.0E-1 1.42E10 6.2E-1 -2.477E2/
PLOG/3.16E-1 1.66E10 6.0E-1 -1.625E2/
PLOG/1.0E0 2.02E10 5.8E-1 3.84E1/
PLOG/3.16E0 9.75E9 6.7E-1 2.48E2/
PLOG/1.0E1 7.34E9 7.2E-1 7.781E2/
PLOG/3.16E1 1.57E9 9.2E-1 1.219E3/
PLOG/1.0E2 7.85E7 1.28E0 1.401E3/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=C2H2+HO2 6.49E6 1.5 5.218E3
DUP
PLOG/1.0E-2 1.08E7 1.28E0 3.322E3/
PLOG/1.0E-1 7.75E6 1.33E0 3.216E3/
PLOG/3.16E-1 1.21E7 1.27E0 3.311E3/
PLOG/1.0E0 2.15E7 1.19E0 3.367E3/
PLOG/3.16E0 1.13E8 1.0E0 3.695E3/
PLOG/1.0E1 1.31E11 1.2E-1 5.872E3/
PLOG/3.16E1 1.19E9 8.2E-1 5.617E3/
PLOG/1.0E2 1.06E17 -1.45E0 1.223E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=C2H2+HO2 6.49E6 1.5 5.218E3
DUP
PLOG/1.0E-2 4.76E1 2.75E0 -7.964E2/
PLOG/1.0E-1 5.16E1 2.73E0 -7.683E2/
PLOG/3.16E-1 5.55E1 2.73E0 -6.585E2/
PLOG/1.0E0 4.6E1 2.76E0 -4.928E2/
PLOG/3.16E0 3.75E0 3.07E0 -6.01E2/
PLOG/1.0E1 5.48E0 3.07E0 8.57E1/
PLOG/3.16E1 4.47E8 0.0E0 9.55E2/
PLOG/1.0E2 2.02E1 2.94E0 1.847E3/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CH2CO+OH 1.17E3 2.43 7.074E3
DUP
PLOG/1.0E-2 8.66E2 2.41E0 6.061E3/
PLOG/1.0E-1 8.91E2 2.41E0 6.078E3/
PLOG/3.16E-1 9.43E2 2.4E0 6.112E3/
PLOG/1.0E0 1.06E3 2.39E0 6.18E3/

PLOG/3.16E0 1.09E3 2.38E0 6.179E3/
PLOG/1.0E1 1.39E3 2.36E0 6.074E3/
PLOG/3.16E1 2.49E6 1.42E0 8.48E3/
PLOG/1.0E2 1.66E10 3.6E-1 1.201E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CH2CO+OH 1.17E3 2.43 7.074E3
DUP
PLOG/1.0E-2 1.82E-1 3.12E0 1.331E3/
PLOG/1.0E-1 2.07E-1 3.11E0 1.383E3/
PLOG/3.16E-1 2.71E-1 3.08E0 1.496E3/
PLOG/1.0E0 5.26E-1 3.01E0 1.777E3/
PLOG/3.16E0 1.37E0 2.9E0 2.225E3/
PLOG/1.0E1 4.19E-1 2.93E0 2.052E3/
PLOG/3.16E1 1.19E-4 4.21E0 2.043E3/
PLOG/1.0E2 1.3E-3 3.97E0 3.414E3/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CH2O+HCO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 2.49E36 -7.6E0 1.264E4/
PLOG/1.0E-1 2.43E36 -7.6E0 1.261E4/
PLOG/3.16E-1 1.95E36 -7.57E0 1.249E4/
PLOG/1.0E0 2.73E35 -7.32E0 1.182E4/
PLOG/3.16E0 1.43E36 -7.47E0 1.246E4/
PLOG/1.0E1 5.18E35 -7.2E0 1.343E4/
PLOG/3.16E1 3.19E20 -2.57E0 5.578E3/
PLOG/1.0E2 2.73E33 -6.28E0 1.6E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CH2O+HCO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 4.54E15 -1.28E0 5.153E2/
PLOG/1.0E-1 4.59E15 -1.28E0 5.13E2/
PLOG/3.16E-1 4.81E15 -1.29E0 5.206E2/
PLOG/1.0E0 6.08E15 -1.31E0 6.457E2/
PLOG/3.16E0 9.45E15 -1.36E0 1.066E3/
PLOG/1.0E1 2.56E15 -1.18E0 1.429E3/
PLOG/3.16E1 1.03E69 -1.923E1 1.476E4/
PLOG/1.0E2 4.21E10 1.9E-1 8.306E2/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=>CH2O+H+CO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 5.82E36 -7.6E0 1.264E4/
PLOG/1.0E-1 5.66E36 -7.6E0 1.261E4/

PLOG/3.16E-1 4.55E36 -7.57E0 1.249E4/
PLOG/1.0E0 6.36E35 -7.32E0 1.182E4/
PLOG/3.16E0 3.35E36 -7.47E0 1.246E4/
PLOG/1.0E1 1.21E36 -7.2E0 1.343E4/
PLOG/3.16E1 7.43E20 -2.57E0 5.578E3/
PLOG/1.0E2 6.36E33 -6.28E0 1.6E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=>CH2O+H+CO 1.16E16 -1.13 3.791E3
DUP
PLOG/1.0E-2 1.06E16 -1.28E0 5.153E2/
PLOG/1.0E-1 1.07E16 -1.28E0 5.13E2/
PLOG/3.16E-1 1.13E16 -1.29E0 5.206E2/
PLOG/1.0E0 1.42E16 -1.31E0 6.457E2/
PLOG/3.16E0 2.2E16 -1.36E0 1.066E3/
PLOG/1.0E1 5.98E15 -1.18E0 1.429E3/
PLOG/3.16E1 2.39E69 -1.923E1 1.476E4/
PLOG/1.0E2 9.81E10 1.9E-1 8.306E2/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CO+CH3O 3.09E13 -0.89 3.682E3
DUP
PLOG/1.0E-2 8.19E18 -2.66E0 3.201E3/
PLOG/1.0E-1 4.06E14 -1.32E0 8.858E2/
PLOG/3.16E-1 4.34E14 -1.33E0 9.006E2/
PLOG/1.0E0 1.03E11 -3.3E-1 -7.478E2/
PLOG/3.16E0 1.89E12 -3.0E0 -8.995E3/
PLOG/1.0E1 1.93E24 -5.63E0 1.8E0/
PLOG/3.16E1 1.1E18 -2.22E0 5.178E3/
PLOG/1.0E2 5.79E32 -6.45E0 1.681E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CO+CH3O 3.09E13 -0.89 3.682E3
DUP
PLOG/1.0E-2 1.29E9 1.8E-1 -1.717E3/
PLOG/1.0E-1 5.99E11 -2.93E0 -9.564E3/
PLOG/3.16E-1 2.91E11 -2.93E0 -1.012E4/
PLOG/1.0E0 5.77E21 -3.54E0 4.772E3/
PLOG/3.16E0 4.99E15 -1.62E0 1.849E3/
PLOG/1.0E1 9.33E16 -1.96E0 3.324E3/
PLOG/3.16E1 1.02E72 -2.069E1 1.586E4/
PLOG/1.0E2 1.1E9 3.1E-1 1.024E3/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CO2+CH3 6.16E13 -1.05 3.743E3
DUP

PLOG/1.0E-2 2.37E35 -7.76E0 1.263E4/
PLOG/1.0E-1 1.73E35 -7.72E0 1.252E4/
PLOG/3.16E-1 4.47E34 -7.55E0 1.214E4/
PLOG/1.0E0 7.25E31 -6.7E0 1.044E4/
PLOG/3.16E0 3.63E35 -7.75E0 1.283E4/
PLOG/1.0E1 2.09E35 -7.53E0 1.405E4/
PLOG/3.16E1 3.84E18 -2.44E0 5.408E3/
PLOG/1.0E2 1.21E32 -6.32E0 1.619E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CO2+CH3 6.16E13 -1.05 3.743E3
DUP
PLOG/1.0E-2 6.27E13 -1.16E0 4.063E2/
PLOG/1.0E-1 6.24E13 -1.16E0 4.014E2/
PLOG/3.16E-1 6.12E13 -1.16E0 3.97E2/
PLOG/1.0E0 5.32E13 -1.14E0 4.467E2/
PLOG/3.16E0 1.45E14 -1.26E0 9.877E2/
PLOG/1.0E1 5.02E13 -1.11E0 1.409E3/
PLOG/3.16E1 1.4E70 -2.011E1 1.543E4/
PLOG/1.0E2 9.21E8 2.5E-1 8.553E2/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=CH2CHO+O 1.22E29 -4.71 4.234E4
DUP
PLOG/1.0E-2 2.7E180 -4.819E1 1.693E5/
PLOG/1.0E-1 3.9E38 -8.69E0 4.277E4/
PLOG/3.16E-1 4.57E47 -1.121E1 4.705E4/
PLOG/1.0E0 7.62E81 -2.128E1 6.508E4/
PLOG/3.16E0 1.86E68 -1.683E1 6.068E4/
PLOG/1.0E1 2.02E55 -1.269E1 5.584E4/
PLOG/3.16E1 1.11E53 -1.179E1 5.669E4/
PLOG/1.0E2 4.3E48 -1.031E1 5.609E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=CH2CHO+O 1.22E29 -4.71 4.234E4
DUP
PLOG/1.0E-2 1.47E30 -6.64E0 4.111E4/
PLOG/1.0E-1 9.65E-12 5.96E0 2.289E4/
PLOG/3.16E-1 3.95E22 -3.71E0 3.627E4/
PLOG/1.0E0 2.39E33 -6.62E0 4.128E4/
PLOG/3.16E0 6.37E31 -5.96E0 4.126E4/
PLOG/1.0E1 2.13E29 -5.1E0 4.071E4/
PLOG/3.16E1 4.66E27 -4.5E0 4.053E4/
PLOG/1.0E2 5.99E25 -3.85E0 4.012E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

C2H3OO=CH2CO+OH 1.55E24 -3.87 4.985E4
DUP
PLOG/1.0E-2 1.15E47 -1.228E1 7.533E4/
PLOG/1.0E-1 8.43E9 -2.06E0 3.372E4/
PLOG/3.16E-1 6.06E4 1.7E-1 3.422E4/
PLOG/1.0E0 1.51E19 -3.61E0 4.306E4/
PLOG/3.16E0 2.13E33 -7.39E0 5.161E4/
PLOG/1.0E1 4.44E36 -7.99E0 5.468E4/
PLOG/3.16E1 1.19E37 -7.8E0 5.646E4/
PLOG/1.0E2 9.08E35 -7.21E0 5.755E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=CH2CO+OH 1.55E24 -3.87 4.985E4
DUP
PLOG/1.0E-2 2.31E2 -7.3E-1 2.571E4/
PLOG/1.0E-1 1.83E-23 7.84E0 2.019E4/
PLOG/3.16E-1 3.82E63 -2.044E1 4.342E4/
PLOG/1.0E0 3.18E27 -7.76E0 3.723E4/
PLOG/3.16E0 2.32E-5 3.47E0 3.156E4/
PLOG/1.0E1 1.06E-1 2.64E0 3.416E4/
PLOG/3.16E1 5.62E2 1.7E0 3.645E4/
PLOG/1.0E2 1.11E7 5.2E-1 3.867E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=CH2O+HCO 1.19E20 -2.29 3.017E4
DUP
PLOG/1.0E-2 1.66E174 -5.552E1 6.032E4/
PLOG/1.0E-1 9.03E66 -1.725E1 4.812E4/
PLOG/3.16E-1 1.82E43 -9.87E0 3.796E4/
PLOG/1.0E0 8.64E33 -6.88E0 3.437E4/
PLOG/3.16E0 7.29E171 -4.353E1 1.919E5/
PLOG/1.0E1 1.03E32 -6.06E0 3.55E4/
PLOG/3.16E1 1.85E34 -6.57E0 3.851E4/
PLOG/1.0E2 5.7E29 -5.19E0 3.68E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=CH2O+HCO 1.19E20 -2.29 3.017E4
DUP
PLOG/1.0E-2 2.27E35 -7.97E0 3.128E4/
PLOG/1.0E-1 2.08E26 -4.96E0 2.878E4/
PLOG/3.16E-1 1.45E20 -3.08E0 2.663E4/
PLOG/1.0E0 1.06E130 -3.938E1 5.47E4/
PLOG/3.16E0 2.35E34 -6.87E0 3.57E4/
PLOG/1.0E1 2.18E175 -5.378E1 6.85E4/
PLOG/3.16E1 1.07E185 -5.422E1 8.899E4/
PLOG/1.0E2 4.68E2 1.81E0 1.81E4/

!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=>CH2O+H+CO 1.19E20 -2.29 3.017E4
DUP
PLOG/1.0E-2 3.88E174 -5.552E1 6.032E4/
PLOG/1.0E-1 2.11E67 -1.725E1 4.812E4/
PLOG/3.16E-1 4.26E43 -9.87E0 3.796E4/
PLOG/1.0E0 2.02E34 -6.88E0 3.437E4/
PLOG/3.16E0 1.7E172 -4.353E1 1.919E5/
PLOG/1.0E1 2.4E32 -6.06E0 3.55E4/
PLOG/3.16E1 4.32E34 -6.57E0 3.851E4/
PLOG/1.0E2 1.33E30 -5.19E0 3.68E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=>CH2O+H+CO 1.19E20 -2.29 3.017E4
DUP
PLOG/1.0E-2 5.29E35 -7.97E0 3.128E4/
PLOG/1.0E-1 4.85E26 -4.96E0 2.878E4/
PLOG/3.16E-1 3.37E20 -3.08E0 2.663E4/
PLOG/1.0E0 2.46E130 -3.938E1 5.47E4/
PLOG/3.16E0 5.49E34 -6.87E0 3.57E4/
PLOG/1.0E1 5.09E175 -5.378E1 6.85E4/
PLOG/3.16E1 2.49E185 -5.422E1 8.899E4/
PLOG/1.0E2 1.09E3 1.81E0 1.81E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3OO=CO+CH3O 1.16E-1 3.16 1.842E4
DUP
PLOG/1.0E-2 5.2E33 -7.92E0 3.132E4/
PLOG/1.0E-1 1.26E98 -2.709E1 6.406E4/
PLOG/3.16E-1 1.8E33 -7.27E0 3.376E4/
PLOG/1.0E0 3.83E33 -7.2E0 3.51E4/
PLOG/3.16E0 1.28E79 -1.961E1 7.487E4/
PLOG/1.0E1 4.07E32 -6.62E0 3.721E4/
PLOG/3.16E1 6.86E44 -1.004E1 4.703E4/
PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: !Refitted by Yang from 500K to 2000K, maximum error is 18.13%
C2H3OO=CO+CH3O 1.16E-1 3.16 1.842E4
DUP
PLOG/1.0E-2 2.31E129 -4.186E1 4.585E4/
PLOG/1.0E-1 2.42E28 -5.99E0 3.054E4/
PLOG/3.16E-1 8.69E-50 1.663E1 -3.9E3/
PLOG/1.0E0 1.19E-39 1.361E1 -1.317E3/
PLOG/3.16E0 8.8E86 -2.308E1 6.101E4/
PLOG/1.0E1 1.27E3 1.44E0 1.866E4/

PLOG/3.16E1 1.97E17 -2.23E0 2.859E4/
PLOG/1.0E2 3.25E4 1.694E0 2.33276E4/
!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:86TSA/ HAM !\COMMENT:
C2H3+H=C2H2+H2 1.7E14 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
C2H3+OH=C2H2+H2O 3.011E13 0.0 0.0E0
!\AUTHOR: !\REF:Tsang, W.; Hampson, R.F., J. Phys. Chem. Ref. Data 15, 1087 (1986) !\COMMENT:
C2H3+CH3=CH4+C2H2 3.92E11 0.0 0.0E0
!\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
2C2H3=C2H2+C2H4 9.6E11 0.0 0.0E0
C2H+H(+M)=C2H2(+M) 1.0E17 0.0 0.0E0
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/3.75E33 -4.8E0 1.9E3/
TROE/6.46E-1 1.32E2 1.315E3 5.566E3/
!!
!\REACTIONCLASS: \RADICAL_ADDITION \A \N \EA
!!
!\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\COMMENT:
C2H2+O=CH2+CO 7.395E8 1.28 2.472E3
!\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\COMMENT:
C2H2+O=HCCO+H 2.958E9 1.28 2.472E3
!\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\COMMENT:
C2H2+HO2=CH2CO+OH 6.03E9 0.0 7.949E3
!\AUTHOR: !\REF:GRI 3.0 AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H2+HCO=C2H3+CO 1.0E7 2.0 6.0E3
!\AUTHOR: !\REF:GRI 3.0 AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H2+CH2=C3H3+H 1.2E13 0.0 6.62E3
!\AUTHOR: !\REF:GRI 3.0 AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H2+HCCO=C3H3+CO 1.0E11 0.0 3.0E3
!!

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!\REACTIONCLASS:    \RADICAL_ADDITION\OH                    \A                  \N
\EA
!!
!\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:
C2H2+OH=C2H+H2O        2.632E6 2.14 1.706E4
!\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:
C2H2+OH=CH2CO+H        1.578E3 2.56 -8.445E2
      PLOG/1.0E-2 1.578E3 2.56E0 -8.445E2/
      PLOG/2.5E-2 1.518E4 2.28E0 -2.921E2/
      PLOG/1.0E-1 3.017E5 1.92E0 5.981E2/
      PLOG/1.0E0 7.528E6 1.55E0 2.106E3/
      PLOG/1.0E1 5.101E6 1.65E0 3.4E3/
      PLOG/1.0E2 1.457E4 2.45E0 4.477E3/
!\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:
C2H2+OH=CH3+CO        4.757E5 1.68 -3.298E2
      PLOG/1.0E-2 4.757E5 1.68E0 -3.298E2/
      PLOG/2.5E-2 4.372E6 1.4E0 2.265E2/
      PLOG/1.0E-1 7.648E7 1.05E0 1.115E3/
      PLOG/1.0E0 1.277E9 7.3E-1 2.579E3/
      PLOG/1.0E1 4.312E8 9.2E-1 3.736E3/
      PLOG/1.0E2 8.25E5 1.77E0 4.697E3/
!\AUTHOR: !\REF:GRI !\COMMENT:
C2H+O2=HCO+CO        5.0E13 0.0 1.5E3
!\AUTHOR: !\REF:GRI !\COMMENT:
C2H+H2=H+C2H2        4.9E5 2.5 5.6E2
!\AUTHOR: !\REF:GRI !\COMMENT:
C2H+OH=H+HCCO        2.0E13 0.0 0.0E0
CH3CHO(+M)=CH3+HCO(+M)        2.45E22 -1.74 8.6355E4
      LOW/1.03E59 -1.13E1 9.59125E4/
      TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
!\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO. 2, 2010 !\COMMENT:
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
CH3CHO(+M)=CH4+CO(+M)        2.72E21 -1.74 8.6355E4
      LOW/1.144E58 -1.13E1 9.59125E4/
      TROE/2.49E-3 7.181E2 6.089E0 3.78E3/
!!
!\REACTIONCLASS:    \RH_ABSTRACTION                    \A                  \N
\EA
!!
!\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:
CH3CHO+O2=CH3CO+HO2        3.01E13 0.0 3.915E4
!\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT IS SOURCE
OF NIST DATA?
CH3CHO+O=CH3CO+OH        5.94E12 0.0 1.868E3
!\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\COMMENT:
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CH3CHO+H=CH3CO+H2 1.31E5 2.58 1.22E3
!\AUTHOR: !\REF:JUAN LI'S PHD THESIS !\COMMENT: WARNING: UNPUBLISHED RESULTS?
CH3CHO+OH=CH3CO+H2O 3.37E12 0.0 -6.19E2
!\AUTHOR: !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT: !\COMMENT:
CH3CHO+HO2=CH3CO+H2O2 3.01E12 0.0 1.192E4
!\AUTHOR: !\REF: GUPTE ET AL.,PROC COMBUST INST 31 (2007) 167?74 !\COMMENT:
CH3CHO+CH3=CH3CO+CH4 7.08E-4 4.58 1.966E3
!\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:
CH3CHO+CH3O2=CH3CO+CH3O2H 3.01E12 0.0 1.192E4
!\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\COMMENT:
CH3CHO+H=CH2CHO+H2 2.72E3 3.1 5.21E3
!\AUTHOR: !\REF:TAYLOR ET AL. 1996 !\COMMENT:
CH3CHO+OH=CH2CHO+H2O 1.72E5 2.4 8.15E2
CH3CO(+M)=CH3+CO(+M) 1.07E12 0.63 1.69E4
LOW/5.65E18 -9.7E-1 1.46E4/
TROE/6.29E-1 8.73E9 5.52E0 7.6E7/
!\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
CH3CO(+M)=CH2CO+H(+M) 9.413E7 1.917 4.49872E4
LOW/1.516E51 -1.027E1 5.539E4/
TROE/6.009E-1 8.103E9 6.677E2 5.0E9/
CH3CO+H=CH2CO+H2 2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE
CH3CO+O=CH2CO+OH 2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE
CH3CO+CH3=CH2CO+CH4 5.0E13 0.0 0.0E0
CH2CHO(+M)=CH2CO+H(+M) 1.43E15 -0.15 4.56E4
LOW/6.0E29 -3.8E0 4.34239E4/
TROE/9.85E-1 3.93E2 9.8E9 5.0E9/
!\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781 !\COMMENT:
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
CH2CHO(+M)=CH3+CO(+M) 2.93E12 0.29 4.03E4
LOW/9.52E33 -5.07E0 4.13E4/
TROE/7.13E-17 1.15E3 4.99E9 1.79E9/
!\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:
CH2CHO+O2=CH2CO+HO2 1.88E5 2.37 2.373E4
PLOG/1.0E-2 1.88E5 2.37E0 2.373E4/
PLOG/1.0E-1 1.88E5 2.37E0 2.737E4/
PLOG/1.0E0 2.51E5 2.33E0 2.38E4/
PLOG/1.0E1 7.05E7 1.63E0 2.529E4/
!\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:

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CH2CHO+O2=>CH2O+CO+OH        2.68E17 -1.84 6.53E3
      PLOG/1.0E-2 2.68E17 -1.84E0 6.53E3/
      PLOG/1.0E-1 1.52E20 -2.58E0 8.98E3/
      PLOG/1.0E0 1.65E19 -2.22E0 1.034E4/
      PLOG/1.0E1 8.953E13 -6.0E-1 1.012E4/
CH2+CO(+M)=CH2CO(+M)        8.1E11 0.0 0.0E0
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      CH4/2.0/
      C2H6/3.0/
      LOW/2.69E33 -5.11E0 7.095E3/
      TROE/5.907E-1 2.75E2 1.226E3 5.185E3/
!!
CH2CO+H=HCCO+H2        1.401E15 -0.171 8.7832E3
!\AUTHOR: !\REF:WKM ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF ESTIMATE?
CH2CO+O=HCCO+OH        1.0E13 0.0 8.0E3
!\AUTHOR: !\REF:WKM ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF ESTIMATE?
CH2CO+OH=HCCO+H2O        1.0E13 0.0 2.0E3
!!
!\REACTIONCLASS:  \RADICAL_ADDITION  \A  \N  \EA
!!
!\AUTHOR: !\REF:WKM (SEE COMMENTS AT BEGINNING OF FILE 15/ 09/ 2011 !\COMMENT: WARNING: SEE COMMENTS IN PREVIOUS VERSION OF MECHANISM
CH2CO+H=CH3+CO        7.704E13 -0.171 4.1832E3
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:
CH2CO+O=CH2+CO2        1.75E12 0.0 1.35E3
!\AUTHOR: !\REF:BROWN ET AL. CHEM. PHYS. LETT. 1989, 161, 491. !\COMMENT:
CH2CO+OH=CH2OH+CO        2.0E12 0.0 -1.01E3
!\AUTHOR: !\REF:WKM CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
CH2CO+CH3=C2H5+CO        4.769E4 2.312 9.468E3
!!
!\REACTIONCLASS:  \RADICAL_ADDITION  \A  \N  \EA
!!
!\AUTHOR: !\REF:WKM CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
HCCO+OH=>H2+2CO        1.0E14 0.0 0.0E0
!\AUTHOR: !\REF:WKM CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
HCCO+O=>H+2CO        8.0E13 0.0 0.0E0
!\AUTHOR: !\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS JOURNAL/ISSUE?
HCCO+O2=>OH+2CO        1.91E11 -0.02 1.02E3
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!\AUTHOR: !\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS JOURNAL/ISSUE?
HCCO+O2=>CO2+CO+H 4.78E12 -0.142 1.15E3
!\AUTHOR: !\REF: CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
CH3+CH2O=C2H5O 3.0E11 0.0 6.336E3
!\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\COMMENT:
CH3CHO+H=C2H5O 4.61E7 1.71 7.09E3
!!
!\REACTIONCLASS: \R+O2 \A \N \EA
!!
!\AUTHOR: !\REF: HARTMANN ET AL. 1990 !\COMMENT:
C2H5O+O2=CH3CHO+HO2 4.28E10 0.0 1.097E3
!\AUTHOR: !\REF:Friedrichs, G.; Davidson, D. F.; Hanson, R. K. Int J. Chem. Kinet. 2004, 36, 157. !\COMMENT: Ultan added 21/08/15
CH3O+HCO=CH3OH+CO 9.0E13 0.0 0.0E0
C3H8(+M)=CH3+C2H5(+M) 1.29E37 -5.84 9.738E4
H2/2.0/
H2O/6.0/
CO/1.5/
CO2/2.0/
CH4/2.0/
C2H6/3.0/
LOW/5.64E74 -1.574E1 9.8714E4/
TROE/3.1E-1 5.0E1 3.0E3 9.0E3/
!\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING
IC3H7+H=C3H8 1.0E14 0.0 0.0E0
!\AUTHOR: !\REF: Ingham,T.; Walker,R.W.; Woolford,R.E., Symp. Int. Combust. Proc. 25, 767-774 (1994) !\COMMENT:
C3H8+O2=IC3H7+HO2 2.0E13 0.0 4.964E4
!\AUTHOR: !\REF:Tsang, W. Chemical kinetic data base for combustion chemistry. Part 3. Propane J. Phys. Chem. Ref. Data 17, 887 (1988) !\COMMENT:
C3H8+H=IC3H7+H2 1.3E6 2.4 4.471E3
!\AUTHOR: !\REF:Tsang, W. Chemical kinetic data base for combustion chemistry. Part 3. Propane J. Phys. Chem. Ref. Data 17, 887 (1988) !\COMMENT:
C3H8+O=IC3H7+OH 5.49E5 2.5 3.14E3
!\AUTHOR: !\REF: Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by OH. 3. Propane, J. Phys. Chem., 90, 1949?954 !\COMMENT:
C3H8+OH=IC3H7+H2O 4.67E7 1.61 -3.5E1
!\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054. !\COMMENT:
C3H8+HO2=IC3H7+H2O2 6.32E1 3.37 1.372E4
!\AUTHOR: !\REF:FIT TO NIST DATABASE !\COMMENT:
C3H8+CH3=IC3H7+CH4 6.4E4 2.17 7.52E3
!\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE PUBLISHED. !\COMMENT: WARNING

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C3H8+C2H3=IC3H7+C2H4        1.0E11 0.0 1.04E4
!\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE PUBLISHED. !\COMMENT: WARNING
C3H8+C2H5=IC3H7+C2H6        1.0E11 0.0 1.04E4
!\AUTHOR: !\REF:DAGAUT ET AL., CST 71, 111(1990) !\COMMENT:
C3H8+C3H5-A=IC3H7+C3H6        7.94E11 0.0 1.62E4
!\AUTHOR: !\REF:DRYER ESTIMATE !\COMMENT:
C3H8+CH3O=IC3H7+CH3OH        3.0E11 0.0 7.0E3
!\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054. !\COMMENT: SCALED AS PER CARSTENSEN ET AL
C3H8+CH3O2=IC3H7+CH3O2H        1.019E1 3.58 1.481E4
!\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054. !\COMMENT: SCALED AS PER CARSTENSEN ET AL
C3H8+C2H5O2=IC3H7+C2H5O2H        1.019E1 3.58 1.481E4
!\AUTHOR: !\REF:ANALOGY TO C2H6+HO2 !\COMMENT:
C3H8+O2CHO=IC3H7+HO2CHO        1.475E4 2.6 1.391E4
!!
!\REACTIONCLASS:    \R_R_RECOMBIN                                    \A                    \N
\EA
!!
!\AUTHOR: !\REF:GLAUDE,P.A. ET AL,PROC. COMBUST. INST !\COMMENT:
IC3H7+H=C2H5+CH3        2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
IC3H7+OH=C3H6+H2O        2.41E13 0.0 0.0E0
!\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
IC3H7+O=CH3CHO+CH3        4.818E13 0.0 0.0E0
!\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE
IC3H7+HO2=IC3H7O+OH        7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE
IC3H7+CH3O2=IC3H7O+CH3O        7.0E12 0.0 -1.0E3
CH3+CH3CHO=IC3H7O        1.0E11 0.0 9.256E3
!\AUTHOR: !\COMMENT: !0512 ADD KWZ
IC3H7+O2=IC3H7O2        1.0E11 0.0 0.0E0
      PLOG/1.0E-2 7.33E5 1.33E0 -6.34564E3/
      PLOG/1.0E-1 2.24E11 -1.05E-1 -3.69787E3/
      PLOG/1.0E0 1.54E18 -2.02E0 -4.98567E2/
      PLOG/1.0E1 6.74E27 -4.85E0 3.77982E3/
      PLOG/1.0E2 1.67E29 -5.15E0 5.03645E3/
!!
IC3H7O2=C3H6+HO2        1.224E9 1.28 3.0E4
!!
!\REACTIONCLASS:    \RO2_R_PRODUCTS                                    \A                    \N
\EA
!!
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2        1.4E16 -1.61 1.86E3
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!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2 1.4E16 -1.61 1.86E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
2IC3H7O2=>O2+2IC3H7O 1.4E16 -1.61 1.86E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+CH3=IC3H7O+CH3O 7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+C2H5=IC3H7O+C2H5O 7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+IC3H7=2IC3H7O 7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+C3H5-A=IC3H7O+C3H5O 7.0E12 0.0 -1.0E3
C2H3+CH3(+M)=C3H6(+M) 2.5E13 0.0 0.0E0
LOW/4.27E58 -1.194E1 9.7698E3/
TROE/1.75E-1 1.341E3 6.0E4 1.014E4/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C2H3+CH3=C3H5-A+H 4.12E29 -4.95 8.0E3
DUP
PLOG/1.0E-2 4.12E29 -4.95E0 8.0E3/
PLOG/1.0E-1 4.86E30 -5.03E0 1.13E4/
PLOG/1.0E0 5.3E29 -4.57E0 1.44E4/
PLOG/1.0E1 1.32E30 -4.54E0 1.93E4/
PLOG/1.0E2 5.16E28 -4.03E0 2.38E4/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C2H3+CH3=C3H5-A+H 5.73E15 -0.77 1.1959E3
DUP
PLOG/1.0E-2 5.73E15 -7.7E-1 1.1959E3/
PLOG/1.0E-1 2.06E13 -7.4E-2 1.4287E3/
PLOG/1.0E0 4.48E10 6.0E-1 1.4216E3/
PLOG/1.0E1 4.1E6 1.71E0 1.0569E3/
PLOG/1.0E2 1.37E-1 3.91E0 -3.5355E2/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6=C2H3+CH3 1.88E78 -18.7 1.3E5
DUP
PLOG/1.0E-2 1.88E78 -1.87E1 1.3E5/
PLOG/1.0E-1 8.73E76 -1.79E1 1.32E5/
PLOG/1.0E0 5.8E75 -1.72E1 1.34E5/
PLOG/1.0E1 8.12E71 -1.58E1 1.36E5/
PLOG/1.0E2 2.15E64 -1.34E1 1.35E5/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6=C2H3+CH3 1.69E59 -13.6 1.1329E5
DUP

PLOG/1.0E-2 1.69E59 -1.36E1 1.1329E5/
PLOG/1.0E-1 2.0E60 -1.37E1 1.1489E5/
PLOG/1.0E0 6.7E54 -1.18E1 1.1384E5/
PLOG/1.0E1 1.06E47 -9.27E0 1.1151E5/
PLOG/1.0E2 7.29E38 -6.7E0 1.0874E5/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6=C3H5-A+H 9.16E74 -17.6 1.2E5
DUP
PLOG/1.0E-2 9.16E74 -1.76E1 1.2E5/
PLOG/1.0E-1 1.73E70 -1.6E1 1.2E5/
PLOG/1.0E0 1.08E71 -1.59E1 1.2486E5/
PLOG/1.0E1 6.4E65 -1.42E1 1.25E5/
PLOG/1.0E2 8.05E56 -1.15E1 1.22E5/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6=C3H5-A+H 2.98E54 -12.3 1.012E5
DUP
PLOG/1.0E-2 2.98E54 -1.23E1 1.012E5/
PLOG/1.0E-1 1.37E43 -8.87E0 9.6365E4/
PLOG/1.0E0 6.28E42 -8.51E0 9.8004E4/
PLOG/1.0E1 4.73E35 -6.26E0 9.5644E4/
PLOG/1.0E2 4.34E28 -4.06E0 9.3114E4/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H5-T+H=C3H6 4.96E60 -15.2 1.8E4
DUP
PLOG/1.0E-2 4.96E60 -1.52E1 1.8E4/
PLOG/1.0E-1 3.2E62 -1.51E1 2.01E4/
PLOG/1.0E0 2.31E60 -1.4E1 2.19E4/
PLOG/1.0E1 3.69E54 -1.2E1 2.21E4/
PLOG/1.0E2 1.15E50 -1.04E1 2.33E4/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H5-T+H=C3H6 1.49E48 -12.0 7.2033E3
DUP
PLOG/1.0E-2 1.49E48 -1.2E1 7.2033E3/
PLOG/1.0E-1 6.76E46 -1.11E1 7.6299E3/
PLOG/1.0E0 1.09E40 -8.66E0 6.4478E3/
PLOG/1.0E1 2.38E31 -5.73E0 4.506E3/
PLOG/1.0E2 5.69E25 -3.83E0 3.2504E3/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H5-T+H=C3H5-A+H 2.11E17 -1.08 1.29E3
DUP
PLOG/1.0E-2 2.11E17 -1.08E0 1.29E3/

PLOG/1.0E-1 9.05E29 -4.91E0 8.54E3/
PLOG/1.0E0 2.98E30 -4.79E0 1.2E4/
PLOG/1.0E1 8.22E28 -4.14E0 1.54E4/
PLOG/1.0E2 2.28E29 -4.12E0 2.09E4/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H5-T+H=C3H5-A+H 6.41E3 2.61 -3.7784E3
DUP
PLOG/1.0E-2 6.41E3 2.61E0 -3.7784E3/
PLOG/1.0E-1 5.19E14 -3.0E-1 1.0904E3/
PLOG/1.0E0 8.17E11 4.9E-1 1.1846E3/
PLOG/1.0E1 2.79E9 1.09E0 1.1875E3/
PLOG/1.0E2 6.75E3 2.7E0 3.738E2/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H5-T+H=C2H3+CH3 3.31E16 -0.69 5.2E3
DUP
PLOG/1.0E-2 3.31E16 -6.9E-1 5.2E3/
PLOG/1.0E-1 9.04E16 -8.1E-1 4.8E3/
PLOG/1.0E0 2.01E24 -2.86E0 1.09E4/
PLOG/1.0E1 2.75E26 -3.31E0 1.58E4/
PLOG/1.0E2 3.15E32 -4.83E0 2.6E4/
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H5-T+H=C2H3+CH3 8.04E13 -0.14 1.15E3
DUP
PLOG/1.0E-2 8.04E13 -1.4E-1 1.15E3/
PLOG/1.0E-1 7.17E10 6.7E-1 6.738E2/
PLOG/1.0E0 9.97E8 1.36E0 1.5964E3/
PLOG/1.0E1 7.41E7 1.57E0 2.1088E3/
PLOG/1.0E2 2.7E12 3.2E-1 6.7918E3/
!\AUTHOR: !\REF: !\COMMENT:
C3H6=C3H5-S+H 7.71E69 -16.09 1.4E5
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6+H=C3H5-A+H2 3.644E5 2.455 4.3612E3
!\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE !\COMMENT:
C3H6+O2=C3H5-A+HO2 5.96E19 -1.67 4.61921E4
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: HAS CAVALOTTI RELEASED UPDATED RATE CONSTANTS FOR THIS?
C3H6+O=C3H5-A+OH 5.24E11 0.7 5.884E3

!\AUTHOR: !\REF: WARNING: NO REFERENCE !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?
C3H6+OH=C3H5-A+H2O 4.46E6 2.072 1.0508E3
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6+HO2=C3H5-A+H2O2 3.07E-2 4.403 1.35472E4
!\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
C3H6+CH3=C3H5-A+CH4 2.21E0 3.5 5.675E3
!\AUTHOR: !\REF: BILL !\COMMENT: !\REF: REDUCED EA BY DIFFERENCE BETWEEN BD FOR SECONDARY ALKYL AND PRIMARY ALL
C3H6+CH3O=C3H5-A+CH3OH 8.4E10 0.0 2.6E3
!\AUTHOR: !\REF: ANALOGY TO C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM
C3H6+CH3O2=C3H5-A+CH3O2H 7.68E-2 4.403 1.35472E4
!\AUTHOR: !\REF: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980) !\COMMENT:
C3H6+C2H5=C3H5-A+C2H6 1.0E11 0.0 9.8E3
!\AUTHOR: !\REF: ANALOGY TO C3H6+HO2 !\COMMENT:
C3H6+C2H5O2=C3H5-A+C2H5O2H 7.68E-2 4.403 1.35472E4
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6+H=C3H5-T+H2 1.498E2 3.381 8.9095E3
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT:
C3H6+O=C3H5-T+OH 6.03E10 0.7 7.632E3
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?
C3H6+OH=C3H5-T+H2O 1.8E6 1.979 2.2352E3
!\AUTHOR: !\REF: C3 NUIG CALCULATION J.M !\COMMENT: WARNING: RESULTS ARE NOW PUBLISHED, UPDATED REFERENCE
C3H6+HO2=C3H5-T+H2O2 1.56E4 2.82 2.44279E4
!\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE !\COMMENT: WARNING: HOW WAS THIS ESTIMATED?
C3H6+O2=C3H5-T+HO2 1.0E13 0.0 5.877E4
!\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
C3H6+CH3=C3H5-T+CH4 8.4E-1 3.5 1.166E4
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6+H=C3H5-S+H2 5.101E2 3.234 1.2357E4
DUP
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
C3H6+H=C3H5-S+H2 3.969E2 3.252 1.2007E4
DUP
!\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE !\COMMENT:
C3H6+O2=C3H5-S+HO2 2.0E13 0.0 6.227E4
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT:

C3H6+O=C3H5-S+OH 1.2E11 0.7 8.9591E3
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?
C3H6+OH=C3H5-S+H2O 1.86E5 2.369 2.502E3
!\AUTHOR: !\REF: C3 NUIG CALCULATION J.M !\COMMENT: WARNING: RESULTS ARE NOW PUBLISHED, UPDATED REFERENCE
C3H6+HO2=C3H5-S+H2O2 9.57E2 3.059 2.07986E4
!\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
C3H6+CH3=C3H5-S+CH4 1.348E0 3.5 1.285E4
!!
!\REACTIONCLASS: \R_ADDITION\O \A \N \EA
!!
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: THE PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.
C3H6+O=C2H5+HCO 7.45E6 1.88 1.83E2
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: THE PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.
C3H6+O=>CH2CO+CH3+H 3.05E6 1.88 1.83E2
!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
C3H6+H=C2H4+CH3 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.54E9 1.35E0 2.542E3/
PLOG/4.0E-2 7.88E10 8.7E-1 3.5996E3/
PLOG/1.0E0 2.67E12 4.7E-1 5.4311E3/
PLOG/1.0E1 9.25E22 -2.6E0 1.2898E4/
PLOG/1.0E2 1.32E23 -2.42E0 1.65E4/
!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
C3H6+H=C2H4+CH3 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.0E-10 0.0E0 0.0E0/
PLOG/4.0E-2 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E1 1.24E5 2.52E0 3.6791E3/
PLOG/1.0E2 2.51E3 2.91E0 3.9809E3/
!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
C3H6+H=IC3H7 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/

!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
C3H6+H=IC3H7 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/
PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
!\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907_C7.inp
C3H6+HO2=IC3H7+O2 8.87E22 -3.09 2.6586E4
PLOG/1.3E-2 1.02E7 1.16E0 1.0273E4/
PLOG/9.869E-1 1.31E20 -2.58E0 1.9078E4/
PLOG/9.87E0 4.14E28 -4.92E0 2.6212E4/
PLOG/9.869E1 8.87E22 -3.09E0 2.6586E4/
!!
!\REACTIONCLASS: \R_DECOMPOSITION \A \N \EA
!!
!! WARNING: PART OF PROPYNE/ALLENE+H PES SO HAS BEEN LOCATED THERE TO KEEP RATE CONSTANTS TOGETHER
!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:KLIPPENSTEIN _ HARDING 2007 !\COMMENT:
C3H5-A+H=C3H4-A+H2 1.232E3 3.035 2.582E3
!\AUTHOR: !\REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\COMMENT:
C3H5-A+OH=C3H4-A+H2O 6.0E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-A+CH3=C3H4-A+CH4 3.0E12 -0.32 -1.31E2
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H5-A+C2H5=C3H4-A+C2H6 4.0E11 0.0 0.0E0
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H5-A+C2H3=C3H4-A+C2H4 1.0E12 0.0 0.0E0
!\AUTHOR: !\REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005) !\COMMENT:
2C3H4-A=C3H5-A+C3H3 5.0E14 0.0 6.47467E4
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H5-S+H=C3H4-A+H2 3.333E12 0.0 0.0E0
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H5-S+CH3=C3H4-A+CH4 1.0E11 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+H=C3H4-P+H2 3.34E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+CH3=C3H4-P+CH4 1.0E11 0.0 0.0E0

!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+H=C3H4-P+H2 3.34E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+CH3=C3H4-P+CH4 1.0E11 0.0 0.0E0
!!
!\REACTIONCLASS: \R_R_RECOMB \A \N
\EA
!!
!\AUTHOR: !\REF: FRIDLYAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776 !\COMMENT:
2C3H5-A=C3H4-A+C3H6 9.55E40 -9.3 1.247E4
PLOG/1.0E0 4.77E40 -9.3E0 1.247E4/
PLOG/4.0E0 3.97E32 -6.8E0 9.18E3/
PLOG/1.0E1 1.46E28 -5.5E0 7.41E3/
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H5-A+C2H5=C2H4+C3H6 4.0E11 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-A+HCO=C3H6+CO 6.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+HCO=C3H6+CO 9.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+HCO=C3H6+CO 9.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+O=C2H4+HCO 6.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+OH=>C2H4+HCO+H 5.0E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+HO2=>C2H4+HCO+OH 2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+O=CH3+CH2CO 6.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+OH=>CH3+CH2CO+H 5.0E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+HO2=>CH3+CH2CO+OH 2.0E13 0.0 0.0E0
!!
!\REACTIONCLASS: \R+O \A \N
\EA
!!
!\AUTHOR: !\REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\COMMENT:
C3H5-A+O=C2H3CHO+H 6.0E13 0.0 0.0E0
!!
!\REACTIONCLASS: \R+OH \A \N
\EA
!!
!\AUTHOR: !\REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\COMMENT:
C3H5-A+OH=>C2H3CHO+2H 5.3E37 -6.71 2.9306E4
PLOG/1.0E-1 5.3E37 -6.71E0 2.9306E4/

PLOG/1.0E0 4.2E32 -5.16E0 3.0126E4/
PLOG/1.0E1 1.6E20 -1.56E0 2.633E4/
!!
!\REACTIONCLASS: \R+O2 \A \N
\EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT: !\AUTHOR: !\REF:!\WANG, J. PHYS. CHEM. REF. DATA 20,
C3H5-A+O2=C3H4-A+HO2 4.99E15 -1.4 2.2428E4
PLOG/1.0E0 4.99E15 -1.4E0 2.2428E4/
PLOG/1.0E1 2.18E21 -2.85E0 3.0755E4/
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT: !\AUTHOR: !\REF:!\WANG, J. PHYS. CHEM. REF. DATA 20,
C3H5-A+O2=CH3CO+CH2O 1.19E15 -1.01 2.0128E4
PLOG/1.0E0 1.19E15 -1.01E0 2.0128E4/
PLOG/1.0E1 7.14E15 -1.21E0 2.1046E4/
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT: !\AUTHOR: !\REF:!\WANG, J. PHYS. CHEM. REF. DATA 20,
C3H5-A+O2=C2H3CHO+OH 1.82E13 -0.41 2.2859E4
PLOG/1.0E0 1.82E13 -4.1E-1 2.2859E4/
PLOG/1.0E1 2.47E13 -4.5E-1 2.3017E4/
!\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:
C3H5-S+O2=CH3CHO+HCO 3.1E31 -5.944 5.7484E3
!\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:
C3H5-S+O2=C2H3CHO+OH 2.7E19 -2.14 5.1429E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+O2=CH3COCH2+O 9.86E25 -3.751 1.12554E4
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+O2=CH3CO+CH2O 2.55E20 -2.608 1.5657E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+O2=C3H4-A+HO2 3.59E10 -0.27 -4.136E2
!!
!\REACTIONCLASS: \R_HO2 \A \N
\EA
!!
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346 \COMMENT:
C3H5-A+HO2=C3H5O+OH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.02E13 -1.58E-1 -1.417E3/
PLOG/1.0E-1 4.98E14 -6.42E-1 -3.491E2/
PLOG/1.0E0 7.77E17 -1.52E0 2.3792E3/
PLOG/1.0E1 2.93E15 -6.84E-1 3.6153E3/
PLOG/1.0E2 1.64E4 2.74E0 1.1444E3/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346 \COMMENT:
C3H5-A+HO2=AC3H5OOH 1.0E11 0.0 0.0E0

PLOG/1.0E-2 1.91E31 -7.23E0 1.3362E3/
PLOG/1.0E-1 6.31E42 -1.03E1 5.5689E3/
PLOG/1.0E0 1.03E45 -1.06E1 7.8515E3/
PLOG/1.0E1 2.79E37 -7.92E0 6.4979E3/
PLOG/1.0E2 1.44E32 -6.01E0 6.0536E3/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346
\COMMENT:
C3H5-A+HO2=C2H3CHO+H2O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.09E0 3.01E0 -3.4211E3/
PLOG/1.0E-1 6.35E1 2.5E0 -2.3414E3/
PLOG/1.0E0 6.05E5 1.39E0 5.951E2/
PLOG/1.0E1 3.1E5 1.59E0 2.6776E3/
PLOG/1.0E2 5.07E-5 4.59E0 9.275E2/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346
\COMMENT:
AC3H5OOH=C2H3CHO+H2O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.99E50 -1.27E1 5.35319E4/
PLOG/1.0E-1 4.72E47 -1.15E1 5.43609E4/
PLOG/1.0E0 1.5E40 -8.84E0 5.31792E4/
PLOG/1.0E1 2.54E28 -5.0E0 4.99194E4/
PLOG/1.0E2 1.48E16 -1.12E0 4.59493E4/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346
\COMMENT:
AC3H5OOH=C3H5O+OH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.49E58 -1.39E1 5.42669E4/
PLOG/1.0E-1 1.8E54 -1.24E1 5.41938E4/
PLOG/1.0E0 3.36E46 -9.81E0 5.24685E4/
PLOG/1.0E1 2.39E36 -6.54E0 4.9429E4/
PLOG/1.0E2 1.28E27 -3.61E0 4.63331E4/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346
\COMMENT:
C3H5O=C2H3+CH2O 1.0E11 0.0 0.0E0
PLOG/1.0E-3 7.26E6 1.82E-1 1.78155E4/
PLOG/1.0E-2 6.97E16 -2.5E0 2.08787E4/
PLOG/1.0E-1 6.64E23 -4.23E0 2.3565E4/
PLOG/1.0E0 1.07E26 -4.56E0 2.46229E4/
PLOG/1.0E1 6.5E29 -5.37E0 2.6645E4/
PLOG/1.0E2 4.63E31 -5.59E0 2.89153E4/
PLOG/1.0E3 8.52E25 -3.61E0 2.78634E4/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346
\COMMENT:
C3H5O=C2H3CHO+H 1.0E11 0.0 0.0E0
PLOG/1.0E-3 3.0E15 -2.31E0 1.46679E4/
PLOG/1.0E-2 1.5E22 -3.96E0 1.8283E4/
PLOG/1.0E-1 1.95E23 -3.99E0 1.91433E4/
PLOG/1.0E0 1.15E25 -4.24E0 2.03112E4/

PLOG/1.0E1 1.76E28 -4.89E0 2.27652E4/
PLOG/1.0E2 1.41E27 -4.28E0 2.37706E4/
PLOG/1.0E3 2.57E20 -2.06E0 2.20401E4/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346 \COMMENT:
C3H5O=C2H4+HCO 1.0E11 0.0 0.0E0
PLOG/1.0E-3 6.62E16 -2.84E0 1.3197E4/
PLOG/1.0E-2 1.26E20 -3.53E0 1.54692E4/
PLOG/1.0E-1 2.13E21 -3.64E0 1.65845E4/
PLOG/1.0E0 1.07E24 -4.16E0 1.8985E4/
PLOG/1.0E1 8.42E25 -4.4E0 2.23826E4/
PLOG/1.0E2 1.86E21 -2.73E0 2.36588E4/
PLOG/1.0E3 4.75E8 1.14E0 2.09225E4/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346 \COMMENT:
C2H3+CH2O=C2H3CHO+H 1.0E11 0.0 0.0E0
PLOG/1.0E-3 2.6E4 2.26E0 1.5103E3/
PLOG/1.0E-2 5.13E4 2.17E0 1.6755E3/
PLOG/1.0E-1 3.99E5 1.91E0 2.2183E3/
PLOG/1.0E0 1.75E7 1.45E0 3.428E3/
PLOG/1.0E1 1.35E9 9.33E-1 5.173E3/
PLOG/1.0E2 2.24E11 3.57E-1 8.0013E3/
PLOG/1.0E3 6.01E5 2.09E0 7.8956E3/
!\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346 \COMMENT:
C2H3+CH2O=C2H4+HCO 1.0E11 0.0 0.0E0
PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
!!
!\REACTIONCLASS: \R+CH3O2 \A \N \EA
!!
!\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2 !\COMMENT:
C3H5-A+CH3O2=C3H5O+CH3O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.33E12 -1.58E-1 -1.417E3/
PLOG/1.0E-1 1.66E14 -6.42E-1 -3.491E2/
PLOG/1.0E0 2.595E17 -1.52E0 2.3792E3/
PLOG/1.0E1 9.78E14 -6.84E-1 3.6153E3/
PLOG/1.0E2 5.47E3 2.74E0 1.1444E3/
!\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040?1053 !\COMMENT:
C3H6+OH=CH3CHO+CH3 6.93E5 1.49 -5.36E2

PLOG/1.3E-3 6.93E5 1.49E0 -5.36E2/
PLOG/1.0E-2 5.94E3 2.01E0 -5.6E2/
PLOG/1.3E-2 1.1E3 2.22E0 -6.8E2/
PLOG/2.5E-2 1.07E2 2.5E0 -7.59E2/
PLOG/1.0E-1 7.83E-1 3.1E0 -9.19E2/
PLOG/1.315E-1 3.07E-1 3.22E0 -9.46E2/
PLOG/1.0E0 3.16E-4 4.05E0 -1.144E3/
PLOG/1.0E1 7.59E-6 4.49E0 -6.8E2/
PLOG/1.0E2 5.45E-5 4.22E0 1.141E3/
!\AUTHOR: !\REF:ACETALDEHYDE ANALOG !\COMMENT:
C3H5O+O2=C2H3CHO+HO2 1.0E12 0.0 6.0E3
C2H+CH3=C3H4-P 8.0E13 0.0 0.0E0
!\AUTHOR: !\REF: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907_C7.INP
C3H4-A=C3H4-P 4.786E48 -10.0 8.8685E4
PLOG/1.0E0 7.762E39 -7.8E0 7.8446E4/
PLOG/1.0E1 4.786E48 -1.0E1 8.8685E4/
!\AUTHOR: !\REF: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907_C7.INP
C3H4-P=C3H3+H 6.48E30 -4.655 9.39252E4
PLOG/1.0E0 6.48E30 -4.655E0 9.39252E4/
PLOG/1.0E1 1.21E25 -2.787E0 9.23761E4/
!\AUTHOR: !\REF: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907_C7.INP
C3H4-A=C3H3+H 1.32E31 -4.749 9.20795E4
PLOG/1.0E0 1.32E31 -4.749E0 9.20795E4/
PLOG/1.0E1 3.65E25 -2.95E0 9.06249E4/
!!
!\REACTIONCLASS: \R_CAT_ISO \A \N \EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-P+C3H3=C3H4-A+C3H3 6.14E6 1.74 1.045E4
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907_C7.INP
C3H4-P+O2=C3H3+HO2 3.0E13 0.0 4.263E4
!\AUTHOR: !\REF:GLAUDE,P.A. ET AL,PROC. COMBUST. INST !\COMMENT:
C3H4-P+O=C3H3+OH 7.65E8 1.5 8.6E3
!\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S !\COMMENT:
C3H4-P+H=C3H3+H2 3.572E4 2.825 4.821E3
!\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S !\COMMENT:
C3H4-P+OH=C3H3+H2O 4.94E6 2.027 1.0596E3

!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-P+HO2=C3H3+H2O2 9.55E-2 4.17 9.6328E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-P+CH3=C3H3+CH4 1.8E12 0.0 7.7E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-P+CH3O2=C3H3+CH3O2H 9.55E-2 4.17 9.6328E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-P+C2H=C2H2+C3H3 1.0E13 0.0 0.0E0
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-P+C2H3=C3H3+C2H4 1.0E12 0.0 7.7E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-P+C3H5-A=C3H3+C3H6 3.0E12 0.0 7.7E3
!\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:
C3H4-A+H=C3H3+H2 6.625E3 3.095 5.522E3
!\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:
C3H4-A+O2=C3H3+HO2 4.0E13 0.0 4.132E4
!\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S !\COMMENT:
C3H4-A+OH=C3H3+H2O 1.482E5 2.492 1.8072E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-A+CH3=C3H3+CH4 1.3E12 0.0 7.7E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-A+HO2=C3H3+H2O2 3.58E-2 4.17 9.6328E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-A+CH3O2=C3H3+CH3O2H 7.161E-2 4.17 9.6328E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-A+C3H5-A=C3H3+C3H6 2.0E11 0.0 7.7E3
!!
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT:
C3H4-A+H=C3H4-P+H 2.44E10 1.04 2.159E3
DUP
PLOG/1.0E-3 8.49E10 8.9E-1 2.503E3/
PLOG/3.9E-2 1.48E13 2.6E-1 4.103E3/
PLOG/1.0E0 2.48E15 -3.3E-1 6.436E3/
PLOG/1.0E1 2.35E25 -3.23E0 1.3165E4/
PLOG/1.0E2 1.02E24 -2.67E0 1.5552E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING:
UNSURE IF CORRECT REFERENCE
C3H4-A+H=C3H4-P+H 2.44E10 1.04 2.159E3
DUP
PLOG/1.0E-3 1.0E-10 0.0E0 0.0E0/
PLOG/3.9E-2 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E0 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E1 1.79E7 1.98E0 4.521E3/
PLOG/1.0E2 4.63E4 2.62E0 4.466E3/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING:
UNSURE IF CORRECT REFERENCE

C3H4-A+H=C3H5-A 2.21E61 -15.25 2.0076E4
DUP
PLOG/1.0E-3 2.21E61 -1.525E1 2.0076E4/
PLOG/3.9E-2 1.24E52 -1.202E1 1.7839E4/
PLOG/1.0E0 4.67E51 -1.145E1 2.134E4/
PLOG/1.0E1 3.75E48 -1.027E1 2.2511E4/
PLOG/1.0E2 4.23E43 -8.61E0 2.2522E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE
C3H4-A+H=C3H5-A 2.21E61 -15.25 2.0076E4
DUP
PLOG/1.0E-3 2.8E38 -8.67E0 8.035E3/
PLOG/3.9E-2 9.33E36 -8.19E0 7.462E3/
PLOG/1.0E0 3.32E30 -5.78E0 6.913E3/
PLOG/1.0E1 2.29E26 -4.32E0 6.163E3/
PLOG/1.0E2 4.38E21 -2.71E0 5.187E3/
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT:
C3H4-A+H=C3H5-S 1.1E30 -6.52 1.52E4
PLOG/1.0E-1 1.1E30 -6.52E0 1.52E4/
PLOG/1.0E0 5.4E29 -6.09E0 1.63E4/
PLOG/1.0E1 2.6E31 -6.23E0 1.87E4/
PLOG/1.0E2 3.2E31 -5.88E0 2.15E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE
C3H4-A+H=C3H5-T 6.44E102 -27.51 5.1768E4
DUP
PLOG/1.0E-3 6.44E102 -2.751E1 5.1768E4/
PLOG/3.9E-2 1.55E53 -1.31E1 1.4472E4/
PLOG/1.0E0 1.9E53 -1.259E1 1.6726E4/
PLOG/1.0E1 7.95E51 -1.182E1 1.8286E4/
PLOG/1.0E2 4.21E52 -1.164E1 2.2262E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-A+H=C3H5-T 6.44E102 -27.51 5.1768E4
DUP
PLOG/1.0E-3 1.1E54 -1.429E1 1.0809E4/
PLOG/3.9E-2 9.88E44 -1.121E1 8.212E3/
PLOG/1.0E0 2.81E40 -9.42E0 7.85E3/
PLOG/1.0E1 2.6E35 -7.57E0 7.147E3/
PLOG/1.0E2 9.88E29 -5.53E0 6.581E3/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-A+H=CH3+C2H2 3.74E1 3.35 5.78E1
DUP
PLOG/1.0E-3 1.23E8 1.53E0 4.737E3/
PLOG/3.9E-2 2.72E9 1.2E0 6.834E3/

PLOG/1.0E0 1.26E20 -1.83E0 1.5003E4/
PLOG/1.0E1 1.68E16 -6.0E-1 1.4754E4/
PLOG/1.0E2 1.37E17 -7.9E-1 1.7603E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-A+H=CH3+C2H2 3.74E1 3.35 5.78E1
DUP
PLOG/1.0E-3 1.0E-10 0.0E0 0.0E0/
PLOG/3.9E-2 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E0 1.23E4 2.68E0 6.335E3/
PLOG/1.0E1 3.31E8 1.14E0 8.886E3/
PLOG/1.0E2 1.28E6 1.71E0 9.774E3/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-P+H=C3H5-T 8.85E51 -13.04 1.2325E4
DUP
PLOG/1.0E-3 8.85E51 -1.304E1 1.2325E4/
PLOG/3.9E-2 3.17E52 -1.269E1 1.4226E4/
PLOG/1.0E0 2.87E53 -1.251E1 1.6853E4/
PLOG/1.0E1 9.51E51 -1.174E1 1.8331E4/
PLOG/1.0E2 4.51E52 -1.158E1 2.2207E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-P+H=C3H5-T 8.85E51 -13.04 1.2325E4
DUP
PLOG/1.0E-3 1.97E46 -1.191E1 7.456E3/
PLOG/3.9E-2 2.59E45 -1.123E1 8.046E3/
PLOG/1.0E0 6.93E39 -9.11E0 7.458E3/
PLOG/1.0E1 6.8E34 -7.29E0 6.722E3/
PLOG/1.0E2 5.65E29 -5.39E0 6.15E3/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-P+H=C3H5-S 3.38E49 -12.75 1.4072E4
DUP
PLOG/1.0E-3 1.0E-10 0.0E0 0.0E0/
PLOG/3.9E-2 3.38E49 -1.275E1 1.4072E4/
PLOG/1.0E0 1.37E51 -1.255E1 1.5428E4/
PLOG/1.0E1 3.88E50 -1.19E1 1.6915E4/
PLOG/1.0E2 2.17E49 -1.11E1 1.8746E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-P+H=C3H5-S 3.38E49 -12.75 1.4072E4
DUP
PLOG/1.0E-3 1.49E38 -1.011E1 7.458E3/
PLOG/3.9E-2 2.98E43 -1.143E1 8.736E3/
PLOG/1.0E0 5.75E39 -9.51E0 8.772E3/

PLOG/1.0E1 4.33E40 -9.6E0 9.401E3/
PLOG/1.0E2 3.44E34 -7.36E0 8.558E3/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO.
C3H4-P+H=CH3+C2H2 2.12E10 1.06 3.945E3
PLOG/1.0E-3 2.44E10 1.04E0 3.98E3/
PLOG/3.9E-2 3.89E10 9.89E-1 4.114E3/
PLOG/1.0E0 3.46E12 4.42E-1 5.463E3/
PLOG/1.0E1 1.72E14 -1.0E-2 7.134E3/
PLOG/1.0E2 1.9E15 -2.9E-1 8.306E3/
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT:
C3H4-P+H=C3H5-A 1.1E60 -14.56 2.81E4
PLOG/1.0E-1 1.1E60 -1.456E1 2.81E4/
PLOG/1.0E0 4.91E60 -1.437E1 3.1644E4/
PLOG/2.0E0 3.04E60 -1.419E1 3.2642E4/
PLOG/5.0E0 9.02E59 -1.389E1 3.3953E4/
PLOG/1.0E1 2.2E59 -1.361E1 3.49E4/
PLOG/1.0E2 1.6E55 -1.207E1 3.75E4/
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:
C3H5-A=C3H5-T 3.9E59 -15.42 7.54E4
PLOG/1.0E-1 3.9E59 -1.542E1 7.54E4/
PLOG/1.0E0 7.06E56 -1.408E1 7.5868E4/
PLOG/2.0E0 4.8E55 -1.359E1 7.5949E4/
PLOG/5.0E0 4.86E53 -1.281E1 7.5883E4/
PLOG/1.0E1 6.4E51 -1.212E1 7.57E4/
PLOG/1.0E2 2.8E43 -9.27E0 7.4E4/
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:
C3H5-A=C3H5-S 1.3E55 -14.53 7.38E4
PLOG/1.0E-1 1.3E55 -1.453E1 7.38E4/
PLOG/1.0E0 5.0E51 -1.302E1 7.33E4/
PLOG/1.0E1 9.7E48 -1.173E1 7.37E4/
PLOG/1.0E2 4.86E44 -9.84E0 7.34E4/
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:
C2H2+CH3=C3H5-T 6.8E20 -4.16 1.8E4
PLOG/1.0E-1 6.8E20 -4.16E0 1.8E4/
PLOG/1.0E0 4.99E22 -4.39E0 1.885E4/
PLOG/2.0E0 6.0E23 -4.6E0 1.9571E4/
PLOG/5.0E0 7.31E25 -5.06E0 2.115E4/
PLOG/1.0E1 9.3E27 -5.55E0 2.29E4/
PLOG/1.0E2 3.8E36 -7.58E0 3.13E4/
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:
C3H5-T=C3H5-S 1.6E44 -12.16 5.22E4
PLOG/1.0E-1 1.6E44 -1.216E1 5.22E4/
PLOG/1.0E0 1.5E48 -1.271E1 5.39E4/
PLOG/1.0E1 5.1E52 -1.337E1 5.72E4/
PLOG/1.0E2 5.8E51 -1.243E1 5.92E4/

!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:
C2H2+CH3=C3H5-A 8.2E53 -13.32 3.32E4
PLOG/1.0E-1 8.2E53 -1.332E1 3.32E4/
PLOG/1.0E0 2.68E53 -1.282E1 3.573E4/
PLOG/2.0E0 3.64E52 -1.246E1 3.6127E4/
PLOG/5.0E0 1.04E51 -1.189E1 3.6476E4/
PLOG/1.0E1 4.4E49 -1.14E1 3.67E4/
PLOG/1.0E2 3.8E44 -9.63E0 3.76E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING:
UNSURE IF CORRECT REFERENCE BASED ON INFO.
CH3+C2H2=C3H5-S 1.78E42 -10.4 1.3647E4
DUP
PLOG/1.0E-3 1.78E42 -1.04E1 1.3647E4/
PLOG/3.9E-2 1.52E44 -1.073E1 1.5256E4/
PLOG/1.0E0 1.19E44 -1.019E1 1.8728E4/
PLOG/1.0E1 6.02E43 -9.74E0 2.0561E4/
PLOG/1.0E2 1.42E42 -8.91E0 2.2235E4/
!\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429?438 !\COMMENT: WARNING:
UNSURE IF CORRECT REFERENCE BASED ON INFO.
CH3+C2H2=C3H5-S 1.78E42 -10.4 1.3647E4
DUP
PLOG/1.0E-3 1.0E-10 0.0E0 0.0E0/
PLOG/3.9E-2 1.0E-10 0.0E0 0.0E0/
PLOG/1.0E0 8.49E35 -8.43E0 1.2356E4/
PLOG/1.0E1 3.04E32 -7.01E0 1.2357E4/
PLOG/1.0E2 1.69E27 -5.07E0 1.169E4/
!!
!\REACTIONCLASS: \R_ADDITION\O \A \N
\EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-P+O=HCCO+CH3 7.3E12 0.0 2.25E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-P+O=C2H4+CO 1.0E13 0.0 2.25E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-P+O=C2H3+HCO 3.2E12 0.0 2.01E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-A+O=C2H4+CO 2.0E7 1.8 1.0E3
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-A+O=C2H2+CH2O 3.0E-3 4.61 -4.243E3
!!
!\REACTIONCLASS: \R_ADDITION\HO2 \A \N
\EA
!!
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-P+HO2=>C2H4+CO+OH 3.0E12 0.0 1.9E4

!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-A+HO2=>C2H4+CO+OH 1.0E11 0.0 1.4E4
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
C3H4-A+HO2=>CH2CO+CH2+OH 4.0E12 0.0 1.9E4
!!
!\REACTIONCLASS: \R_ADDITION\CH2 \A \N \EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H4-A+C2H=C2H2+C3H3 1.0E13 0.0 0.0E0
C3H3+O=CH2O+C2H 2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H3+HO2=>OH+CO+C2H3 8.0E11 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H3+HCO=C3H4-A+CO 2.5E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H3+HCO=C3H4-P+CO 2.5E13 0.0 0.0E0
!\AUTHOR: !\REF:Tsang, W.; Hampson, R.F., J. Phys. Chem. Ref. Data 15, 1087 (1986) !\COMMENT:
C2H5+C2H=C3H3+CH3 1.81E13 0.0 0.0E0
!\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE
C3H3+O2=CH2CO+HCO 1.7E5 1.7 1.5E3
!!
!\REACTIONCLASS: \R+HO2 \A \N \EA
!!
!\AUTHOR: !\REF: ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS. CHEM. A, 2012, 116 (13), PP 3325?346 !\COMMENT:
C3H3+HO2=C3H3O+OH 1.0E11 0.0 0.0E0
PLOG/1.0E-2 1.02E13 -1.58E-1 -1.417E3/
PLOG/1.0E-1 4.98E14 -6.42E-1 -3.491E2/
PLOG/1.0E0 7.77E17 -1.52E0 2.3792E3/
PLOG/1.0E1 2.93E15 -6.84E-1 3.6153E3/
PLOG/1.0E2 1.64E4 2.74E0 1.1444E3/
!\AUTHOR: !\REF: !\COMMENT:
C2H+CH2O=C3H3O 1.0E11 0.0 0.0E0
PLOG/1.0E-3 5.925E-4 2.609E0 -4.2973E3/
PLOG/1.0E-2 5.688E6 -7.3E-2 -1.2341E3/
PLOG/1.0E-1 5.39E13 -1.803E0 1.4522E3/
PLOG/1.0E0 8.733E15 -2.074E0 2.5101E3/
PLOG/1.0E1 5.305E19 -2.943E0 4.5322E3/
PLOG/1.0E2 3.779E21 -3.163E0 6.8025E3/
!\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE
C3H3+OH=CH2O+C2H2 2.0E12 0.0 0.0E0

!\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE
C3H3+OH=C2H3+HCO 1.0E13 0.0 0.0E0
!\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE
C3H3+OH=C2H4+CO 1.0E13 0.0 0.0E0
!\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006 !\COMMENT:
CH2CO+CH3=CH3COCH2 1.76E4 2.48 6.13E3
C2H3+HCO=C2H3CHO 1.81E13 0.0 0.0E0
!\AUTHOR: !\REF:BASED ON CH3CHO+H !\COMMENT:
C2H3CHO+H=C2H3CO+H2 1.34E13 0.0 3.3E3
!\AUTHOR: !\REF:BASED ON CH3CHO+H !\COMMENT:
C2H3CHO+O=C2H3CO+OH 5.94E12 0.0 1.868E3
!\AUTHOR: !\REF:TAYLOR ET AL. 1996 !\COMMENT:
C2H3CHO+OH=C2H3CO+H2O 9.24E6 1.5 -9.62E2
!\AUTHOR: !\REF:TAYLOR ET AL. 1996 !\COMMENT:
C2H3CHO+O2=C2H3CO+HO2 1.005E13 0.0 4.07E4
!\AUTHOR: !\REF:BASED ON CH3CHO+HO2 !\COMMENT:
C2H3CHO+HO2=C2H3CO+H2O2 3.01E12 0.0 1.192E4
!\AUTHOR: !\REF:BASED ON CH3CHO+HO2 !\COMMENT:
C2H3CHO+CH3=C2H3CO+CH4 2.608E6 1.78 5.911E3
!\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE. !\COMMENT:
C2H3CHO+C2H3=C2H3CO+C2H4 1.74E12 0.0 8.44E3
!\AUTHOR: !\REF:ANALOGY WITH CH3CHO+CH3O !\COMMENT:
C2H3CHO+CH3O=C2H3CO+CH3OH 1.0E12 0.0 3.3E3
!\AUTHOR: !\REF:BASED ON CH3CHO+HO2 !\COMMENT:
C2H3CHO+CH3O2=C2H3CO+CH3O2H 3.01E12 0.0 1.192E4
C2H3+CO=C2H3CO 1.51E11 0.0 4.81E3
IC4H9=TC4H9 3.56E10 0.88 3.46E4
IC4H9=C3H6+CH3 1.0E0 1.0 1.0E0
PLOG/1.0E-1 3.15E41 -9.5E0 3.3486E4/
PLOG/1.0E0 6.75E44 -1.007E1 3.7209E4/
PLOG/1.0E1 7.79E44 -9.7E0 3.9751E4/
PLOG/1.0E2 3.61E39 -7.78E0 3.9583E4/
IC3H5CO=C3H5-T+CO 1.278E20 -1.89 3.446E4
TC4H9+O2=IC4H8+HO2 8.37E-1 3.59 1.196E4
!\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:
IC4H9+O2=IC4H8+HO2 1.07E0 3.71 9.322E3
!!
!\REACTIONCLASS: \R_O2_RO2 \A \N \EA
!!
!\AUTHOR: !\REF: F. GOLDSMITH JPCA, 2012 !\COMMENT:
IC4H9+O2=IC4H9O2 6.6946E13 -0.3 -1.872E2
!\AUTHOR: !\REF: F. GOLDSMITH JPCA, 2012 !\COMMENT:
TC4H9+O2=TC4H9O2 6.6946E13 -0.3 -1.872E2

!!
!\REACTIONCLASS: \RO2_ALKENE_HO2 \A \N
\EA
!!
!\AUTHOR: !\ ALL USE DEAN'S DATA FIRST TWO 2011, SECOND TWO 2013 !\COMMENT:
IC4H9O2=IC4H8+HO2 1.94E8 1.27 2.96E4
!!
!\REACTIONCLASS: \RO2_QOOH \A \N
\EA
!!
!\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701 !\COMMENT:
IC4H9O2=IC4H8O2H-I 9.82E7 1.3 2.15E4
!\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701 !\COMMENT:
IC4H9O2=IC4H8O2H-T 2.31E9 0.8 2.71E4
!\AUTHOR: !\REF:GREEN 2003 !\COMMENT:
IC4H8O2H-I=>OH+CH2O+C3H6 8.451E15 -0.68 2.917E4
IC4H8=IC4H7-I1+H 7.71E69 -16.09 1.4E5
IC4H8=C3H5-T+CH3 1.42E93 -22.79 1.33825E5
PLOG/1.0E-1 1.26E94 -2.299E1 1.34024E5/
PLOG/1.0E0 6.76E93 -2.251E1 1.37933E5/
PLOG/3.5E0 3.14E90 -2.137E1 1.37866E5/
PLOG/1.0E1 9.2E85 -1.994E1 1.36498E5/
PLOG/3.5E1 6.05E78 -1.776E1 1.33437E5/
PLOG/1.0E2 4.87E71 -1.565E1 1.29919E5/
IC4H8=IC4H7+H 4.66E92 -22.45 1.29059E5
PLOG/1.0E-1 7.51E95 -2.338E1 1.29214E5/
PLOG/1.0E0 3.59E88 -2.099E1 1.27813E5/
PLOG/3.5E0 2.96E82 -1.912E1 1.25456E5/
PLOG/1.0E1 2.13E76 -1.727E1 1.22629E5/
PLOG/3.5E1 1.13E68 -1.482E1 1.18416E5/
PLOG/1.0E2 4.73E60 -1.266E1 1.14404E5/
IC4H8+OH=IC4H7+H2O 4.3950169E4 2.67841 -8.27103E2
!AUTHOR: !REF: C ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY ! MULTIPLY BY 2 FROM THE CALCULATION
IC4H8+OH=IC4H7-I1+H2O 1.0930095E4 2.81477 1.1141999E3
!AUTHOR: !REF: YASUNAGA, PROC. COMBUST INST., 2009, 32, 453-460. INCREASED BY 40% AT 800-1000 K.
IC4H8+O2=IC4H7+HO2 3.12E13 0.0 3.745E4
!AUTHOR: !REF: C-J CHEN AND J. W. BOZZELLI J. PHYS. CHEM. A, 2000, 104, 9715-9732.
IC4H8+O2=IC4H7-I1+HO2 2.0E13 0.0 6.227E4
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=IC4H7+H2 7.29E5 2.455 4.3612E3
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=IC4H7-I1+H2 8.621E2 3.25 1.216698E4

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!AUTHOR: !REF: ANALOGY WITH C2H4
IC4H8+O=IC4H7+OH        1.05E12 0.7 5.884E3
!AUTHOR: !REF: ANALOGY WITH C2H4
IC4H8+O=IC4H7-I1+OH        1.2E11 0.7 8.9591E3
!AUTHOR: !REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
IC4H8+HO2=IC4H7+H2O2        2.92E-1 4.12 1.2802E4
!AUTHOR: !REF: C3 NUIG CALCULATION J.MENDES
IC4H8+HO2=IC4H7-I1+H2O2        9.7038941E4 2.54892 2.4733172E4
!AUTHOR: !REF: YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.
IC4H8+CH3=IC4H7+CH4        3.2E12 0.0 1.0E4
!AUTHOR: !REF: YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.
IC4H8+CH3=IC4H7-I1+CH4        2.0E12 0.0 1.5E4
!AUTHOR: !REF: ANALOGY TO C3H6+CH3O
IC4H8+CH3O=IC4H7+CH3OH        1.68E11 0.0 2.6E3
! AUTHOR: !REF:WESTBROOK AND PITZ ESTIMATE 1983
IC4H8+C3H5-A=IC4H7+C3H6        7.94E11 0.0 2.05E4
! AUTHOR: !REF:WESTBROOK AND PITZ ESTIMATE 1983
IC4H8+C3H5-S=IC4H7+C3H6        7.94E11 0.0 2.05E4
! AUTHOR: !REF:WESTBROOK AND PITZ ESTIMATE 1983
IC4H8+C3H5-T=IC4H7+C3H6        7.94E11 0.0 2.05E4
!AUTHOR: !REF:ANALOGY TO C3H6+CH3O2
IC4H8+CH3O2=IC4H7+CH3O2H        1.54E-1 4.403 1.35472E4
!AUTHOR: !REF:ANALOGY WITH RH+RO2 --) R+RO2H
IC4H8+O2CHO=IC4H7+HO2CHO        1.928E4 2.6 1.391E4
!!
!\REACTIONCLASS:    \RA_DECOMPOSITION                                    \A                    \N
\EA
!!
!\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT:
IC4H7=IC4H7-I1        1.3E55 -14.53 7.38E4
      PLOG/1.0E-1 1.3E55 -1.453E1 7.38E4/
      PLOG/1.0E0 5.0E51 -1.302E1 7.33E4/
      PLOG/1.0E1 9.7E48 -1.173E1 7.37E4/
      PLOG/1.0E2 4.86E44 -9.84E0 7.34E4/
!\AUTHOR: !\REF: C ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF
THEORY !\COMMENT:
C3H4-A+CH3=IC4H7        4.02097E4 2.5 8.8475E3
!!
!\REACTIONCLASS:    \RA_HO2_PRODUCTS                                    \A                    \N
\EA
!!
!AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP
3325-3346
IC4H7+HO2=IC4H7O+OH        1.0E11 0.0 0.0E0
      PLOG/1.0E-2 1.02E13 -1.58E-1 -1.417E3/
      PLOG/1.0E-1 4.98E14 -6.42E-1 -3.491E2/
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PLOG/1.0E0 7.77E17 -1.52E0 2.3792E3/
PLOG/1.0E1 2.93E15 -6.84E-1 3.6153E3/
PLOG/1.0E2 1.64E4 2.74E0 1.1444E3/
!AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
IC4H7O=C3H5-T+CH2O 1.0E11 0.0 0.0E0
PLOG/1.0E-3 7.26E6 1.82E-1 1.78155E4/
PLOG/1.0E-2 6.97E16 -2.5E0 2.08787E4/
PLOG/1.0E-1 6.64E23 -4.23E0 2.3565E4/
PLOG/1.0E0 1.07E26 -4.56E0 2.46229E4/
PLOG/1.0E1 6.5E29 -5.37E0 2.6645E4/
PLOG/1.0E2 4.63E31 -5.59E0 2.89153E4/
PLOG/1.0E3 8.52E25 -3.61E0 2.78634E4/
!AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
IC4H7O=C3H6+HCO 1.0E11 0.0 0.0E0
PLOG/1.0E-3 6.62E16 -2.84E0 1.3197E4/
PLOG/1.0E-2 1.26E20 -3.53E0 1.54692E4/
PLOG/1.0E-1 2.13E21 -3.64E0 1.65845E4/
PLOG/1.0E0 1.07E24 -4.16E0 1.8985E4/
PLOG/1.0E1 8.42E25 -4.4E0 2.23826E4/
PLOG/1.0E2 1.86E21 -2.73E0 2.36588E4/
PLOG/1.0E3 4.75E8 1.14E0 2.09225E4/
!AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
C3H5-T+CH2O=C3H6+HCO 1.0E11 0.0 0.0E0
PLOG/1.0E-3 1.11E7 1.09E0 1.8072E3/
PLOG/1.0E-2 2.47E7 9.93E-1 1.9949E3/
PLOG/1.0E-1 2.47E8 7.04E-1 2.5962E3/
PLOG/1.0E0 1.42E10 2.09E-1 3.9342E3/
PLOG/1.0E1 3.45E13 -7.26E-1 6.9443E3/
PLOG/1.0E2 3.31E14 -8.66E-1 1.09657E4/
PLOG/1.0E3 1.65E1 3.17E0 9.3998E3/
!!
!\REACTIONCLASS: \R_CH3O2_PRODUCTS \A \N \EA
!!
!\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2 !\COMMENT:
IC4H7+CH3O2=IC4H7O+CH3O 1.0E11 0.0 0.0E0
PLOG/1.0E-2 3.33E12 -1.58E-1 -1.417E3/
PLOG/1.0E-1 1.66E14 -6.42E-1 -3.491E2/
PLOG/1.0E0 2.595E17 -1.52E0 2.3792E3/
PLOG/1.0E1 9.78E14 -6.84E-1 3.6153E3/
PLOG/1.0E2 5.47E3 2.74E0 1.1444E3/
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC4H7+IC3H7O2=IC4H7O+IC3H7O 7.0E12 0.0 -1.0E3

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!!
!\REACTIONCLASS:  \RS_R_PRODUCTS                                    \A          \N
\EA
!!
!\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990). !\COMMENT:
IC4H7-I1+H=C3H4-A+CH4       3.333E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
IC4H7-I1+H=C3H4-P+CH4       3.34E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
IC4H7-I1+O=C3H6+HCO       6.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
IC4H7-I1+OH=>C3H6+HCO+H       5.0E12 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
IC4H7-I1+HO2=>C3H6+HCO+OH       2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
IC4H7-I1+HCO=IC4H8+CO       9.0E13 0.0 0.0E0
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
IC4H7-I1+CH3=C3H4-P+C2H6       1.0E11 0.0 0.0E0
!!
!\REACTIONCLASS:  \RADICAL_ADDITION\H                               \A          \N
\EA
!!
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=IC4H9       1.0E0 1.0 0.0E0
     DUP
     PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
     PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
     PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
     PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=IC4H9       1.0E0 1.0 0.0E0
     DUP
     PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
     PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
     PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
     PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
     PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=TC4H9       1.0E0 1.0 1.0E0
     DUP
     PLOG/1.3E-3 1.35E44 -1.068E1 8.1964E3/
     PLOG/4.0E-2 2.11E57 -1.423E1 1.5147E4/
     PLOG/1.0E0 3.26E61 -1.494E1 2.0161E4/
     PLOG/1.0E1 5.3E56 -1.312E1 2.0667E4/
     PLOG/1.0E2 1.11E50 -1.08E1 2.0202E4/
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
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```
IC4H8+H=TC4H9        1.0E0 1.0 1.0E0
      DUP
      PLOG/1.3E-3 2.17E130 -3.258E1 1.3614E5/
      PLOG/4.0E-2 2.25E29 -5.84E0 4.2419E3/
      PLOG/1.0E0 1.06E30 -5.63E0 5.6134E3/
      PLOG/1.0E1 6.11E26 -4.44E0 5.1823E3/
      PLOG/1.0E2 2.73E23 -3.26E0 4.597E3/
!DIVIDED BY 3 TO HAVE BETTER PREDICTION OF PROPENE IN FR
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=C3H6+CH3        1.0E0 1.0 1.0E0
      DUP
      PLOG/1.3E-3 5.13E8 1.35E0 2.542E3/
      PLOG/4.0E-2 2.63E10 8.7E-1 3.5996E3/
      PLOG/1.0E0 8.9E11 4.7E-1 5.4311E3/
      PLOG/1.0E1 3.08E22 -2.6E0 1.2898E4/
      PLOG/1.0E2 4.4E22 -2.42E0 1.65E4/
!AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727
IC4H8+H=C3H6+CH3        1.0E0 1.0 1.0E0
      DUP
      PLOG/1.3E-3 7.7E2 1.35E0 2.542E3/
      PLOG/4.0E-2 3.94E4 8.7E-1 3.5996E3/
      PLOG/1.0E0 1.34E6 4.7E-1 5.4311E3/
      PLOG/1.0E1 4.13E4 2.52E0 3.6791E3/
      PLOG/1.0E2 8.37E2 2.91E0 3.9809E3/
!!
!\REACTIONCLASS:    \RADICAL_ADDITION\HO2                    \A                    \N
\EA
!!
!\AUTHOR: !\REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218) !\COMMENT:
IC4H8+HO2=TC4H9O2        1.04E-1 3.45 4.338E3
!\AUTHOR: !\ REF: VILLANO, S, M.; CARSTENSEN, H-H.; DEAN, A. M. J. PHYS. CHEM. A., 2013,
117, 6458. !\COMMENT:
IC4H8+HO2=IC4H8O2H-T        1.64E4 2.43 8.3E3
!!
!\REACTIONCLASS:    \RADICAL_ADDITION\O                    \A                    \N
\EA
!!
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT:
IC4H8+O=IC3H7+HCO        7.45E6 1.88 1.83E2
!\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT:
IC4H8+O=>CH2CO+2CH3        3.05E6 1.88 1.83E2
C3H5-A+CH3(+M)=C4H8-1(+M)        1.0E14 -0.32 -2.623E2
      H2/2.0/
      H2O/6.0/
      CH4/2.0/
      CO/1.5/
```

CO2/2.0/
C2H6/3.0/
LOW/3.91E60 -1.281E1 6.25E3/
TROE/1.04E-1 1.606E3 6.0E4 6.1184E3/
C2H5+C2H3(+M)=C4H8-1(+M) 1.5E13 0.0 0.0E0
H2/2.0/
H2O/6.0/
CH4/2.0/
CO/1.5/
CO2/2.0/
C2H6/3.0/
LOW/1.55E56 -1.179E1 8.9845E3/
TROE/1.98E-1 2.2779E3 6.0E4 5.7232E3/
!\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325? 3346 !\COMMENT:
C2H3+CH3CHO=C2H4+CH3CO 1.65E1 3.17 9.3998E3
!\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325? 3346 !\COMMENT:
C3H5-S+CH2O=C3H6+HCO 1.65E1 3.17 9.3998E3
C4H8-1+H=C2H4+C2H5 1.0E0 1.0 1.0E0
DUP
PLOG/1.0E-3 2.55E6 1.93E0 5.564E3/
PLOG/1.0E-2 5.56E6 1.83E0 5.802E3/
PLOG/1.0E-1 1.21E9 1.18E0 7.472E3/
PLOG/1.0E0 9.47E16 -1.03E0 1.3413E4/
PLOG/1.0E1 4.5E28 -4.24E0 2.3618E4/
PLOG/1.0E2 7.02E32 -5.22E0 3.1754E4/
!\AUTHOR: !\REF: !\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=C2H4+C2H5 1.0E0 1.0 1.0E0
DUP
PLOG/1.0E-3 3.45E7 1.81E0 2.263E3/
PLOG/1.0E-2 8.06E7 1.71E0 2.522E3/
PLOG/1.0E-1 1.18E10 1.1E0 4.077E3/
PLOG/1.0E0 6.02E15 -4.9E-1 8.452E3/
PLOG/1.0E1 7.58E21 -2.14E0 1.4245E4/
PLOG/1.0E2 2.29E21 -1.87E0 1.7243E4/
!\AUTHOR: !\REF: !\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=C3H6+CH3 1.0E0 1.0 1.0E0
DUP
PLOG/1.0E-3 7.83E9 1.17E0 1.442E3/
PLOG/1.0E-2 3.39E10 1.0E0 1.895E3/
PLOG/1.0E-1 3.7E13 1.4E-1 4.127E3/
PLOG/1.0E0 4.57E19 -1.54E0 9.061E3/
PLOG/1.0E1 8.57E23 -2.66E0 1.414E4/
PLOG/1.0E2 1.32E20 -1.46E0 1.5383E4/
!\AUTHOR: !\REF: !\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS

```
C4H8-1+H=C3H6+CH3        1.0E0 1.0 1.0E0
        DUP
        PLOG/1.0E-3 1.8E6 1.76E0 5.9E3/
        PLOG/1.0E-2 3.46E6 1.68E0 6.1E3/
        PLOG/1.0E-1 4.02E8 1.1E0 7.574E3/
        PLOG/1.0E0 1.21E16 -9.9E-1 1.3175E4/
        PLOG/1.0E1 7.14E27 -4.23E0 2.3319E4/
        PLOG/1.0E2 1.0E33 -5.49E0 3.1922E4/
!\AUTHOR: !\REF:ANALOGY WITH C3H6+O
C4H8-1+O=>CH2CO+C2H5+H        3.05E6 1.88 1.83E2
!!
!\REACTIONCLASS:    \R_ADDITION\H                                   \A          \N
\EA
!!
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN
ET AL.
C4H6+H=C2H4+C2H3        1.46E30 -4.34 2.1647E4
        PLOG/1.0E0 1.46E30 -4.34E0 2.1647E4/
        PLOG/1.0E1 5.45E30 -4.51E0 2.1877E4/
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN
ET AL.
C4H6+H=C3H4-P+CH3        2.0E12 0.0 7.0E3
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN
ET AL.
C4H6+H=C3H4-A+CH3        2.0E12 0.0 7.0E3
!!
!\REACTIONCLASS:    \R_ADDITION\OH                                  \A          \N
\EA
!!
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL. !\COMMENT: TEST, 0525 KWZ
C4H6+OH=C2H3CHO+CH3        1.37E12 0.0 -1.04E3
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL. !\COMMENT: TEST, 0525 KWZ
C4H6+OH=C3H5-A+CH2O        1.37E12 0.0 -1.04E3
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL. !\COMMENT: WARNING: THIS REACTION IS IN THE WRONG PLACE!!
2C2H3=C4H6        7.0E57 -13.82 1.7629E4
        PLOG/2.63E-2 7.0E57 -1.382E1 1.7629E4/
        PLOG/1.2E-1 1.5E52 -1.197E1 1.6056E4/
        PLOG/1.0E0 1.5E42 -8.84E0 1.2483E4/
C6H101-5=2C3H5-A        4.9E22 -2.06 6.33555E4
        PLOG/1.0E0 5.07E47 -9.7E0 7.268E4/
        PLOG/4.0E0 4.22E39 -7.3E0 6.939E4/
        PLOG/1.0E1 2.12E35 -6.0E0 6.762E4/
!!
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!\REACTIONCLASS:    \RH_R_ABSTRACTION                                  \A                    \N
\EA
!!
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+H=C6H9-A+H2       6.752E5 2.36 2.07E2
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+O2=C6H9-A+HO2       4.0E14 0.0 3.889E4
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+O=C6H9-A+OH       1.32E6 2.43 1.21E3
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+OH=C6H9-A+H2O       5.528E4 2.64 -1.919E3
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+CH3=C6H9-A+CH4       7.38E0 3.31 4.002E3
!!
!\REACTIONCLASS:    \RADICAL_DECOMPOSITION                             \A                    \N
\EA
!!
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C4H6+C2H3=C6H9-A       8.8E5 2.5 6.13E3
!!
!\REACTIONCLASS:    \RADICAL_ADDITION\H                                \A                    \N
\EA
!!
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+H=>C3H4-A+C3H5-A+H2       1.0E12 0.0 0.0E0
!\AUTHOR: !\REF: WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+H=C3H5-A+C3H6       1.0E13 0.0 0.0E0
!!!!!!!!!!!!!!!!!!!!!!!C8H18-25!!!!!!!!!
!C8H18-25        +O2         (=)C8H17       +HO2                     5.000E+15    0.00    46000.0
!REV                                                      / 1.000E+12    0.00          0.0 /
C8H18-25+OH=>C8H17+H2O       1.6E14 0.0 3.0E3
!2.300E+13
C8H18-25+HO2=>C8H17+H2O2       12.3E13 0.0 1.695E4    !6.3E13
C8H18-25+H=C8H17+H2       3.34E6 2.8 8.147E3
!*3
C8H18-25+O2=C8H17+HO2       6.0E16 0.0 4.6E4
!C8H18-25        +OH          =)C8H17       +H2O                     5.63E+6    1.8      1431
!C8H18-25        +HO2         =)C8H17       +H2O2                    1.000E+14    0.00    16010
C8H17+O2=C8H17-OO       4.52E12 0.0 0.0E0
!C8H17-OO                 (=)C8-QOOH                           7.5E+11    0.00    24000
C8H17-OO=C8-QOOH       2.5E11 0.0 2.4E4
C8-QOOH+O2=C8-OOQOOH       4.52E12 0.0 0.0E0
!C8-OOQOOH              =)C8-KET       +OH                     5.5E+11    0.00    21000
C8-OOQOOH=>C8-KET+OH       3.5E11 0.0 2.1E4
C8-KET=>C6H13CO+CH2O+OH       1.78E15 0.0 3.91E4
C6H13CO+O2=>IC3H7+C3H5-A+CO+HO2       3.16E13 0.0 1.0E4
```

!*3
C8H17=2C3H6+C2H5 9.0E14 -0.1 2.678E4
!*3
C8H17=IC4H8+IC4H9 4.0E14 -0.1 2.678E4

!!!!!NC12!!!!!!

!\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING
NC3H7+H=C3H8 1.0E14 0.0 0.0E0
!\AUTHOR: !\REF: ANALOGY WITH C4H10+O2(=)PC4H9+HO2 !\COMMENT:
C3H8+O2=NC3H7+HO2 6.0E13 0.0 5.229E4
!\AUTHOR: !\REF:Curran estimate, 15% lower than Tsang, W. Chemical kinetic data base for combustion chemistry. Part 3. Propane J. Phys. Chem.
C3H8+H=NC3H7+H2 3.49E5 2.69 6.45E3
!\AUTHOR: !\REF:Tsang, W. Chemical kinetic data base for combustion chemistry. Part 3. Propane J. Phys. Chem. Ref. Data 17, 887 (1988) !\COMMENT:
C3H8+O=NC3H7+OH 3.71E6 2.4 5.505E3
!\AUTHOR: !\REF: Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by OH. 3. Propane, J. Phys. Chem., 90, 1949?954 !\COMMENT:
C3H8+OH=NC3H7+H2O 1.054E10 0.97 1.586E3
!\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054. !\COMMENT:
C3H8+HO2=NC3H7+H2O2 4.08E1 3.59 1.716E4
!\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
C3H8+CH3=NC3H7+CH4 9.04E-1 3.65 7.154E3
!\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE PUBLISHED. !\COMMENT: WARNING
C3H8+C2H3=NC3H7+C2H4 1.0E11 0.0 1.04E4
!\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE PUBLISHED. !\COMMENT: WARNING
C3H8+C2H5=NC3H7+C2H6 1.0E11 0.0 1.04E4
!\AUTHOR: !\REF:DAGAUT ET AL., CST 71, 111(1990) !\COMMENT:
C3H8+C3H5-A=NC3H7+C3H6 7.94E11 0.0 2.05E4
!\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054. !\COMMENT: SCALED AS PER CARSTENSEN ET AL
C3H8+CH3O2=NC3H7+CH3O2H 1.386E0 3.97 1.828E4
!!
!\REACTIONCLASS: \R+RO2 \A \N \EA
!!
!\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE
NC3H7+HO2=NC3H7O+OH 7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE
NC3H7+CH3O2=NC3H7O+CH3O 7.0E12 0.0 -1.0E3
C2H5+CH2O=NC3H7O 1.0E11 0.0 3.496E3
NC3H7+O2=C3H6+HO2 3.0E-19 0.0 3.0E3

```
!\AUTHOR: !\COMMENT: !0512 ADD KWZ
NC3H7+O2=NC3H7O2        1.0E11 0.0 0.0E0
      PLOG/1.0E-2 9.2E8 4.05E-1 -4.39865E3/
      PLOG/1.0E-1 1.45E14 -9.84E-1 -1.7108E3/
      PLOG/1.0E0 2.09E13 -4.99E-1 -9.38423E2/
      PLOG/1.0E1 1.15E20 -2.42E0 2.45126E3/
      PLOG/1.0E2 2.07E16 -1.3E0 8.03419E2/
!\AUTHOR: !\REF: \VLN 2011 !\COMMENT: WARNING: CANNOT TELL WHAT REFERENCE IS
NC3H7O2=C3H6+HO2        6.24E8 1.25 2.96E4
!!
!\REACTIONCLASS:    \RO2_QOOH                                   \A          \N
\EA
!!
!\AUTHOR: !\REF:Sharma !\COMMENT: WARNING: KPS-NO CLUE AS TO SOURCE
NC3H7O2=C3H6OOH1-2        4.09E8 1.1 3.01E4
!!
!\REACTIONCLASS:    \QOOH_PRODUCTS                              \A          \N
\EA
!!
!\AUTHOR: !\REF:HIGH PRESSURE RATE RULES FOR ALKYL+O2 REACTIONS 2
VLN2012 !\COMMENT:
C3H6OOH1-2=C3H6O1-2+OH        1.21E9 1.05 1.13E4
!\AUTHOR: !\REF:Villano !\COMMENT:
C3H6OOH1-2=C3H6+HO2        2.34E10 0.77 1.53E4
!\AUTHOR: !\REF:Villano !\COMMENT:
C3H6OOH1-2=>C2H4+CH2O+OH        1.31E33 -7.01 4.812E4
2NC3H7O2=>2NC3H7O+O2        1.4E16 -1.61 1.86E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
NC3H7O2+CH3=NC3H7O+CH3O        7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
NC3H7O2+C2H5=NC3H7O+C2H5O        7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
NC3H7O2+NC3H7=2NC3H7O        7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
NC3H7O2+C3H5-A=NC3H7O+C3H5O        7.0E12 0.0 -1.0E3
!\AUTHOR: !\REF:ESTIMATE !\COMMENT:
NC3H7O2+CH3O2=>NC3H7O+CH3O+O2        1.4E16 -1.61 1.86E3
C3H6O1-2=C2H4+CH2O        6.0E14 0.0 6.0E4
!\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT: WARNING: WHAT ARE SOURCES OF
RATE CONSTANTS?
C3H6O1-2+OH=>CH2O+C2H3+H2O        5.0E12 0.0 0.0E0
!\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+H=>CH2O+C2H3+H2        2.63E7 2.0 5.0E3
!\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+O=>CH2O+C2H3+OH        8.43E13 0.0 5.2E3
!\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
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C3H6O1-2+HO2=>CH2O+C2H3+H2O2 1.0E13 0.0 1.5E4
!\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H 1.0E13 0.0 1.9E4
!\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+CH3=>CH2O+C2H3+CH4 2.0E11 0.0 1.0E4
C3H6+O=>CH3CHCO+2H 3.05E6 1.88 1.83E2
FROM MILLER/KLIPPENSTEIN??
C3H6+H=NC3H7 1.0E0 1.0 0.0E0
DUP
PLOG/1.3E-3 7.99E81 -2.3161E1 2.2239E4/
PLOG/4.0E-2 4.24E68 -1.8427E1 1.9665E4/
PLOG/1.0E0 1.04E49 -1.15E1 1.5359E4/
PLOG/1.0E1 6.2E41 -8.892E0 1.4637E4/
PLOG/1.0E2 1.0E-10 0.0E0 0.0E0/
!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
C3H6+H=NC3H7 1.0E0 1.0 0.0E0
DUP
PLOG/1.3E-3 1.85E26 -5.83E0 3.8658E3/
PLOG/4.0E-2 2.82E30 -6.49E0 5.4708E3/
PLOG/1.0E0 3.78E28 -5.57E0 5.6251E3/
PLOG/1.0E1 1.46E25 -4.28E0 5.2478E3/
PLOG/1.0E2 4.22E27 -4.39E0 9.3458E3/

!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??

C2H4+CH3=NC3H7 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 8.67E48 -1.254E1 1.8206E4/
PLOG/4.0E-2 1.06E49 -1.204E1 2.0001E4/
PLOG/1.0E0 7.67E47 -1.117E1 2.2366E4/
PLOG/1.0E1 1.81E45 -1.003E1 2.3769E4/
PLOG/1.0E2 2.04E40 -8.25E0 2.4214E4/
!\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
C2H4+CH3=NC3H7 1.0E0 1.0 1.0E0
DUP
PLOG/1.3E-3 1.12E43 -1.13E1 1.308E4/
PLOG/4.0E-2 7.28E39 -9.88E0 1.3164E4/
PLOG/1.0E0 2.6E33 -7.46E0 1.2416E4/
PLOG/1.0E1 3.85E27 -5.38E0 1.1455E4/
PLOG/1.0E2 1.66E21 -3.17E0 1.0241E4/
!\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907_C7.inp
C3H6+HO2=C3H6O1-2+OH 1.13E19 -1.68 2.3587E4

PLOG/1.3E-2 3.73E3 2.64E0 1.1173E4/
PLOG/9.869E-1 1.78E12 1.1E-1 1.6137E4/
PLOG/9.87E0 3.9E17 -1.4E0 2.0077E4/
PLOG/9.869E1 1.13E19 -1.68E0 2.3587E4/
C3H5-S+O2=CH3CHCHO+O 5.38E18 -2.14 5.1429E3
!CH3CHCHO(=)C2H3CHO+H 4.164E+012 -0.020 32410.0 !\AUTHOR: !\REF: PELUCCHI ECM 2013 !\COMMENT:
!IC3H7(=)C3H6+H 1.0 1.0 1.0
CH3CHCHO=C2H3CHO+H 1.0E0 1.0 1.0E0
PLOG/1.0E-2 1.74E50 -1.173E1 5.287E4/
PLOG/1.0E-1 1.13E47 -1.057E1 5.0479E4/
PLOG/1.0E0 2.94E43 -9.29E0 4.881E4/
PLOG/2.5E0 1.16E42 -8.78E0 4.8382E4/
PLOG/5.0E0 9.48E40 -8.4E0 4.8095E4/
PLOG/1.0E1 7.19E39 -8.01E0 4.7818E4/
PLOG/2.5E1 2.13E38 -7.49E0 4.7438E4/
PLOG/5.0E1 1.42E37 -7.09E0 4.7128E4/
!\AUTHOR: !\REF: PELUCCHI ECM 2013 !\COMMENT:
CH3CHCHO=CH3CHCO+H 8.328E12 -0.02 3.241E4
CH3CHCO+OH=C2H5+CO2 1.73E12 0.0 -1.01E3
CH3CHCO+H=C2H5+CO 4.4E12 0.0 1.459E3

!\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:
PC4H9+O2=C4H8-1+HO2 8.37E-1 3.59 1.196E4
!C4H71-1,4OOH(=)NC4KET14+OH 9.000E+014 0.000 1500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:
!C4H72-2,3OOH(=)NC4KET23+OH 9.000E+014 0.000 1500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:
!C4H72-2,4OOH(=)NC4KET24+OH 9.000E+014 0.000 1500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:
!!
!\REACTIONCLASS: \ALKENEKHP_DECOMP \A \N \EA
!!
!\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:
C4H72-1OOH=>CH2O+C3H5-S+OH 1.5E16 0.0 4.2E4
!16_03 !C4H71-4OOH=)CH2O+C3H5-A+OH 1.500E+016 0.000 42000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:
!\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:
C4H71-3OOH=>C2H3CHO+CH3+OH 1.05E16 0.0 4.16E4
C4H71-3+H=C4H8-1 5.0E13 0.0 5.0E3
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
C4H8-1+OH=C4H71-3+H2O 7.769E5 2.2 -4.3718E2
!\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A 2011, 115, 2549–2556 !\COMMENT:

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C4H8-1+OH=C4H71-1+H2O        6.93E6 1.92 4.96204E3
C4H8-1+HO2=C4H71-3+H2O2        7.82E-1 3.97 1.1702E4
!\AUTHOR: !\REF:ANALOGY WITH C3H6+HO2
C4H8-1+HO2=C4H71-1+H2O2        9.57E2 3.059 2.07986E4
!\AUTHOR: !\REF:KPS, TST/RRHO+HRS
C4H8-1+H=C4H71-3+H2        2.42E3 3.05 1.995E3
!\AUTHOR: !\REF:KPS, TST/RRHO+HRS
C4H8-1+H=C4H71-1+H2        2.63E4 2.83 1.205E4
      DUP
!\AUTHOR: !\REF:KPS, TST/RRHO+HRS
C4H8-1+H=C4H71-1+H2        2.23E4 2.85 1.171E4
      DUP
!\AUTHOR: !\REF:IN ARAMCO
C4H8-1+O=C4H71-3+OH        1.75E11 0.7 5.884E3
!\AUTHOR: !\REF: ANALOGY WITH C2H4+O
C4H8-1+O=C4H71-1+OH        1.2E11 0.7 8.9591E3
!\AUTHOR: !\REF:IN ARAMCO !*5
C4H8-1+O2=C4H71-3+HO2        1.0E14 0.0 3.719E4
!\AUTHOR: !\REF: ANALOGY WITH C3H6+O2
C4H8-1+O2=C4H71-1+HO2        2.0E13 0.0 6.227E4
!\AUTHOR: !\REF:IN ARAMCO (TSANG '91)
C4H8-1+CH3=C4H71-3+CH4        2.21E0 3.5 5.675E3
!\AUTHOR: !\REF:ANALOGY WITH C3H6+CH3
C4H8-1+CH3=C4H71-1+CH4        1.348E0 3.5 1.285E4
!\AUTHOR: !\REF:IN ARAMCO (TSANG '91)
C4H8-1+CH3O2=C4H71-3+CH3O2H        2.7E4 0.7 5.884E3
!\AUTHOR: !\REF:IN ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))
C4H8-1+C3H5-A=C4H71-3+C3H6        7.9E10 0.0 1.24E4
!\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)
C4H71-3+C2H5=C4H8-1+C2H4        2.59E12 0.0 -1.31E2
!\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)
C4H71-3+CH3O=C4H8-1+CH2O        2.41E13 0.0 0.0E0
!\AUTHOR: !\REF:YANG CALCULATIONS
C4H71-1=C2H5+C2H2        2.85E12 0.68 3.3178291E4
!\AUTHOR: !\REF:YANG CALCULATIONS
C4H71-3=C4H6+H        8.53E7 1.95 4.7490106E4
C4H71-3+HO2=C4H71-3OOH        1.0E0 1.0 1.0E0
      PLOG/1.0E-2 2.05E1 1.24E0 -2.2589E4/
      PLOG/1.0E-1 3.69E6 8.0E-2 -1.8331E4/
      PLOG/1.0E0 2.02E13 -1.45E0 -1.1709E4/
      PLOG/2.0E0 1.49E15 -1.87E0 -9.604E3/
      PLOG/5.0E0 1.85E17 -2.31E0 -6.991E3/
      PLOG/1.0E1 2.88E18 -2.55E0 -5.26E3/
      PLOG/3.0E1 3.45E19 -2.71E0 -3.14E3/
      PLOG/5.0E1 5.33E19 -2.7E0 -2.438E3/
C4H71-3+HO2=C4H72-1OOH        1.0E0 1.0 1.0E0
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PLOG/1.0E-2 1.0E7 -3.3E-1 -1.7896E4/
PLOG/1.0E-1 1.15E11 -1.16E0 -1.4831E4/
PLOG/1.0E0 2.95E16 -2.33E0 -9.451E3/
PLOG/2.0E0 7.68E17 -2.62E0 -7.705E3/
PLOG/5.0E0 2.21E19 -2.89E0 -5.556E3/
PLOG/1.0E1 1.14E20 -2.99E0 -4.159E3/
PLOG/3.0E1 2.8E20 -2.96E0 -2.503E3/
PLOG/5.0E1 2.4E20 -2.88E0 -1.971E3/

!\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)
C4H71-3+O=C2H3CHO+CH3 6.03E13 0.0 0.0E0
!!
!\REACTIONCLASS: \RA_R_ABSTRACTION \A \N
\EA
!!
!\AUTHOR: !\REF: J. D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427 !\COMMENT:!*2
C4H71-3+O2=C4H6+HO2 1.07E0 3.71 9.322E3
!\AUTHOR: !\REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)
H+C4H71-3=C4H6+H2 3.16E13 0.0 0.0E0
!\AUTHOR: !\REF:EDELSON AND ALLARA, 1980
C2H5+C4H71-3=C4H6+C2H6 3.98E12 0.0 0.0E0
!\AUTHOR: !\REF:EDELSON AND ALLARA, 1980
C2H3+C4H71-3=C2H4+C4H6 3.98E12 0.0 0.0E0
!\AUTHOR: !\REF:EDELSON AND ALLARA, 1980
C3H5-A+C4H71-3=C3H6+C4H6 6.31E12 0.0 0.0E0
!!
!\REACTIONCLASS: \RSP_O2 \A \N
\EA
!!
!\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A
C4H71-1+O2=C4H71-1O2 4.07E27 -4.67 5.222E3
!\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A
C4H71-1O2=C3H6CHO-3+O 1.22E29 -4.71 4.234E4
!16_03 !CH3CHCO+CH3(=)C4H7O2-2 7.26E+03 2.43 8960 !FROM PRAJAKTA PARAB'S CALCULATION FOR CH2CO+CH3(=)CH3COCH2
!!
!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
\EA
C4H8-1+H=PC4H9 1.0E0 1.0 1.0E0
DUP
PLOG/1.0E-3 1.35E15 -2.81E0 1.57E3/
PLOG/1.0E-2 5.2E16 -2.97E0 1.992E3/
PLOG/1.0E-1 1.91E21 -3.97E0 4.636E3/
PLOG/1.0E0 1.9E31 -6.46E0 1.1968E4/
PLOG/1.0E1 2.1E40 -8.6E0 2.1058E4/

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      PLOG/1.0E2 1.44E37 -7.21E0 2.4896E4/
!\AUTHOR: !\REF: !\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
C4H8-1+H=PC4H9        1.0E0 1.0 1.0E0
      DUP
      PLOG/1.0E-3 4.33E20 -4.16E0 -2.63E2/
      PLOG/1.0E-2 1.78E22 -4.33E0 1.86E2/
      PLOG/1.0E-1 1.98E26 -5.18E0 2.518E3/
      PLOG/1.0E0 3.78E32 -6.63E0 7.265E3/
      PLOG/1.0E1 8.79E34 -6.91E0 1.0952E4/
      PLOG/1.0E2 7.8E28 -4.79E0 1.0355E4/
!\AUTHOR: !\REF: !\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PC4H9=C2H4+C2H5        1.0E0 1.0 1.0E0
      PLOG/1.0E-3 3.44E34 -8.1E0 2.8397E4/
      PLOG/1.0E-2 1.11E39 -9.05E0 3.1891E4/
      PLOG/1.0E-1 7.74E42 -9.78E0 3.5771E4/
      PLOG/1.0E0 7.47E43 -9.67E0 3.8722E4/
      PLOG/1.0E1 2.06E39 -7.97E0 3.8955E4/
      PLOG/1.0E2 1.48E29 -4.71E0 3.595E4/
!\AUTHOR: !\REF: !\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PC4H9=C3H6+CH3        1.0E0 1.0 1.0E0
      PLOG/1.0E-3 3.71E25 -5.81E0 3.4965E4/
      PLOG/1.0E-2 1.85E27 -6.01E0 3.5481E4/
      PLOG/1.0E-1 2.46E32 -7.16E0 3.8637E4/
      PLOG/1.0E0 2.05E42 -9.61E0 4.6415E4/
      PLOG/1.0E1 4.98E48 -1.097E1 5.4456E4/
      PLOG/1.0E2 2.23E42 -8.68E0 5.6601E4/
!!
!\REACTIONCLASS:    \RADICAL_ADDITION\O                                    \A                    \N
\EA
!!
!\AUTHOR: !\REF:ANALOGY WITH C3H6+O
C4H8-1+O=NC3H7+HCO        7.45E6 1.88 1.83E2

!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:
C2H3CHO+CH3=C3H6CHO-3        1.23E11 0.0 7.8E3
!!!!!!!!!!NC12H26!!!!!
NC12H26+O2=>C12H25+HO2        8.0E14 0.0 4.5E4
NC12H26+OH=>C12H25+H2O        8.787E6 2.0 -2.25983E3
NC12H26+H=>C12H25+H2        5.295E7 2.0 3.95057E3
NC12H26+O=>C12H25+OH        2.977E7 2.0 2.57954E3
NC12H26+CH3=>C12H25+CH4        8.587E5 2.0 4.87129E3
!3.1850e+06
NC12H26+HO2=>C12H25+H2O2        4.5E6 2.0 1.188773E4
!----- low temperature oxidation reactions
C12H25+O2=C12H25-OO        2.0E12 0.0 0.0E0
      REV/5.0E13 0.0E0 3.1E4/
```

```
C12H25-OO=C12-QOOH        3.0E12 0.0 2.4E4
      REV/2.0E10 0.0E0 1.61E4/
C12-QOOH+O2=C12-OOQOOH        2.0E12 0.0 0.0E0
      REV/2.0E14 0.0E0 2.9E4/
!6.0000e+12
C12-OOQOOH=>C12-KET+OH        3.0E12 0.0 2.6E4 !2.5E12
C12-KET=>OH+CH2O+C3H6+C4H8-1+NC3H7+CO        8.15E14 0.0 3.9E4
C12-QOOH=>C12H24+HO2        1.945E13 0.0 2.4E4
!----- high temperature pyrolysis reactions
NC12H26=>PC4H9+NC3H7+C3H6+C2H4        2.0E16 0.0 8.1E4
C12H25=>3C2H4+C4H8-1+C2H5        0.5E13 0.0 3.0E4                    !3.0E13
!1.0000e+12
C12H25=>2C4H8-1+C2H4+C2H5        4.0E13 0.0 3.0E4                    !1.5E13
!C12H25=)2C5H10-1+C2H5                                2.0000e+13        0.000          30000.00
!----- C12H24 sub-mechanism
C12H24+OH=>C12H23+H2O        5.62E8 1.61 -3.489E1
C12H24+HO2=>C12H23+H2O2        7.58E2 3.37 1.371989E4
C12H24+H=>C12H23+H2        1.56E7 2.4 4.47108E3
C12H24+O=>C12H23+OH        6.62E6 2.45 2.83007E3
C12H23=>2C4H8-1+C4H71-1        2.0E12 0.0 2.997132E4

!!!!!C9H12!!!!!!!!

H+O+M=OHV+M        1.5E13 0.0 5.975E3
      H2/1.0/
      H2O/6.5/
      O2/0.4/
      N2/0.4/
!!
!\REACTIONCLASS:    \DEACTIVATION                                                \A                    \N
\EA
!!
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+H2O=OH+H2O        5.93E12 0.5 -8.6E2
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+H2=OH+H2        2.95E12 0.5 -4.44E2
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+N2=OH+N2        1.08E11 0.5 -1.242E3
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+OH=2OH        6.01E12 0.5 -7.64E2
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+H=OH+H        1.31E12 0.5 -1.67E2
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV=OH        1.45E6 0.0 0.0E0
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+O2=OH+O2        2.1E12 0.5 -4.78E2
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!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+CO2=OH+CO2 2.75E12 0.5 -9.68E2
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+CO=OH+CO 3.23E12 0.5 -7.87E2
!\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
OHV+CH4=OH+CH4 3.36E12 0.5 -6.35E2
!H2O2(+H2O)(=)OH+OH(+H2O) 2.000E+012 0.900 48749.0 !\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601 (2011)!\COMMENT: RATE CONSTANT IS FOR N2
!LOW/ 1.865E+025 -2.300 48749.0/
!TROE/ 5.100E-001 1.000E-030 1.000E+030/
!\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601 (2011)!\COMMENT: RATE CONSTANT IS FOR N2, !\COMMENT: EFFICIENCIS OF H2O FROM THE SAME REF,
!LOW-PRESSURE-LIMIT
!TROE PARAMETERS
!3RD BODY COLLIDER EFFICIENCIES
!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: KPS !\REF: NOT A CLUE WHAT REFERENCE IS HERE AS MECHANISM IS A MESS !\COMMENT: WARNING
!!
!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N \EA
!!
!\AUTHOR: ?? !\REF: JOSHI AND WANG IJCK (2006), 38, (1), 57-73. !\COMMENT:

!!
!\REACTIONCLASS: \RADICAL_ADDITION\HO2 \A \N \EA
!!
!\AUTHOR: ?? !\REF: YOU ET AL. J. PHYS. CHEM. A 2007, 111, 4031-4042 !\COMMENT:

H+CO2=OCHO 7.5E13 0.0 2.9E4
CH2(S)+N2=CH2+N2 1.5E13 0.0 6.0E2
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+H2O=CH2+H2O 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+CO=CH2+CO 9.0E12 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+CO2=CH2+CO2 7.0E12 0.0 0.0E0
!!
!\REACTIONCLASS: \RADICAL_RECOMBINATIONS \A \N \EA
!!

!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+O2=>H+OH+CO 2.8E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+O2=CO+H2O 1.2E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+O=CO+H2 1.5E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+O=HCO+H 1.5E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+H2=CH3+H 7.0E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+H=CH+H2 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+OH=CH2O+H 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT: WARNING
CH2(S)+CO2=CH2O+CO 1.4E13 0.0 0.0E0
CH2+H=CH+H2 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT:
CH2+OH=CH+H2O 1.13E7 2.0 3.0E3
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+H2O=CH+H2O 5.3E13 0.0 0.0E0
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+CO=CH+CO 2.44E12 0.5 0.0E0
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+CO2=CH+CO2 2.41E-1 4.3 -1.694E3
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+O2=CH+O2 2.48E6 2.14 -1.72E3
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+H2=CH+H2 1.47E14 0.0 1.361E3
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+CH4=CH+CH4 1.73E13 0.0 1.67E2
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV=CH 1.86E6 0.0 0.0E0
!\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:
CHV+N2=CH+N2 3.03E2 3.4 -3.81E2
!!
!\REACTIONCLASS: \RADICAL_RECOMBINATIONS \A \N \EA

!!
!\AUTHOR: !\REF:KATHROTIA ET AL. COMB _ FLAME 2010 !\COMMENT:
CH+O2=CO+OHV 4.04E13 0.0 0.0E0
!\AUTHOR: !\REF: GRI 3.0 !\COMMENT:
CH+O2=HCO+O 3.3E13 0.0 0.0E0
!\AUTHOR: !\REF: MESSING ET AL.,J. CHEM. PHYS. 74, 3874 (1981) !\COMMENT:
CH+O=CO+H 5.7E13 0.0 0.0E0
!\AUTHOR: !\REF: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985) !\COMMENT:
CH+OH=HCO+H 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF:BERGEAT ET AL., CHEM. PHYS. LETT. 480, 21 (2009) !\COMMENT:
CH+H2O=H+CH2O 1.774E16 -1.22 2.38E1
!\AUTHOR: !\REF: BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB. P. 73, 1982 !\COMMENT: X0.5
CH+CO2=HCO+CO 1.7E12 0.0 6.85E2
CH3+OH=CH2(S)+H2O 4.936E14 -0.669 -4.458E2
PLOG/1.0E-2 4.936E14 -6.69E-1 -4.458E2/
PLOG/1.0E-1 1.207E15 -7.78E-1 -1.756E2/
PLOG/1.0E0 5.282E17 -1.518E0 1.772E3/
PLOG/1.0E1 4.788E23 -3.155E0 7.003E3/
PLOG/1.0E2 8.433E19 -1.962E0 8.244E3/
!\AUTHOR: ?? !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:
CH3+OH=HCOH+H2 8.674E8 0.787 -3.046E3
PLOG/1.0E-2 8.674E8 7.87E-1 -3.046E3/
PLOG/1.0E-1 3.115E9 6.3E-1 -2.669E3/
PLOG/1.0E0 1.557E11 1.56E-1 -1.368E3/
PLOG/1.0E1 1.704E21 -2.641E0 6.412E3/
PLOG/1.0E2 7.25E20 -2.402E0 9.639E3/
!\AUTHOR: ?? !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:
!\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:
CH2OH+HO2=HOCH2O+OH 1.0E13 0.0 0.0E0
HCOH+O2=>CO2+H+OH 5.0E12 0.0 0.0E0
!\AUTHOR: !\REF:MARINOV 1996 !\COMMENT:
HCOH+O2=CO2+H2O 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF:MARINOV 1996 !\COMMENT:
HCOH+O=>CO2+2H 5.0E13 0.0 0.0E0
!\AUTHOR: !\REF:MARINOV 1996 !\COMMENT:
HCOH+O=>CO+OH+H 3.0E13 0.0 0.0E0
!\AUTHOR: !\REF:MARINOV 1996 !\COMMENT:
HCOH+H=CH2O+H 2.0E14 0.0 0.0E0
!\AUTHOR: !\REF:MARINOV 1996 !\COMMENT:
HCOH+OH=HCO+H2O 2.0E13 0.0 0.0E0
CH2O+OCHO=HCO+HOCHO 5.6E12 0.0 1.36E4
!!
!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N \EA

!!
!\AUTHOR: !\REF: LI ET AL. IJCK 2007 !\COMMENT: X1.2
!3RD BODY COLLIDER EFFICIENCIES
CH2O+OH=HOCH2O 4.5E15 -1.1 0.0E0
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
HOCH2O=HOCHO+H 1.0E14 0.0 1.49E4
HOCHO=CO+H2O 2.45E12 0.0 6.047E4
!\AUTHOR: !\REF:BLAKE ET AL. J. CHEM. SOC. B: 10, 1923 (1971) !\COMMENT:
HOCHO=CO2+H2 2.95E9 0.0 4.852E4
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
OCHO+HO2=HOCHO+O2 3.5E10 0.0 -3.275E3
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:
OCHO+H2O2=HOCHO+HO2 2.4E12 0.0 1.0E4
!!
!\REACTIONCLASS: \LUMPED_BIMOLECULAR \A \N \EA
!!
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+H=>H2+CO2+H 4.24E6 2.1 4.868E3
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+H=>H2+CO+OH 6.03E13 -0.35 2.988E3
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+O=>CO+2OH 1.77E18 -1.9 2.975E3
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+OH=>H2O+CO2+H 2.62E6 2.06 9.16E2
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+OH=>H2O+CO+OH 1.85E7 1.51 -9.62E2
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+CH3=>CH4+CO+OH 3.9E-7 5.8 2.2E3
!\AUTHOR: !\REF:MARINOV ESTIMATE !\COMMENT:
HOCHO+HO2=>H2O2+CO+OH 1.0E12 0.0 1.192E4
!!
!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N \EA
!!
!\AUTHOR: !\REF:WKM ESTIMATE !\COMMENT: WHAT IS SOURCE OF RATE CONSTANT?
OCHO+OH=HO2CHO 2.0E13 0.0 0.0E0
C2H3+O2=CHCHO+OH 2.84E14 -0.8 7.232E3
DUP
PLOG/1.0E-2 3.91E11 -1.1E-1 2.131E3/

PLOG/1.0E-1 1.13E9 5.5E-1 4.6E1/
PLOG/3.16E-1 8.46E8 5.6E-1 7.0E-1/
PLOG/1.0E0 2.75E14 -1.83E0 4.6E0/
PLOG/3.16E0 2.58E20 -2.84E0 7.53E3/
PLOG/1.0E1 9.18E14 -2.26E0 -4.0E-1/
PLOG/3.16E1 6.11E25 -4.21E0 1.305E4/
PLOG/1.0E2 1.65E30 -5.35E0 1.843E4/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
C2H3+O2=CHCHO+OH 2.84E14 -0.8 7.232E3
DUP
PLOG/1.0E-2 9.91E11 -6.6E-1 -6.0E-1/
PLOG/1.0E-1 6.94E14 -1.16E0 4.542E3/
PLOG/3.16E-1 2.79E13 -7.2E-1 3.479E3/
PLOG/1.0E0 4.99E11 -1.4E-1 1.995E3/
PLOG/3.16E0 2.35E10 2.3E-1 1.573E3/
PLOG/1.0E1 1.7E14 -8.2E-1 4.45E3/
PLOG/3.16E1 1.42E11 5.0E-2 3.774E3/
PLOG/1.0E2 3.17E11 -2.0E-2 5.338E3/
!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

!\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

!!
!\REACTIONCLASS: \R_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:86TSA/ HAM !\COMMENT:
C2H2+CH2(S)=C3H3+H 2.0E13 0.0 0.0E0
!\AUTHOR: !\REF:GRI 3.0 AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H+O2=CO2+CHV 2.17E10 0.0 0.0E0

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!\AUTHOR: !\REF:GRI !\COMMENT:
C2H+O=CO+CHV        6.2E12 0.0 0.0E0
!\AUTHOR: !\REF:GRI !\COMMENT:
C2H+O=CO+CH        5.0E13 0.0 0.0E0
!\AUTHOR: !\REF:GRI !\COMMENT:
CH3CHO+OH=CH3+HOCHO        3.0E15 -1.076 0.0E0
CH+CH2O=H+CH2CO        9.46E13 0.0 -5.15E2
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:
CH+CO+M=HCCO+M        7.57E22 -1.9 0.0E0
!!
!\REACTIONCLASS:    \RADICAL_ADDITION                                    \A                    \N
\EA
!!
!\AUTHOR: !\REF:GRI !\COMMENT:
HCCO+H=CH2(S)+CO        1.0E14 0.0 0.0E0
!\AUTHOR: !\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS JOURNAL/ISSUE?
CH+HCCO=CO+C2H2        5.0E13 0.0 0.0E0

!!!!!!!!!!!!!!!!!!!!T135MB!!!!!!!!!!!!!!!
C9H12+H=CH3+C8H10        2.848E6 2.0 9.44E2
C9H12(+M)=H+C8H9CH2(+M)        1.1E10 1.694 8.36559E4
      LOW/5.855E103 -2.3904E1 1.096403E5/
      TROE/1.31E-1 4.793E2 4.688E2 4.6848E3/
C9H12+O2=C8H9CH2+HO2        6.54E7 2.5 4.6045E4
C9H12+H=C8H9CH2+H2        1.941E1 3.98 3.384E3
C9H12+OH=C8H9CH2+H2O        5.31E5 2.39 -6.02E2
C9H12+O=C8H9CH2+OH        1.89E12 0.0 0.0E0
C8H9CH2+O=C8H9CHO+H        5.2E13 0.0 0.0E0
C8H9CH2+O=C8H9+CH2O        1.19E14 0.0 0.0E0
C8H9CH2+HO2=C8H9CH2O+OH        3.0E12 0.0 0.0E0
C8H9CH2O=>C8H9CHO+H        1.99E13 0.0 1.8728E4
C8H9CH2O=>C8H9+CH2O        8.55E13 0.0 2.6017E4
C8H9CHO=C8H9CO+H        4.0E15 0.0 8.37E4
C8H9CO=>C8H9+CO        4.0E14 0.0 2.95E4
C8H9CHO+H=C8H9CO+H2        4.0E13 0.0 3.2E3
C8H9CHO+CH3=C8H9CO+CH4        2.0E-6 5.6 1.5E3
C8H9CHO+OH=C8H9CO+H2O        7.8E12 0.0 0.0E0
C8H9CHO+HO2=C8H9CO+H2O2        3.0E12 0.0 1.1E4
C8H10+O=C8H9+OH        1.328E13 0.0 1.47E4
C8H10+OH=C8H9+H2O        1.064E8 1.42 1.45E4
C8H9+O2=C8H9O+O        2.6E13 0.0 6.1E3
C8H9+O=C8H9O        1.0E14 0.0 0.0E0
C8H9+O2=C8H9OO        1.86E13 -0.22 -7.11E2
C8H9OO=C8H9O+O        1.27E15 -0.246 3.8536E4
C8H9O=>CO+C7H9        7.6E11 0.0 4.38E4
C7H9+O=C6H9+CO        3.2E13 -0.17 4.4E2
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C7H9+HO2=C7H9O+OH 6.3E29 -4.69 1.165E4
C7H9O=C6H9+CO 1.1E79 -19.62 6.625E4
C6H9=C3H4-P+C3H5-S 1.0E14 0.0 4.392E4

!!!!!Decalin!!!!!

C2H4+OH=PC2H4OH 1.74E43 -10.461 7.6987E3
PLOG/1.0E-2 1.74E43 -1.0461E1 7.6987E3/
PLOG/2.5E-2 3.25E37 -8.629E0 5.2147E3/
PLOG/1.0E-1 1.84E35 -7.75E0 4.9089E3/
PLOG/1.0E0 2.56E36 -7.752E0 6.9461E3/
PLOG/1.0E1 3.7E33 -6.573E0 7.6059E3/
PLOG/1.0E2 1.12E26 -4.101E0 5.757E3/

O2C2H4OH=PC2H4OH+O2 3.9E16 -1.0 3.0E4
!\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
O2C2H4OH=>OH+2CH2O 1.25E11 0.0 1.89E4

2C3H3=C6H6 1.8189E74 -18.14 3.1896E4
PLOG/3.947E-2 1.64E66 -1.5902E1 2.7529E4/
PLOG/1.0E0 3.1609E55 -1.255E1 2.2264E4/
PLOG/1.0E1 3.8888E50 -1.101E1 2.032E4/

C4H6=C4H5-N+H 5.3E44 -8.62 1.23608E5
!!
!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N \EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C4H6+H=C4H5-N+H2 1.33E6 2.53 1.224E4
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING SOURCE UNCLEAR DEFINED IN WRONG DIRECTION
C4H5-N+HO2=C4H6+O2 6.0E11 0.0 0.0E0
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.
C4H6+O=C4H5-N+OH 7.5E6 1.9 3.74E3
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.
C4H6+OH=C4H5-N+H2O 6.2E6 2.0 3.43E3
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING SOURCE UNCLEAR DEFINED IN WRONG DIRECTION
C4H5-N+H2O2=C4H6+HO2 1.21E10 0.0 -5.96E2
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.
C4H6+C2H3=C4H5-N+C2H4 5.0E13 0.0 2.28E4

!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.
C4H6+C3H5-A=C4H5-N+C3H6 1.0E13 0.0 2.25E4
!!
!\REACTIONCLASS: \R_ADDITION\H \A \N \EA
!!
!\AUTHOR: !\REF: WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.

C2H3+C2H2=C4H5-N 1.1E31 -7.14 5.6E3
PLOG/1.32E-2 1.1E31 -7.14E0 5.6E3/
PLOG/2.63E-2 1.1E32 -7.33E0 6.2E3/
PLOG/1.2E-1 2.4E31 -6.95E0 5.6E3/
PLOG/1.0E0 9.3E38 -8.76E0 1.2E4/
PLOG/1.0E1 8.1E37 -8.09E0 1.34E4/
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: WARNING: THIS REACTION IS IN THE WRONG PLACE!!

2C2H3=C4H5-N+H 1.1E24 -3.28 1.2395E4
PLOG/2.63E-2 1.1E24 -3.28E0 1.2395E4/
PLOG/1.2E-1 4.6E24 -3.38E0 1.465E4/
PLOG/1.0E0 2.4E20 -2.04E0 1.5361E4/
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
C4H5-N+HCO=C4H6+CO 5.0E12 0.0 0.0E0
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
C4H5-N+HO2=>C2H3+CH2CO+OH 6.6E12 0.0 0.0E0
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
C4H5-N+O2=HCO+C2H3CHO 9.2E16 -1.39 1.01E3
!(BASED ON C2H3+O2 FROM KLIPPENSTEIN)
C4H5-N+O2=>H+CO+C2H3CHO 5.19E15 -1.26 3.31262E3
!!
!\REACTIONCLASS: \AROMATIC_GROWTH \A \N \EA
!!
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C4H6+C2H3=>C6H6+H2+H 5.62E11 0.0 3.24E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C4H5-N+C2H2=C6H6+H 1.6E16 -1.33 5.4E3
!\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C4H5-N+C2H3=C6H6+H2 1.84E-13 7.07 -3.611E3
!!!!!!!!!!!!!!!!!!!!Decalin!!!!!!!!!!!!!!!
Decalin+O2=>RDecalin+HO2 5.0E14 0.0 4.46969E4

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Decalin+OH=>RDecalin+H2O        7.988E6 2.0 -2.25983E3
Decalin+H=>RDecalin+H2        4.813E7 2.0 3.95057E3
Decalin+O=>RDecalin+OH        2.707E7 2.0 2.57954E3
Decalin+HO2=>RDecalin+H2O2        9.6E13 0.0 1.5862E4
!----- low temperature oxidation reactions
RDecalin+O2=RDec-OO        1.0E12 0.0 0.0E0
        REV/3.0E13 0.0E0 2.9E4/
RDec-OO=Dec-QOOH        1.0E12 0.0 2.65E4
        REV/3.0E11 0.0E0 1.35E4/
Dec-QOOH+O2=Dec-OOQOOH        6.0E11 0.0 0.0E0
        REV/3.0E13 0.0E0 2.9E4/
Dec-OOQOOH=>Dec-KET+OH        1.0E12 0.0 2.65E4
Dec-KET=>OH+CH2CO+C2H4+C4H6+CH2CHO        2.0E21 0.0 6.0E4
RDec-OO=DCYC10H16+HO2        6.5E5 2.5 3.5E4
!----- high temperature pyrolysis reactions
Decalin=>CYC6H10+2C2H4        4.0E16 0.0 8.1E4
RDecalin=>C2H5+C8H12        4.0E12 0.0 3.0E4
RDecalin=>2C2H4+CYC6H9-3        1.0E12 0.0 3.0E4
RDecalin=>C4H7+CYC6H10        1.0E12 0.0 3.0E4
!----- DCYC10H16 sub-mechanism
DCYC10H16+OH=DCLD1-3R+H2O        6.91E4 2.6 -1.919E3
DCYC10H16+HO2=DCLD1-3R+H2O2        1.7E4 2.5 8.92E3
DCYC10H16+H=DCLD1-3R+H2        8.44E5 2.4 2.07E2
DCYC10H16+O=DCLD1-3R+OH        1.65E6 2.4 1.21E3
DCLD1-3R(+M)=>2C2H4+X135C6H7-3R(+M)        3.55E12 0.29 2.82969E4
        H2/2.0/
        H2O/6.0/
        CO/1.5/
        CO2/2.0/
        LOW/4.5E-26 1.309E1 -6.005E2/
        TROE/-7.4E-1 3.08E2 2.8E1 5.0E4/
!----- A1-C6H6
C6H6+H=X135C6H7-3R        1.22E22 -1.87 3.12E4
!----- C8H12 sub-mechanism
C8H12=LC5H7+C3H5-A        3.4712E118 -30.1379504 1.24456738E5
        PLOG/6.6E-3 3.4712E118 -3.01379504E1 1.24456738E5/
        PLOG/3.95E-2 1.4318E111 -2.77647395E1 1.23078036E5/
        PLOG/1.0E-1 2.0999E107 -2.65327E1 1.22362291E5/
        PLOG/1.0E0 6.76031E97 -2.348216E1 1.20645383E5/
        PLOG/1.0E1 4.95722E76 -1.725025E1 1.09498886E5/
        PLOG/1.0E2 2.4478E50 -9.68228E0 9.29912889E4/
        PLOG/1.0E5 3.21454E23 -2.03E0 7.4957588E4/
C8H12+H=C3H6+LC5H7        1.76E17 -1.05 6.461E3
        PLOG/1.0E-1 1.76E17 -1.05E0 6.461E3/
        PLOG/1.0E0 1.6E22 -2.39E0 1.118E4/
        PLOG/1.0E1 6.6E24 -3.04E0 1.561E4/
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CYC6H10=C4H6+C2H4        5.0E78 -18.94 9.8386E4
      PLOG/3.9E-2 5.0E78 -1.894E1 9.8386E4/
      PLOG/1.97E-1 2.6E70 -1.636E1 9.551E4/
      PLOG/1.0E0 3.81E25 -3.58E0 6.4034E4/
      PLOG/1.0E5 8.31E13 3.87E-1 6.4116E4/
CYC6H9-3+H(+M)=CYC6H10(+M)        4.0E14 0.0 0.0E0
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      LOW/2.66E60 -1.2E1 5.9678E3/
      TROE/2.0E-2 1.0966E3 1.0966E3 6.8595E3/
CYC6H10=CYC6H8-13+H2        1.0E14 0.0 6.9E4
CYC6H10+H=CYC6H9-3+H2        6.752E5 2.36 2.07E2
CYC6H10+O=CYC6H9-3+OH        1.32E6 2.43 1.21E3
CYC6H10+OH=CYC6H9-3+H2O        5.528E4 2.64 -1.919E3
CYC6H9-3=C6H9-13-6        8.92E18 -2.94 1.9897E4
      PLOG/3.9E-2 8.92E18 -2.94E0 1.9897E4/
      PLOG/1.97E-1 6.83E22 -3.82E0 2.3511E4/
      PLOG/1.0E0 1.56E29 -5.39E0 2.9211E4/
      PLOG/1.0E1 4.15E37 -7.44E0 3.7753E4/
      PLOG/1.0E2 1.92E39 -7.58E0 4.2286E4/
      PLOG/1.0E5 2.53E13 1.6E-1 2.9785E4/
CYC6H9-3=CYC6H8-13+H        8.14E14 -2.42 2.1719E4
      PLOG/3.9E-2 8.14E14 -2.42E0 2.1719E4/
      PLOG/1.97E-1 1.23E20 -3.61E0 2.6095E4/
      PLOG/1.0E0 1.18E28 -5.58E0 3.2946E4/
      PLOG/1.0E1 1.31E39 -8.28E0 4.3693E4/
      PLOG/1.0E2 4.67E42 -8.87E0 5.0298E4/
      PLOG/1.0E5 1.6E11 5.9E-1 3.5447E4/
CYC6H9-3+O2=CYC6H8-13+HO2        1.0E9 0.0 0.0E0
C2H4+C4H5-N=C6H9-13-6        1.23E35 -7.76 9.93E3
      PLOG/3.9E-2 6.15E34 -7.76E0 9.93E3/
      PLOG/1.0E-1 1.23E35 -7.76E0 9.93E3/
      PLOG/1.0E0 7.93E38 -8.47E0 1.422E4/
      PLOG/1.0E1 2.99E36 -7.4E0 1.548E4/
CYC6H8-13=C6H6+H2        1.0E14 0.0 6.0E4
C6H6+O=CYC5H6+CO        6.02E15 -0.49 1.4993E4
      PLOG/1.0E-1 7.22E13 1.2E-1 1.17769E4/
      PLOG/1.0E0 6.02E15 -4.9E-1 1.4993E4/
      PLOG/1.0E1 1.38E38 -6.71E0 3.46314E4/
      PLOG/5.0E1 1.57E31 -4.73E0 3.35684E4/
      PLOG/5.0E2 2.23E56 -1.169E1 5.55982E4/
CYC5H6+H=LC5H7        8.27E126 -32.3 8.2348E4
C3H5-A+C2H2=LC5H7        8.38E30 -6.2 1.2824E4
LC5H7+OH=C2H3CHO+C2H4        2.0E13 0.0 0.0E0
```

```
CYC5H5+H(+M)=CYC5H6(+M)        2.6E14 0.0 0.0E0
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
      LOW/1.144E81 -1.828E1 1.2994E4/
      TROE/6.8E-2 4.007E2 4.1358E3 5.5019E3/
CYC5H6+H=CYC5H5+H2        3.03E8 1.71 5.59E3
CYC5H6+H=C2H2+C3H5-A        7.74E36 -6.2 3.289E4
CYC5H6+C2H3=CYC5H5+C2H4        6.0E12 0.0 0.0E0
CYC5H6+O=CYC5H5+OH        4.77E4 2.7 1.106E3
CYC5H6+OH=CYC5H5+H2O        3.08E6 2.0 0.0E0
CYC5H6+O2=CYC5H5+HO2        4.0E13 0.0 3.715E4
CYC5H6+O=C4H5-N+CO+H        8.7E51 -11.1 3.324E4
CYC5H6+O=>C2H4+C2H2+CO        3.89E8 1.36 8.8671E2
CYC5H6+OH=>C2H4+C2H2+HCO        3.75E36 -7.8 7.06023E3
CYC5H5+O2=C5H4O+OH        7.0E11 0.08 1.8E4
CYC5H5+HO2=C5H4O+H2O        1.19E33 -6.52 1.34E4
CYC5H5+O=C5H4O+H        5.81E13 0.0 2.0E1
OH+CYC5H5=>CO+C4H6        1.25E13 0.25 4.35E3
C5H4O+O=CO+HCO+C3H3        1.2E8 1.4 -8.58E2
C4H7=C4H6+H        1.27E24 -4.75 2.3777E4
      PLOG/3.3E-2 1.27E24 -4.75E0 2.3777E4/
      PLOG/6.6E-2 1.38E26 -5.221E0 2.5729E4/
      PLOG/1.32E-1 1.75E28 -5.709E0 2.7764E4/
      PLOG/1.97E-1 3.16E29 -6.003E0 2.8985E4/
      PLOG/2.63E-1 2.69E30 -6.222E0 2.989E4/
C2H4+C2H3=C4H7        1.23E35 -7.76 9.93E3
      PLOG/3.3E-2 6.15E34 -7.76E0 9.93E3/
      PLOG/1.0E-1 1.23E35 -7.76E0 9.93E3/
      PLOG/1.0E0 7.93E38 -8.47E0 1.422E4/
      PLOG/1.0E1 2.99E36 -7.4E0 1.548E4/
C4H7+O2=C4H6+HO2        1.0E9 0.0 0.0E0
C4H7+HO2=CH2O+OH+C3H5-A        2.4E13 0.0 0.0E0
OH+C2H3CHO=>CO2+C2H4+H        8.0E12 0.0 0.0E0
HO2+C2H3CHO=>CH2CO+CH2O+OH        5.0E12 0.0 1.5E4
C2H3CHO+H=C2H4+HCO        2.0E13 0.0 3.5E3



! NOX REACTIONS

N+NO=N2+O        8.0E12 0.0 3.55E2      !2.7E13L
N+O2=NO+O        9.0E8 1.0 6.5E3    !9.0E9
N+OH=NO+H        3.36E11 0.0 3.85E2    !3.36E13
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/
      CO/1.5/
      CO2/2.0/
      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/
      CO/1.5/
      CO2/2.0/
      AR/0.7/
NO2+O=NO+O2      3.9E12 0.0 -2.4E2
NO2+H=NO+OH      1.32E14 0.0 3.6E2
NH+O=NO+H        4.0E13 0.0 0.0E0
NH+H=N+H2        3.2E13 0.0 3.3E2
NH+OH=HNO+H      2.0E13 0.0 0.0E0
NH+OH=N+H2O      2.0E9 1.2 0.0E0
NH+O2=HNO+O      4.61E5 2.0 6.5E3
NH+O2=NO+OH      1.28E6 1.5 1.0E2
NH+N=N2+H        1.5E13 0.0 0.0E0
NH+H2O=HNO+H2    2.0E13 0.0 1.385E4
NH+NO=N2+OH      2.16E13 -0.23 0.0E0
NH+NO=N2O+H      3.65E12 -0.45 0.0E0     !!!3.65E14
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/
      CO/1.5/
      CO2/2.0/
      AR/0.7/
NNH+O2=HO2+N2    5.0E12 0.0 0.0E0
NNH+O=OH+N2      2.5E13 0.0 0.0E0
NNH+O=NH+NO      7.0E11 0.0 0.0E0    !!7.0E13
NNH+H=H2+N2      5.0E13 0.0 0.0E0
NNH+OH=H2O+N2    2.0E13 0.0 0.0E0
H+NO+M=HNO+M     4.48E19 -1.32 7.4E2
      H2/2.0/
      H2O/6.0/
      CO/1.5/
      CO2/2.0/
```

```
      AR/0.7/
HNO+O=NO+OH       2.5E13 0.0 0.0E0
HNO+H=H2+NO       9.0E11 0.72 6.6E2
HNO+OH=NO+H2O       1.3E7 1.9 -9.5E2
HNO+O2=HO2+NO       1.0E13 0.0 1.3E4
HCN+O=NH+CO       5.07E3 2.64 4.98E3
CH+N2=HCN+N       3.12E7 0.88 2.013E4    !3.12E9
CH2+N2=HCN+NH       1.0E13 0.0 7.4E4
CH+NO=HCN+O       4.1E14 0.0 0.0E0    !4.1E13
CH+NO=N+HCO       2.46E14 0.0 0.0E0    !2.46E13
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
NH+CO2=HNO+CO       1.0E13 0.0 1.435E4
N+CO2=NO+CO       3.0E12 0.0 1.13E4

END
```

S2. The thermodynamic data

```
THERMO
    300.000   1000.000   5000.000
N2                      G 8/02N   2       0       0       0G    200.000   6000.00   1000.00          1
 2.95257637E+00 1.39690040E-03-4.92631603E-07 7.86010195E-11-4.60755204E-15       2
-9.23948688E+02 5.87188762E+00 3.53100528E+00-1.23660988E-04-5.02999433E-07       3
 2.43530612E-09-1.40881235E-12-1.04697628E+03 2.96747038E+00 0.00000000E+00       4
HE                      000000HE  1                G       300.00    5000.00 1000.00          1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00       2
-7.45375000E+02 9.15348900E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00       3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 9.15348800E-01                      4
H2                      TPIS78H   2       0       0       0G    200.000   6000.00   1000.00          1
 2.93286575E+00 8.26608026E-04-1.46402364E-07 1.54100414E-11-6.88804800E-16       2
-8.13065581E+02-1.02432865E+00 2.34433112E+00 7.98052075E-03-1.94781510E-05       3
 2.01572094E-08-7.37611761E-12-9.17935173E+02 6.83010238E-01 0.00000000E+00       4
H                       L 6/94H   1       0       0       0G    200.000   6000.00   1000.00          1
 0.25000000E+01 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00       2
 0.25473660E+05-0.44668285E+00 0.25000000E+01 0.00000000E+00 0.00000000E+00       3
 0.00000000E+00 0.00000000E+00 0.25473660E+05-0.44668285E+00 0.26219035E+05       4
O2                      RUS 89O   2       0       0       0G    200.000   6000.00   1000.00          1
 3.66096065E+00 6.56365811E-04-1.41149627E-07 2.05797935E-11-1.29913436E-15       2
-1.21597718E+03 3.41536279E+00 3.78245636E+00-2.99673416E-03 9.84730201E-06       3
-9.68129509E-09 3.24372837E-12-1.06394356E+03 3.65767573E+00 0.00000000E+00       4
O                       L 1/90O   1       0       0       0G    200.000   6000.00   1000.00          1
 2.54363697E+00-2.73162486E-05-4.19029520E-09 4.95481845E-12-4.79553694E-16       2
 2.92260120E+04 4.92229457E+00 3.16826710E+00-3.27931884E-03 6.64306396E-06       3
-6.12806624E-09 2.11265971E-12 2.91222592E+04 2.05193346E+00 2.99687009E+04       4
OHV                     121286O   1H    1               G   0300.00    5000.00   1000.00          1
+2.88273000E+00+1.01397430E-03-2.27687700E-07+2.17468300E-11-5.12630500E-16       2
+5.02650000E+04+5.59571200E+00+3.63726600E+00+1.85091000E-04-1.67616460E-06       3
+2.38720200E-09-8.43144200E-13+5.00213000E+04+1.35886050E+00+0.00000000E+00       4
H2O                     L 5/89H   2 O   1       0       0G    200.000   6000.00   1000.00          1
 0.26770389E+01 0.29731816E-02-0.77376889E-06 0.94433514E-10-0.42689991E-14       2
-0.29885894E+05 0.68825500E+01 0.41986352E+01-0.20364017E-02 0.65203416E-05       3
-0.54879269E-08 0.17719680E-11-0.30293726E+05-0.84900901E+00-0.29084817E+05       4
OH                      IU3/03O   1 H   1       0       0G    200.000   6000.00   1000.00          1
 2.83853033E+00 1.10741289E-03-2.94000209E-07 4.20698729E-11-2.42289890E-15       2
 3.69780808E+03 5.84494652E+00 3.99198424E+00-2.40106655E-03 4.61664033E-06       3
-3.87916306E-09 1.36319502E-12 3.36889836E+03-1.03998477E-01 4.48613328E+03       4
H2O2                    T 8/03H   2O    2       0       0G    200.000   6000.00   1000.00          1
 4.57977305E+00 4.05326003E-03-1.29844730E-06 1.98211400E-10-1.13968792E-14       2
-1.80071775E+04 6.64970694E-01 4.31515149E+00-8.47390622E-04 1.76404323E-05       3
-2.26762944E-08 9.08950158E-12-1.77067437E+04 3.27373319E+00-1.63425145E+04       4
HO2                     T 1/09H   1O    2       0       0G    200.000   5000.00   1000.00          1
 4.17228741E+00 1.88117627E-03-3.46277286E-07 1.94657549E-11 1.76256905E-16       2
```

3.10206839E+01 2.95767672E+00 4.30179807E+00-4.74912097E-03 2.11582905E-05 3
-2.42763914E-08 9.29225225E-12 2.64018485E+02 3.71666220E+00 1.47886045E+03 4
CO RUS 79C 1O 1 0 0G 200.000 6000.00 1000.00 1
0.30484859E+01 0.13517281E-02-0.48579405E-06 0.78853644E-10-0.46980746E-14 2
-0.14266117E+05 0.60170977E+01 0.35795335E+01-0.61035369E-03 0.10168143E-05 3
0.90700586E-09-0.90442449E-12-0.14344086E+05 0.35084093E+01-0.13293628E+05 4
CO2 L 7/88C 1O 2 0 0G 200.000 6000.00 1000.00 1
0.46365111E+01 0.27414569E-02-0.99589759E-06 0.16038666E-09-0.91619857E-14 2
-0.49024904E+05-0.19348955E+01 0.23568130E+01 0.89841299E-02-0.71220632E-05 3
0.24573008E-08-0.14288548E-12-0.48371971E+05 0.99009035E+01-0.47328105E+05 4
CH4 G 8/99C 1 H 4 0 0 G 200.000 6000.00 1000.00 1
1.65326226E+00 1.00263099E-02-3.31661238E-06 5.36483138E-10-3.14696758E-14 2
-1.00095936E+04 9.90506283E+00 5.14911468E+00-1.36622009E-02 4.91453921E-05 3
-4.84246767E-08 1.66603441E-11-1.02465983E+04-4.63848842E+00-8.97226656E+03 4
CH3 IU0702C 1 H 3 0 0 G 200.000 6000.00 1000.00 1
0.29781206E+01 0.57978520E-02-0.19755800E-05 0.30729790E-09-0.17917416E-13 2
0.16509513E+05 0.47224799E+01 0.36571797E+01 0.21265979E-02 0.54583883E-05 3
-0.66181003E-08 0.24657074E-11 0.16422716E+05 0.16735354E+01 0.17643935E+05 4
CH2 IU3/03C 1 H 2 0 0 G 200.000 6000.00 1000.00 1
3.14631886E+00 3.03671259E-03-9.96474439E-07 1.50483580E-10-8.57335515E-15 2
4.60412605E+04 4.72341711E+00 3.71757846E+00 1.27391260E-03 2.17347251E-06 3
-3.48858500E-09 1.65208866E-12 4.58723866E+04 1.75297945E+00 4.70504920E+04 4
CH IU3/03C 1 H 1 0 0 G 200.000 6000.00 1000.00 1
+2.52093690E+00+1.76536390E-03-4.61476600E-07+5.92896750E-11-3.34745010E-15 2
+7.09467690E+04+7.40518290E+00+3.48975830E+00+3.24321600E-04-1.68997510E-06 3
+3.16284200E-09-1.40618030E-12+7.06126460E+04+2.08428410E+00+7.16581880E+04 4
CH3O2H A 7/05C 1 H 4 O 2 0 G 200.000 6000.00 1000.00 1
7.76538058E+00 8.61499712E-03-2.98006935E-06 4.68638071E-10-2.75339255E-14 2
-1.82979984E+04-1.43992663E+01 2.90540897E+00 1.74994735E-02 5.28243630E-06 3
-2.52827275E-08 1.34368212E-11-1.68894632E+04 1.13741987E+01-1.52423685E+04 4
CH3O2 H 3C 1O 2 0G 300.000 5000.000 1374.000 11
6.47970487E+00 7.44401080E-03-2.52348555E-06 3.89577296E-10-2.25182399E-14 2
-1.56285441E+03-8.19477074E+00 1.97339205E+00 1.53542340E-02-6.37314891E-06 3
3.19930565E-10 2.82193915E-13 2.54278835E+02 1.69194215E+01 4
CH3OH T06/02C 1H 4 O 1 0 G 200.000 6000.00 1000.00 1
3.52726795E+00 1.03178783E-02-3.62892944E-06 5.77448016E-10-3.42182632E-14 2
-2.60028834E+04 5.16758693E+00 5.65851051E+00-1.62983419E-02 6.91938156E-05 3
-7.58372926E-08 2.80427550E-11-2.56119736E+04-8.97330508E-01-2.41746056E+04 4
CH3O IU1/03C 1 H 3 O 1 0 G 200.000 6000.00 1000.00 1
4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-14 2
3.78111940E+02-1.96680028E+00 3.71180502E+00-2.80463306E-03 3.76550971E-05 3
-4.73072089E-08 1.86588420E-11 1.29569760E+03 6.57240864E+00 2.52571660E+03 4
CH2OH IU2/03C 1 H 3 O 1 0 G 200.000 6000.00 1000.00 1
5.09314370E+00 5.94761260E-03-2.06497460E-06 3.23008173E-10-1.88125902E-14 2
-4.03409640E+03-1.84691493E+00 4.47834367E+00-1.35070310E-03 2.78484980E-05 3
-3.64869060E-08 1.47907450E-11-3.50072890E+03 3.30913500E+00-2.04462770E+03 4

CH2O T 5/11H 2C 1O 1 0G 200.000 6000.00 1000.00 1
3.16952665E+00 6.19320560E-03-2.25056366E-06 3.65975660E-10-2.20149458E-14 2
-1.45486831E+04 6.04207898E+00 4.79372312E+00-9.90833322E-03 3.73219990E-05 3
-3.79285237E-08 1.31772641E-11-1.43791953E+04 6.02798058E-01-1.31293365E+04 4
HCO T 5/03C 1 H 1 O 1 0 G 200.000 6000.00 1000.00 1
3.92001542E+00 2.52279324E-03-6.71004164E-07 1.05615948E-10-7.43798261E-15 2
3.65342928E+03 3.58077056E+00 4.23754610E+00-3.32075257E-03 1.40030264E-05 3
-1.34239995E-08 4.37416208E-12 3.87241185E+03 3.30834869E+00 5.08749163E+03 4
HO2CHO 6/26/95 THERMC 1H 2O 3 0G 300.000 5000.000 1378.00 21
9.87503878E+00 4.64663708E-03-1.67230522E-06 2.68624413E-10-1.59595232E-14 2
-3.80502496E+04-2.24939155E+01 2.42464726E+00 2.19706380E-02-1.68705546E-05 3
6.25612194E-09-9.11645843E-13-3.54828006E+04 1.75027796E+01 4
O2CHO 6/26/95 THERMC 1H 1O 3 0G 300.000 5000.000 1368.00 11
7.24075139E+00 4.63312951E-03-1.63693995E-06 2.59706693E-10-1.52964699E-14 2
-1.87027618E+04-6.49547212E+00 3.96059309E+00 1.06002279E-02-5.25713351E-06 3
1.01716726E-09-2.87487602E-14-1.73599383E+04 1.17807483E+01 4
C2H6 G 8/88C 2H 6 0 0G 200.000 6000.00 1000.00 1
4.04666411E+00 1.53538802E-02-5.47039485E-06 8.77826544E-10-5.23167531E-14 2
-1.24473499E+04-9.68698313E-01 4.29142572E+00-5.50154901E-03 5.99438458E-05 3
-7.08466469E-08 2.68685836E-11-1.15222056E+04 2.66678994E+00-1.00849652E+04 4
C2H5 8/ 4/ 4 THERMC 2H 5 0 0G 300.000 5000.000 1387.000 11
5.88784390E+00 1.03076793E-02-3.46844396E-06 5.32499257E-10-3.06512651E-14 2
1.15065499E+04-8.49651771E+00 1.32730217E+00 1.76656753E-02-6.14926558E-06 3
-3.01143466E-10 4.38617775E-13 1.34284028E+04 1.71789216E+01 4
C2H5O2H 9/ 1/12 C 2H 6O 2 0G 300.000 5000.000 1390.000 31
1.04823538E+01 1.34779879E-02-4.62179078E-06 7.18618519E-10-4.17307436E-14 2
-2.46578171E+04-2.84294243E+01 1.83755328E+00 3.38053586E-02-2.37548140E-05 3
9.31974865E-09-1.58003428E-12-2.15814086E+04 1.80977584E+01 4
C2H5O2 9/ 1/12 C 2H 5O 2 0G 300.000 5000.000 1389.000 21
9.50282570E+00 1.20429839E-02-4.09491581E-06 6.33049241E-10-3.66133788E-14 2
-7.37069391E+03-2.21717130E+01 3.90351912E+00 2.22599212E-02-1.01610079E-05 3
1.71709751E-09 1.88166738E-14-5.09654081E+03 8.98722750E+00 4
C2H4 8/12/15 C 2H 4 0 0G 300.000 5000.000 1392.000 01
5.07061289E+00 9.11140768E-03-3.10506692E-06 4.80733851E-10-2.78321396E-14 2
3.66391217E+03-6.64501414E+00 4.81118223E-01 1.83778060E-02-9.99633565E-06 3
2.73211039E-09-3.01837289E-13 5.44386648E+03 1.85867157E+01 4
C2H3 8/12/15 C 2H 3 0 0G 300.000 5000.000 1400.000 01
4.99675415E+00 6.55838271E-03-2.20921909E-06 3.39300272E-10-1.95316926E-14 2
3.34604382E+04-3.01451097E+00 1.25545094E+00 1.57481597E-02-1.12218328E-05 3
4.50915682E-09-7.74861577E-13 3.47435574E+04 1.69664043E+01 4
C2H3OO H 3C 2O 2 G 298.150 2000.000 1000.00 1
6.04483828E+00 1.45511127E-02-7.50974622E-06 1.83488280E-09-1.66689681E-13 2
1.01699244E+04-3.71144913E+00 1.09784776E+00 2.95333237E-02-2.27744360E-05 3
7.20559155E-09-3.07929092E-13 1.13996101E+04 2.13563583E+01 4
C2H2 G 1/91C 2 H 2 0 0 G 200.000 6000.00 1000.00 1
4.65878489E+00 4.88396667E-03-1.60828888E-06 2.46974544E-10-1.38605959E-14 2

2.57594042E+04-3.99838194E+00 8.08679682E-01 2.33615762E-02-3.55172234E-05 3
2.80152958E-08-8.50075165E-12 2.64289808E+04 1.39396761E+01 2.74459950E+04 4
C2H T 5/10C 2 H 1 0 0 G 200.000 6000.00 1000.00 1
3.66270248E+00 3.82492252E-03-1.36632500E-06 2.13455040E-10-1.23216848E-14 2
6.71683790E+04 3.92205792E+00 2.89867676E+00 1.32988489E-02-2.80733327E-05 3
2.89484755E-08-1.07502351E-11 6.70616050E+04 6.18547632E+00 6.83210436E+04 4
C2H5O 8/12/15 C 2H 5O 1 0G 300.000 5000.000 1467.000 11
8.19120635E+00 1.10391986E-02-3.75270536E-06 5.80275784E-10-3.35735146E-14 2
-5.66847208E+03-1.90131344E+01 2.90353584E+00 1.77256708E-02-2.69624757E-06 3
-3.45830533E-09 1.25224784E-12-3.28930290E+03 1.13545591E+01 4
CH3CHO L 8/88C 2 H 4 O 1 0 G 200.000 6000.00 1000.00 1
0.54041108E+01 0.11723059E-01-0.42263137E-05 0.68372451E-09-0.40984863E-13 2
-0.22593122E+05-0.34807917E+01 0.47294595E+01-0.31932858E-02 0.47534921E-04 3
-0.57458611E-07 0.21931112E-10-0.21572878E+05 0.41030159E+01-0.19987949E+05 4
CH3CO IU2/03C 2 H 3 O 1 0 G 200.000 6000.00 1000.00 1
0.53137165E+01 0.91737793E-02-0.33220386E-05 0.53947456E-09-0.32452368E-13 2
-0.36450414E+04-0.16757558E+01 0.40358705E+01 0.87729487E-03 0.30710010E-04 3
-0.39247565E-07 0.15296869E-10-0.26820738E+04 0.78617682E+01-0.12388039E+04 4
CH2CHO T03/10C 2 H 3 O 1 0 G 200.000 6000.00 1000.00 1
6.53928338E+00 7.80238629E-03-2.76413612E-06 4.42098906E-10-2.62954290E-14 2
-1.18858659E+03-8.72091393E+00 2.79502600E+00 1.01099472E-02 1.61750645E-05 3
-3.10303145E-08 1.39436139E-11 1.62944975E+02 1.23646657E+01 1.53380440E+03 4
CH2CO H 2C 2O 1 0G 300.00 5000.00 1000.00 1
5.35869367E+00 6.95641586E-03-2.64802637E-06 4.65067592E-10-3.08641820E-14 2
-7.90294013E+03-3.98525731E+00 1.81422511E+00 1.99008590E-02-2.21416008E-05 3
1.45028521E-08-3.98877068E-12-7.05394926E+03 1.36079359E+01 4
HCCO T 4/09H 1 C 2 O 1 0 G 200.000 6000.00 1000.00 1
5.91479333E+00 3.71408730E-03-1.30137010E-06 2.06473345E-10-1.21476759E-14 2
1.93596301E+04-5.50567269E+00 1.87607969E+00 2.21205418E-02-3.58869325E-05 3
3.05402541E-08-1.01281069E-11 2.01633840E+04 1.36968290E+01 2.14444387E+04 4
C3H8 8/12/15 C 3H 8 0 0G 300.000 5000.000 1390.000 21
9.15541310E+00 1.72574139E-02-5.85614868E-06 9.04190155E-10-5.22523772E-14 2
-1.75762439E+04-2.77418510E+01 2.40878470E-01 3.39548599E-02-1.60930874E-05 3
2.83480628E-09 2.78195172E-14-1.40362853E+04 2.16500800E+01 4
IC3H7 8/12/15 C 3H 7 0 0G 298.0 6000.0 1000.0 1
6.70775549E+00 1.74048076E-02-6.07615926E-06 9.60084351E-10-5.65656490E-14 2
7.55377821E+03-1.03686516E+01-8.97467137E-01 4.15744022E-02-4.94778349E-05 3
4.56493655E-08-1.79085437E-11 9.93950407E+03 2.92641758E+01 4
NC3H7 8/12/15 C 3H 7 0 0G 298.0 6000.0 1000.0 1
7.48614243E+00 1.65769478E-02-5.74876481E-06 9.04103694E-10-5.30867231E-14 2
8.93710008E+03-1.42595379E+01-2.20120865E+00 5.29641653E-02-7.23640506E-05 3
6.36996940E-08-2.29332581E-11 1.15130744E+04 3.43669174E+01 4
NC3H7O2 8/12/15 C 3H 7O 2 0G 300.000 5000.000 1390.000 31
1.32753283E+01 1.61303126E-02-5.52348308E-06 8.58197168E-10-4.98172586E-14 2
-1.16032968E+04-4.15091215E+01 2.13311681E+00 3.96692045E-02-2.37570127E-05 3
6.96020417E-09-7.82576856E-13-7.46687112E+03 1.92444565E+01 4

NC3H7O 8/12/15 C 3H 7O 1 0G 300.000 5000.000 1386.000 21
1.15279177E+01 1.53775991E-02-5.23946272E-06 8.11382512E-10-4.69927603E-14 2
-9.85099867E+03-3.54233008E+01 2.57486880E+00 3.07100600E-02-1.20048836E-05 3
3.40807108E-12 7.25275283E-13-6.20913350E+03 1.45966401E+01 4
IC3H7O2 8/12/15 C 3H 7O 2 0G 300.000 5000.000 1407.000 31
1.35268120E+01 1.54306581E-02-5.17464218E-06 7.92548669E-10-4.55415379E-14 2
-1.33946348E+04-4.40461451E+01 2.58517502E+00 4.16107259E-02-2.92193877E-05 3
1.08614807E-08-1.66312005E-12-9.67013161E+03 1.44731300E+01 4
IC3H7O 8/12/15 C 3H 7O 1 0G 300.000 5000.000 1527.000 21
1.19648494E+01 1.42943974E-02-4.71413211E-06 7.14027066E-10-4.07161162E-14 2
-1.17519389E+04-3.88860959E+01 2.36108410E+00 3.45650027E-02-1.94579631E-05 3
4.71536901E-09-2.64704937E-13-8.28791395E+03 1.33112436E+01 4
C3H6 8/12/15 C 3H 6 0 0G 298.000 6000.000 1000.000 01
6.59032304E+00 1.52592866E-02-5.30369441E-06 8.35510888E-10-4.91215549E-14 2
-2.47481113E+02-1.15748238E+01-1.54606737E+00 4.36553128E-02-5.61392417E-05 3
4.98421927E-08-1.84798923E-11 2.07056233E+03 2.99232495E+01 4
C3H6CHO-3 C 4H 7O 1 0G 300.0000 5000.0000 1678.00 1
1.21729663e+01 1.80056550e-02-6.43783092e-06 1.03362049e-09-6.14850407e-14 2
-1.08762913e+04-3.80454831e+01 7.31671476e-01 4.17195442e-02-2.21538951e-05 3
4.18563988e-09 6.57157083e-14-6.89768622e+03 2.40278065e+01 4
C3H6OOH1-2 9/ 1/12 C 3H 7O 2 0G 300.000 5000.000 1387.000 41
1.38088686E+01 1.43845650E-02-4.74440961E-06 7.19308280E-10-4.10654123E-14 2
-5.14352831E+03-4.20210765E+01 2.83631132E+00 3.88229894E-02-2.47944364E-05 3
7.85644898E-09-9.58634300E-13-1.26002528E+03 1.72549973E+01 4
C3H6O1-2 A01/05C 3 H 6 O 1 0 G 200.000 6000.00 1000.00 1
8.01491079E+00 1.73919953E-02-6.26027968E-06 1.01188256E-09-6.06239111E-14 2
-1.51980838E+04-1.88279964E+01 3.42806676E+00 6.25176642E-03 6.13196311E-05 3
-8.60387185E-08 3.51371393E-11-1.28446646E+04 1.04244994E+01-1.11564001E+04 4
C3H5-A 8/12/15 C 3H 5 0 0G 298.000 6000.000 1000.000 01
7.37604097E+00 1.23449782E-02-4.26463882E-06 6.69045835E-10-3.92202554E-14 2
1.77332960E+04-1.61758204E+01-3.32899442E+00 5.38423469E-02-7.65500752E-05 3
6.35512285E-08-2.14283003E-11 2.03420628E+04 3.68038362E+01 4
C3H5-S 8/12/15 C 3H 5 0 0G 300.000 5000.000 1390.000 11
7.95954498E+00 1.11163183E-02-3.75197834E-06 5.77246260E-10-3.32768957E-14 2
2.80567891E+04-1.79800372E+01 1.61793372E+00 2.44803904E-02-1.41856503E-05 3
4.16402233E-09-4.90904795E-13 3.04291037E+04 1.66341443E+01 4
C3H5-T 8/12/15 C 3H 5 0 0G 300.000 5000.000 1376.000 11
7.69949212E+00 1.17803985E-02-4.07791749E-06 6.38119222E-10-3.72229675E-14 2
2.61747145E+04-1.68305890E+01 2.29256998E+00 1.98527646E-02-6.42635654E-06 3
-5.90016395E-10 5.05491095E-13 2.85773377E+04 1.39407124E+01 4
C3H5O KPS12 C 3H 5O 1 0G 300.000 5000.000 1402.000 01
1.02638186E+01 1.17609932E-02-3.89837957E-06 5.92650815E-10-3.38867417E-14 2
7.25938472E+03-2.75108651E+01 8.24068673E-01 3.46749909E-02-2.51786795E-05 3
9.56781953E-09-1.48085302E-12 1.04203725E+04 2.28283070E+01 4
AC3H5OOH GOLDSMITH C 3H 6O 2 0G 298.0 6000.0 1000.000 31
1.20838649E+01 1.47946591E-02-5.13212591E-06 8.07504999E-10-4.74394983E-14 2

-1.02184463E+04-3.36434791E+01 3.18124993E+00 4.35233041E-02-5.16277353E-05 3
4.32011427E-08-1.57714983E-11-7.63521503E+03 1.21725683E+01 4
C3H4-P T 2/90H 4 C 3 0 0 G 200.000 6000.00 1000.00 1
0.60252400E+01 0.11336542E-01-0.40223391E-05 0.64376063E-09-0.38299635E-13 2
0.19620942E+05-0.86043785E+01 0.26803869E+01 0.15799651E-01 0.25070596E-05 3
-0.13657623E-07 0.66154285E-11 0.20802374E+05 0.98769351E+01 0.22302059E+05 4
C3H4-A L 8/89C 3 H 4 0 0 G 200.000 6000.00 1000.00 1
0.63168722E+01 0.11133728E-01-0.39629378E-05 0.63564238E-09-0.37875540E-13 2
0.20117495E+05-0.10995766E+02 0.26130445E+01 0.12122575E-01 0.18539880E-04 3
-0.34525149E-07 0.15335079E-10 0.21541567E+05 0.10226139E+02 0.22962267E+05 4
HOCHO L 8/88H 2C 1O 2 0G 200.0000 6000.0000 1000.00 1
4.61383160e+00 6.44963640e-03-2.29082510e-06 3.67160470e-10-2.18736750e-14 2
-4.75055381e+04 8.57943900e-01 2.94556779e+00 4.50339570e-03 1.19287605e-05 3
-1.55602334e-08 5.30043911e-12-4.66866299e+04 1.11969030e+01 4
C3H2 T12/00C 3 H 2 0 0 G 200.000 6000.00 1000.00 1
6.67324762E+00 5.57728845E-03-1.99180164E-06 3.20289156E-10-1.91216272E-14 2
7.57571184E+04-9.72894405E+00 2.43417332E+00 1.73013063E-02-1.18294047E-05 3
1.02756396E-09 1.62626314E-12 7.69074892E+04 1.21012230E+01 7.83005132E+04 4
C3H2(S) 0C 3H 2 0 0G 200.000 5000.000 900.00 0 1
0.77642570E+01 0.47112774E-02-0.16170637E-05 0.25472406E-09-0.15038572E-13 2
0.66849672E+05-0.15098549E+02 0.52976482E+01 0.16987466E-01-0.24266517E-04 3
0.18653681E-07-0.55763001E-11 0.67240466E+05-0.37540041E+01 4
SC3H4OH 3/28/13 C 3H 5O 1 0G 300.000 5000.000 1407.000 21
1.20968484E+01 9.43976596E-03-3.10773897E-06 4.69609188E-10-2.67165710E-14 2
-3.85854894E+02-3.76795997E+01 1.72870561E+00 4.41015870E-02-4.72013860E-05 3
2.52073596E-08-5.13375710E-12 2.22720503E+03 1.43928257E+01 4
C3H3 T 7/11C 3 H 3 0 0 G 200.0000 6000.0000 1000.00 1
7.14221719e+00 7.61902211e-03-2.67460030e-06 4.24914904e-10-2.51475443e-14 2
3.95710114e+04-1.25848129e+01 1.34577939e+00 3.27862238e-02-4.75146981e-05 3
3.77892566e-08-1.19201553e-11 4.07684638e+04 1.52273795e+01 4
C3H3O 2/17/14 CZHOUH 3C 3O 1 G 298.150 2000.000 1000.00 1
4.19355696E+00 1.95625103E-02-1.22336450E-05 3.90615061E-09-5.08539231E-13 2
3.14931737E+04 5.03216224E+00 8.75023836E-01 3.51184068E-02-3.89901356E-05 3
2.40255750E-08-6.10883631E-12 3.20427921E+04 2.04717253E+01 4
C2H3CHO KPS12 C 3H 4O 1 0G 300.000 5000.000 1398.000 01
9.99155394E+00 9.82348001E-03-3.31203088E-06 5.09524422E-10-2.93821890E-14 2
-1.25303509E+04-2.85168883E+01 7.33844455E-01 3.17482671E-02-2.29599468E-05 3
8.42104232E-09-1.23613478E-12-9.38473548E+03 2.10308851E+01 4
C2H3CO KPS12 C 3H 3O 1 0G 300.000 5000.000 1395.000 01
8.86032735E+00 8.48985205E-03-2.90350080E-06 4.50763986E-10-2.61524281E-14 2
7.73489171E+03-2.06978792E+01 1.65335195E+00 2.57402596E-02-1.89009911E-05 3
7.29174972E-09-1.16083226E-12 1.02020654E+04 1.78705872E+01 4
CH3COCH2 2/14/13 THERMC 3H 5O 1 0G 300.000 5000.000 1387.000 21
1.09524298E+01 1.11458668E-02-3.86262877E-06 6.05088857E-10-3.53293362E-14 2
-9.60833727E+03-3.15622776E+01 1.13381826E+00 3.25095045E-02-2.10424651E-05 3
6.64421151E-09-8.12618901E-13-6.04868361E+03 2.17158655E+01 4

CH3CHCHO C 3H 5O 1 0G 300.0000 5000.0000 1424.00 1
1.06781476e+01 1.12805711e-02-3.89010759e-06 6.07617268e-10-3.54120848e-14 2
-7.73356095e+03-3.24986051e+01 1.50820655e+00 2.66659824e-02-9.43206175e-06 3
-1.66802213e-09 1.19759861e-12-4.04506558e+03 1.87193427e+01 4
CH3CHCO 8/8/12 GMGH 4C 3O 1 G 100.000 5000.000 1106.37 1
5.96288513E+00 1.50316128E-02-6.05409922E-06 1.11097563E-09-7.67696576E-14 2
-1.04134572E+04-4.59703062E+00 3.00496509E+00 1.83622137E-02-5.86273596E-07 3
-8.19950383E-09 3.38640683E-12-9.30827849E+03 1.20089218E+01 4
IC4H9 8/12/15 C 4H 9 0 0G 300.000 5000.000 1397.000 31
1.23261837E+01 1.92057770E-02-6.52063623E-06 1.00704497E-09-5.82038734E-14 2
2.50995714E+03-4.13478742E+01 1.20802408E-01 4.73187324E-02-3.16440251E-05 3
1.14229699E-08-1.74784642E-12 6.84032915E+03 2.44291032E+01 4
TC4H9 8/12/15 C 4H 9 0 0G 300.000 5000.000 1380.000 31
1.02682832E+01 2.09965262E-02-7.14945754E-06 1.10648358E-09-6.40498314E-14 2
1.57542675E+02-3.00960941E+01 1.05841769E+00 3.41133739E-02-9.03156779E-06 3
-2.95313136E-09 1.41436845E-12 4.22699258E+03 2.23965051E+01 4
IC3H5CO C 4H 5O 1 0G 300.000 5000.000 1396.000 21
1.29634401E+01 1.17954996E-02-4.04361488E-06 6.28771516E-10-3.65209867E-14 2
-8.26519462E+02-4.20562575E+01 1.87306990E+00 3.95188508E-02-3.11404053E-05 3
1.28844447E-08-2.18165308E-12 2.85270691E+03 1.68774016E+01 4
IC4H9O2 9/ 1/12 C 4H 9O 2 0G 300.000 5000.000 1432.000 41
1.78793870E+01 1.82474607E-02-6.01252193E-06 9.11106794E-10-5.20018932E-14 2
-1.74569774E+04-6.61552973E+01 1.77219624E+00 5.34032789E-02-3.31041810E-05 3
9.24465657E-09-8.01706642E-13-1.17768774E+04 2.09581481E+01 4
TC4H9O2 9/ 1/12 C 4H 9O 2 0G 300.000 5000.000 1380.000 41
1.80863238E+01 1.99282971E-02-6.98287309E-06 1.10171726E-09-6.46381057E-14 2
-2.04420664E+04-6.97533212E+01 2.63892371E+00 5.44717499E-02-3.75504698E-05 3
1.40479250E-08-2.27968600E-12-1.47598933E+04 1.40325533E+01 4
IC4H8O2H-I 9/ 1/12 C 4H 9O 2 0G 300.000 5000.000 1414.000 51
1.83915486E+01 1.73042831E-02-5.66841018E-06 8.55414265E-10-4.86781778E-14 2
-9.48569748E+03-6.67673286E+01 1.86432620E-01 6.26430177E-02-4.83690886E-05 3
1.88657148E-08-2.91189385E-12-3.59086611E+03 2.97635367E+01 4
IC4H8O2H-T 9/ 1/12 C 4H 9O 2 0G 300.000 5000.000 1413.000 51
1.69753885E+01 1.85198010E-02-6.09075415E-06 9.21673609E-10-5.25502501E-14 2
-1.14812757E+04-5.88259039E+01 3.84374544E+00 4.36800978E-02-2.07599526E-05 3
2.51709167E-09 5.41306513E-13-6.50766215E+03 1.34244877E+01 4
IC4H8 8/12/15 C 4H 8 0 0G 300.0000 5000.0000 1392.00 1
1.11444028e+01 1.81609265e-02-6.17791116e-06 9.55481871e-10-5.52826092e-14 2
-7.83360374e+03-3.68427105e+01-1.58177255e-01 4.33182744e-02-2.84827170e-05 3
1.08143707e-08-1.94336997e-12-3.70029021e+03 2.44698953e+01 4
IC4H7 8/12/15 C 4H 7 0 0G 300.0000 5000.0000 1384.00 1
1.18999143e+01 1.51569859e-02-5.09995449e-06 7.83722199e-10-4.51660275e-14 2
1.00412972e+04-4.02225555e+01-3.93867491e-01 4.29625224e-02-2.94297021e-05 3
1.09428139e-08-1.82173503e-12 1.44109428e+04 2.61658302e+01 4
IC4H7-I1 5/13/15 C 4H 7 0 0G 300.0000 5000.0000 1396.00 1
1.11158752e+01 1.55127192e-02-5.23769366e-06 8.05998394e-10-4.64703390e-14 2

2.19546869e+04-3.41368426e+01 7.23581491e-01 4.02155569e-02-2.88825033e-05 3
1.19333399e-08-2.22819625e-12 2.55823066e+04 2.16527592e+01 4
IC4H7O 4/ 3/ 0 THERMC 4H 7O 1 0G 300.0000 5000.0000 1386.00 1
1.33457615e+01 1.61218588e-02-5.44376403e-06 8.38199374e-10-4.83608280e-14 2
6.16344043e+02-4.36758305e+01 1.58484533e+00 4.19406786e-02-2.71769161e-05 3
9.54715871e-09-1.52856249e-12 4.88586206e+03 2.01308525e+01 4
C4H8-1 C 4H 8 0 0G 300.0000 5000.0000 1388.00 1
1.10189295e+01 1.82714177e-02-6.21801907e-06 9.62038611e-10-5.56791341e-14 2
-5.80393315e+03-3.47867626e+01-3.61777665e-02 4.15291809e-02-2.51105967e-05 3
8.50487415e-09-1.40258913e-12-1.63431991e+03 2.56471981e+01 4
C4H6 C 4H 6 0 0G 300.000 5000.000 1388.000 11
1.01064561E+01 1.46248415E-02-5.01373934E-06 7.79510645E-10-4.52675769E-14 2
9.96133753E+03-2.97310638E+01 1.01356056E+00 3.35722771E-02-1.96279376E-05 3
5.74803850E-09-6.75029065E-13 1.33956759E+04 1.99957382E+01 4
PC4H9 8/12/15 C 4H 9 0 0G 300.0000 5000.0000 1393.00 1
1.18547949e+01 1.96962095e-02-6.71054229e-06 1.03891144e-09-6.01513573e-14 2
3.38823494e+03-3.72264496e+01 2.01470162e-01 4.44403445e-02-2.71094585e-05 3
9.31612022e-09-1.54895901e-12 7.76384720e+03 2.64009986e+01 4
C4H72-1OOH C 4H 8O 2 0G 300.0000 5000.0000 1381.00 1
1.80122740e+01 1.70340943e-02-5.89884086e-06 9.23962123e-10-5.39539803e-14 2
-1.74485924e+04-6.55086671e+01 9.64840717e-01 5.83131973e-02-4.64513227e-05 3
2.06106668e-08-4.03209051e-12-1.15717503e+04 2.57513285e+01 4
C4H71-3OOH C 4H 8O 2 0G 300.0000 5000.0000 1392.00 1
1.92985494e+01 1.54534427e-02-5.25460431e-06 8.13772446e-10-4.71689947e-14 2
-1.84918728e+04-7.49822387e+01-1.78454606e+00 7.05029324e-02-6.20768013e-05 3
2.84904671e-08-5.39904245e-12-1.17746358e+04 3.61899577e+01 4
C4H5OH-13 9/24/15 C 4H 6O 1 0G 300.0000 5000.0000 1405.00 1
1.40975061e+01 1.29826578e-02-4.36356696e-06 6.69260196e-10-3.84920001e-14 2
-1.40973972e+04-4.94187354e+01-1.99457801e+00 6.40503996e-02-6.83762138e-05 3
3.73891978e-08-8.02932171e-12-9.73513998e+03 3.24814285e+01 4
C4H5-N H6W/94C 4H 5 0 0G 300.000 3000.00 1000.00 1
0.98501978E+01 0.10779008E-01-0.13672125E-05-0.77200535E-09 0.18366314E-12 2
0.38840301E+05-0.26001846E+02 0.16305321E+00 0.39830137E-01-0.34000128E-04 3
0.15147233E-07-0.24665825E-11 0.41429766E+05 0.23536163E+02 4
C4H3-N H6W/94C 4H 3 0 0G 300.000 3000.00 1000.00 1
0.54328279E+01 0.16860981E-01-0.94313109E-05 0.25703895E-08-0.27456309E-12 2
0.61600680E+05-0.15673981E+01-0.31684113E+00 0.46912100E-01-0.68093810E-04 3
0.53179921E-07-0.16523005E-10 0.62476199E+05 0.24622559E+02 4
C4H2 D11/99C 4H 2 0 0G 300.000 3000.000 1000. 1
0.91576328E+01 0.55430518E-02-0.13591604E-05 0.18780075E-10 0.23189536E-13 2
0.52588039E+05-0.23711460E+02 0.10543978E+01 0.41626960E-01-0.65871784E-04 3
0.53257075E-07-0.16683162E-10 0.54185211E+05 0.14866591E+02 4
H2C4O 120189H 2C 4O 1 G 0300.00 4000.00 1000.00 1
0.01026888E+03 0.04896164E-01-0.04885081E-05-0.02708566E-08 0.05107013E-12 2
0.02346903E+06-0.02815985E+03 0.04810971E+02 0.01313999E+00 0.09865073E-05 3
-0.06120720E-07 0.01640003E-10 0.02545803E+06 0.02113424E+02 4

C-C6H4 H6W/94C 6H 4 0 0G 300.000 3000.00 1000.00 1
0.13849209E+02 0.78807920E-02 0.18243836E-05-0.21169166E-08 0.37459977E-12 2
0.47446340E+05-0.50404953E+02-0.30991268E+01 0.54030564E-01-0.40839004E-04 3
0.10738837E-07 0.98078490E-12 0.52205711E+05 0.37415207E+02 4
C4H71-1 C 4H 7 0 0G 300.000 5000.000 1390.000 21
1.10531750E+01 1.55668782E-02-5.25853044E-06 8.09627095E-10-4.67015477E-14 2
2.39455759E+04-3.31548457E+01 8.97231085E-01 3.77003788E-02-2.33194855E-05 3
7.38468124E-09-9.50027900E-13 2.76498158E+04 2.19835413E+01 4
C4H71-3 1/13/16 C 4H 7 0 0G 300.000 5000.000 1367.000 11
1.16977564E+01 1.53404517E-02-5.16928607E-06 7.95431212E-10-4.58914150E-14 2
1.07395001E+04-3.82992966E+01 9.40350126E-01 3.56830321E-02-1.74384567E-05 3
2.78964567E-09 1.78068599E-13 1.49303203E+04 2.11349333E+01 4
C4H71-1O2 9/29/15 C 4H 7O 2 0G 300.000 5000.000 1390.000 31
1.63738534E+01 1.62685376E-02-5.62192103E-06 8.78982520E-10-5.12510706E-14 2
-1.06318473E+03-5.69005716E+01 2.02223104E+00 4.85577506E-02-3.30293697E-05 3
1.13406677E-08-1.57078109E-12 4.04143594E+03 2.06106646E+01 4
C6H101-5 4/12/13 THERMC 6H 10 0 0G 300.0000 5000.0000 1413.00 1
1.60456030e+01 2.34774145e-02-7.85797929e-06 1.20200542e-09-6.90100029e-14 2
2.12537311e+03-5.88374564e+01-1.21046499e+00 6.52237687e-02-4.72810055e-05 3
1.87420247e-08-3.20571254e-12 7.95992435e+03 3.33283154e+01 4
C6H9-A 12/ 5/12 THERMC 6H 9 0 0G 300.000 5000.000 1400.000 21
1.70842767E+01 2.08842788E-02-7.14529004E-06 1.10943563E-09-6.43676989E-14 2
2.01040204E+04-6.39326012E+01-2.66715213E+00 7.26196475E-02-6.05323920E-05 3
2.66000571E-08-4.74613408E-12 2.64415017E+04 4.02220332E+01 4
C8H18-25 12/15/12 THERMC 8H 18 0 0G 300.000 5000.000 1392.000 71
2.54549930E+01 3.96534052E-02-1.36162044E-05 2.11932528E-09-1.23169412E-13 2
-3.99732909E+04-1.11331149E+02-2.48400000E+00 1.01584567E-01-6.59154027E-05 3
2.22814321E-08-3.13617796E-12-2.98376225E+04 4.00669711E+01 4
C8H17 12/15/12 THERMC 8H 17 0 0G 300.000 5000.000 1392.000 71
2.50528860E+01 3.75424475E-02-1.29087897E-05 2.01103405E-09-1.16949199E-13 2
-1.49296270E+04-1.04979739E+02-2.20231551E+00 9.91224727E-02-6.64580522E-05 3
2.34921991E-08-3.48441290E-12-5.14931643E+03 4.23154141E+01 4
C8H17-OO 12/12 THERMC 8H 17O 2 0G 300.000 5000.000 1393.000 91
2.93041783E+01 3.81477400E-02-1.31116317E-05 2.04214228E-09-1.18740222E-13 2
-3.66435601E+04-1.23570485E+02 1.76077843E-01 1.05080844E-01-7.24414803E-05 3
2.63052810E-08-3.98759611E-12-2.63323923E+04 3.33999909E+01 4
C8-QOOH 12/12 THERMC 8H 17O 2 0G 300.000 5000.000 1397.000 91
3.08469483E+01 3.66472441E-02-1.25522210E-05 1.95048773E-09-1.13228730E-13 2
-3.03655555E+04-1.31024666E+02 3.32952494E-01 1.10303073E-01-8.17355603E-05 3
3.20089396E-08-5.18458745E-12-1.99621147E+04 3.20842468E+01 4
C8-OOQOOH 1212 THERMC 8H 17O 4 0G 300.000 5000.000 1392.000 91
3.61352084E+01 3.69959669E-02-1.28081851E-05 2.00491973E-09-1.16994942E-13 2
-5.11210723E+04-1.54312332E+02 2.88820077E+00 1.12415349E-01-7.75570077E-05 3
2.70847142E-08-3.82475488E-12-3.93610240E+04 2.50245710E+01 4
C8-KET 1212 THERMC 8H 16O 3 0G 300.000 5000.000 1397.000 91
3.34809894E+01 3.47621921E-02-1.19833298E-05 1.87043640E-09-1.08930292E-13 2

-6.45979401E+04-1.44426807E+02 2.91696872E-01 1.13808624E-01-8.42781606E-05 3
3.20829993E-08-4.97097770E-12-5.32590508E+04 3.32229986E+01 4
C6H13CO C 7H 13O 1 G 0300.00 5000.00 1000.00 1
1.94783812E+01 2.50466029E-02-8.54861346E-06 1.32557944E-09-7.68503296E-14 2
-2.07923937E+04-7.21995578E+01 2.14479069E+00 6.17863563E-02-3.74134690E-05 3
1.13283795E-08-1.36917698E-12-1.43451172E+04 2.23128045E+01 4
NC12H26 H 26O 0C 12 0G 300 5000 1000 1
9.97283422E+00 1.07615296E-01-4.89001251E-05 8.23896743E-09 0.00000000E+00 2
-4.31954165E+04-1.35346202E+01-2.62181594E+00 1.47237711E-01-9.43970271E-05 3
3.07441268E-08-4.03602230E-12-4.00654253E+04 5.00994626E+01 4
C12H25 H 25O 0C 12 0G 300 5000 1000 1
1.05038381E+01 1.03781439E-01-4.72009520E-05 7.95823570E-09 0.00000000E+00 2
-1.85218187E+04-1.30420516E+01-1.85028741E+00 1.42670708E-01-9.18916555E-05 3
3.00883392E-08-3.97454300E-12-1.54530435E+04 4.93702421E+01 4
C12H25-OO H 25O 2C 12 0G 300 5000 1000 1
1.23894782E+01 1.08048928E-01-4.88652961E-05 8.15401282E-09 0.00000000E+00 2
-3.76523809E+04-1.71146487E+01 1.58304260E+00 1.42768096E-01-8.97641809E-05 3
2.90200208E-08-3.87985556E-12-3.50130986E+04 3.72784659E+01 4
C12-QOOH H 25O 2C 12 0G 300 5000 1000 1
1.27466803E+01 1.09092599E-01-5.04380562E-05 8.60701975E-09 0.00000000E+00 2
-3.13603674E+04-1.67749779E+01 1.42078475E+00 1.44039473E-01-8.95663728E-05 3
2.73266131E-08-3.21225523E-12-2.85025839E+04 4.06420206E+01 4
C12-OOQOOH H 25O 4C 12 0G 300 5000 1000 1
1.51871349E+01 1.15993054E-01-5.46645659E-05 9.41993241E-09 0.00000000E+00 2
-5.13250050E+04-2.70027681E+01 3.14841764E+00 1.53204599E-01-9.64230273E-05 3
2.94570879E-08-3.45152229E-12-4.82915577E+04 3.40092586E+01 4
C12-KET H 24O 3C 12 0G 300 5000 1000 1
1.68711079E+01 1.02964968E-01-4.66434716E-05 7.80054730E-09 0.00000000E+00 2
-6.72051106E+04-3.91545673E+01 2.09319905E+00 1.50718255E-01-1.03321455E-04 3
3.70082886E-08-5.50513600E-12-6.36120922E+04 3.51536853E+01 4
C12H24 H 24O 0C 12 0G 300 5000 1000 1
9.89916240E+00 1.01613270E-01-4.62099791E-05 7.79130314E-09 0.00000000E+00 2
-2.92166047E+04-1.15674133E+01-2.43874931E+00 1.40512846E-01-9.10032977E-05 3
3.00308587E-08-4.00790141E-12-2.61556835E+04 5.07457348E+01 4
C12H23 H 23O 0C 12 0G 300 5000 1000 1
8.98672959E+00 1.00339497E-01-4.62145144E-05 7.88149275E-09 0.00000000E+00 2
-5.42684121E+03-3.84845990E+00-2.11314538E+00 1.34620184E-01-8.46497174E-05 3
2.63093386E-08-3.17345456E-12-2.62784580E+03 5.24144232E+01 4
C6H6 G 6/01C 6H 6 0 0G 200.000 6000.000 1000.000 1
1.10809576E+01 2.07176746E-02-7.52145991E-06 1.22320984E-09-7.36091279E-14 2
4.30641035E+03-4.00413310E+01 5.04818632E-01 1.85020642E-02 7.38345881E-05 3
-1.18135741E-07 5.07210429E-11 8.55247913E+03 2.16412893E+01 9.96811598E+03 4
C6H5 T04/02C 6H 5 0 0G 200.000 6000.000 1000. 1
1.08444762E+01 1.73212473E-02-6.29233249E-06 1.02369961E-09-6.16216828E-14 2
3.55598475E+04-3.53735134E+01 2.10306633E-01 2.04745507E-02 5.89743006E-05 3
-1.01534255E-07 4.47105660E-11 3.95468722E+04 2.52910455E+01 4.08610970E+04 4

C6H5OH L 4/84C 6H 6O 1 0G 300.000 5000.000 1000. 1
0.14912073E+02 0.18378135E-01-0.61983128E-05 0.91983221E-09-0.49209565E-13 2
-0.18375199E+05-0.55924103E+02-0.16956539E+01 0.52271299E-01-0.72024050E-05 3
-0.35859603E-07 0.20449073E-10-0.13284121E+05 0.32542160E+02-0.11594207E+05 4
C6H5O T05/02C 6H 5O 1 0G 200.000 6000.000 1000. 1
1.37221720E+01 1.74688771E-02-6.35504520E-06 1.03492308E-09-6.23410504E-14 2
2.87274751E+02-4.88181680E+01-4.66204455E-01 4.13443975E-02 1.32412991E-05 3
-5.72872769E-08 2.89763707E-11 4.77858391E+03 2.76990274E+01 6.49467016E+03 4
C5H5 TAK0505C 5H 5 0 0G 298.150 3500.000 969.35 1
1.33675715E+00 3.24793912E-02-1.67587774E-05 4.03514137E-09-3.70739036E-13 2
3.00730524E+04 1.60315806E+01-3.97555452E+00 7.41370991E-02-1.11803345E-04 3
9.04628776E-08-2.80999747E-11 3.01769405E+04 3.67153636E+01 4
C3H5-S H 5C 3 G 300.0 5000.0 1390.0 1
7.95954498E0 1.11163183E-2 -3.75197834E-6 5.7724626E-10-3.32768957E-14 2
2.80567891E4 -1.79800372E1 1.61793372E0 2.44803904E-2 -1.41856503E-5 3
4.16402233E-9-4.90904795E-13 3.04291037E4 1.66341443E1 4
C8H9 H 9C 8 G 298.0 5000.0 1384.0 1
1.78733446E1 2.58674252E-2 -8.99034932E-6 1.41079575E-9-8.24625224E-14 2
2.328925E4 -7.07794812E1 -2.38189244E0 7.20549781E-2 -5.03283046E-5 3
1.8869002E-8-3.01760355E-12 3.0583665E4 3.86532413E1 4
C8H9O H 9O 1C 8 G 300.0 5000.0 1398.0 1
2.13847355E1 2.3953936E-2 -8.0177241E-6 1.22754526E-9-7.05549832E-14 2
-1.16892915E4 -8.84209016E1 -3.63403106E0 8.80898074E-2 -7.1667001E-5 3
3.01294215E-8-5.10086525E-12 -3.64481803E3 4.38023349E1 4
C8H9OO H 9O 2C 8 G 300.0 5000.0 1392.0 1
2.20747829E1 2.62304897E-2 -8.95585441E-6 1.38908492E-9-8.05473928E-14 2
-2.75188213E3 -8.72984931E1 -2.23167844E0 8.71497326E-2 -6.89429495E-5 3
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C9H12 H 12C 9 G 298.0 5000.0 1392.0 1
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1.70244194E-8-1.86084863E-12 -4.16066788E3 4.63565635E1 4
C8H9CH2 H 11C 9 G 300.0 5000.0 1392.0 1
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5.13256E3 -1.04769621E2 -3.79062417E0 9.28655286E-2 -6.77602501E-5 3
2.49733918E-8-3.69121942E-12 1.46246024E4 4.39198526E1 4
C7H9 H 9C 7 G 300.0 5000.0 1385.0 1
1.58794665E1 2.47334017E-2 -8.53285789E-6 1.33212022E-9-7.75762212E-14 2
1.54411482E4 -6.02035236E1 2.28626781E0 5.31316327E-2 -3.16146307E-5 3
1.02857614E-8-1.50423055E-12 2.06890843E4 1.43119441E1 4
C8H9CH2O H 11O 1C 9 G 300.0 5000.0 1379.0 1
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2.31358247E1 2.81807117E-2 -9.62221828E-6 1.49399799E-9-8.67401397E-14 2

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C8H9CO H 9O 1C 9 G 300.0 5000.0 1374.0 1
2.32503E1 2.55969013E-2 -8.74279116E-6 1.3578281E-9-7.88519658E-14 2
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C7H9O H 9O 1C 7 G 300.0 5000.0 1372.0 1
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C8H10 H 10C 8 G 298.0 5000.0 1393.0 1
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Decalin H 18C 10 G 300.0 3500.0 1750.0 1
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-3.79226289E4 -1.35167747E2 -1.45870783E1 1.41956207E-1 -9.78878828E-5 3
3.36726212E-8-4.59507321E-12 -2.33632912E4 8.87980358E1 4
RDecalin H 17C 10 G 300.0 3500.0 1800.0 1
2.85620333E1 4.11366392E-2 -1.3602411E-5 2.01592783E-9-1.09376626E-13 2
-1.53025063E4 -1.39641687E2 -1.39601308E1 1.35630337E-1 -9.23471594E-5 3
3.11806495E-8-4.16003241E-12 5.47278088E0 9.04971362E1 4
RDec-OO H 17O 2C 10 G 300.0 3500.0 1800.0 1
1.72379174E1 3.76978745E-2 -1.66331315E-5 3.54555182E-9-3.00284988E-13 2
-1.92027471E4 -7.01676462E1 -6.00367537E0 8.93458584E-2 -5.96731181E-5 3
1.94862876E-8-2.51427606E-12 -1.08357738E4 5.56207021E1 4
Dec-QOOH H 17O 2C 10 G 300.0 3500.0 1800.0 1
1.72379174E1 3.76978745E-2 -1.66331315E-5 3.54555182E-9-3.00284988E-13 2
-1.92027471E4 -7.01676462E1 -6.00367537E0 8.93458584E-2 -5.96731181E-5 3
1.94862876E-8-2.51427606E-12 -1.08357738E4 5.56207021E1 4
Dec-OOQOOH H 17O 4C 10 G 300.0 3500.0 1800.0 1
1.72379174E1 3.76978745E-2 -1.66331315E-5 3.54555182E-9-3.00284988E-13 2
-1.92027471E4 -7.01676462E1 -6.00367537E0 8.93458584E-2 -5.96731181E-5 3
1.94862876E-8-2.51427606E-12 -1.08357738E4 5.56207021E1 4
Dec-KET H 16O 3C 10 G 300.0 3500.0 1460.0 1
1.16022418E1 3.57303662E-2 -1.34415883E-5 2.50437459E-9-1.89510289E-13 2
-3.63821557E4 -4.98532958E1 -8.02402159E0 8.95009509E-2 -6.86853396E-5 3
2.77298318E-8 -4.5089379E-12 -3.06512867E4 5.22593733E1 4
CYC6H10 H 10C 6 G 300.0 5000.0 1393.0 1
1.69201625E1 2.48608737E-2 -8.61766278E-6 1.35001194E-9-7.88190989E-14 2
-9.88586866E3 -7.27056327E1 -6.97415769E0 8.26568084E-2 -6.3042846E-5 3
2.50749274E-8-4.09857788E-12 -1.75447984E3 5.49728305E1 4

```
!------------------------------ C6H9 FROM Z.D.WANG
CYC6H9-3                T-2-92H      9C      6                G        298.15       3000.0    1000.0          1
      2.6295828E1     8.6828857E-3    -1.5770376E-6              0.0E0              0.0E0       2
      2.0863563E3     -1.2573825E2        -3.57143E0     6.1696043E-2    -2.6928803E-5       3
            0.0E0              0.0E0       1.3657039E4        3.998625E1                      4
C4H7                    H      7C      4                G        300.0        5000.0    1392.0          1
     1.12103578E1    1.60483196E-2 -5.46502292E-6 8.45941053E-10-4.89772739E-14       2
     1.09041937E4    -3.55593015E1 -3.50508352E-1    4.26511243E-2 -2.90979373E-5       3
    1.05403914E-8-1.60059854E-12      1.49933591E4      2.67295696E1                      4
DCYC10H16               H     16C     10                G        300.0        5000.0    1391.0          1
     3.05217184E1    3.97463189E-2 -1.39776808E-5    2.21121412E-9-1.29991361E-13       2
    -2.54153937E4    -1.53290995E2      -1.6542703E1    1.48067434E-1 -1.07756098E-4       3
     3.8503536E-8-5.42883606E-12    -9.05931339E3      9.98013349E1                      4
DCLD1-3R                H     15C     10                G        300.0        5000.0    1378.0          1
     3.03440494E1    3.80059782E-2 -1.35288736E-5    2.15742935E-9-1.27533348E-13       2
    -9.75573088E3    -1.53898607E2    -1.62174834E1    1.39435172E-1 -9.44648383E-5       3
    2.99826664E-8-3.54694362E-12      7.01419628E3       9.855346E1                      4
C8H12                   H     12C      8                G        300.0        5000.0    1000.0          1
       1.976428E1      2.9963946E-2    -9.7380325E-6     1.5051418E-9 -9.0761525E-14       2
      7.7515449E3      -7.3911842E1       -1.546801E0       8.393272E-2    -5.4211614E-5       3
     1.2875682E-8     3.4034136E-13       1.3973911E4       3.766996E1                      4
X135C6H7-3R             H      7C      6                G        300.0        5000.0    1398.0          1
     1.62688437E1    1.6985742E-2 -5.81636908E-6 9.03502401E-10-5.24327982E-14       2
     4.00858043E4    -6.00702658E1    -1.53698406E0    6.84728803E-2    -6.4766571E-5       3
    3.18058294E-8-6.17696288E-12      4.53855976E4      3.22250772E1                      4
!------------------------------ C5H7 FROM Z.D.WANG
LC5H7                   L-1-05H      7C      5                G        200.0        6000.0    1000.0          1
     1.00547248E1      2.099234E-2 -7.61351868E-6    1.23001919E-9-7.35400707E-14       2
     1.98179446E4    -2.63876649E1      3.25248853E0      1.8069592E-2    4.89541094E-5       3
  -7.98199491E-8 3.41337844E-11       2.2646706E4      1.37042774E1                      4
CYC5H5                  -ITTEDH      5C      5                G        300.0        3000.0    1000.0          1
     4.21464919E0    2.71834728E-2 -1.33173209E-5    3.08980119E-9-2.77879873E-13       2
     2.88952416E4 -3.05999781E-2    -7.37844042E0    9.72391818E-2 -1.69579138E-4       3
    1.51818667E-7-5.12075479E-11      3.05514662E4      5.12829539E1                      4
CYC5H6                  T-1-90H      6C      5                G        200.0        6000.0    1000.0          1
      9.9757848E0      1.8905543E-2    -6.8411461E-6      1.109934E-9 -6.6680236E-14       2
      1.1081693E4      -3.2209454E1      8.6108957E-1      1.4804031E-2    7.2108895E-5       3
    -1.1338055E-7    4.8689972E-11       1.4801755E4       2.1353453E1                      4
!--------------------------- C6H8 FROM Z.D.WANG
CYC6H8-13               T-2-90H      8C      6                G        200.0        6000.0    1000.0          1
       1.177987E1      2.551998E-2    -9.2666947E-6     1.5068122E-9 -9.0658701E-14       2
      6.5486686E3      -4.1618805E1       1.7265319E0      1.4887612E-2    9.480923E-5       3
    -1.4083394E-7    5.8859873E-11       1.1021297E4       1.9130886E1                      4
C6H9-13-6               A05-05H      9C      6                G        200.0        6000.0    1000.0          1
     1.29128125E1    2.49789213E-2 -8.89951453E-6    1.42497072E-9-8.47614769E-14       2
     2.59325675E4    -3.64160038E1      1.8554664E0    4.92225637E-2 -2.28412959E-5       3
```

8.06990651E-10 1.28870367E-12 2.93951548E4 2.25553124E1 4
CH2(S) IU6/03C 1 H 2 0 0 G 200.000 6000.00 1000.00 1
3.13501686E+00 2.89593926E-03-8.16668090E-07 1.13572697E-10-6.36262835E-15 2
5.05040504E+04 4.06030621E+00 4.19331325E+00-2.33105184E-03 8.15676451E-06 3
-6.62985981E-09 1.93233199E-12 5.03662246E+04-7.46734310E-01 5.15727280E+04 4
CHV 073003C 1H 1 G 0300.00 5000.00 1000.00 1
0.02196223E+02 0.02340381E-01-0.07058201E-05 0.09007582E-09-0.03855040E-13 2
0.10419559E+06 0.09178373E+02 0.03200202E+02 0.02072875E-01-0.05134431E-04 3
0.05733890E-07-0.01955533E-10 0.10393714E+06 0.03331587E+02 4
HCOH MAR94 C 1H 2O 1 0G 300. 5000. 1398. 1
9.18749272E+00 1.52011152E-03-6.27603516E-07 1.09727989E-10-6.89655128E-15 2
7.81364593E+03-2.73434214E+01-2.82157421E+00 3.57331702E-02-3.80861580E-05 3
1.86205951E-08-3.45957838E-12 1.12956672E+04 3.48487757E+01 4
HOCH2O2H 9/ 1/12 C 1H 4O 3 0G 300.000 5000.000 1398.000 21
1.24531886E+01 7.18221110E-03-2.47029548E-06 3.85611737E-10-2.24774193E-14 2
-4.24862928E+04-3.58745197E+01 5.35189713E-01 3.73266553E-02-3.15299511E-05 3
1.30352583E-08-2.11473264E-12-3.86609415E+04 2.71776082E+01 4
OCHO ATCT/AC 1 O 2 H 1 0 G 200.000 6000.000 1000.00 1
4.14394211E+00 5.59738818E-03-1.99794019E-06 3.16179193E-10-1.85614483E-14 2
-1.72459887E+04 5.07778617E+00 4.68825921E+00-4.14871834E-03 2.55066010E-05 3
-2.84473900E-08 1.04422559E-11-1.69867041E+04 4.28426480E+00-1.55992356E+04 4
CHCHO H 2C 2O 1 G 298.150 2000.000 1000.00 1
4.92632910E+00 9.71712147E-03-5.54855980E-06 1.53068537E-09-1.64742462E-13 2
2.89499494E+04 5.27874677E-01 2.33256751E+00 1.62952986E-02-9.72052177E-06 3
5.15124155E-10 1.03836514E-12 2.96585452E+04 1.39904923E+01 4
PC2H4OH 8/12/15 C 2H 5O 1 0G 300.000 5000.000 1395.000 21
8.06750150E+00 1.06143554E-02-3.57999360E-06 5.50363760E-10-3.17051769E-14 2
-6.92747939E+03-1.53833428E+01 2.59479867E+00 2.27100669E-02-1.39473846E-05 3
4.70095591E-09-6.90044236E-13-4.91486975E+03 1.43240718E+01 4
O2C2H4OH 9/ 1/12 THERMC 2H 5O 3 0G 300.000 5000.000 1506.000 41
1.27503881E+01 1.11514325E-02-3.83473891E-06 5.98155829E-10-3.48372108E-14 2
-2.52770876E+04-3.54317608E+01 7.04009800E+00 1.59564166E-02 2.21097416E-06 3
-7.05197355E-09 2.08266026E-12-2.24524432E+04-1.75361758E+00 4
C5H4O T 8/99C 5H 4O 1 0G 200.000 6000.000 1000. 1
1.00806824E+01 1.61143465E-02-5.83314509E-06 9.46759320E-10-5.68972206E-14 2
1.94364771E+03-2.94521623E+01 2.64576497E-01 3.34873827E-02 1.67738470E-06 3
-2.96207455E-08 1.54431476E-11 5.11159287E+03 2.35409513E+01 6.64245999E+03 4
HOCH2O 000000H 3O 2C 1 G 300.00 5000.00 1000.00 1
1.72976110E+00 1.61486804E-02-7.75692098E-06 1.37089042E-09 0.00000000E+00 2
-2.22802407E+04 1.91890617E+01 4.11183145E+00 7.53850697E-03 3.77337370E-06 3
-5.38746005E-09 1.45615887E-12-2.28023001E+04 7.46807254E+00 4
RP3 121286O 1H 1 G 0300.00 5000.00 1000.00 1
+2.88273000E+00+1.01397430E-03-2.27687700E-07+2.17468300E-11-5.12630500E-16 2
+5.02650000E+04+5.59571200E+00+3.63726600E+00+1.85091000E-04-1.67616460E-06 3
+2.38720200E-09-8.43144200E-13+5.00213000E+04+1.35886050E+00+0.00000000E+00 4

H2CN 41687H 2C 1N 1 G 300.00 4000.000 1000.000 1
0.52097030E+01 0.29692911E-02-0.28555891E-06-0.16355500E-09 0.30432589E-13 2
0.27677109E+05-0.44444780E+01 0.28516610E+01 0.56952331E-02 0.10711400E-05 3
-0.16226120E-08-0.23511081E-12 0.28637820E+05 0.89927511E+01 4
HCN GRI/98H 1C 1N 1 G 200.000 6000.000 1000.000 1
0.38022392E+01 0.31464228E-02-0.10632185E-05 0.16619757E-09-0.97997570E-14 2
0.14407292E+05 0.15754601E+01 0.22589886E+01 0.10051170E-01-0.13351763E-04 3
0.10092349E-07-0.30089028E-11 0.14712633E+05 0.89164419E+01 4
HNO And93 H 1N 1O 1 G 200.000 6000.000 1000.000 1
0.29792509E+01 0.34944059E-02-0.78549778E-06 0.57479594E-10-0.19335916E-15 2
0.11750582E+05 0.86063728E+01 0.45334916E+01-0.56696171E-02 0.18473207E-04 3
-0.17137094E-07 0.55454573E-11 0.11548297E+05 0.17498417E+01 4
N L 6/88N 1 G 200.000 6000.000 1000.000 1
0.24159429E+01 0.17489065E-03-0.11902369E-06 0.30226245E-10-0.20360982E-14 2
0.56133773E+05 0.46496096E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 0.56104637E+05 0.41939087E+01 4
NNH T07/93N 2H 1 G 200.000 6000.000 1000.000 1
0.37667544E+01 0.28915082E-02-0.10416620E-05 0.16842594E-09-0.10091896E-13 2
0.28650697E+05 0.44705067E+01 0.43446927E+01-0.48497072E-02 0.20059459E-04 3
-0.21726464E-07 0.79469539E-11 0.28791973E+05 0.29779410E+01 4
N2O L 7/88N 2O 1 G 200.000 6000.000 1000.000 1
0.48230729E+01 0.26270251E-02-0.95850874E-06 0.16000712E-09-0.97752303E-14 2
0.80734048E+04-0.22017207E+01 0.22571502E+01 0.11304728E-01-0.13671319E-04 3
0.96819806E-08-0.29307182E-11 0.87417744E+04 0.10757992E+02 4
NH And94 N 1H 1 G 200.000 6000.000 1000.000 1
0.27836928E+01 0.13298430E-02-0.42478047E-06 0.78348501E-10-0.55044470E-14 2
0.42120848E+05 0.57407799E+01 0.34929085E+01 0.31179198E-03-0.14890484E-05 3
0.24816442E-08-0.10356967E-11 0.41880629E+05 0.18483278E+01 4
NH2 And89 N 1H 2 G 200.000 6000.000 1000.000 1
0.28347421E+01 0.32073082E-02-0.93390804E-06 0.13702953E-09-0.79206144E-14 2
0.22171957E+05 0.65204163E+01 0.42040029E+01-0.21061385E-02 0.71068348E-05 3
-0.56115197E-08 0.16440717E-11 0.21885910E+05-0.14184248E+00 4
NH3 J 6/77N 1H 3 G 200.000 6000.000 1000.000 1
0.26344521E+01 0.56662560E-02-0.17278676E-05 0.23867161E-09-0.12578786E-13 2
-0.65446958E+04 0.65662928E+01 0.42860274E+01-0.46605230E-02 0.21718513E-04 3
-0.22808887E-07 0.82638046E-11-0.67417285E+04-0.62537277E+00 4
NO RUS 78N 1O 1 G 200.000 6000.000 1000.000 1
0.32606056E+01 0.11911043E-02-0.42917048E-06 0.69457669E-10-0.40336099E-14 2
0.99209746E+04 0.63693027E+01 0.42184763E+01-0.46389760E-02 0.11041022E-04 3
-0.93361354E-08 0.28035770E-11 0.98446230E+04 0.22808464E+01 4
NO2 L 7/88N 1O 2 G 200.000 6000.000 1000.000 1
0.48847542E+01 0.21723956E-02-0.82806906E-06 0.15747510E-09-0.10510895E-13 2
0.23164983E+04-0.11741695E+00 0.39440312E+01-0.15854290E-02 0.16657812E-04 3
-0.20475426E-07 0.78350564E-11 0.28966179E+04 0.63119917E+01 4

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HCNO                BDEA94H   1N   1C   1O   1G   300.000  5000.000  1382.000       1
 6.59860456E+00 3.02778626E-03-1.07704346E-06 1.71666528E-10-1.01439391E-14       2
 1.79661339E+04-1.03306599E+01 2.64727989E+00 1.27505342E-02-1.04794236E-05       3
 4.41432836E-09-7.57521466E-13 1.92990252E+04 1.07332972E+01                      4
HOCN                BDEA94H   1N   1C   1O   1G   300.000  5000.000  1368.000       1
 5.89784885E+00 3.16789393E-03-1.11801064E-06 1.77243144E-10-1.04339177E-14       2
-3.70653331E+03-6.18167825E+00 3.78604952E+00 6.88667922E-03-3.21487864E-06       3
 5.17195767E-10 1.19360788E-14-2.82698400E+03 5.63292162E+00                      4
HNCO                BDEA94H   1N   1C   1O   1G   300.000  5000.000  1478.000       1
 6.22395134E+00 3.17864004E-03-1.09378755E-06 1.70735163E-10-9.95021955E-15       2
-1.66599344E+04-8.38224741E+00 3.63096317E+00 7.30282357E-03-2.28050003E-06       3
-6.61271298E-10 3.62235752E-13-1.55873636E+04 6.19457727E+00                      4
NCO                 EA 93 N   1C   1O   1        G   200.000  6000.000  1000.000       1
 0.51521845E+01 0.23051761E-02-0.88033153E-06 0.14789098E-09-0.90977996E-14       2
 0.14004123E+05-0.25442660E+01 0.28269308E+01 0.88051688E-02-0.83866134E-05       3
 0.48016964E-08-0.13313595E-11 0.14682477E+05 0.95504646E+01                      4
CN                  HBH92 C   1N   1        G   200.000  6000.000  1000.000       1
 0.37459805E+01 0.43450775E-04 0.29705984E-06-0.68651806E-10 0.44134173E-14       2
 0.51536188E+05 0.27867601E+01 0.36129351E+01-0.95551327E-03 0.21442977E-05       3
-0.31516323E-09-0.46430356E-12 0.51708340E+05 0.39804995E+01                      4
HCNN                SRI/94C   1N   2H   1        G   300.000  5000.000  1000.000       1
 0.58946362E+01 0.39895959E-02-0.15982380E-05 0.29249395E-09-0.20094686E-13       2
 0.53452941E+05-0.51030502E+01 0.25243194E+01 0.15960619E-01-0.18816354E-04       3
 0.12125540E-07-0.32357378E-11 0.54261984E+05 0.11675870E+02                      4
AR                  120186AR  1                 G   300.000  5000.000  1000.000       1
 0.02500000E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00       2
-0.07453750E+04 0.04366000E+02 0.02500000E+02 0.00000000E+00 0.00000000E+00       3
 0.00000000E+00 0.00000000E+00-0.07453750E+04 0.04366000E+02                      4
C3H8                L 4/85C   3H   8        G   300.000  5000.000  1000.000       1
 0.75341368E+01 0.18872239E-01-0.62718491E-05 0.91475649E-09-0.47838069E-13       2
-0.16467516E+05-0.17892349E+02 0.93355381E+00 0.26424579E-01 0.61059727E-05       3
-0.21977499E-07 0.95149253E-11-0.13958520E+05 0.19201691E+02                      4
C3H7                L 9/84C   3H   7        G   300.000  5000.000  1000.000       1
 0.77026987E+01 0.16044203E-01-0.52833220E-05 0.76298590E-09-0.39392284E-13       2
 0.82984336E+04-0.15480180E+02 0.10515518E+01 0.25991980E-01 0.23800540E-05       3
-0.19609569E-07 0.93732470E-11 0.10631863E+05 0.21122559E+02                      4

END
```

S3. The transport data

N2		1	97.530	3.621	0.000	1.760	4.000 !
HE		0	10.200	2.576	0.000	0.000	0.000 !
AR	0	136.500	3.330	0.000	0.000	0.000	
H2		1	38.000	2.920	0.000	0.790	280.000 !
H		0	145.000	2.050	0.000	0.000	0.000 !
O2		1	107.400	3.458	0.000	1.600	3.800 !
O		0	80.000	2.750	0.000	0.000	0.000 !
H2O		2	572.400	2.605	1.844	0.000	4.000 !
OH		1	80.000	2.750	0.000	0.000	0.000 !
OHV		1	80.000	2.750	0.000	0.000	0.000 !
H2O2		2	107.400	3.458	0.000	0.000	3.800 !
HO2		2	107.400	3.458	0.000	0.000	1.000 !
CO		1	98.100	3.650	0.000	1.950	1.800 !
CO2		1	244.000	3.763	0.000	2.650	2.100 !
HOCO		2	498.000	3.590	0.000	0.000	2.000 !
CH4		2	141.400	3.746	0.000	2.600	13.000 !
CH3		1	144.000	3.800	0.000	0.000	0.000 !
CH2		1	144.000	3.800	0.000	0.000	0.000 !
CH		1	80.000	2.750	0.000	0.000	0.000 !
CH3O2H		2	481.800	3.626	0.000	0.000	1.000 !
CH3O2		2	481.800	3.626	0.000	0.000	1.000 !
CH3OH		2	481.800	3.626	0.000	0.000	1.000 !
CH3O		2	417.000	3.690	1.700	0.000	2.000 !
CH2OH		2	417.000	3.690	1.700	0.000	2.000 !
CH2O		2	498.000	3.590	0.000	0.000	2.000 !
HCO		2	498.000	3.590	0.000	0.000	0.000 !
HO2CHO		2	436.000	3.970	0.000	0.000	2.000 !
O2CHO		2	436.000	3.970	0.000	0.000	2.000 !
C2H6		2	247.500	4.350	0.000	0.000	1.500 !
C2H5		2	247.500	4.350	0.000	0.000	1.500 !
C2H5O2H		2	470.600	4.410	0.000	0.000	1.500 !
C2H5O2		2	470.600	4.410	0.000	0.000	1.500 !
C2H4		2	238.400	3.496	0.000	0.000	1.500 !
C2H3		2	265.300	3.721	0.000	0.000	1.000 !
C2H3OO		2	436.000	3.970	0.000	0.000	2.000 !
C2H2		1	265.300	3.721	0.000	0.000	2.500 !
C2H		1	265.300	3.721	0.000	0.000	2.500 !
C2H5O		2	470.600	4.410	0.000	0.000	1.500 !
CH3CHO		2	436.000	3.970	0.000	0.000	2.000 !
CH3CO		2	436.000	3.970	0.000	0.000	2.000 !
CH2CHO		2	436.000	3.970	0.000	0.000	2.000 !
CH2CO		2	436.000	3.970	0.000	0.000	2.000 !
HCCO		2	150.000	2.500	0.000	0.000	1.000 !
C3H8		2	303.400	4.810	0.000	0.000	1.000 !

IC3H7	2	303.400	4.810	0.000	0.000	1.000 !
NC3H7	2	303.400	4.810	0.000	0.000	1.000 !
NC3H7O2	2	481.500	4.997	1.700	0.000	1.000 !
IC3H7O2	2	459.500	5.036	1.700	0.000	1.000 !
NC3H7O	2	481.500	4.997	1.700	0.000	1.000 !
IC3H7O	2	459.500	5.036	1.700	0.000	1.000 !
C3H6	2	307.800	4.140	0.000	0.000	1.000 !
C3H5-A	2	316.000	4.220	0.000	0.000	1.000 !
C3H5-S	2	316.000	4.220	0.000	0.000	1.000 !
C3H5-T	2	316.000	4.220	0.000	0.000	1.000 !
C3H5O	2	411.000	4.820	0.000	0.000	1.000 !
AC3H5OOH	2	481.500	4.997	1.700	0.000	1.000 !
C3H4-P	1	324.800	4.290	0.000	0.000	1.000 !
C3H4-A	1	324.800	4.290	0.000	0.000	1.000 !
C2H3CHO	2	428.800	4.958	2.900	0.000	1.000 !
C2H3CO	2	443.200	4.120	0.000	0.000	1.000 !
CH3COCH2	2	435.500	4.860	0.000	0.000	1.000 !
C4H72-1OOH	2	496.000	5.200	0.000	0.000	1.000 !
C4H71-3OOH	2	496.000	5.200	0.000	0.000	1.000 !
C4H5OH-13	2	436.400	5.352	0.000	0.000	1.000 !
C4H5-N	2	357.000	5.180	0.000	0.000	1.000 !
C4H3-N	2	357.000	5.180	0.000	0.000	1.000 !
C4H2	1	357.000	4.720	0.000	0.000	1.000 !
CH2CHCHCHO	1	357.000	5.180	0.000	0.000	1.000 !
H2C4O	2	357.000	5.180	0.000	0.000	1.000 !
C3H6CHO-3	2	464.200	5.009	2.600	0.000	1.000 !
C-C6H4	2	464.800	5.290	0.000	10.320	0.000 !
C6H6	2	468.500	5.230	0.000	10.300	1.000 !
C6H5	2	412.300	5.349	0.000	0.000	1.000 !
C6H5OH	2	450.000	5.500	0.000	0.000	1.000 !
C6H5O	2	450.000	5.500	0.000	0.000	1.000 !
C5H5	1	408.000	5.200	0.000	0.000	1.000 !
HOCHO	2	436.000	3.970	0.000	0.000	2.000 !
C3H6OOH1-2	2	435.200	4.662	2.700	0.000	1.000 !
C3H6O1-2	2	403.600	4.968	2.000	0.000	1.000 !
CH3CHCHO	2	387.860	4.687	0.000	0.000	0.000 !
CH3CHCO	2	443.200	4.120	0.000	0.000	1.000 !
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 !
SC3H4OH	2	298.893	5.345	0.000	0.000	1.000 !
IC4H9	2	352.000	5.240	0.000	0.000	1.000 !
TC4H9	2	352.000	5.240	0.000	0.000	1.000 !
IC3H5CO	2	436.400	5.352	0.000	0.000	1.000 !
IC4H9O2	2	502.252	5.430	0.000	0.000	0.000 !
TC4H9O2	2	502.252	5.430	0.000	0.000	0.000 !
IC4H8O2H-I	2	502.200	5.356	1.800	0.000	1.000 !

IC4H8O2H-T 2 502.200 5.356 1.800 0.000 1.000 !
IC4H7O 2 496.000 5.200 0.000 0.000 1.000 !
IC4H8 2 344.500 5.089 0.500 0.000 1.000 !
IC4H7 2 355.000 4.650 0.000 0.000 1.000 !
IC4H7-I1 2 380.022 4.633 0.000 0.000 0.000 !
C4H8-1 2 355.000 4.650 0.000 0.000 1.000 !
C4H71-1 2 357.100 4.720 0.000 0.000 1.000 !
C4H71-3 2 357.100 4.720 0.000 0.000 1.000 !
C4H71-1O2 2 436.400 5.352 0.000 0.000 1.000 !
C4H6 2 357.000 4.720 0.000 0.000 1.000 !
C6H101-5 2 337.788 5.608 0.000 0.000 1.000 !
C6H9-A 2 346.876 5.564 0.000 0.000 1.000 !
C8H18-25 2 578.34 6.21 0 15.9 1 !CALC
C8H17 2 578.34 6.21 0 15.9 1 !SAME AS C8H18-25
C3H3 0 311.261 4.136 0.000 0.000 0.000
PC4H9 0 388.026 4.689 0.000 0.000 0.000
C8H17-OO 0 666.695 6.379 0.000 0.000 0.000
C8-QOOH 0 666.695 6.379 0.000 0.000 0.000
C8-OOQOOH 0 748.325 6.813 0.000 0.000 0.000
C8-KET 0 705.790 6.590 0.000 0.000 0.000
C3H3O 2.000 301.263 5.055 0.000 0.000 1.000 !!
NC12H26 2 789.160 7.060 0.000 22.750 1.000
C12H25 2 789.160 7.060 0.000 22.750 1.000
C12H25-OO 2 789.160 7.060 0.000 22.750 1.000
C12-QOOH 2 789.160 7.060 0.000 22.750 1.000
C12-OOQOOH 2 789.160 7.060 0.000 22.750 1.000
C12-KET 2 789.160 7.060 0.000 22.750 1.000
C12H24 2 787.050 6.930 0.000 22.520 1.000
C12H23 2 787.050 6.930 0.000 22.520 1.000
C6H13CO 2 581.3 6.506 2.0 0.0 1.0
C8H9 2 439.519 5.851 0.000 0.000 1.000
C8H9O 2 472.173 6.102 0.000 0.000 1.000
C8H9OO 2 502.757 6.331 0.000 14.750 1.000
C9H12 2 547.900 6.335 0.100 15.630 1.000
C8H9CH2 2 547.900 6.335 0.100 15.630 1.000
C8H9CH2O 2 499.085 6.304 0.000 0.000 1.000
C8H9CHO 2 497.198 6.290 0.000 0.000 1.000
C8H9CO 2 495.305 6.276 0.000 0.000 1.000
C7H9 2 413.357 5.644 0.000 12.100 1.000
C7H9O 2 447.877 5.916 0.000 12.670 1.000
C6H9 2 385.468 5.417 0.000 10.590 1.000
C8H10 2 441.646 5.867 0.000 0.000 1.000
C7H8O 2 447.877 5.916 0.000 12.670 1.000
Decalin 2 630.4 6.18 0.0 16.5 1.0
RDecalin 2 630.4 6.18 0.0 16.5 1.0
RDec-OO 2 630.4 6.18 0.0 16.5 1.0

Dec-QOOH 2 630.4 6.18 0.0 16.5 1.0
Dec-OOQOOH 2 630.4 6.18 0.0 16.5 1.0
Dec-KET 2 630.4 6.18 0.0 16.5 1.0
CYC6H10 2 387.884 5.437 0.0 10.76 1.0
CYC6H9-3 2 464.8 5.29 0.0 0.0 1.0
C4H7 2 357.0 5.176 0.0 0.0 1.0
DCYC10H16 2 630.4 6.18 0.0 16.5 1.0
DCLD1-3R 2 630.4 6.18 0.0 16.5 1.0
C8H12 2 630.4 6.18 0.0 16.5 1.0
X135C6H7-3R 2 630.4 6.18 0.0 16.5 1.0
LC5H7 1 357.0 5.18 0.0 0.0 1.0
CYC5H5 2 408.0 5.2 0.0 0.0 1.0
CYC5H6 2 408.0 5.2 0.0 0.0 1.0
CYC6H8-13 2 504.629 5.628 0.0 0.0 1.0
C6H9-13-6 2 504.629 5.628 0.0 0.0 1.0
CH2(S) 1 144.000 3.800 0.000 0.000 0.000
CHV 1.000 80.000 2.750 0.000 0.000 0.000
HCOH 2 267.2436266 3.79218336 0 4.56 1
HOCH2O 2 470.600 4.410 0.000 0.000 1.500
OCHO 2 498.000 3.590 0.000 0.000 2.000
CHCHO 2 436.000 3.970 0.000 0.000 2.000
PC2H4OH 2 470.600 4.410 0.000 0.000 1.500
O2C2H4OH 2 523.200 5.664 1.700 0.000 1.000
C5H4O 2 450.000 5.500 0.000 0.000 1.000
N 0 71.400 3.298 0.000 0.000 0.000 ! *
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 ! *
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
HCN 1 569.000 3.630 0.000 0.000 1.000