

```
!+++++
+++++
+++++
!\START_SPECIES_LIST
!+++++
+++++
+++++
ELEMENTS
C
H
N
O
AR
HE
CL
END
!+++++
+++++
+++++
SPECIES
!+++++
+++++
+++++
!\SPECIES_MODULE: DILUENTS
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
AR
N2
HE
!\END_SPECIES_MODULE: DILUENTS
!+++++
+++++
+++++
!\SPECIES_MODULE: \H2_O2
!\MODCOMMENTS: A. Keromnes, W.K. Metcalfe, K.A. Heufer, N. Donohoe, A.K.
Das, C.J. Sung, J. Herzler, C. Naumann, P. Griebel,
!\MODCOMMENTS: O. Mathieu, M.C. Krejci, E.L. Petersen, W.J. Pitz, H.J.
Curran
!\MODCOMMENTS: An Experimental and Detailed Chemical Kinetic Modelling
Study of Hydrogen and Syngas Mixtures at Elevated Pressures"
!\MODCOMMENTS: Combustion and Flame (2013) 160 995-1011.
!\MODWARNINGS:
!\MODSUBMECHS: \H2 \O2 \H2O \H2O2
!+++++
+++++
+++++
!-----
-----
!\SUBMECH: \H2
!-----
-----
!\PYROSPEC:
H2
```

```
H
!-----
-----
!-----
-----
!\SUBMECH: \O2
!-----
-----
!\PYROSPEC:
O2
O
!-----
-----
!-----
-----
!\SUBMECH: \H2O
!-----
-----
!\PYROSPEC:
H2O
OH
OHV
!-----
-----
!-----
-----
!\SUBMECH: \H2O2
!-----
-----
!\PYROSPEC:
H2O2
HO2
!-----
-----
!+++++
+++++
+++++
!\END_SPECIES_MODULE: \H2_O2
!+++++
+++++
+++++
!+++++
+++++
+++++
!\SPECIES_MODULE: \C1
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS: \CO \CH4 \CH3OH \CH2O
!+++++
+++++
+++++
!-----
-----
!\SUBMECH: \CO
!\MODCOMMENTS: A. Keromnes, W.K. Metcalfe, K.A. Heufer, N. Donohoe, A.K.
Das, C.J. Sung, J. Herzler, C. Naumann, P. Griebel,
!\MODCOMMENTS: O. Mathieu, M.C. Krejci, E.L. Petersen, W.J. Pitz, H.J.
Curran
```

!\MODCOMMENTS: An Experimental and Detailed Chemical Kinetic Modelling  
Study of Hydrogen and Syngas Mixtures at Elevated Pressures"  
!\MODCOMMENTS: Combustion and Flame (2013) 160 995-1011.

!-----  
-----

!\PYROSPEC:

CO  
CO2

!\OXIDSPEC:

HOCO

!-----  
-----

! C1--C2 Mechanism from:

! W.K. Metcalfe, S.M. Burke, S.S. Ahmed, H.J. Curran

! A hierarchical and comparative kinetic modeling study of C1-C2  
hydrocarbon and oxygenated fuels

! Int. J. Chem. Kinet. (2013) 45(10) 638-675.

!-----  
-----

!\SUBMECH: \CH4

!-----  
-----

!\PYROSPEC:

CH4  
CH3  
CH2  
CH2(S)

C  
CH  
CHV

!\OXIDSPEC:

CH3O2H  
CH3O2  
CH2O2H

!-----  
-----

!-----  
-----

!\SUBMECH: \CH3OH

! U. Burke, W.K. Metcalfe, S.M. Burke, K.A. Heufer, P. Dagaut, H.J.  
Curran

! A Detailed Chemical Kinetic Modeling, Ignition Delay time and Jet-  
Stirred Reactor Study of Methanol Oxidation

! Combust. Flame (2016) 165 125-136.

!-----  
-----

!\PYROSPEC:

CH3OH  
CH3O  
CH2OH

!\OXIDSPEC:

!-----  
-----

!-----  
-----

!\SUBMECH: \CH2O

! C1--C2 Mechanism from:

! W.K. Metcalfe, S.M. Burke, S.S. Ahmed, H.J. Curran

! A hierarchical and comparative kinetic modeling study of C1-C2 hydrocarbon and oxygenated fuels  
! Int. J. Chem. Kinet. (2013) 45(10) 638-675.

!-----  
-----

!\PYROSPEC:

CH2O

HCO

HCOH

!\OXIDSPEC:

HO2CHO

HOCH2O2H

HOCH2O2

OCH2O2H

HOCH2O

O2CHO

HOCHO

OCHO

!-----  
-----

!+++++  
+++++  
+++++

!\END\_SPECIES\_MODULE: \C1

!+++++  
+++++  
+++++

!+++++  
+++++  
+++++

!\SPECIES\_MODULE: \C2

!\MODCOMMENTS:

!\MODWARNINGS:

!\MODSUBMECHS: \C2H6 \CH3CHO \CH2CO \C2H4 \C2H2 \C2H5OH \CH3OCH3 \CH3OCHO

!+++++  
+++++  
+++++

!-----  
-----

!\SUBMECH: \C2H6

! C1--C2 Mechanism from:

! W.K. Metcalfe, S.M. Burke, S.S. Ahmed, H.J. Curran

! A hierarchical and comparative kinetic modeling study of C1-C2 hydrocarbon and oxygenated fuels

! Int. J. Chem. Kinet. (2013) 45(10) 638-675.

!-----  
-----

!\PYROSPEC:

C2H6

C2H5

!\OXIDSPEC:

C2H5O2H

C2H5O2

!-----  
-----

!-----  
-----

!\SUBMECH: \C2H4

! M.M. Kopp, N.S. Donato, E.L. Petersen, W.K. Metcalfe, S.M. Burke, H.J. Curran

! Ignition and oxidation of ethylene-air mixtures at elevated pressures.  
Part 1: Experimental results

! J. Propul. Power (2014) 30(3) 790-798.

!

! M.M. Kopp, E.L. Petersen, W.K. Metcalfe, S.M. Burke, H.J. Curran

! Ignition and oxidation of ethylene-air mixtures at elevated pressures.  
Part 2: chemical kinetics

! J. Propul. Power (2014) 30(3) 799-811.

!-----

! \PYROSPEC:

C2H4

C2H3

! \OXIDSPEC:

CHOCHO

C2H3OOH

C2H3OO

CHCHO

!-----

!-----

!-----

!-----

! \SUBMECH: \C2H2

!-----

!-----

! \PYROSPEC:

C2H2

C2H

H2CC

! \OXIDSPEC:

!-----

!-----

!-----

!-----

! \SUBMECH: \C2H5OH

! G. Mittal, S.M. Burke, V.A. Davies, B. Parajuli, W.K. Metcalfe, H.J. Curran

! Autoignition of ethanol in a rapid compression machine

! Combust. Flame (2014) 161(5) 1164-1171.

!-----

!-----

! \PYROSPEC:

C2H5OH

C2H5O

PC2H4OH

SC2H4OH

! \OXIDSPEC:

O2C2H4OH

C2H4O2H

C2H4O1-2

C2H3O1-2

!-----

!-----

!-----

!-----

! \SUBMECH: \CH3CHO

!-----  
-----  
!\PYROSPEC:  
CH3CHO  
CH3CO  
CH2CHO  
!\OXIDSPEC:  
O2CH2CHO  
HO2CH2CO  
!-----  
-----  
!  
-----  
!\SUBMECH: \C2H3OH  
!-----  
-----  
!\PYROSPEC:  
C2H3OH  
C2H2OH  
!\OXIDSPEC:  
!-----  
-----  
!  
-----  
!\SUBMECH: \CH2CO  
!-----  
-----  
!\PYROSPEC:  
CH2CO  
HCCO  
HCCOH  
!\OXIDSPEC:  
!-----  
-----  
!  
-----  
!\SUBMECH: \ACID  
!-----  
-----  
!\PYROSPEC:  
!\OXIDSPEC:  
CH3CO3H  
CH3CO3  
CH3CO2  
!-----  
-----  
!  
-----  
!\SUBMECH: \CH3OCH3  
! U. Burke, K.P. Somers, P. O'Toole, C.M. Zinner, N. Marquet, G. Bourque,  
E.L. Petersen, W.K. Metcalfe, Z. Serinyel, H.J. Curran  
! An ignition delay and kinetic modeling study of methane, dimethyl  
ether, and their mixtures at high pressures  
! Combust. Flame (2015) 162(2) 315-330.  
!-----  
-----  
!\PYROSPEC:  
CH3OCH3

```

CH3OCH2
!\OXIDSPEC:
CH3OCH2O2H
CH3OCH2O2
CH2OCH2O2H
O2CH2OCH2O2H
HO2CH2OCHO
OCH2OCHO
HOCH2OCO
CH3OCH2O
!-----
!-----
!-----
!\SUBMECH: \CH3OCHO
! U. Burke, K.P. Somers, P. O'Toole, C.M. Zinner, N. Marquet, G. Bourque,
E.L. Petersen, W.K. Metcalfe, Z. Serinyel, H.J. Curran
! An ignition delay and kinetic modeling study of methane, dimethyl
ether, and their mixtures at high pressures
! Combust. Flame (2015) 162(2) 315-330.
!-----
!-----
!\PYROSPEC:
CH3OCHO
CH3OCO
CH2OCHO
!\OXIDSPEC:
!-----
!+++++
!+++++
!+++++
!\END_SPECIES_MODULE: \C2
!+++++
!+++++
!+++++
!\SPECIES_MODULE: \C3
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS: \CH3COCH3 \C2H3CHO \C2H5CHO \C3H8 \C3H6 \C3H4-A \C3H4-P
!+++++
!+++++
!+++++
!-----
!-----
!\SUBMECH: \C3H8
!-----
!-----
!\PYROSPEC:
C3H8
IC3H7
NC3H7
!\OXIDSPEC:
NC3H7O2H
NC3H7O2

```

IC3H7O2H  
IC3H7O2  
NC3H7O  
IC3H7O  
C3H6OOH1-2  
C3H6OOH1-3  
C3H6OOH2-1  
C3H6OOH1-2O2  
C3H6OOH1-3O2  
C3H6OOH2-1O2  
C3KET12  
C3KET13  
C3H51-2,3OOH  
C3H52-1,3OOH  
C3H5O1-2OOH-3  
C3H5O1-3OOH-2  
C3H6O1-2  
C3H6O1-3

!-----  
-----  
!-----  
-----

!\SUBMECH: \C3H6

! S.M. Burke, W.K. Metcalfe, O. Herbinet, F. Battin-Leclerc, F.M. Haas,  
J. Santner, F.L. Dryer, H.J. Curran

! An experimental and modeling study of propene oxidation. Part 1:  
Speciation measurements in jet-stirred and flow reactors

! Combust. Flame (2014) 161(11) 2765-2784.

!

! S.M. Burke, U. Burke, O. Mathieu, I. Osorio, C. Keesee, A. Morones, E.  
Petersen, W. Wang, T. DeVerter, M. Oehlschlaeger, B. Rhodes,

! R. Hanson, D. Davidson, B. Weber, C-J. Sung, J. Santner, Y. Ju, F.

Haas, F. Dryer, E. Volkov, E. Nilsson, A. Konnov, M. Alrefae,

! F. Khaled, A. Farooq, P. Dirrenberger, P-A. Glaude, F. Battin-Leclerc

! An experimental and modeling study of propene oxidation. Part 2:

Ignition delay time and flame speed measurements

! Combust. Flame (2015) 162(2) 296-314.

!-----  
-----

!\PYROSPEC:

C3H6

C3H5-A

C3H5-S

C3H5-T

CC3H6

!\OXIDSPEC:

C3H5O

CH2CHOCH2

CH3CHCHO

AC4H7OOH

C3H6OH1-2

CH3CHCO

AC3H5OOH

C3H6OH2-1

HOC3H6O2

!TQJC3H6OH TQC3H6OI QC3H5OHP CCY(COC)OH IQJC3H6OH IQC3H6OT CY(COC)COH

CHOCOCH3 CY(CCOC)OH



!TQC3H5OHI TQC3H5OHIO2 TQC3H5OHIQ-I TQC3H5OHIQ-P C2H3COHOOH COHOOH CY(COC)  
OH CY(COCC)OOH  
!TQC3H5OHTO2 OHCOCO OHCH3 IQC3H5OHPJ IQC3H5OHPJO2 IQC3H5OTQ-I HO2CH2CHO  
IQC3H5OHQ-SJ  
SC3H5OH  
IC3H5OH  
C3H5OH  
CH2CCH2OH  
!CHOCO HCH2OOH

!-----  
-----  
!-----  
-----

!\SUBMECH: \C3H4-A\C3H4-P  
! S.M. Burke, W.K. Metcalfe, O. Herbinet, F. Battin-Leclerc, F.M. Haas,  
J. Santner, F.L. Dryer, H.J. Curran  
! An experimental and modeling study of propene oxidation. Part 1:  
Speciation measurements in jet-stirred and flow reactors  
! Combust. Flame (2014) 161(11) 2765-2784.  
!  
! S.M. Burke, U. Burke, O. Mathieu, I. Osorio, C. Keesee, A. Morones, E.  
Petersen, W. Wang, T. DeVerter, M. Oehlschlaeger, B. Rhodes,  
! R. Hanson, D. Davidson, B. Weber, C-J. Sung, J. Santner, Y. Ju, F.  
Haas, F. Dryer, E. Volkov, E. Nilsson, A. Konnov, M. Alrefae,  
! F. Khaled, A. Farooq, P. Dirrenberger, P-A. Glaude, F. Battin-Leclerc  
! An experimental and modeling study of propene oxidation. Part 2:  
Ignition delay time and flame speed measurements  
! Combust. Flame (2015) 162(2) 296-314.  
!-----

!\PYROSPEC:  
C3H4-P  
C3H4-A  
C3H3  
CC3H4  
C3H2  
H2CCC(S)  
C3H2(S)  
C3H2C  
!\OXIDSPEC:  
PC3H4OH-2  
SC3H4OH  
C3H3O  
C3H3O2H  
C2HCHO  
!-----  
-----  
!-----  
-----

!\SUBMECH: \C2H5CHO  
!-----  
-----

!\PYROSPEC:  
C2H5CHO  
C2H5CO  
CH2CH2CHO  
C2H3CHO  
C2H3CO

```
!\OXIDSPEC:
!-----
!-----
!-----
!\SUBMECH: \CH3COCH3
!-----
!-----
!\PYROSPEC:
CH3COCH3
CH3COCH2
!\OXIDSPEC:
CH3COCH2O2
CH3COCH2O
C3KET21
!-----
!-----
!+++++
!+++++
!+++++
!\END_SPECIES_MODULE: \C3
!+++++
!+++++
!+++++
!+++++
!+++++
!\SPECIES_MODULE: \C4
!\MODCOMMENTS: TC3H6OH/IC3H5Q/CH3COCHO ARE (?) C3 SPECIES BUT ARE UNIQUE
TO I-C4H8 SO IS INCLUDED IN C4 MODULE
!\MODWARNINGS:
!\MODSUBMECHS: \C4H10 \IC4H10 \IC4H8 \C4H8-1 \C4H8-2 \C4H6 \C4H612 \C4H6-
2 \C4H4 \C4H2 \NC3H7CHO \C2H5COCH3
!+++++
!+++++
!+++++
!-----
!-----
!\SUBMECH: \C4H10
!-----
!-----
!\PYROSPEC:
C4H10
PC4H9
SC4H9
!\OXIDSPEC:
PC4H9O
SC4H9O
PC4H9O2
SC4H9O2
PC4H9O2H
SC4H9O2H
C4H8OOH1-2
C4H8OOH1-3
C4H8OOH1-4
C4H8OOH2-1
C4H8OOH2-3
C4H8OOH2-4
```

C4H8O1-2  
C4H8O1-3  
C4H8O1-4  
C4H8O2-3  
C4H8OOH1-2O2  
C4H8OOH1-3O2  
C4H8OOH1-4O2  
C4H8OOH2-1O2  
C4H8OOH2-3O2  
C4H8OOH2-4O2  
C4H71-2, 4OOH  
C4H72-1, 3OOH  
C4H72-1, 4OOH  
C4H71-2, 3OOH  
C4H7O1-3OOH-4  
C4H7O1-3OOH-2  
C4H7O1-2OOH-4  
C4H7O1-4OOH-2  
C4H7O1-2OOH-3  
C4H7O2-3OOH-1  
C4H72-1OOH  
NC4KET12  
NC4KET13  
NC4KET14  
NC4KET21  
NC4KET23  
NC4KET24  
C4H71-3OOH  
C4H71-3, 4OOH  
C4H72-3, 4OOH  
HO2CH2CHO

!-----  
-----

!-----  
-----

!\SUBMECH: \IC4H10  
!-----  
-----

!\PYROSPEC:

IC4H10  
IC4H9  
TC4H9

!\OXIDSPEC:

TC4H9O  
IC4H9O  
IC4H8O  
IC3H7CHO  
IC3H7CO  
IC3H6CHO  
TC3H6CHO  
IC3H5CHO  
TC3H6O2CHO  
IC3H5O2HCHO  
TC3H6O2HCO  
TC3H6OCHO  
IC3H6CO  
IC3H5CO  
IC3H4CHO-A

SC4H7OH-I  
IC4H9O2  
TC4H9O2  
IC4H8O2H-I  
IC4H8O2H-T  
TC4H8O2H-I  
CC4H8O  
IC4H8OOH-IO2  
IC4H8OOH-TO2  
TC4H8OOH-IO2  
IC4KETII  
IC4KETIT  
TIC4H7Q2-I  
IIC4H7Q2-I  
IIC4H7Q2-T  
IC4H7OOH  
IC4H9O2H  
TC4H9O2H

!-----  
-----  
!-----  
-----

!\SUBMECH: \IC4H8  
! C-W. Zhou, Y. Li, E. O'Connor, K.P. Somers, S. Thion, C. Keesee, O.  
Mathieu, E.L. Petersen, T. A. DeVerter, M.A. Oehlschlaeger,  
! G. Kukkadapu, C-J. Sung, M. Alrefae, F. Khaled, A. Farooq, P.  
Dirrenberger, P-A. Glaude, F. Battin-Leclerc, J. Santner, Y. Ju,  
! T. Held, F.M. Haas, F.L. Dryer, H.J. Curran, Comprehensive experimental  
and modeling study of isobutene oxidation  
! Combust. Flame (2016) accepted.

!-----  
-----

!\PYROSPEC:  
IC4H8  
IC4H7  
IC4H7-I1  
!\OXIDSPEC:  
IC4H7O2  
IC4H6OOH-I  
CCYCCOOC-T1  
C2CYCOOC-I1  
IC4H7O  
CVCYCCOC  
CCYC2OCO  
CCYCCOOC-I2  
CHOIC3H6O  
IC3H5OOCH2  
CCYCCO-T1  
IC4H8OH-IT  
IC4H8OH-TI  
IC4H7OH  
IC4H8OH  
IC4H6OH  
TQJC4H8OH  
TQC4H8OI  
QC4H7OHP  
TQC4H7OHI  
CCY (CCO) COH

C2CY (COC) OH  
IQJC4H8OH  
IC3H6OHCHO  
IQC4H8OT  
IQC4H7OHT  
CCY (CCOC) OH  
CH2COHCH2OOH  
TC3H6OH  
TQC4H7OHIO2  
TQC4H7OHTO2  
TQC4H7OHIQ-I  
TQC4H7OHIQ-P  
IC3H5COHQ  
CH2CQCOHQ  
IC3H5Q  
COHQCYC (COC)  
QCYC (CCOC) OH  
HOCOCQ (CH3) 2  
IQC4H7OHTO2  
IQC4H8OTQ-I  
IQC4H7OHTQ-P  
CHOC (CH3) OHCH2Q  
CO (CH2OOH) 2  
CH3COCHO  
IC3H5OCH2  
IC4H7OOCH3  
IC4H7OOIC4H7

!-----

-----

!-----

-----

!\SUBMECH: \C4H8-1\C4H8-2  
! Y. Li, C-W. Zhou, K.P. Somers, K. Zhang, H.J. Curran  
! The Oxidation of 2-Butene: A High Pressure Ignition Delay, Kinetic  
Modeling Study and Reactivity Comparison with Isobutene and 1-Butene  
! Proc. Combust. Inst. (2017) submitted.

!-----

-----

!\PYROSPEC:

C4H8-1

C4H8-2

C4H71-1

C4H71-2

C4H71-3

C4H71-4

C4H72-2

!\OXIDSPEC:

C4H71-O

PC4H8OH-2

SC4H8OH-1

SC4H8OH-3

C4H71-3OH

C4H71-4OH

C4H71-1OH

C4H71-2OH

C4H72-1OH

C4H72-2OH

SQC4H8OP

PQC4H8OS  
PQC4H7OHS-3  
NC4KET12OH  
SQC4H7OHS-4  
SQC4H8OS  
NC4KET23OH  
SC4H8OH-3O2  
CCY (COCC) OH  
C4H7O2-1  
C4H6-1  
AC3H5OCH2  
IC4H6Q2-II  
C5H10-2  
CC5H10  
C6H10D24  
C5H91-3  
C5H92-4  
C5H92-5  
C5H91-4  
C5H91-5  
C5H9O2-4  
SC3H5OCH2-1  
C8H141-5, 3-4  
C8H141-5, 3  
C8H142-6  
C8H131-5, 3-4, TA  
C8H131-5, 3, TA  
C8H131-5, 3, SA  
C8H131-5, 3, PA  
C8H132-6, SA  
C8H132-6, PA  
C6H101-3, 3  
C8H131-5, 3-4, TAO  
C8H131-5, 3, TAO  
C8H131-5, 3, SAO  
C8H131-5, 3, PAO  
C8H132-6, SAO  
C8H132-6, PAO  
C7H111-5, 3, 6P  
C7H111-5, 1P  
!NEW 24092915 ADDED  
C4H64, 2-1OH  
C4H63, 1-1OH  
C4H63, 1-3OH  
C4H63, 1-2OH  
C4H5OH-13  
SQC4H7OHP-4  
CY (CCCO) COH  
NC4KET21OH  
C2H5CHOHCO  
CH3COCOHCH3  
C2H4COCH2OH  
CH3COHCO  
CH2COHCHO  
SQC4H7OHP-4O2  
PQC4H7OHS-3O2  
SQC4H7OHS-4O2  
C4H7O2-1, 3OOH

NC4KET13OH-2  
NC4KET24OH-1  
NC4KET24OH-3  
C4H6OHOH1-4-3  
C4H6OHOH2-2-1  
C4H6OHOH1-3-4  
C4H6OHOH1-2-3  
HOCH2CHO  
C4H71-4OOH  
C4H71-4O2  
C4H61-3OOH4  
C4H6O1-3OOH4  
C4H6O2-1OOH4  
HOCH2COCH2  
HOCH2CO  
HOCHCHO  
PC3H4OH-3  
PC3H4OH-1  
CH3COCHOH  
SC2H2OH  
PC4H8OH-1  
PC4H8OH-3  
C4H7O1-4  
PC4H8OH-4  
SC4H8OH-2  
CH2COHCO  
C4H72-2O2  
C4H71-1O2  
C4H71-2O2  
C3H6OH1-1  
PC4H8OH-2O2  
SC4H8OH-1O2  
C4H71-3OOCH3  
C4H72-1OOCH3

!-----  
-----

!-----  
-----

!\SUBMECH: \C4H6\C4H612\C4H6-2\C4H4\C4H2  
! C.-W. Zhou under development

!-----  
-----

!\PYROSPEC:

C4H6  
C4H612  
C4H6-2  
C4H5-I  
C4H5-N  
C4H5-2  
C4H4  
C4H3-I  
C4H3-N  
C4H2

!\OXIDSPEC:

C4H6O25  
C2H3CHOCH2  
C4H4O  
C4H6O23

CH2CHCHCHO  
H2C4O

!-----  
-----  
!-----  
-----

!\SUBMECH: \NC3H7CHO

!-----  
-----

!\PYROSPEC:

NC3H7CHO  
NC3H7CO  
C3H6CHO-1  
C3H6CHO-2  
C3H6CHO-3

SC3H5CHO  
SC3H5CO

!\OXIDSPEC:

!-----  
-----  
!-----  
-----

!\SUBMECH: \C2H5COCH3

!-----  
-----

!\PYROSPEC:

C2H5COCH3  
C2H5COCH2  
CH2CH2COCH3  
CH3CHCOCH3  
C2H3COCH3

!\OXIDSPEC:

CH3CHOOCH3  
CH2CHOOHCOCH3

!-----  
-----  
!-----  
-----

!\SUBMECH: \C2H5CHCO

!-----  
-----

!\PYROSPEC:

C2H5CHCO

!\OXIDSPEC:

!-----  
-----

!++++  
++++  
++++

!\END\_SPECIES\_MODULE: \C4

!++++  
++++  
++++

!++++  
++++  
++++

!\SPECIES\_MODULE: \C5



! J. Bugler, B. Marks, O. Mathieu, R. Archuleta, A. Camou, C. Gregoire,  
K.A. Heufer, E.L. Petersen, H.J. Curran  
! An Ignition Delay Time and Chemical Kinetic Modelling Study of the  
Pentane Isomers  
! Combust. Flame (2016) 163(1) 136-156.

!  
! J. Bugler, K.P. Somers, E.J. Silke, H.J. Curran  
! Revisiting the kinetics and thermodynamics of the low-temperature  
oxidation pathways of alkanes: A case study of the three pentane isomers  
! J. Phys. Chem. A (2015) 119(28) 7510-7527.

!  
!\MODCOMMENTS:  
!\MODWARNINGS: KPS, 22/07/2015 JBS PENTANE SPECIES LIST HAS TO BE ADDED  
AND COMBINED WITH CWS AC5H10 AS THERE ARE 1/2/3 SPECIES WHICH ARE IN BOTH  
MECHANISMS

!\MODWARNINGS: SEARCH FOR "\\WARNING: DUPLICATED KINETICS" FOR MORE INFO.  
!\MODWARNINGS: Following species in C5 submech but are not C5 species:  
OCH2CHO CH2OCH2CHO C2H4OCHO C4H7O1-4 C4H7O2-1

!\MODSUBMECHS: \NC5H12 \IC5H12 \NEOC5H12 \AC5H10 \BC5H10 \CC5H10 \B13DE2M  
\TC4H8CHO \PC4H8CHO-1 \PC4H8CHO-2 \PC4H8CHO-3 \C5H9O12-5 \C5H9O13-5 \C5H9O14-  
5 \C5H9O23-1 \C5H9O23-5 \C5H9O24-1 \NC3H7COCH3 \C2H5COC2H5

!++++  
!++++  
!++++

!-----  
-----  
!\SUBMECH: \C5H10-1\C5H10-2  
!-----  
-----

!\PYROSPEC:  
C5H10-1  
C5H10-2  
C5H81-3  
C5H91-3  
C5H91-4  
C5H91-5  
C5H92-4  
C5H92-5  
!\OXIDSPEC:  
C5H9O1-3  
C5H9O2-4

!-----  
-----  
!-----  
-----  
-----

!\SUBMECH: \CC5H10\BC5H10  
!-----  
-----

!\PYROSPEC:  
BC5H10  
CC5H10  
CC5H9-A  
CC5H9-B  
!\OXIDSPEC:  
AC5H9O-C  
CC5H9O-B

```
!-----
!-----
!-----
!\SUBMECH: \AC5H10
!-----
!-----
!\PYROSPEC:
AC5H10
AC5H9-A2
AC5H9-C
AC5H9-D
!\OXIDSPEC:
B2E2M1OJ
!-----
!-----
!\SUBMECH: \B13DE2M
!-----
!-----
!\PYROSPEC:
B13DE2M
B13DE2MJ
B12DE3M
!\OXIDSPEC:
B2E3M1OJ
!-----
!-----
!\SUBMECH: \TC4H8CHO
!-----
!-----
!\PYROSPEC:
TC4H8CHO
!\OXIDSPEC:
O2C4H8CHO
O2HC4H8CO
!-----
!-----
!+++++
!+++++
!+++++
!\END_SPECIES_MODULE: \C5
!+++++
!+++++
!+++++
!+++++
!+++++
!\SPECIES_MODULE: \C6
! K. Zhang, C. Banyon, C. Togbe P. Dagaut, J. Bugler, H.J. Curran
! An experimental and kinetic modelling study of n-hexane oxidation
! Combust. Flame (2015) 162(11) 4194-4207
!
!\MODCOMMENTS:
!\MODWARNINGS:
```

```
!\MODSUBMECHS: \NC6H14 \C6H12-1\C6H12-2\C6H12-3 \NC5H11CHO
\C6H10D13\C6H10D24 \C6H10-15
!+++++
!-----
!\SUBMECH: \C6H10D13\C6H10D24
!-----
!\PYROSPEC:
C6H10D24
!\OXIDSPEC:
!-----
!\SUBMECH: \C6H101-5
!-----
!\PYROSPEC:
C6H101-5
C6H9-A
!\OXIDSPEC:
!-----
!+++++
!\END_SPECIES_MODULE: \C6
!+++++
!\SPECIES_MODULE: \C8
!\MODCOMMENTS: IC4H7CHO IS UNIQUE DECOMPOSITION PRODUCT OF H15DE2M, SO IS
NOT INCLUDED IN C4 MECHANISM YET.
!\MODWARNINGS:
!\MODSUBMECHS: \H15DE25DM
!+++++
!\SUBMECH: \H15DE25DM
! C-W. Zhou, Y. Li, E. O'Connor, K.P. Somers, S. Thion, C. Keese, O.
Mathieu, E.L. Petersen, T. A. DeVerter, M.A. Oehlschlaeger,
! G. Kukkadapu, C-J. Sung, M. Alrefae, F. Khaled, A. Farooq, P.
Dirrenberger, P-A. Glaude, F. Battin-Leclerc, J. Santner, Y. Ju,
! T. Held, F.M. Haas, F.L. Dryer, H.J. Curran, Comprehensive experimental
and modeling study of isobutene oxidation
! Combust. Flame (2016) accepted.
!-----
!\PYROSPEC:
H15DE25DM
```

H15DE25DM-S  
H15DE25DM-A  
!\OXIDSPEC:  
H15DE25DM-AO  
H15DE25DM-SO  
H15DE2M-T  
IC4H7CHO  
!-----  
-----  
!++++  
++++  
++++  
!\END\_SPECIES\_MODULE: \C8  
!++++  
++++  
++++  
!++++  
++++  
++++  
!\SPECIES\_MODULE: \AROMATIC  
!\MODCOMMENTS:  
!\MODWARNINGS:  
!\MODSUBMECHS: \CORE\_TO\_AROMATIC\_LINKERS \C6H6 \C6H5OH \C5H6  
!++++  
++++  
++++  
!-----  
-----  
!\SUBMECH: \CORE\_TO\_AROMATIC\_LINKERS  
!-----  
-----  
!\PYROSPEC:  
L-C6H4  
C-C6H4  
C6H3  
C6H2  
!\OXIDSPEC:  
!-----  
-----  
!-----  
-----  
!\SUBMECH: \C6H6  
!-----  
-----  
!\PYROSPEC:  
C6H6  
FULVENE  
C6H5  
!\OXIDSPEC:  
C6H5OO  
C6H5OOH  
!-----  
-----  
!-----  
-----  
!\SUBMECH: \C6H5OH  
!-----  
-----

!\PYROSPEC:

C6H5OH

C6H5O

C6H4OH

!\OXIDSPEC:

OC6H4OH

O-C6H4O2

P-C6H4O2

O-OC6H5OJ

P-OC6H5OJ

P-C6H3O2

!

!

!\SUBMECH: \C5H6

!

!\PYROSPEC:

C5H6

C5H5

C5H6-L

C#CCVCCJ

C5H7

CVCCJCVC

CVCCVCCJ

!\OXIDSPEC:

CVCCJCVCOH

HOCVCCVO

CVCCVCCOH

OC5H7O

OC4H6O

OC4H5O

O2CCHOOJ

HOCVCCJVO

C5H5OH

C5H5O

C5H4OH

C5H4O

C5H3O

CJVCCVCCVO

CVCCVCCJVO

CJVCCVO

!Sub mech : chloroacetate de méthyle

CH3OCOCH2CL

CH2OCOCH2CL

CH3OCOCHCL

CH2CL !radical chlorométhane

CH3CL !chlorométhane

COCH2CL

COCHCL !chloroketene

OCOCH2CL

CH3COOCH3

CH2COOCH3

CH3COOCH2

CH3COOH

HCL

```

CL2
C2H5CL !Chloroéthane
CH2CLCH2CL !1,2-dichloroéthane
CH3CHCL2 !1,1-dichloroéthane
CL
CH2CL2
CH2CH2CL !radical chloroethane
CH3CHCL !radical chloroéthane 2
CH2CHCL ! chloroéthène
CH2CCL !radical chloroéthène
CHCL2 !radical dichloromethane
CHCL !chloromethylene
!CH2CLCHCL !radical dichloroethane
!-----
!-----
!+++++
!+++++
!+++++
!\END_SPECIES_MODULE: \AROMATIC
!+++++
!+++++
!+++++
END
!\END_SPECIES_LIST
!\END_SPECIES_LIST
!\START_KINETICS_INPUT
REACTIONS
!+++++
!+++++
!+++++
!\KINETICS_MODULE: \H2_O2
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
!+++++
!+++++
!+++++
!-----
!-----
!\SUBMECH: \H2
!-----
!-----
!-----
!-----
!\REACTIONCLASS: \UNIMOL \A
\N \EA
!-----
H2+M<=>H+H+M
+4.5770000E+019 -1.4000000E+000 +1.0440000E+005 !\AUTHOR: AK !\REF:
TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
H2 / 2.500 / H2O / 12.000 / CO / 1.900 / CO2 / 3.800 / HE / 0.830 / CH4
/ 2.000 / C2H6 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES
!-----
!\REACTIONCLASS: \ABSTRACTION \A
\N \EA

```

```

!
-----
!\SITE: \UNDEF
H2+O<=>H+OH
+5.0800000E+004 +2.6700000E+000 +6.2920000E+003 !\AUTHOR: AK
!\REF:SUTHERLAND ET AL., 21ST SYMPOSIUM, P. 929 (1986) !\COMMENT:
H2+OH<=>H+H2O
+4.3800000E+013 +0.0000000E+000 +6.9900000E+003 !\AUTHOR: AK !\REF:LAM
ET AL. SUBMITTED IJCK !\COMMENT
!-----
!-----
!\ENDSUBMECH: \H2
!-----
!-----
!\SUBMECH: \O2
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!-----
!\REACTIONCLASS: \UNIMOL \A
\N \EA
!-----
O+O+M<=>O2+M
+6.1650000E+015 -5.0000000E-001 +0.0000000E+000 !\AUTHOR: AK !\REF:
TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:
H2 / 2.500 / H2O / 12.000 / AR / 0.830 / CO / 1.900 / CO2 / 3.800 / HE /
0.830 / CH4 / 2.000 / C2H6 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES
!-----
!\REACTIONCLASS: \RADICAL_ADDITION\H \A
\N \EA
!-----
O2+H<=>O+OH
+1.0400000E+014 +0.0000000E+000 +1.5286000E+004 !\AUTHOR: AK !\REF:
HONG ET AL. PROC. OF THE COMB. INST. 33 (2011) 309-316 !\COMMENT: 2
PARAMETER FIT
!-----
!-----
!\ENDSUBMECH: \O2
!-----
!-----
!\SUBMECH: \H2O
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!-----
!\REACTIONCLASS: \UNIMOL \A
\N \EA

```

!  
-----  
H+OH+M<=>H2O+M  
+3.5000000E+022 -2.0000000E+000 +0.0000000E+000 !\AUTHOR: AK !\REF: LI  
IJCK 36: 566-575, 2004 !\COMMENT:OPTIMISED TO FIT H2 AND CH4 FLAMES DATA  
H2 / 0.730 / H2O / 3.650 / CH4 / 2.000 / C2H6 / 3.000 / AR / 0.380 /  
!3RD BODY COLLIDER EFFICIENCIES  
!

-----  
!\REACTIONCLASS: \ABSTRACTION \A  
\N \EA  
!

-----  
O+H2O<=>OH+OH  
+6.7000000E+007 +1.7040000E+000 +1.4986800E+004 !\AUTHOR: AK !\REF:  
SUTHERLAND ET AL., 23RD SYMPOSIUM, P. 51 (1990) !\COMMENT:  
!

-----  
!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

-----  
O+H+M<=>OH+M  
+4.7140000E+018 -1.0000000E+000 +0.0000000E+000 !\AUTHOR: AK !\REF:  
TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
H2 / 2.500 / H2O / 12.000 / AR / 0.750 / CO / 1.500 / CO2 / 2.000 / HE /  
0.750 / CH4 / 2.000 / C2H6 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
!=====

!\SUBSPECIES: \OHV  
!=====

!

-----  
!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

-----  
H+O+M<=>OHV+M  
+1.5000000E+013 +0.0000000E+000 +5.9750000E+003 !\AUTHOR: AK  
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:  
H2 / 1.000 / H2O / 6.500 / O2 / 0.400 / N2 / 0.400 / AR / 0.350 / !3RD  
BODY COLLIDER EFFICIENCIES  
!

-----  
!\REACTIONCLASS: \DEACTIVATION \A  
\N \EA  
!

-----  
OHV+H2O<=>OH+H2O  
+5.9300000E+012 +5.0000000E-001 -8.6000000E+002 !\AUTHOR: AK  
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:  
OHV+H2<=>OH+H2  
+2.9500000E+012 +5.0000000E-001 -4.4400000E+002 !\AUTHOR: AK  
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:  
OHV+N2<=>OH+N2  
+1.0800000E+011 +5.0000000E-001 -1.2420000E+003 !\AUTHOR: AK  
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:



```

OHV+OH<=>OH+OH
+6.0100000E+012 +5.0000000E-001 -7.6400000E+002 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV+H<=>OH+H
+1.3100000E+012 +5.0000000E-001 -1.6700000E+002 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV+AR<=>OH+AR
+1.6900000E+012 +0.0000000E+000 +4.1350000E+003 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV<=>OH
+1.4500000E+006 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV+O2<=>OH+O2
+2.1000000E+012 +5.0000000E-001 -4.7800000E+002 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV+CO2<=>OH+CO2
+2.7500000E+012 +5.0000000E-001 -9.6800000E+002 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV+CO<=>OH+CO
+3.2300000E+012 +5.0000000E-001 -7.8700000E+002 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
OHV+CH4<=>OH+CH4
+3.3600000E+012 +5.0000000E-001 -6.3500000E+002 !\AUTHOR: AK
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
!=====
!=====
!\ENDSUBSPECIES: \OHV
!=====
!=====
!-----
!-----
!\ENDSUBMECH: \H2O
!-----
!-----
!-----
!\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/
H2O2 (+M)<=>OH+OH(+M)
+2.0000000E+012 +9.0000000E-001 +4.8749000E+004 !\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 /
+2.4900000E+024 -2.3000000E+000 +4.8749000E+004 / !LOW-PRESSURE-LIMIT

```

TROE / +4.3000000E-001 +1.0000000E-030 +1.0000000E+030 / !TROE PARAMETERS  
H2O / 7.650 / CO2 / 1.600 / N2 / 1.500 / O2 / 1.200 / HE / 0.650 / H2O2 / 7.700 / H2 / 3.700 / CO / 2.800 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

H2O2+H<=>H2O+OH  
+2.4100000E+013 +0.0000000E+000 +3.9700000E+003 !\AUTHOR: AK  
!\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
!\COMMENT:  
H2O2+H<=>H2+HO2  
+2.1500000E+010 +1.0000000E+000 +6.0000000E+003 !\AUTHOR: AK !\REF:  
ELLINGSON J. PHYS. CHEM. (2007) 111, (51), 13554-13566 !\COMMENT:  
H2O2+O<=>OH+HO2  
+9.5500000E+006 +2.0000000E+000 +3.9700000E+003 !\AUTHOR: AK  
!\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
!\COMMENT:  
H2O2+OH<=>H2O+HO2  
+1.7400000E+012 +0.0000000E+000 +3.1800000E+002 !\AUTHOR: AK !\REF:  
HONG ET AL. J. PHYS. CHEM. A 114 (2010) 5718-5727 !\COMMENT:  
DUP  
H2O2+OH<=>H2O+HO2  
+7.5900000E+013 +0.0000000E+000 +7.2690000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
DUP  
!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA  
!

---

HO2+H<=>OH+OH  
+7.0790000E+013 +0.0000000E+000 +2.9500000E+002 !\AUTHOR: KPS !\REF:  
NOT A CLUE WHAT REFERENCE IS HERE AS MECHANISM IS A MESS !\COMMENT:  
WARNING  
HO2+H<=>H2+O2  
+1.1402000E+010 +1.0827000E+000 +5.5378000E+002 !\AUTHOR: AK  
!\REF:MICHAEL SUTHERLAND 2000 !\COMMENT:  
HO2+O<=>OH+O2  
+3.2500000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: AK  
!\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)  
OH+HO2<=>H2O+O2  
+7.0000000E+012 +0.0000000E+000 -1.0929600E+003 !\AUTHOR: ?? !\REF:  
hong pci 2013 1015C !\COMMENT: WARNING  
DUP  
OH+HO2<=>H2O+O2  
+4.5000000E+014 +0.0000000E+000 +1.0929600E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
DUP  
HO2+HO2<=>H2O2+O2  
+1.0000000E+014 +0.0000000E+000 +1.1040883E+004 !\AUTHOR: AK !\REF:  
hong pci 2013, kapel 2002 !\COMMENT: WARNING  
DUP

HO2+HO2<=>H2O2+O2  
+1.9000000E+011 +0.0000000E+000 -1.4089248E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
DUP  
!

---

!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

---

---

H+O2 (+M) <=> HO2 (+M)  
+4.6500000E+012 +4.4000000E-001 +0.0000000E+000 !\AUTHOR: AK  
!\REF:FERNANDES PCCP 2008 !COMMENT: Efficiencis of AR and HE derived from  
seperated reactions,  
LOW /  
+1.7370000E+019 -1.2300000E+000 +0.0000000E+000 / !LOW-PRESSURE-LIMIT  
TROE / +6.7000000E-001 +1.0000000E-  
030 +1.0000000E+030 +1.0000000E+030 / !TROE PARAMETERS  
H2 / 1.300 / CO / 1.900 / CO2 / 3.800 / HE / 0.640 / H2O / 10.000 / AR /  
0.500 / CH4 / 2.000 / C2H6 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
!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/  
!

!\ENDSUBMECH: \H2O2

!\KINETICS\_MODULE: \H2\_O2  
!\MODCOMMENTS:  
!\MODWARNINGS:  
!\MODSUBMECHS: CO, CH2O, CH4,  
!\KINETICS\_MODULE: \C1

!\SUBMECH: \CO  
!\MECHCOMMENTS:  
!\MECHWARNINGS:

!-----  
-----  
!

!\REACTIONCLASS: \RADICAL\_ADDITION\O \A  
\N \EA  
!

CO+O(+M)<=>CO2(+M)  
+1.3620000E+010 +0.0000000E+000 +2.3840000E+003 !\AUTHOR: ?? !\REF:  
MEULLER 99 \* 0.76  
LOW /  
+1.1730000E+024 -2.7900000E+000 +4.1910000E+003 / !LOW-PRESSURE-LIMIT  
H2 / 2.000 / H2O / 12.000 / CO / 1.750 / CO2 / 3.600 / AR / 0.700 / HE /  
0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

CO+OH<=>CO2+H  
+7.0150000E+004 +2.0530000E+000 -3.5570000E+002 !\AUTHOR: ?? !\REF:  
JOSHI AND WANG IJCK (2006), 38, (1), 57-73. !\COMMENT:  
DUP  
CO+OH<=>CO2+H  
+5.7570000E+012 -6.6400000E-001 +3.3180000E+002 !\AUTHOR: !\REF:  
!\COMMENT:  
DUP  
!

!\REACTIONCLASS: \RADICAL\_ADDITION\HO2 \A  
\N \EA  
!

CO+HO2<=>CO2+OH  
+1.5700000E+005 +2.1800000E+000 +1.7940000E+004 !\AUTHOR: ?? !\REF: YOU  
ET AL. J. PHYS. CHEM. A 2007, 111, 4031-4042 !\COMMENT:  
!

!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

CO+O2<=>CO2+O  
+1.1190000E+012 +0.0000000E+000 +4.7700000E+004 !\AUTHOR: ?? !\REF:  
86TSA/ HAM \* 0.44 !\COMMENT:  
!=====  
=====  
!\SUBSPECIES: \CO2  
!=====  
=====  
!

!\REACTIONCLASS: \RADICAL\_ADIDTION\H \A  
\N \EA  
!

```

H+CO2<=>OCHO
+7.5000000E+013 +0.0000000E+000 +2.9000000E+004   !\AUTHOR: ?? !\REF:
CURRAN ESTIMATE !\COMMENT: WARNING
!=====
=====
!\ENDSUBSPECIES: \CO2
!=====
=====
!=====
=====
!\SUBSPECIES: \HOCO
!=====
=====
HOCO<=>CO+OH
+6.3000000E+032 -5.9600000E+000 +3.2470000E+004   !\AUTHOR: ?? !\REF:
JOHN R. BARKER CALCULATION 7/ 3/ 2013 !\COMMENT: WARNING: RATE CONSTANTS
FROM PRIVATE COMMUNICATION WITH JOHN BARKER.
PLOG /                               +1.0000000E-003 +1.5500000E-
008 +2.9300000E+000 +8.7680000E+003 /
PLOG /                               +3.0000000E-003
+1.7700000E+003 +3.4000000E-001 +1.8076000E+004 /
PLOG /                               +2.9600000E-002
+2.0200000E+013 -1.8700000E+000 +2.2755000E+004 /
PLOG /                               +9.8700000E-002
+1.6800000E+018 -3.0500000E+000 +2.4323000E+004 /
PLOG /                               +2.9610000E-001
+2.5000000E+024 -4.6300000E+000 +2.7067000E+004 /
PLOG /                               +9.8690000E-001
+4.5400000E+026 -5.1200000E+000 +2.7572000E+004 /
PLOG /                               +2.9607000E+000
+7.1200000E+028 -5.6000000E+000 +2.8535000E+004 /
PLOG /                               +9.8690000E+000
+5.4800000E+029 -5.7000000E+000 +2.8899000E+004 /
PLOG /                               +2.9607000E+001
+9.8900000E+031 -6.1900000E+000 +3.0518000E+004 /
PLOG /                               +9.8690000E+001
+5.7400000E+033 -6.5300000E+000 +3.2068000E+004 /
PLOG /                               +2.9607000E+002
+2.6100000E+033 -6.2900000E+000 +3.2231000E+004 /
PLOG /                               +9.8690000E+002
+6.3000000E+032 -5.9600000E+000 +3.2470000E+004 /
HOCO<=>CO2+H
+1.8970000E+038 -8.0470000E+000 +3.4240000E+004   !\AUTHOR: ?? !\REF:
JOHN R. BARKER CALCULATION 7/ 3/ 2013 !\COMMENT: WARNING: RATE CONSTANTS
FROM PRIVATE COMMUNICATION WITH JOHN BARKER.
PLOG /                               +1.0000000E-003
+4.7580000E+018 -3.8170000E+000 +1.7676000E+004 /
PLOG /                               +3.0000000E-003
+2.2250000E+020 -4.1490000E+000 +1.9037000E+004 /
PLOG /                               +9.9000000E-003
+7.5640000E+021 -4.4340000E+000 +2.0325000E+004 /
PLOG /                               +2.9600000E-002
+9.1070000E+024 -5.1890000E+000 +2.2419000E+004 /
PLOG /                               +9.8700000E-002
+3.1440000E+029 -6.3760000E+000 +2.5233000E+004 /
PLOG /                               +2.9610000E-001
+1.1500000E+032 -7.0370000E+000 +2.6662000E+004 /

```

PLOG / +9.8690000E-001  
+1.0690000E+036 -8.1070000E+000 +2.9064000E+004 /  
PLOG / +2.9607000E+000  
+2.4380000E+036 -8.1530000E+000 +2.9336000E+004 /  
PLOG / +9.8690000E+000  
+6.6630000E+035 -7.9190000E+000 +2.9217000E+004 /  
PLOG / +2.9607000E+001  
+1.7230000E+038 -8.5060000E+000 +3.1273000E+004 /  
PLOG / +9.8690000E+001  
+3.0070000E+041 -9.2900000E+000 +3.3966000E+004 /  
PLOG / +2.9607000E+002  
+6.7670000E+036 -7.8320000E+000 +3.1613000E+004 /  
PLOG / +9.8690000E+002  
+1.8970000E+038 -8.0470000E+000 +3.4240000E+004 /

!=====  
=====

!\ENDUBSPECIES: \HOCO

!=====  
=====

!-----  
-----

!\ENDSUBMECH: \CO

!-----  
-----

!-----  
-----

!\SUBMECH: \CH4

!\MECHCOMMENTS:

!\MECHWARNINGS:

!-----  
-----

!-----  
-----

!\REACTIONCLASS: \UNIMOL

\A

\N \EA

!-----  
-----

CH3+H(+M) <=> CH4(+M)

+1.2700000E+016 -6.3000000E-001 +3.8300000E+002 !\AUTHOR: ?? !\REF: GRI  
MECHANISM !\COMMENT: WARNING: WHAT IS REFERENCE FOR GRI MECHANISM?

LOW /

+2.4770000E+033 -4.7600000E+000 +2.4400000E+003 / !LOW-PRESSURE-LIMIT

TROE / +7.8300000E-001

+7.4000000E+001 +2.9410000E+003 +6.9640000E+003 / !TROE PARAMETERS

H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES

!-----  
-----

!\REACTIONCLASS: \RH\_R\_ABSTRACTION

\A

\N \EA

!-----  
-----

CH4+H<=>CH3+H2

+6.1400000E+005 +2.5000000E+000 +9.5870000E+003 !\AUTHOR: !\REF:

BAULCH, D.L.; ET AL., J. PHYS. CHEM. REF. DATA (2005) !\COMMENT:

CH4+O<=>CH3+OH

+1.0200000E+009 +1.5000000E+000 +8.6000000E+003 !\AUTHOR: !\REF:

!REF:GRI 3.0 !\COMMENT: WARNING: WHAT IS REFERENCE FOR GRI MECHANISM?

CH4+OH<=>CH3+H2O  
+5.8300000E+004 +2.6000000E+000 +2.1900000E+003 !\AUTHOR: !\REF: CURRAN  
ESTIMATE, FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT ARE REFERENCES TO  
RATE CONSTANTS IN NIST?  
CH4+HO2<=>CH3+H2O2  
+1.1300000E+001 +3.7400000E+000 +2.1010000E+004 !\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+CH3O2<=>CH3+CH3O2H +9.6000000E-  
001 +3.7700000E+000 +1.7810000E+004 !\AUTHOR: !\REF: NEW FIT FROM HJC  
!\COMMENT: WARNING: WHAT IS SOURCE OF THIS RATE CONSTANT??  
CH3+HO2<=>CH4+O2  
+1.1600000E+005 +2.2300000E+000 -3.0220000E+003 !\AUTHOR: !\REF:  
JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279-286 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\CH2 \A  
\N \EA  
!

---

CH4+CH2<=>CH3+CH3  
+2.4600000E+006 +2.0000000E+000 +8.2700000E+003 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
!=====  
!=====  
!\SUBSPECIES: \CH2(S)  
!=====  
!=====  
!

---

!\REACTIONCLASS: \DEACTIVATION \A  
\N \EA  
!

---

CH2(S)+N2<=>CH2+N2  
+1.5000000E+013 +0.0000000E+000 +6.0000000E+002 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2(S)+AR<=>CH2+AR  
+9.0000000E+012 +0.0000000E+000 +6.0000000E+002 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2(S)+H2O<=>CH2+H2O  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2(S)+CO<=>CH2+CO  
+9.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2(S)+CO2<=>CH2+CO2  
+7.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
!

---

!\REACTIONCLASS: \RADICAL\_RECOMBINATIONS \A  
\N \EA  
!

---

CH2(S)+O2=>H+OH+CO  
+2.8000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING

CH2 (S) +O2<=>CO+H2O  
+1.2000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2 (S) +O<=>CO+H2  
+1.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2 (S) +O<=>HCO+H  
+1.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2 (S) +H2<=>CH3+H  
+7.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2 (S) +H<=>CH+H2  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2 (S) +OH<=>CH2O+H  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING  
CH2 (S) +CO2<=>CH2O+CO  
+1.4000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT: WARNING

!=====  
=====

!\ENDSUBSPECIES: \CH2 (S)

!=====  
=====

!=====  
=====

!\SUBSPECIES: \CH2

!=====  
=====

CH2+H (+M) <=>CH3 (+M)  
+2.5000000E+016 -8.0000000E-001 +0.0000000E+000 !\AUTHOR: !\REF: LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
LOW /  
+3.2000000E+027 -3.1400000E+000 +1.2300000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +6.8000000E-001  
+7.8000000E+001 +1.9950000E+003 +5.5900000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

!\REACTIONCLASS: \RADICAL\_RECOMBINATIONS \A

\N \EA

!=====  
=====

CH2+O2<=>HCO+OH  
+1.0600000E+013 +0.0000000E+000 +1.5000000E+003 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT:  
CH2+O2=>CO2+H+H  
+2.6400000E+012 +0.0000000E+000 +1.5000000E+003 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT:  
CH2+O=>CO+H+H  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT:  
CH2+H<=>CH+H2  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:



GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)

!\COMMENT:

CH2+OH<=>CH+H2O

+1.1300000E+007 +2.0000000E+000 +3.0000000E+003 !\AUTHOR: !\REF: GRI

3.0 !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \CH2

!=====  
=====

!=====  
=====

!\SUBSPECIES: \CHV

!=====  
=====

!\_\_\_\_\_

!\REACTIONCLASS: \DEACTIVATION

\A

\N \EA

!\_\_\_\_\_

CHV+AR<=>CH+AR

+4.0000000E+011 +5.0000000E-001 +0.0000000E+000 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT: CHV+M<=>CH+M

CHV+H2O<=>CH+H2O

+5.3000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

CHV+CO<=>CH+CO

+2.4400000E+012 +5.0000000E-001 +0.0000000E+000 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

CHV+CO2<=>CH+CO2

+2.4100000E-

001 +4.3000000E+000 -1.6940000E+003 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987) !\COMMENT:

CHV+O2<=>CH+O2

+2.4800000E+006 +2.1400000E+000 -1.7200000E+003 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

CHV+H2<=>CH+H2

+1.4700000E+014 +0.0000000E+000 +1.3610000E+003 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

CHV+CH4<=>CH+CH4

+1.7300000E+013 +0.0000000E+000 +1.6700000E+002 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

CHV<=>CH

+1.8600000E+006 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

CHV+N2<=>CH+N2

+3.0300000E+002 +3.4000000E+000 -3.8100000E+002 !\AUTHOR: ??

!\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

!\COMMENT:

```

C+H+M<=>CHV+M
+6.0000000E+014 +0.0000000E+000 +6.9400000E+003   !\AUTHOR: ??
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
!
=====
!\REACTIONCLASS:  \RADICAL_RECOMBINATIONS           \A
\N                \EA
!
=====
CH+O2<=>CO+OHV
+4.0400000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR:
!\REF:KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
CH+O2<=>HCO+O
+3.3000000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF: GRI
3.0 !\COMMENT:
CH+O<=>CO+H
+5.7000000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:
MESSING ET AL., J. CHEM. PHYS. 74, 3874 (1981) !\COMMENT:
CH+H<=>C+H2
+1.1000000E+014 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF: GRI
3.0 !\COMMENT:
CH+OH<=>HCO+H
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:
GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)
!\COMMENT:
CH+H2O<=>H+CH2O
+1.7740000E+016 -1.2200000E+000 +2.3800000E+001   !\AUTHOR: !\REF:BERGEAT
ET AL., CHEM. PHYS. LETT. 480, 21 (2009) !\COMMENT:
CH+CO2<=>HCO+CO
+1.7000000E+012 +0.0000000E+000 +6.8500000E+002   !\AUTHOR: !\REF:
BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB. P. 73, 1982 !\COMMENT:
X0.5
!=====
!=====
!\ENDSUBSPECIES:  \CHV
!=====
!=====
!\SUBSPECIES:  \C
!=====
!=====
C+OH<=>CO+H
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:
GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)
!\COMMENT:
C+O2<=>CO+O
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:
GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)
!\COMMENT:
!=====
!=====
!\ENDSUBSPECIES:  \C
!=====
!=====
!\SUBSPECIES:  \CH3

```

!=====  
=====

!  
-----  
!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

-----  
CH3+O2 (+M) <=> CH3O2 (+M)  
+7.8120000E+009 +9.0000000E-001 +0.0000000E+000 !\AUTHOR: ?? !\REF:  
R.X. FERNANDES ET AL., J. PHYS. CHEM. A, (2006) 110:4442-4449. !\COMMENT:  
LOW /  
+6.8500000E+024 -3.0000000E+000 +0.0000000E+000 / !LOW-PRESSURE-LIMIT  
TROE / +6.0000000E-001  
+1.0000000E+003 +7.0000000E+001 +1.7000000E+003 / !TROE PARAMETERS  
CH3+O2 <=> CH3O+O  
+7.5460000E+012 +0.0000000E+000 +2.8320000E+004 !\AUTHOR: ?? !\REF:N.  
K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109, 7902-7914 (2005) !\COMMENT:  
CH3+O2 <=> CH2O+OH  
+2.6410000E+000 +3.2830000E+000 +8.1050000E+003 !\AUTHOR: ?? !\REF:  
PERSONAL COMMUNICATION, STEVE KLIPPENSTEIN !\COMMENT: WARNING: HAS THIS  
BEEN PUBLISHED?

!  
-----  
!\REACTIONCLASS: \RADICAL\_ADDITION\O \A  
\N \EA  
!

-----  
CH3+O <=> CH2O+H  
+5.5400000E+013 +5.0000000E-002 -1.3600000E+002 !\AUTHOR: !\REF:HARDING  
AND KLIPPENSTEIN 2B04, 30TH SYMP 2004. !\COMMENT:

!  
-----  
!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

-----  
CH3+OH <=> CH2(S)+H2O  
+4.9360000E+014 -6.6900000E-001 -4.4580000E+002 !\AUTHOR: ?? !\REF:FROM  
JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950 !\COMMENT: ONLY INCLUDING  
TRANS HCOH FOR SIMPLICITY,  
PLOG / +1.0000000E-002  
+4.9360000E+014 -6.6900000E-001 -4.4580000E+002 /  
PLOG / +1.0000000E-001  
+1.2070000E+015 -7.7800000E-001 -1.7560000E+002 /  
PLOG / +1.0000000E+000  
+5.2820000E+017 -1.5180000E+000 +1.7720000E+003 /  
PLOG / +1.0000000E+001  
+4.7880000E+023 -3.1550000E+000 +7.0030000E+003 /  
PLOG / +1.0000000E+002  
+8.4330000E+019 -1.9620000E+000 +8.2440000E+003 /  
CH3+OH <=> CH2O+H2  
+3.5020000E+005 +1.4410000E+000 -3.2440000E+003 !\AUTHOR: ?? !\REF:FROM  
JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950 !\COMMENT:  
PLOG / +1.0000000E-002  
+3.5020000E+005 +1.4410000E+000 -3.2440000E+003 /  
PLOG / +1.0000000E-001  
+8.8540000E+005 +1.3270000E+000 -2.9750000E+003 /

PLOG / +1.0000000E+000  
 +1.6500000E+007 +9.7300000E-001 -2.0100000E+003 /  
 PLOG / +1.0000000E+001  
 +5.3740000E+009 +2.8700000E-001 +2.8000000E+002 /  
 PLOG / +1.0000000E+002  
 +9.4940000E+018 -2.1990000E+000 +9.7690000E+003 /  
 CH3+OH<=>CH2OH+H  
 +1.6210000E+010 +9.6500000E-001 +3.2100000E+003 !\AUTHOR: ?? !\REF:FROM  
 JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT: INCREASED BY  
 FACTOR OF 2  
 PLOG / +1.0000000E-002  
 +1.6210000E+010 +9.6500000E-001 +3.2140000E+003 /  
 PLOG / +1.0000000E-001  
 +1.8070000E+010 +9.5000000E-001 +3.2470000E+003 /  
 PLOG / +1.0000000E+000  
 +4.6860000E+010 +8.3300000E-001 +3.5660000E+003 /  
 PLOG / +1.0000000E+001  
 +1.5250000E+013 +1.3400000E-001 +5.6410000E+003 /  
 PLOG / +1.0000000E+002  
 +3.5900000E+014 -1.8600000E-001 +8.6010000E+003 /  
 CH3+OH<=>H+CH3O  
 +1.1860000E+009 +1.0160000E+000 +1.1940000E+004 !\AUTHOR: ?? !\REF:FROM  
 JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +1.1860000E+009 +1.0160000E+000 +1.1940000E+004 /  
 PLOG / +1.0000000E-001  
 +1.1880000E+009 +1.0160000E+000 +1.1940000E+004 /  
 PLOG / +1.0000000E+000  
 +1.2300000E+009 +1.0110000E+000 +1.1950000E+004 /  
 PLOG / +1.0000000E+001  
 +1.7980000E+009 +9.6500000E-001 +1.2060000E+004 /  
 PLOG / +1.0000000E+002  
 +5.2420000E+010 +5.5100000E-001 +1.3070000E+004 /  
 CH3+OH<=>HCOH+H2  
 +8.6740000E+008 +7.8700000E-001 -3.0460000E+003 !\AUTHOR: ?? !\REF:FROM  
 JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +8.6740000E+008 +7.8700000E-001 -3.0460000E+003 /  
 PLOG / +1.0000000E-001  
 +3.1150000E+009 +6.3000000E-001 -2.6690000E+003 /  
 PLOG / +1.0000000E+000  
 +1.5570000E+011 +1.5600000E-001 -1.3680000E+003 /  
 PLOG / +1.0000000E+001  
 +1.7040000E+021 -2.6410000E+000 +6.4120000E+003 /  
 PLOG / +1.0000000E+002  
 +7.2500000E+020 -2.4020000E+000 +9.6390000E+003 /  
 CH3+OH<=>CH2+H2O  
 +4.2930000E+004 +2.5680000E+000 +3.9978000E+003 !\AUTHOR: ?? !\REF:FROM  
 JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279-286 !\COMMENT:  
 !

---

!\REACTIONCLASS: \R+HO2 \A  
 \N \EA  
 !

---

CH3+HO2<=>CH3O+OH  
 +1.0000000E+012 +2.6900000E-001 -6.8750000E+002 !\AUTHOR: ?? !\REF:  
 JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279-286 !\COMMENT:

```
!=====
=====
!\ENDSUBSPECIES: \CH3
!=====
=====
!=====
=====
!\SUBSPECIES: \CH3O2
!=====
=====
!
-----
!\REACTIONCLASS: \RADICAL_RECOMBINATIONS \A
\N \EA
!
```

```
CH3O2+O<=>CH3O+O2
+3.6000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--
3220. !\COMMENT:
CH3O2+H<=>CH3O+OH
+9.6000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--
3220. !\COMMENT:
CH3O2+OH<=>CH3OH+O2
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--
3220. !\COMMENT:
CH3O2+HO2<=>CH3O2H+O2
+2.4700000E+011 +0.0000000E+000 -1.5700000E+003 !\AUTHOR:
!\REF:LIGHTFOOT,P.D. ETAL., ATMOS. ENVIRON. PART A: 26, 1805-1961 (1992)
!\COMMENT:
CH3O2+H2O2<=>CH3O2H+HO2
+2.4100000E+012 +0.0000000E+000 +9.9360000E+003 !\AUTHOR:
!\REF:REF:Tsang, W., J. Phys. Chem. Ref. Data 15, 1087 (1986) !\COMMENT:
ADDED 29/07/2015
CH3O2+CH3<=>CH3O+CH3O
+5.0800000E+012 +0.0000000E+000 -1.4110000E+003 !\AUTHOR:
!\REF:KEIFFER, M. ET AL., J. CHEM. SOC. FARADAY TRANS. 2: 84, 505 (1988)
!\COMMENT:
CH3O2+CH3O2=>CH2O+CH3OH+O2
+3.1100000E+014 -1.6100000E+000 -1.0510000E+003 !\AUTHOR:
!\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--
3220. !\COMMENT:
CH3O2+CH3O2=>O2+CH3O+CH3O
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:
!\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--
3220. !\COMMENT:
!
```

```
!\REACTIONCLASS: \RH_R_ABSTRACTION \A
\N \EA
!
```

```
H2+CH3O2<=>H+CH3O2H
+1.5000000E+014 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG &
HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:
```

!  
-----  
!\REACTIONCLASS: \KHP\_DECOMP \A  
\N \EA  
!

CH3O2H<=>CH3O+OH  
+6.3100000E+014 +0.0000000E+000 +4.2300000E+004 !\AUTHOR:  
!\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--  
3220. !\COMMENT:  
CH2O2H<=>CH2O+OH  
+9.0000000E+014 +0.0000000E+000 +1.5000000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: KPS: THIS REACTION WAS MOVED FROM THE C4 MECHANISM!!  
!=====  
!=====  
!\ENDSUBSPECIES: \CH3O2  
!=====  
!=====  
!-----  
!-----  
!\ENDSUBMECH: \CH4  
!-----  
!-----  
!-----  
!\SUBMECH: \CH3OH  
!\MECHCOMMENTS: HCOH IS FORMED FROM CH3+OH, IT IS NOT NECESSARY FOR  
FORMALDEHYDE OXIDATION, AND MINOR FOR CH4/CH3OH  
!\MECHWARNINGS:  
!-----  
!-----  
!

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

CH3OH(+M)<=>CH3+OH(+M)  
+2.0840000E+018 -6.1500000E-001 +9.2540600E+004 !\AUTHOR: !\REF:FROM  
JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950 !\COMMENT: NEGLECTING HCOH  
CHANNELS AS THEY ARE NOT IMPORTANT  
LOW /  
+1.5000000E+043 -6.9950000E+000 +9.7992200E+004 / !LOW-PRESSURE-LIMIT  
TROE / -4.7480000E-001  
+3.5580000E+004 +1.1160000E+003 +9.0230000E+003 / !TROE PARAMETERS  
CH3OH(+M)<=>CH2(S)+H2O(+M)  
+3.1210000E+018 -1.0170000E+000 +9.1712000E+004 !\AUTHOR: !\REF:FROM  
JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950 !\COMMENT: NEGLECTING HCOH  
CHANNELS AS THEY ARE NOT IMPORTANT  
LOW /  
+1.4300000E+047 -8.2270000E+000 +9.9417100E+004 / !LOW-PRESSURE-LIMIT  
TROE / +2.5450000E+000  
+3.2900000E+003 +4.7320000E+004 +4.7110000E+004 / !TROE PARAMETERS  
CH3OH(+M)<=>CH2OH+H(+M) +7.8960000E-  
003 +5.0380000E+000 +8.4467400E+004 !\AUTHOR: !\REF:FROM JASPER/  
KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950 !\COMMENT: NEGLECTING HCOH CHANNELS  
AS THEY ARE NOT IMPORTANT

LOW /  
+3.3900000E+042 -7.2440000E+000 +1.0523030E+005 / !LOW-PRESSURE-LIMIT  
TROE / -7.3910000E+001  
+3.7050000E+004 +4.1500000E+004 +5.2200000E+003 / !TROE PARAMETERS  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTIONS \A  
\N \EA  
!

---

---

CH3OH+H<=>CH3O+H2  
+1.9900000E+005 +2.5600000E+000 +1.0300000E+004 !\AUTHOR: !\REF:J.  
CHEM. PHYS. 134, 094302 (2011) !\COMMENT: WARNING INCOMPLETE REFERENCE  
CH3OH+H<=>CH2OH+H2  
+3.0700000E+005 +2.5500000E+000 +5.4400000E+003 !\AUTHOR: !\REF:J.  
CHEM. PHYS. 134, 094302 (2011) !\COMMENT: WARNING INCOMPLETE REFERENCE  
CH3OH+O<=>CH3O+OH  
+3.8800000E+004 +2.5000000E+000 +3.0800000E+003 !\AUTHOR: !\REF:TSANG,  
JPC REF. DATA, 16:471 (1987)!\COMMENT: reduced by an order of magnitude  
from abstraction from the methyl site  
CH3OH+O<=>CH2OH+OH  
+3.8800000E+005 +2.5000000E+000 +3.0800000E+003 !\AUTHOR: !\REF:TSANG,  
JPC REF. DATA, 16:471 (1987) !\COMMENT:  
CH3OH+OH<=>CH3O+H2O  
+1.5000000E+002 +3.0300000E+000 -7.6300000E+002 !\AUTHOR: !\REF:XU ET  
AL. PROC 31 2007 159-166 !\COMMENT:  
CH3OH+OH<=>CH2OH+H2O  
+3.0800000E+004 +2.6500000E+000 -8.0670000E+002 !\AUTHOR: !\REF:XU ET  
AL. PROC 31 2007 159-166 !\COMMENT:  
!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  
CH3OH+O2<=>CH3O+HO2  
+3.5800000E+004 +2.2700000E+000 +4.2764500E+004 !\AUTHOR: !\REF:S. J.  
Klippenstein, L. B. Harding, M. J. Davis, A. S. Tomlin, R. T. Skodje,  
PCI, 33 (2011) 351-357  
!\COMMENT:(above)reduced by an order of magnitude from abstraction from  
the methyl site due to increased bond strengths, Ultan added 21/08/15  
CH3OH+O2<=>CH2OH+HO2  
+3.5800000E+005 +2.2700000E+000 +4.2764500E+004 !\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+HO2<=>CH2OH+H2O2 1.080E+004 2.550 10530.0 !\AUTHOR: !\REF: CURRAN  
ESTIMATE !\COMMENT: WARNING: Ultan removed 21/08/15  
CH3OH+HO2<=>CH3O+H2O2  
+1.2200000E+012 +0.0000000E+000 +2.0070700E+004 !\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  
+3.2600000E+013 +0.0000000E+000 +1.8782200E+004 !\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+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  
CH3OH+CH3<=>CH2OH+CH4 +2.1300000E-  
001 +3.9530000E+000 +7.0551000E+003 !\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

+3.2200000E+003 +2.4250000E+000 +8.5795000E+003 !\AUTHOR: !\REF:I. M. Alecu, D. G. Truhlar, J. Phys. Chem. A, 115 (2011) 14599-14611 !\COMMENT: Ultan added 21/08/15

CH3OH+HCO<=>CH2OH+CH2O

+9.6300000E+003 +2.9000000E+000 +1.3110000E+004 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:

CH3OH+CH3O<=>CH2OH+CH3OH

+3.0000000E+011 +0.0000000E+000 +4.0740000E+003 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:

CH3OH+CH3O2<=>CH2OH+CH3O2H

+1.8100000E+012 +0.0000000E+000 +1.3710000E+004 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)

!=====

=====

!\SUBSPECIES: \CH2OH

!=====

=====

!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTIONS

\A

\N \EA

!

---

CH2OH+O2<=>CH2O+HO2

+1.5100000E+015 -1.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GROTHER, H. H. ET AL., J. PHYS. CHEM. 92: 4028 (1988). !\COMMENT: DUP

CH2OH+O2<=>CH2O+HO2

+2.4100000E+014 +0.0000000E+000 +5.0170000E+003 !\AUTHOR: !\REF: !\COMMENT: DUP

CH2OH+H<=>CH2O+H2

+6.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:

CH2OH+HO2<=>CH2O+H2O2

+1.2000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991). !\COMMENT:

CH2OH+HCO<=>CH2O+CH2O

+1.8000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998) !\COMMENT: Ultan removed 21/08/15

CH2OH+HCO<=>CH3OH+CO

+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: !\COMMENT: WARNING, NO REF

CH2OH+CH3O<=>CH2O+CH3OH

+2.4000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991). !\COMMENT:

CH2OH+OH<=>H2O+CH2O

+2.4000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:

CH2OH+O<=>OH+CH2O

+4.2000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:

CH2OH+CH2OH<=>CH2O+CH3OH

+3.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)



!  
-----  
!\REACTIONCLASS: \R+HO2 \A  
\N \EA  
!

-----  
CH2OH+HO2<=>HOCH2O+OH  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT??  
!=====

!\ENDSUBSPECIES: \CH2OH  
!=====

!\SUBSPECIES: \CH3O  
!=====

!

-----  
!\REACTIONCLASS: \R\_R\_ABSTRACTIONS \A  
\N \EA  
!

-----  
CH3O+O2<=>CH2O+HO2 +4.3800000E-019  
+9.5000000E+000 -5.5010000E+003 !\AUTHOR: !\REF:WANTUCK, P.J. E AL.  
J. PHYS. CHEM. 91, 4653 (1987) !\COMMENT:  
CH3O+H<=>CH2O+H2  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:HOYERMANN ET AL., 18TH SYMPOSIUM !\COMMENT:  
CH3O+HO2<=>CH2O+H2O2  
+3.0100000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
CH3O+CH3<=>CH2O+CH4  
+1.2000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING: NO REFERENCE !\COMMENT: WARNING: NO REFERENCE  
CH3O+CH3O<=>CH3OH+CH2O  
+6.0300000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
!=====

!\ENDSUBSPECIES: \CH3O  
!=====

!\SUBSPECIES: \HCOH  
!=====

!

-----  
!\REACTIONCLASS: \LUMPED\_BIMOLECULAR \A  
\N \EA  
!

HCOH+O2=>CO2+H+OH  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
1996 !\COMMENT:  
HCOH+O2<=>CO2+H2O  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
1996 !\COMMENT:  
HCOH+O=>CO2+H+H  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
1996 !\COMMENT:  
HCOH+O=>CO+OH+H  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
1996 !\COMMENT:  
HCOH+H<=>CH2O+H  
+2.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
1996 !\COMMENT:  
HCOH+OH<=>HCO+H2O  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
1996 !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \CH3O

!=====  
=====

!-----  
-----

!\ENDSUBMECH: \CH3OH

!-----  
-----

!-----  
-----

!\SUBMECH: \CH2O

!\MECHCOMMENTS: THE REACTION OCHO+OH<=>HO2CHO SEEMS TO BE A DEAD END OF  
SORTS, HO2CHO HAS A LIMITED SET OF CONSUMPTION/CROSS-REACTIONS (KPS,  
28/06/2015)

!\MECHCOMMENTS: THE REACTION SEQUENCE H+CO2=OCHO=>PRODUCTS MEANS THAT THE  
THE CO/CH2O MECHANISMS ARE INEXTRICABLY LINKED "IN THEORY". I AM NOT SURE  
ABOUT "IN PRACTICE". (KPS, 28/06/2015)

!\MECHWARNINGS:

!-----  
-----

!-----  
-----

!\REACTIONCLASS: \UNIMOL

\A

\N \EA

!-----  
-----

HCO+H(+M)<=>CH2O(+M)

+1.0900000E+012 +4.8000000E-001 -2.6000000E+002 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

LOW /

+1.3500000E+024 -2.5700000E+000 +1.4250000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +7.8240000E-001

+2.7100000E+002 +2.7550000E+003 +6.5700000E+003 / !TROE PARAMETERS

H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES

CO+H2(+M)<=>CH2O(+M)

+4.3000000E+007 +1.5000000E+000 +7.9600000E+004 !\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 /  
+5.0700000E+027 -3.4200000E+000 +8.4348000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +9.3200000E-001  
+1.9700000E+002 +1.5400000E+003 +1.0300000E+004 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

CH2O+O2<=>HCO+HO2  
+8.0700000E+015 +0.0000000E+000 +5.3420000E+004 !\AUTHOR: !\REF: N. K.  
SRINIVASAN ET AL., J. PHYS. CHEM. A 109, 7902-7914 (2005) !\COMMENT:  
CH2O+O<=>HCO+OH  
+6.2600000E+009 +1.1500000E+000 +2.2600000E+003 !\AUTHOR: !\REF: CURRAN  
FIT TO NIST DATABASE !\COMMENT:  
CH2O+H<=>HCO+H2  
+5.7400000E+007 +1.9000000E+000 +2.7400000E+003 !\AUTHOR: !\REF: IRDAM  
ET AL., IJCK 1993, 25, 285 !\COMMENT:  
CH2O+OH<=>HCO+H2O  
+7.8200000E+007 +1.6300000E+000 -1.0550000E+003 !\AUTHOR: !\REF: V.  
VASUDEVAN ET AL. IJCK. 37: 98--109 (2005). !\COMMENT:  
CH2O+HO2<=>HCO+H2O2  
+1.8800000E+004 +2.7000000E+000 +1.1520000E+004 !\AUTHOR: !\REF: J.  
PHYS. CHEM. A 109, 12027-12035, 2005 !\COMMENT:  
CH2O+CH3<=>HCO+CH4  
+3.8300000E+001 +3.3600000E+000 +4.3120000E+003 !\AUTHOR: !\REF: BAULCH  
ET AL. JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA, 34, 3, 757-1397  
2005 !\COMMENT:  
CH2O+O2CHO<=>HCO+HO2CHO  
+1.9900000E+012 +0.0000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986 !\COMMENT:  
CH2O+OCHO<=>HCO+HOCHO  
+5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF: CURRAN  
ESTIMATE !\COMMENT:  
CH2O+CH3O<=>HCO+CH3OH  
+6.6200000E+011 +0.0000000E+000 +2.2940000E+003 !\AUTHOR:  
!\REF: FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998). !\COMMENT:  
CH2O+CH3O2<=>HCO+CH3O2H  
+1.9900000E+012 +0.0000000E+000 +1.1660000E+004 !\AUTHOR: !\REF: TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

---

HCO+M<=>H+CO+M  
+5.7000000E+011 +6.6000000E-001 +1.4870000E+004 !\AUTHOR: !\REF: LI ET  
AL. IJCK 2007 !\COMMENT: X1.2  
H2 / 2.000 / H2O / 6.000 / CO / 1.500 / CO2 / 2.000 / CH4 / 2.000 / C2H6  
/ 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
!

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

HCO+O2<=>CO+HO2  
+7.5800000E+012 +0.0000000E+000 +4.1000000E+002 !\AUTHOR: !\REF:TIMONEN  
ET AL., JPC, 92:651 (1988) !\COMMENT:  
HCO+O<=>CO+OH  
+3.0200000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
HCO+H<=>CO+H2  
+7.3400000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TIMONEN  
ET AL., JPC, 92:651 (1988) !\COMMENT:  
HCO+OH<=>CO+H2O  
+3.0110000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
HCO+CH3<=>CH4+CO  
+2.6500000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987) !\COMMENT:  
HCO+HCO<=>CH2O+CO  
+1.8000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
!

---

!\REACTIONCLASS: \LUMPED\_BIMOLECULAR \A  
\N \EA  
!

---

HCO+O<=>CO2+H  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
HCO+HO2=>CO2+H+OH  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
HCO+HCO=>H2+CO+CO  
+3.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA  
!

---

CH2O+H(+M)<=>CH2OH(+M)  
+5.4000000E+011 +4.5400000E-001 +3.6000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000  
LOW /  
+1.2700000E+032 -4.8200000E+000 +6.5300000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +7.1870000E-001  
+1.0300000E+002 +1.2910000E+003 +4.1600000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CO / 1.500 / CO2 / 2.000 / CH4 / 2.000 / C2H6  
/ 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
CH3O(+M)<=>CH2O+H(+M)  
+6.8000000E+013 +0.0000000E+000 +2.6170000E+004 !\AUTHOR: !\REF:HIPPLER  
ET AL. PCCP. 3: 3450--2458 (2001).  
LOW /  
+1.8670000E+025 -3.0000000E+000 +2.4307000E+004 / !LOW-PRESSURE-LIMIT

TROE / +9.0000000E-001  
+2.5000000E+003 +1.3000000E+003 +1.0000000E+099 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CO / 1.500 / CO2 / 2.000 / CH4 / 2.000 / C2H6  
/ 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

CH2O+OH<=>HOCH2O  
+4.5000000E+015 -1.1000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:26TH  
INTL. COMBUSTION SYMP. P 497--504. !\COMMENT:  
HOCH2O<=>HOCHO+H  
+1.0000000E+014 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\HO2 \A  
\N \EA  
!

---

CH2O+HO2<=>OCH2O2H  
+1.5000000E+011 +0.0000000E+000 +1.1900000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
OCH2O2H<=>HOCH2O2  
+3.0000000E+011 +0.0000000E+000 +8.6000000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
HOCH2O2+HO2<=>HOCH2O2H+O2  
+3.5000000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
HOCH2O+OH<=>HOCH2O2H  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

---

HCO+O2<=>O2CHO  
+1.2000000E+011 +0.0000000E+000 -1.1000000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
!=====  
!\\SUBSPECIES: \HOCHO  
!=====  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

HOCHO<=>CO+H2O  
+2.4500000E+012 +0.0000000E+000 +6.0470000E+004 !\AUTHOR: !\REF:BLAKE  
ET AL. J. CHEM. SOC. B: 10, 1923 (1971) !\COMMENT:

HOCHO<=>CO2+H2  
+2.9500000E+009 +0.0000000E+000 +4.8520000E+004 !\AUTHOR: !\REF:BLAKE  
ET AL. J. CHEM. SOC. B: 10, 1923 (1971) !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

OCHO+HO2<=>HOCHO+O2  
+3.5000000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
OCHO+H2O2<=>HOCHO+HO2  
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \LUMPED\_BIMOLECULAR \A  
\N \EA  
!

---

HOCHO+H=>H2+CO2+H  
+4.2400000E+006 +2.1000000E+000 +4.8680000E+003 !\AUTHOR: !\REF:MARINOV  
ESTIMATE !\COMMENT:  
HOCHO+H=>H2+CO+OH  
+6.0300000E+013 -3.5000000E-001 +2.9880000E+003 !\AUTHOR: !\REF:MARINOV  
ESTIMATE !\COMMENT:  
HOCHO+O=>CO+OH+OH  
+1.7700000E+018 -1.9000000E+000 +2.9750000E+003 !\AUTHOR: !\REF:MARINOV  
ESTIMATE !\COMMENT:  
HOCHO+OH=>H2O+CO2+H  
+2.6200000E+006 +2.0600000E+000 +9.1600000E+002 !\AUTHOR: !\REF:MARINOV  
ESTIMATE !\COMMENT:  
HOCHO+OH=>H2O+CO+OH  
+1.8500000E+007 +1.5100000E+000 -9.6200000E+002 !\AUTHOR: !\REF:MARINOV  
ESTIMATE !\COMMENT:  
HOCHO+CH3=>CH4+CO+OH +3.9000000E-  
007 +5.8000000E+000 +2.2000000E+003 !\AUTHOR: !\REF:MARINOV ESTIMATE  
!\COMMENT:  
HOCHO+HO2=>H2O2+CO+OH  
+1.0000000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:MARINOV  
ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

OCHO+OH<=>HO2CHO  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WKM  
ESTIMATE !\COMMENT: WHAT IS SOURCE OF RATE CONSTANT?  
!

!\ENDSUBSPECIES: \HOCHO

!-----  
-----  
!-----  
-----

```

!\ENDSUBMECH: \CH2O
!-----
!+++++
!+++++
!+++++
!\END_KINETICS_MODULE: \C1
!+++++
!+++++
!+++++
!\KINETICS_MODULE: \C2
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
!+++++
!+++++
!+++++
!-----
!\SUBMECH: \C2H6
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!-----
!\REACTIONCLASS: \UNIMOL \A
\N \EA
!-----
CH3+CH3 (+M) <=> C2H6 (+M)
+2.2770000E+015 -6.9000000E-001 +1.7490000E+002 !\AUTHOR: !\REF:WANG ET
AL., JPC A 107:11414 (2003) !\COMMENT:
LOW /
+8.0540000E+031 -3.7500000E+000 +9.8160000E+002 / !LOW-PRESSURE-LIMIT
TROE / +0.0000000E+000
+5.7000000E+002 +1.0000000E+030 +1.0000000E+030 / !TROE PARAMETERS
H2O / 5.000 / CO / 2.000 / CO2 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES
C2H5+H (+M) <=> C2H6 (+M)
+5.2100000E+017 -9.9000000E-001 +1.5800000E+003 !\AUTHOR: !\REF:WANG ET
AL., JPC A 107:11414 (2003) !\COMMENT:
LOW /
+1.9900000E+041 -7.0800000E+000 +6.6850000E+003 / !LOW-PRESSURE-LIMIT
TROE / +8.4200000E-001
+1.2500000E+002 +2.2190000E+003 +6.8820000E+003 / !TROE PARAMETERS
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES
!-----
!\REACTIONCLASS: \RH_R_ABSTRACTION \A
\N \EA
!-----

```

C2H6+O2<=>C2H5+HO2  
+6.0300000E+013 +0.0000000E+000 +5.1870000E+004 !\AUTHOR: !\REF:BAULCH  
ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:  
C2H6+O<=>C2H5+OH  
+3.5500000E+006 +2.4000000E+000 +5.8300000E+003 !\AUTHOR: !\REF:  
MIYOSHI,A. ET AL., CHEM. PHYS. LETT. 204, 241-247 (1993) !\COMMENT:  
C2H6+H<=>C2H5+H2  
+1.1500000E+008 +1.9000000E+000 +7.5300000E+003 !\AUTHOR: !\REF:WANG ET  
AL., JPC A 107:11414 (2003) !\COMMENT:  
C2H6+OH<=>C2H5+H2O  
+1.4800000E+007 +1.9000000E+000 +9.5000000E+002 !\AUTHOR: !\REF:CURRAN,  
FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT IS ORIGINAL SOURCE OF NIST  
DATA?  
C2H6+HO2<=>C2H5+H2O2  
+3.4600000E+001 +3.6100000E+000 +1.6920000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
C2H6+CH<=>C2H5+CH2  
+1.1000000E+014 +0.0000000E+000 -2.6000000E+002 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
C2H6+CH2(S)<=>C2H5+CH3  
+1.2000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:MECHANISM AND MODELING OF NITROGEN CHEMISTRY IN COMBUSTION, WSS/  
CI, AUTUMN 1988 !\COMMENT: WARNING: SOURCE SEEMS DATED  
C2H6+CH3<=>C2H5+CH4 +5.5500000E-  
004 +4.7200000E+000 +3.2310000E+003 !\AUTHOR: !\REF:TSANG AND HAMPSON,  
J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
C2H6+CH3O<=>C2H5+CH3OH  
+2.4100000E+011 +0.0000000E+000 +7.0900000E+003 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
C2H6+CH3O2<=>C2H5+CH3O2H  
+1.9400000E+001 +3.6400000E+000 +1.7100000E+004 !\AUTHOR:  
!\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003 !\COMMENT:  
C2H6+C2H5O2<=>C2H5+C2H5O2H  
+8.6000000E+000 +3.7600000E+000 +1.7200000E+004 !\AUTHOR:  
!\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_BETA\_SCISSION \A  
\N \EA  
!

---

C2H4+H(+M)<=>C2H5(+M)  
+9.5690000E+008 +1.4630000E+000 +1.3550000E+003 !\AUTHOR: !\REF:MILLER  
KLIPPENSTEIN PCCP 2004, 6, 1192-1202 !\COMMENT: :HP AND LP LIMIT\*0.7  
LOW /  
+1.4190000E+039 -6.6420000E+000 +5.7690000E+003 / !LOW-PRESSURE-LIMIT  
TROE / -5.6900000E-001  
+2.9900000E+002 -9.1470000E+003 +1.5240000E+002 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA  
!

---



C2H5+H<=>C2H4+H2  
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
CURRAN: FIT TO PRATT/ WOOD 84 AND PRATT/ VELDMAN 76 !\COMMENT: WHAT IS  
SOURCE OF ORIGINAL DATA? EXPERIMENT? THEORY?  
C2H4+C2H4<=>C2H5+C2H3  
+4.8200000E+014 +0.0000000E+000 +7.1530000E+004 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
C2H5+CH3<=>CH4+C2H4  
+1.1800000E+004 +2.4500000E+000 -2.9210000E+003 !\AUTHOR: !\REF:ZHU,  
R.S. ET AL., J. CHEM. PHYS. 120:6566:6573 (2004) !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

C2H5+O<=>CH3CHO+H  
+1.1000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI 3.0  
!\COMMENT:  
C2H5+HO2<=>C2H5O+OH  
+1.1000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN.  
BASED ON CH3+HO2<=>PRODUCTS !\COMMENT:  
C2H5+CH3O2<=>C2H5O+CH3O  
+8.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:CURRAN.  
BASED ON CH3+HO2<=>PRODUCTS !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

CH3+CH3<=>H+C2H5  
+4.7400000E+012 +1.0500000E-001 +1.0664300E+004 !\AUTHOR: !\REF:STEWART  
ET AL C&F 1989 !\COMMENT:  
PLOG / +1.0000000E-002  
+4.7400000E+012 +1.0500000E-001 +1.0664300E+004 /  
PLOG / +1.0000000E-001  
+2.5700000E+013 -9.6000000E-002 +1.1406100E+004 /  
PLOG / +1.0000000E+000  
+3.1000000E+014 -3.6200000E-001 +1.3372500E+004 /  
PLOG / +1.0000000E+001  
+2.1500000E+010 +8.8500000E-001 +1.3532500E+004 /  
PLOG / +1.0000000E+002  
+1.0320000E+002 +3.2300000E+000 +1.1236100E+004 /  
!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

---

C2H5+O2<=>C2H5O2  
+3.3980000E+053 -1.3900000E+001 +9.2790000E+003 !\AUTHOR: !\REF:John D.  
DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
PLOG / +4.0000000E-002  
+3.3980000E+053 -1.3900000E+001 +9.2790000E+003 /  
PLOG / +1.0000000E+000  
+9.3620000E+059 -1.5280000E+001 +1.4240000E+004 /

PLOG / +1.0000000E+001  
 +1.2620000E+060 -1.4910000E+001 +1.6240000E+004 /  
 C2H5+O2<=>C2H4O2H  
 +2.1030000E+034 -9.0100000E+000 +5.4440000E+003 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +2.1030000E+034 -9.0100000E+000 +5.4440000E+003 /  
 PLOG / +1.0000000E+000  
 +4.8840000E+033 -8.3100000E+000 +7.7100000E+003 /  
 PLOG / +1.0000000E+001  
 +1.7050000E+045 -1.1490000E+001 +1.4590000E+004 /  
 C2H5+O2<=>C2H4+HO2  
 +2.0940000E+009 +4.9000000E-001 -3.9140000E+002 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +2.0940000E+009 +4.9000000E-001 -3.9140000E+002 /  
 PLOG / +1.0000000E+000  
 +1.8430000E+007 +1.1300000E+000 -7.2060000E+002 /  
 PLOG / +1.0000000E+001  
 +7.5610000E+014 -1.0100000E+000 +4.7490000E+003 /  
 !C2H5+O2<=>C2H4+HO2 6.609E+000 3.510 14160.0 !\AUTHOR: !\REF:\COMMENT:  
 RMVD BECAUSE THIS WILL NEVER BE USED BY CHEMKIIN  
 !DUP  
 C2H5+O2<=>C2H4O1-2+OH  
 +1.3030000E+003 +1.9300000E+000 -5.0270000E+002 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +1.3030000E+003 +1.9300000E+000 -5.0270000E+002 /  
 PLOG / +1.0000000E+000  
 +2.4380000E+002 +2.1800000E+000 -6.2500000E+001 /  
 PLOG / +1.0000000E+001  
 +4.6210000E+009 +1.5000000E-001 +5.4090000E+003 /  
 C2H5+O2<=>CH3CHO+OH +4.9080000E-  
 006 +4.7600000E+000 +2.5430000E+002 !\AUTHOR: !\REF:John D. DeSain, J.  
 Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002 +4.9080000E-  
 006 +4.7600000E+000 +2.5430000E+002 /  
 PLOG / +1.0000000E+000 +6.8030000E-  
 002 +3.5700000E+000 +2.6430000E+003 /  
 PLOG / +1.0000000E+001  
 +8.2650000E+002 +2.4100000E+000 +5.2850000E+003 /  
 C2H4O2H<=>C2H5O2 +2.6530000E-  
 016 +6.9600000E+000 +2.3960000E+003 !\AUTHOR: !\REF:John D. DeSain, J.  
 Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002 +2.6530000E-  
 016 +6.9600000E+000 +2.3960000E+003 /  
 PLOG / +1.0000000E+000  
 +1.0640000E+041 -1.0100000E+001 +2.6030000E+004 /  
 PLOG / +1.0000000E+001  
 +1.2030000E+036 -8.1300000E+000 +2.7020000E+004 /  
 C2H5O2<=>CH3CHO+OH  
 +1.2370000E+035 -9.4200000E+000 +3.6360000E+004 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +1.2370000E+035 -9.4200000E+000 +3.6360000E+004 /  
 PLOG / +1.0000000E+000  
 +1.6870000E+036 -9.2200000E+000 +3.8700000E+004 /

PLOG / +1.0000000E+001  
 +2.5200000E+041 -1.0200000E+001 +4.3710000E+004 /  
 C2H5O2<=>C2H4+HO2  
 +1.7820000E+032 -7.1000000E+000 +3.2840000E+004 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +1.7820000E+032 -7.1000000E+000 +3.2840000E+004 /  
 PLOG / +1.0000000E+000  
 +2.7010000E+037 -8.4700000E+000 +3.5840000E+004 /  
 PLOG / +1.0000000E+001  
 +1.9800000E+038 -8.4600000E+000 +3.7900000E+004 /  
 C2H5O2<=>C2H4O1-2+OH  
 +5.7780000E+045 -1.1900000E+001 +4.1120000E+003 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +5.7780000E+045 -1.1900000E+001 +4.1120000E+003 /  
 PLOG / +1.0000000E+000  
 +1.9160000E+043 -1.0750000E+001 +4.2400000E+004 /  
 PLOG / +1.0000000E+001  
 +3.9650000E+043 -1.0460000E+001 +4.5580000E+004 /  
 C2H4O2H<=>C2H4O1-2+OH  
 +8.9590000E+038 -9.4000000E+000 +2.0660000E+004 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +8.9590000E+038 -9.4000000E+000 +2.0660000E+004 /  
 PLOG / +1.0000000E+000  
 +1.2240000E+037 -8.3200000E+000 +2.1460000E+004 /  
 PLOG / +1.0000000E+001  
 +8.8480000E+030 -6.0800000E+000 +2.0660000E+004 /  
 C2H4O2H<=>C2H4+HO2  
 +3.9180000E+040 -1.0200000E+001 +2.2250000E+004 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +3.9180000E+040 -1.0200000E+001 +2.2250000E+004 /  
 PLOG / +1.0000000E+000  
 +6.8250000E+040 -9.6100000E+000 +2.3840000E+004 /  
 PLOG / +1.0000000E+001  
 +3.9800000E+034 -7.2500000E+000 +2.3250000E+004 /  
 C2H4O2H<=>CH3CHO+OH  
 +5.8190000E+026 -7.9700000E+000 +2.0860000E+004 !\AUTHOR: !\REF:John D.  
 DeSain, J. Phys. Chem. A, 2003, 107 (22), pp 4415-4427 !\COMMENT:  
 PLOG / +4.0000000E-002  
 +5.8190000E+026 -7.9700000E+000 +2.0860000E+004 /  
 PLOG / +1.0000000E+000  
 +5.5200000E+034 -9.8800000E+000 +2.6230000E+004 /  
 PLOG / +1.0000000E+001  
 +1.1880000E+034 -9.0200000E+000 +2.9210000E+004 /  
 !

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
 \N \EA  
 !

---

H2+C2H5O2<=>H+C2H5O2H  
 +1.5000000E+014 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG &  
 HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:  
 !=====

!\SUBSPECIES: \C2H5O2H  
!  
=====

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

C2H5O2+HO2<=>C2H5O2H+O2  
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:TSANG,  
JPC REF. DATA, 16:471 (1987) !\COMMENT:  
C2H5O2+CH2O<=>C2H5O2H+HCO  
+1.9900000E+012 +0.0000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
C2H5O2+CH4<=>C2H5O2H+CH3  
+1.8100000E+011 +0.0000000E+000 +1.8480000E+004 !\AUTHOR: !\REF:BASED  
ON CH4+CH3O2 !\COMMENT: WARNING:  
C2H5O2+CH3OH<=>C2H5O2H+CH2OH  
+1.8100000E+012 +0.0000000E+000 +1.3710000E+004 !\AUTHOR: !\REF:TSANG,  
JPC REF. DATA, 16:471 (1987) !\COMMENT:  
!

!\REACTIONCLASS: \KHP\_DECOMP \A  
\N \EA  
!

C2H5O2H<=>C2H5O+OH  
+6.3100000E+014 +0.0000000E+000 +4.2300000E+004 !\AUTHOR:  
!\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003 !\COMMENT:  
!  
=====

!\ENDSUBSPECIES: \C2H5O2H  
!  
=====

!\SUBSPECIES: C2H4O1-2  
!  
=====

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

C2H4O1-2<=>CH3+HCO  
+3.6300000E+013 +0.0000000E+000 +5.7200000E+004 !\AUTHOR:  
!\REF:LIFSHITZ ET AL. 1983 !\COMMENT:  
C2H4O1-2<=>CH3CHO  
+7.4070000E+012 +0.0000000E+000 +5.3800000E+004 !\AUTHOR: !\REF:CURRAN,  
FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT IS SOURCE OF NIST DATA?  
!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

C2H4O1-2+H<=>C2H3O1-2+H2  
+8.0000000E+013 +0.0000000E+000 +9.6800000E+003 !\AUTHOR: !\REF:BALDWIN  
ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984) !\COMMENT:  
C2H4O1-2+OH<=>C2H3O1-2+H2O  
+1.7800000E+013 +0.0000000E+000 +3.6100000E+003 !\AUTHOR: !\REF:BALDWIN  
ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984) !\COMMENT:  
C2H4O1-2+HO2<=>C2H3O1-2+H2O2  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH ETHENE !\COMMENT: WARNING: KPS: WHAT IS JUSTIFICATION FOR THIS  
ANALOGY??  
C2H4O1-2+CH3<=>C2H3O1-2+CH4  
+1.0700000E+012 +0.0000000E+000 +1.1830000E+004 !\AUTHOR: !\REF:BALDWIN  
ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984) !\COMMENT:  
C2H4O1-2+CH3O<=>C2H3O1-2+CH3OH  
+1.2000000E+011 +0.0000000E+000 +6.7500000E+003 !\AUTHOR: !\REF:BALDWIN  
ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984) !\COMMENT:  
C2H4O1-2+CH3O2<=>C2H3O1-2+CH3O2H  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH ETHENE !\COMMENT: WARNING: KPS: WHAT IS JUSTIFICATION FOR THIS  
ANALOGY??  
C2H4O1-2+C2H5O2<=>C2H3O1-2+C2H5O2H  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH ETHENE !\COMMENT: WARNING: KPS: WHAT IS JUSTIFICATION FOR THIS  
ANALOGY??  
!  
\_\_\_\_\_

!\REACTIONCLASS: \RADICAL\_ISOMERISATION \A  
\N \EA

!-----  
-----

C2H3O1-2<=>CH3CO  
+8.5000000E+014 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:BALDWIN  
ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984) !\COMMENT:  
C2H3O1-2<=>CH2CHO  
+1.0000000E+014 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:BALDWIN  
ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984) !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \C2H4O1-2

!=====  
=====

!-----  
-----

!\ENDSUBMECH: \C2H6

!-----  
-----

!-----  
-----

!\SUBMECH: \C2H4

!\MECHCOMMENTS:

!\MECHWARNINGS:

!-----  
-----

!  
\_\_\_\_\_

!\REACTIONCLASS: \UNIMOL \A  
\N \EA

!  
-----  
C2H3+H(+M)<=>C2H4(+M)  
+6.0800000E+012 +2.7000000E-001 +2.8000000E+002 !\AUTHOR: !\REF:GRI 3.0  
!\COMMENT:  
LOW /  
+1.4000000E+030 -3.8600000E+000 +3.3200000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +7.8200000E-001  
+2.0750000E+002 +2.6630000E+003 +6.0950000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
C2H4(+M)<=>H2+H2CC(+M)  
+8.0000000E+012 +4.4000000E-001 +8.8770000E+004 !\AUTHOR: !\REF:GRI  
!\COMMENT: WARNING: IS THIS FROM SAME VERSION OF GRI AS ABOVE? IF NOT  
FALL-OFF EFFECTS MAY BE INCORRECT.  
LOW /  
+7.0000000E+050 -9.3100000E+000 +9.9860000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +7.3450000E-001  
+1.8000000E+002 +1.0350000E+003 +5.4170000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

-----  
!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

-----  
C2H4+O2<=>C2H3+HO2  
+4.2200000E+013 +0.0000000E+000 +5.7623100E+004 !\AUTHOR: !\REF:CHECK  
EFFECT!!\!\!\!\!\ !\COMMENT: WARNING: SOURCE OF REFERENCE IS CONFUSING  
C2H4+H<=>C2H3+H2  
+5.0700000E+007 +1.9300000E+000 +1.2950000E+004 !\AUTHOR:  
!\REF:KNYAZEV,V.D. ET AL.,J. PHYS. CHEM. 100, 11346-1135 (1996)  
!\COMMENT:  
C2H4+OH<=>C2H3+H2O  
+2.2300000E+004 +2.7450000E+000 +2.2155000E+003 !\AUTHOR: !\REF: FROM  
STANFORD !\COMMENT: WARNING: SOURCE OF RATE CONSTANT IS UNCLEAR  
C2H4+CH3O<=>C2H3+CH3OH  
+1.2000000E+011 +0.0000000E+000 +6.7500000E+003 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
C2H4+CH3O2<=>C2H3+CH3O2H  
+8.5900000E+000 +3.7540000E+000 +2.7132000E+004 !\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  
+8.5900000E+000 +3.7540000E+000 +2.7132000E+004 !\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+CH3CO3<=>C2H3+CH3CO3H  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:BAULCH  
ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:  
C2H4+CH3<=>C2H3+CH4  
+9.7600000E+002 +2.9470000E+000 +1.5148000E+004 !\AUTHOR: !\REF:  
WARNING REFERENCE UNCLEAR !\COMMENT: WARNING: SOURCE OF RATE CONSTANT  
UNCLEAR IN MECHANISM  
DUP  
C2H4+CH3<=>C2H3+CH4 +8.1300000E-  
005 +4.4170000E+000 +8.8358000E+003 !\AUTHOR: !\REF: !\COMMENT:

DUP

!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

C2H4+O<=>CH3+HCO

+7.4530000E+006 +1.8800000E+000 +1.8300000E+002 !\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

+6.0980000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF: BAULCH  
ET AL. JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA: 34, 3, 757-1397  
2005 !\COMMENT: MAKING BRANCHING RATIO 55:45 WARNING:

CH+CH4<=>C2H4+H

+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: BUTLER,  
FLEMING, GOSS, LIN, ACS SYMP. SER. 134 (1980). !\COMMENT:

CH2(S)+CH3<=>C2H4+H

+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: MARINOV  
ESTIMATE. !\COMMENT: WARNING: IS RATE CONSTANT MOST UP TO DATE? WHAT IS  
ESTIMATE BA

!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

C2H4+OH<=>CH3+CH2O

+5.3500000E+000 +2.9200000E+000 -1.7327000E+003 !\AUTHOR: !\REF: SJK, J  
PHYS CHEM 110 2006 6960-6970 !\COMMENT:

PLOG / +1.0000000E-002

+5.3500000E+000 +2.9200000E+000 -1.7327000E+003 /

PLOG / +2.5000000E-002

+3.1900000E+001 +2.7100000E+000 -1.1723000E+003 /

PLOG / +1.0000000E-001

+5.5500000E+002 +2.3600000E+000 -1.8080000E+002 /

PLOG / +1.0000000E+000

+1.7800000E+005 +1.6800000E+000 +2.0605000E+003 /

PLOG / +1.0000000E+001

+2.3700000E+009 +5.6000000E-001 +6.0067000E+003 /

PLOG / +1.0000000E+002

+2.7600000E+013 -5.0000000E-001 +1.1455100E+004 /

C2H4+OH<=>CH3CHO+H +2.3700000E-  
007 +5.3000000E+000 -2.0506000E+003 !\AUTHOR: !\REF: SJK, J PHYS CHEM  
110 2006 6960-6970 !\COMMENT:

PLOG / +1.0000000E-002 +2.3700000E-

007 +5.3000000E+000 -2.0506000E+003 /

PLOG / +2.5000000E-002 +8.7300000E-

005 +4.5700000E+000 -6.1800000E+002 /

PLOG / +1.0000000E-001 +4.0300000E-

001 +3.5400000E+000 +1.8817000E+003 /

PLOG / +1.0000000E+000 +2.3800000E-

002 +3.9100000E+000 +1.7227000E+003 /

PLOG / +1.0000000E+001

+8.2500000E+008 +1.0100000E+000 +1.0507300E+004 /

PLOG / +1.0000000E+002

+6.8000000E+009 +8.1000000E-001 +1.3867300E+004 /

C2H4+OH<=>C2H3OH+H  
+1.0400000E+004 +2.6000000E+000 +4.1210000E+003 !\AUTHOR: !\REF:SJK, J  
PHYS CHEM 110 2006 6960-6970 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.0400000E+004 +2.6000000E+000 +4.1210000E+003 /  
PLOG / +2.5000000E-002  
+1.0700000E+004 +2.6000000E+000 +4.1290000E+003 /  
PLOG / +1.0000000E-001  
+1.5200000E+004 +2.5600000E+000 +4.2383000E+003 /  
PLOG / +1.0000000E+000  
+3.1900000E+005 +2.1900000E+000 +5.2556000E+003 /  
PLOG / +1.0000000E+001  
+1.9400000E+008 +1.4300000E+000 +7.8288000E+003 /  
PLOG / +1.0000000E+002  
+8.5500000E+010 +7.5000000E-001 +1.1490800E+004 /  
C2H4+OH<=>PC2H4OH  
+1.7400000E+043 -1.0461000E+001 +7.6987000E+003 !\AUTHOR: !\REF:SJK, J  
PHYS CHEM 110 2006 6960-6970 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.7400000E+043 -1.0461000E+001 +7.6987000E+003 /  
PLOG / +2.5000000E-002  
+3.2500000E+037 -8.6290000E+000 +5.2147000E+003 /  
PLOG / +1.0000000E-001  
+1.8400000E+035 -7.7500000E+000 +4.9089000E+003 /  
PLOG / +1.0000000E+000  
+2.5600000E+036 -7.7520000E+000 +6.9461000E+003 /  
PLOG / +1.0000000E+001  
+3.7000000E+033 -6.5730000E+000 +7.6059000E+003 /  
PLOG / +1.0000000E+002  
+1.1200000E+026 -4.1010000E+000 +5.7570000E+003 /  
!

---

!\REACTIONCLASS: \ALKENE\_RO2\_CYC\_ETH\_RO \A  
\n \EA  
!

---

C2H4+HO2<=>C2H4O1-2+OH  
+3.3450000E+012 +0.0000000E+000 +1.7190000E+004 !\AUTHOR: !\REF:BAULCH  
AND COBOS !\COMMENT: A\*1.5"  
C2H4+CH3O2<=>C2H4O1-2+CH3O  
+2.8200000E+012 +0.0000000E+000 +1.7110000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF ESTIMATE?  
C2H4+C2H5O2<=>C2H4O1-2+C2H5O  
+2.8200000E+012 +0.0000000E+000 +1.7110000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF ESTIMATE?

!\SUBSPECIES: \C2H3

---

!\REACTIONCLASS: \RADICAL\_BETA\_SCISSION \A  
\n \EA  
!



C2H2+H(+M)<=>C2H3(+M)  
+1.7100000E+010 +1.2660000E+000 +2.7090000E+003 !\AUTHOR: !\REF:MILLER  
KLIPPENSTEIN PCCP 2004, 6, 1192-1202 !\COMMENT:  
LOW /  
+6.3460000E+031 -4.6640000E+000 +3.7800000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +7.8800000E-001 -  
1.0200000E+004 +1.0000000E-030 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

---

C2H3+O2<=>C2H3OO  
+4.0700000E+027 -4.6700000E+000 +5.2220000E+003 ! !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
PLOG / +1.0000000E-002  
+1.5500000E+024 -5.4500000E+000 +9.6620000E+003 /  
PLOG / +1.0000000E-001  
+3.4800000E+056 -1.5010000E+001 +1.9160000E+004 /  
PLOG / +3.1600000E-001  
+1.2500000E+064 -1.6970000E+001 +2.1290000E+004 /  
PLOG / +1.0000000E+000  
+3.3400000E+061 -1.5790000E+001 +2.0150000E+004 /  
PLOG / +3.1600000E+000  
+7.3400000E+053 -1.3110000E+001 +1.7300000E+004 /  
PLOG / +1.0000000E+001  
+4.1600000E+048 -1.1210000E+001 +1.6000000E+004 /  
PLOG / +3.1600000E+001  
+2.3300000E+043 -9.3800000E+000 +1.4810000E+004 /  
PLOG / +1.0000000E+002  
+3.4100000E+039 -8.0400000E+000 +1.4360000E+004 /

DUP

C2H3+O2<=>C2H3OO  
+4.0700000E+027 -4.6700000E+000 +5.2220000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
PLOG / +1.0000000E-002 +1.7800000E-  
009 +4.1500000E+000 -4.7070000E+003 /  
PLOG / +1.0000000E-001  
+2.3600000E+022 -4.5200000E+000 +2.8390000E+003 /  
PLOG / +3.1600000E-001  
+2.0000000E+026 -5.4300000E+000 +2.7250000E+003 /  
PLOG / +1.0000000E+000  
+6.1300000E+028 -5.8900000E+000 +3.1540000E+003 /  
PLOG / +3.1600000E+000  
+2.1400000E+029 -5.8000000E+000 +3.5200000E+003 /  
PLOG / +1.0000000E+001  
+3.4800000E+028 -5.3700000E+000 +3.6360000E+003 /  
PLOG / +3.1600000E+001  
+3.3200000E+027 -4.9500000E+000 +3.6100000E+003 /  
PLOG / +1.0000000E+002  
+1.0300000E+027 -4.7200000E+000 +3.6800000E+003 /

DUP

C2H3+O2<=>CHCHO+OH

+2.8400000E+014 -8.0000000E-001 +7.2320000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+3.9100000E+011 -1.1000000E-001 +2.1310000E+003 /  
PLOG / +1.0000000E-001  
+1.1300000E+009 +5.5000000E-001 +4.6000000E+001 /  
PLOG / +3.1600000E-001  
+8.4600000E+008 +5.6000000E-001 +7.0000000E-001 /  
PLOG / +1.0000000E+000  
+2.7500000E+014 -1.8300000E+000 +4.6000000E+000 /  
PLOG / +3.1600000E+000  
+2.5800000E+020 -2.8400000E+000 +7.5300000E+003 /  
PLOG / +1.0000000E+001  
+9.1800000E+014 -2.2600000E+000 -4.0000000E-001 /  
PLOG / +3.1600000E+001  
+6.1100000E+025 -4.2100000E+000 +1.3050000E+004 /  
PLOG / +1.0000000E+002  
+1.6500000E+030 -5.3500000E+000 +1.8430000E+004 /

DUP

C2H3+O2<=>CHCHO+OH

+2.8400000E+014 -8.0000000E-001 +7.2320000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+9.9100000E+011 -6.6000000E-001 -6.0000000E-001 /  
PLOG / +1.0000000E-001  
+6.9400000E+014 -1.1600000E+000 +4.5420000E+003 /  
PLOG / +3.1600000E-001  
+2.7900000E+013 -7.2000000E-001 +3.4790000E+003 /  
PLOG / +1.0000000E+000  
+4.9900000E+011 -1.4000000E-001 +1.9950000E+003 /  
PLOG / +3.1600000E+000  
+2.3500000E+010 +2.3000000E-001 +1.5730000E+003 /  
PLOG / +1.0000000E+001  
+1.7000000E+014 -8.2000000E-001 +4.4500000E+003 /  
PLOG / +3.1600000E+001  
+1.4200000E+011 +5.0000000E-002 +3.7740000E+003 /  
PLOG / +1.0000000E+002  
+3.1700000E+011 -2.0000000E-002 +5.3380000E+003 /

DUP

C2H3+O2<=>CH2CHO+O

+1.7600000E+012 +1.5000000E-001 +4.2050000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+7.8800000E+020 -2.6700000E+000 +6.7420000E+003 /  
PLOG / +1.0000000E-001  
+7.7200000E+020 -2.6700000E+000 +6.7130000E+003 /  
PLOG / +3.1600000E-001  
+9.8700000E+020 -2.7000000E+000 +6.7240000E+003 /  
PLOG / +1.0000000E+000  
+7.1000000E+020 -2.6500000E+000 +6.4890000E+003 /  
PLOG / +3.1600000E+000  
+4.5000000E+020 -2.5300000E+000 +6.4060000E+003 /  
PLOG / +1.0000000E+001  
+1.7600000E+023 -3.2200000E+000 +8.6970000E+003 /

PLOG / +3.1600000E+001  
 +3.1400000E+025 -3.7700000E+000 +1.1530000E+004 /  
 PLOG / +1.0000000E+002  
 +1.0200000E+026 -3.8000000E+000 +1.3910000E+004 /  
 DUP  
 C2H3+O2<=>CH2CHO+O  
 +1.7600000E+012 +1.5000000E-001 +4.2050000E+003 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +1.3600000E+010 +6.2000000E-001 -2.7760000E+002 /  
 PLOG / +1.0000000E-001  
 +1.4200000E+010 +6.2000000E-001 -2.4770000E+002 /  
 PLOG / +3.1600000E-001  
 +1.6600000E+010 +6.0000000E-001 -1.6250000E+002 /  
 PLOG / +1.0000000E+000  
 +2.0200000E+010 +5.8000000E-001 +3.8400000E+001 /  
 PLOG / +3.1600000E+000  
 +9.7500000E+009 +6.7000000E-001 +2.4800000E+002 /  
 PLOG / +1.0000000E+001  
 +7.3400000E+009 +7.2000000E-001 +7.7810000E+002 /  
 PLOG / +3.1600000E+001  
 +1.5700000E+009 +9.2000000E-001 +1.2190000E+003 /  
 PLOG / +1.0000000E+002  
 +7.8500000E+007 +1.2800000E+000 +1.4010000E+003 /  
 DUP  
 C2H3+O2<=>C2H2+HO2  
 +6.4900000E+006 +1.5000000E+000 +5.2180000E+003 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +1.0800000E+007 +1.2800000E+000 +3.3220000E+003 /  
 PLOG / +1.0000000E-001  
 +7.7500000E+006 +1.3300000E+000 +3.2160000E+003 /  
 PLOG / +3.1600000E-001  
 +1.2100000E+007 +1.2700000E+000 +3.3110000E+003 /  
 PLOG / +1.0000000E+000  
 +2.1500000E+007 +1.1900000E+000 +3.3670000E+003 /  
 PLOG / +3.1600000E+000  
 +1.1300000E+008 +1.0000000E+000 +3.6950000E+003 /  
 PLOG / +1.0000000E+001  
 +1.3100000E+011 +1.2000000E-001 +5.8720000E+003 /  
 PLOG / +3.1600000E+001  
 +1.1900000E+009 +8.2000000E-001 +5.6170000E+003 /  
 PLOG / +1.0000000E+002  
 +1.0600000E+017 -1.4500000E+000 +1.2230000E+004 /  
 DUP  
 C2H3+O2<=>C2H2+HO2  
 +6.4900000E+006 +1.5000000E+000 +5.2180000E+003 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +4.7600000E+001 +2.7500000E+000 -7.9640000E+002 /  
 PLOG / +1.0000000E-001  
 +5.1600000E+001 +2.7300000E+000 -7.6830000E+002 /  
 PLOG / +3.1600000E-001  
 +5.5500000E+001 +2.7300000E+000 -6.5850000E+002 /

```

PLOG / +1.0000000E+000
+4.6000000E+001 +2.7600000E+000 -4.9280000E+002 /
PLOG / +3.1600000E+000
+3.7500000E+000 +3.0700000E+000 -6.0100000E+002 /
PLOG / +1.0000000E+001
+5.4800000E+000 +3.0700000E+000 +8.5700000E+001 /
PLOG / +3.1600000E+001
+4.4700000E+008 +0.0000000E+000 +9.5500000E+002 /
PLOG / +1.0000000E+002
+2.0200000E+001 +2.9400000E+000 +1.8470000E+003 /
DUP
!\DUP\PDEPP
C2H3+O2<=>CHOCHO+H
+3.0800000E+012 -2.6000000E-001 +3.2770000E+003 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002
+4.7900000E+014 -1.0300000E+000 +9.1200000E+002 /
PLOG / +1.0000000E-001
+5.0300000E+014 -1.0400000E+000 +9.2250000E+002 /
PLOG / +3.1600000E-001
+6.4300000E+014 -1.0700000E+000 +9.8290000E+002 /
PLOG / +1.0000000E+000
+3.7300000E+015 -1.2900000E+000 +1.4410000E+003 /
PLOG / +3.1600000E+000
+2.4400000E+018 -2.1300000E+000 +3.2340000E+003 /
PLOG / +1.0000000E+001
+1.3000000E+015 -1.0900000E+000 +2.3930000E+003 /
PLOG / +3.1600000E+001
+3.5700000E+033 -6.5000000E+000 +1.4910000E+004 /
PLOG / +1.0000000E+002
+3.2800000E+031 -5.7600000E+000 +1.6250000E+004 /
DUP
C2H3+O2<=>CHOCHO+H
+3.0800000E+012 -2.6000000E-001 +3.2770000E+003 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002 +2.8000000E-
004 +4.0400000E+000 -7.0190000E+003 /
PLOG / +1.0000000E-001 +3.4500000E-
004 +4.0100000E+000 -6.9780000E+003 /
PLOG / +3.1600000E-001 +9.7300000E-
004 +3.8900000E+000 -6.7680000E+003 /
PLOG / +1.0000000E+000 +4.9800000E-
001 +3.1500000E+000 -5.4960000E+003 /
PLOG / +3.1600000E+000
+1.3400000E+005 +1.6700000E+000 -2.9310000E+003 /
PLOG / +1.0000000E+001
+4.5000000E+015 -3.0800000E+000 -4.8360000E+003 /
PLOG / +3.1600000E+001
+3.8400000E+010 +2.2000000E-001 +9.4130000E+002 /
PLOG / +1.0000000E+002
+2.7500000E+008 +8.3000000E-001 +8.5760000E+002 /
DUP
C2H3+O2<=>CH2CO+OH
+1.1700000E+003 +2.4300000E+000 +7.0740000E+003 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

```

PLOG / +1.0000000E-002  
+8.6600000E+002 +2.4100000E+000 +6.0610000E+003 /  
PLOG / +1.0000000E-001  
+8.9100000E+002 +2.4100000E+000 +6.0780000E+003 /  
PLOG / +3.1600000E-001  
+9.4300000E+002 +2.4000000E+000 +6.1120000E+003 /  
PLOG / +1.0000000E+000  
+1.0600000E+003 +2.3900000E+000 +6.1800000E+003 /  
PLOG / +3.1600000E+000  
+1.0900000E+003 +2.3800000E+000 +6.1790000E+003 /  
PLOG / +1.0000000E+001  
+1.3900000E+003 +2.3600000E+000 +6.0740000E+003 /  
PLOG / +3.1600000E+001  
+2.4900000E+006 +1.4200000E+000 +8.4800000E+003 /  
PLOG / +1.0000000E+002  
+1.6600000E+010 +3.6000000E-001 +1.2010000E+004 /

DUP

C2H3+O2<=>CH2CO+OH

+1.1700000E+003 +2.4300000E+000 +7.0740000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002 +1.8200000E-  
001 +3.1200000E+000 +1.3310000E+003 /  
PLOG / +1.0000000E-001 +2.0700000E-  
001 +3.1100000E+000 +1.3830000E+003 /  
PLOG / +3.1600000E-001 +2.7100000E-  
001 +3.0800000E+000 +1.4960000E+003 /  
PLOG / +1.0000000E+000 +5.2600000E-  
001 +3.0100000E+000 +1.7770000E+003 /  
PLOG / +3.1600000E+000  
+1.3700000E+000 +2.9000000E+000 +2.2250000E+003 /  
PLOG / +1.0000000E+001 +4.1900000E-  
001 +2.9300000E+000 +2.0520000E+003 /  
PLOG / +3.1600000E+001 +1.1900000E-  
004 +4.2100000E+000 +2.0430000E+003 /  
PLOG / +1.0000000E+002 +1.3000000E-  
003 +3.9700000E+000 +3.4140000E+003 /

DUP

C2H3+O2<=>CH2O+HCO

+1.1600000E+016 -1.1300000E+000 +3.7910000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+2.4900000E+036 -7.6000000E+000 +1.2640000E+004 /  
PLOG / +1.0000000E-001  
+2.4300000E+036 -7.6000000E+000 +1.2610000E+004 /  
PLOG / +3.1600000E-001  
+1.9500000E+036 -7.5700000E+000 +1.2490000E+004 /  
PLOG / +1.0000000E+000  
+2.7300000E+035 -7.3200000E+000 +1.1820000E+004 /  
PLOG / +3.1600000E+000  
+1.4300000E+036 -7.4700000E+000 +1.2460000E+004 /  
PLOG / +1.0000000E+001  
+5.1800000E+035 -7.2000000E+000 +1.3430000E+004 /  
PLOG / +3.1600000E+001  
+3.1900000E+020 -2.5700000E+000 +5.5780000E+003 /  
PLOG / +1.0000000E+002  
+2.7300000E+033 -6.2800000E+000 +1.6000000E+004 /

DUP

C2H3+O2<=>CH2O+HCO

+1.1600000E+016 -1.1300000E+000 +3.7910000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+4.5400000E+015 -1.2800000E+000 +5.1530000E+002 /  
PLOG / +1.0000000E-001  
+4.5900000E+015 -1.2800000E+000 +5.1300000E+002 /  
PLOG / +3.1600000E-001  
+4.8100000E+015 -1.2900000E+000 +5.2060000E+002 /  
PLOG / +1.0000000E+000  
+6.0800000E+015 -1.3100000E+000 +6.4570000E+002 /  
PLOG / +3.1600000E+000  
+9.4500000E+015 -1.3600000E+000 +1.0660000E+003 /  
PLOG / +1.0000000E+001  
+2.5600000E+015 -1.1800000E+000 +1.4290000E+003 /  
PLOG / +3.1600000E+001  
+1.0300000E+069 -1.9230000E+001 +1.4760000E+004 /  
PLOG / +1.0000000E+002  
+4.2100000E+010 +1.9000000E-001 +8.3060000E+002 /

DUP

C2H3+O2=>CH2O+H+CO

+1.1600000E+016 -1.1300000E+000 +3.7910000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+5.8200000E+036 -7.6000000E+000 +1.2640000E+004 /  
PLOG / +1.0000000E-001  
+5.6600000E+036 -7.6000000E+000 +1.2610000E+004 /  
PLOG / +3.1600000E-001  
+4.5500000E+036 -7.5700000E+000 +1.2490000E+004 /  
PLOG / +1.0000000E+000  
+6.3600000E+035 -7.3200000E+000 +1.1820000E+004 /  
PLOG / +3.1600000E+000  
+3.3500000E+036 -7.4700000E+000 +1.2460000E+004 /  
PLOG / +1.0000000E+001  
+1.2100000E+036 -7.2000000E+000 +1.3430000E+004 /  
PLOG / +3.1600000E+001  
+7.4300000E+020 -2.5700000E+000 +5.5780000E+003 /  
PLOG / +1.0000000E+002  
+6.3600000E+033 -6.2800000E+000 +1.6000000E+004 /

DUP

C2H3+O2=>CH2O+H+CO

+1.1600000E+016 -1.1300000E+000 +3.7910000E+003 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+1.0600000E+016 -1.2800000E+000 +5.1530000E+002 /  
PLOG / +1.0000000E-001  
+1.0700000E+016 -1.2800000E+000 +5.1300000E+002 /  
PLOG / +3.1600000E-001  
+1.1300000E+016 -1.2900000E+000 +5.2060000E+002 /  
PLOG / +1.0000000E+000  
+1.4200000E+016 -1.3100000E+000 +6.4570000E+002 /  
PLOG / +3.1600000E+000  
+2.2000000E+016 -1.3600000E+000 +1.0660000E+003 /

```

PLOG / +1.0000000E+001
+5.9800000E+015 -1.1800000E+000 +1.4290000E+003 /
PLOG / +3.1600000E+001
+2.3900000E+069 -1.9230000E+001 +1.4760000E+004 /
PLOG / +1.0000000E+002
+9.8100000E+010 +1.9000000E-001 +8.3060000E+002 /
DUP
C2H3+O2<=>CO+CH3O
+3.0900000E+013 -8.9000000E-001 +3.6820000E+003 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002
+8.1900000E+018 -2.6600000E+000 +3.2010000E+003 /
PLOG / +1.0000000E-001
+4.0600000E+014 -1.3200000E+000 +8.8580000E+002 /
PLOG / +3.1600000E-001
+4.3400000E+014 -1.3300000E+000 +9.0060000E+002 /
PLOG / +1.0000000E+000
+1.0300000E+011 -3.3000000E-001 -7.4780000E+002 /
PLOG / +3.1600000E+000
+1.8900000E+012 -3.0000000E+000 -8.9950000E+003 /
PLOG / +1.0000000E+001
+1.9300000E+024 -5.6300000E+000 +1.8000000E+000 /
PLOG / +3.1600000E+001
+1.1000000E+018 -2.2200000E+000 +5.1780000E+003 /
PLOG / +1.0000000E+002
+5.7900000E+032 -6.4500000E+000 +1.6810000E+004 /
DUP
C2H3+O2<=>CO+CH3O
+3.0900000E+013 -8.9000000E-001 +3.6820000E+003 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002
+1.2900000E+009 +1.8000000E-001 -1.7170000E+003 /
PLOG / +1.0000000E-001
+5.9900000E+011 -2.9300000E+000 -9.5640000E+003 /
PLOG / +3.1600000E-001
+2.9100000E+011 -2.9300000E+000 -1.0120000E+004 /
PLOG / +1.0000000E+000
+5.7700000E+021 -3.5400000E+000 +4.7720000E+003 /
PLOG / +3.1600000E+000
+4.9900000E+015 -1.6200000E+000 +1.8490000E+003 /
PLOG / +1.0000000E+001
+9.3300000E+016 -1.9600000E+000 +3.3240000E+003 /
PLOG / +3.1600000E+001
+1.0200000E+072 -2.0690000E+001 +1.5860000E+004 /
PLOG / +1.0000000E+002
+1.1000000E+009 +3.1000000E-001 +1.0240000E+003 /
DUP
C2H3+O2<=>CO2+CH3
+6.1600000E+013 -1.0500000E+000 +3.7430000E+003 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002
+2.3700000E+035 -7.7600000E+000 +1.2630000E+004 /
PLOG / +1.0000000E-001
+1.7300000E+035 -7.7200000E+000 +1.2520000E+004 /

```

PLOG / +3.1600000E-001  
 +4.4700000E+034 -7.5500000E+000 +1.2140000E+004 /  
 PLOG / +1.0000000E+000  
 +7.2500000E+031 -6.7000000E+000 +1.0440000E+004 /  
 PLOG / +3.1600000E+000  
 +3.6300000E+035 -7.7500000E+000 +1.2830000E+004 /  
 PLOG / +1.0000000E+001  
 +2.0900000E+035 -7.5300000E+000 +1.4050000E+004 /  
 PLOG / +3.1600000E+001  
 +3.8400000E+018 -2.4400000E+000 +5.4080000E+003 /  
 PLOG / +1.0000000E+002  
 +1.2100000E+032 -6.3200000E+000 +1.6190000E+004 /  
 DUP  
 C2H3+O2<=>CO2+CH3  
 +6.1600000E+013 -1.0500000E+000 +3.7430000E+003 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +6.2700000E+013 -1.1600000E+000 +4.0630000E+002 /  
 PLOG / +1.0000000E-001  
 +6.2400000E+013 -1.1600000E+000 +4.0140000E+002 /  
 PLOG / +3.1600000E-001  
 +6.1200000E+013 -1.1600000E+000 +3.9700000E+002 /  
 PLOG / +1.0000000E+000  
 +5.3200000E+013 -1.1400000E+000 +4.4670000E+002 /  
 PLOG / +3.1600000E+000  
 +1.4500000E+014 -1.2600000E+000 +9.8770000E+002 /  
 PLOG / +1.0000000E+001  
 +5.0200000E+013 -1.1100000E+000 +1.4090000E+003 /  
 PLOG / +3.1600000E+001  
 +1.4000000E+070 -2.0110000E+001 +1.5430000E+004 /  
 PLOG / +1.0000000E+002  
 +9.2100000E+008 +2.5000000E-001 +8.5530000E+002 /  
 DUP  
 C2H3OO<=>CHCHO+OH  
 +5.8900000E+036 -7.1000000E+000 +5.1440000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +3.6400000E+049 -1.2130000E+001 +6.7420000E+004 /  
 PLOG / +1.0000000E-001  
 +1.4400000E+036 -9.9200000E+000 +4.1220000E+004 /  
 PLOG / +3.1600000E-001  
 +4.1800000E+040 -1.0530000E+001 +4.3670000E+004 /  
 PLOG / +1.0000000E+000  
 +3.7900000E+046 -1.0720000E+001 +5.1900000E+004 /  
 PLOG / +3.1600000E+000  
 +1.6000000E+049 -1.1240000E+001 +5.4150000E+004 /  
 PLOG / +1.0000000E+001  
 +2.3800000E+051 -1.1640000E+001 +5.6980000E+004 /  
 PLOG / +3.1600000E+001  
 +2.0000000E+054 -1.2220000E+001 +6.1840000E+004 /  
 PLOG / +1.0000000E+002  
 +9.5400000E+195 -5.2270000E+001 +1.6350000E+005 /  
 DUP  
 C2H3OO<=>CHCHO+OH  
 +5.8900000E+036 -7.1000000E+000 +5.1440000E+004 !\AUTHOR: !\REF:



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

PLOG / +1.0000000E-002  
+1.1700000E+056 -1.4810000E+001 +6.0700000E+004 /  
PLOG / +1.0000000E-001  
+2.3200000E+040 -9.3900000E+000 +5.0420000E+004 /  
PLOG / +3.1600000E-001  
+1.6100000E+043 -9.9900000E+000 +5.0290000E+004 /  
PLOG / +1.0000000E+000  
+2.3300000E+124 -3.6770000E+001 +7.0100000E+004 /  
PLOG / +3.1600000E+000  
+1.8800000E+103 -2.9490000E+001 +6.5410000E+004 /  
PLOG / +1.0000000E+001  
+5.9600000E+086 -2.3810000E+001 +6.2170000E+004 /  
PLOG / +3.1600000E+001  
+1.5100000E+057 -1.3940000E+001 +5.5390000E+004 /  
PLOG / +1.0000000E+002  
+1.7900000E+034 -6.4000000E+000 +5.0000000E+004 /

DUP

C2H3OO<=>CH2CHO+O

+1.2200000E+029 -4.7100000E+000 +4.2340000E+004 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+2.7000000E+180 -4.8190000E+001 +1.6930000E+005 /  
PLOG / +1.0000000E-001  
+3.9000000E+038 -8.6900000E+000 +4.2770000E+004 /  
PLOG / +3.1600000E-001  
+4.5700000E+047 -1.1210000E+001 +4.7050000E+004 /  
PLOG / +1.0000000E+000  
+7.6200000E+081 -2.1280000E+001 +6.5080000E+004 /  
PLOG / +3.1600000E+000  
+1.8600000E+068 -1.6830000E+001 +6.0680000E+004 /  
PLOG / +1.0000000E+001  
+2.0200000E+055 -1.2690000E+001 +5.5840000E+004 /  
PLOG / +3.1600000E+001  
+1.1100000E+053 -1.1790000E+001 +5.6690000E+004 /  
PLOG / +1.0000000E+002  
+4.3000000E+048 -1.0310000E+001 +5.6090000E+004 /

DUP

C2H3OO<=>CH2CHO+O

+1.2200000E+029 -4.7100000E+000 +4.2340000E+004 !\AUTHOR: !\REF:  
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+1.4700000E+030 -6.6400000E+000 +4.1110000E+004 /  
PLOG / +1.0000000E-001 +9.6500000E-  
012 +5.9600000E+000 +2.2890000E+004 /  
PLOG / +3.1600000E-001  
+3.9500000E+022 -3.7100000E+000 +3.6270000E+004 /  
PLOG / +1.0000000E+000  
+2.3900000E+033 -6.6200000E+000 +4.1280000E+004 /  
PLOG / +3.1600000E+000  
+6.3700000E+031 -5.9600000E+000 +4.1260000E+004 /  
PLOG / +1.0000000E+001  
+2.1300000E+029 -5.1000000E+000 +4.0710000E+004 /  
PLOG / +3.1600000E+001  
+4.6600000E+027 -4.5000000E+000 +4.0530000E+004 /

PLOG / +1.0000000E+002  
 +5.9900000E+025 -3.8500000E+000 +4.0120000E+004 /  
 DUP  
 C2H3OO<=>CHOCHO+H  
 +4.7200000E+020 -2.6900000E+000 +3.2320000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +6.4100000E+080 -2.2200000E+001 +5.1750000E+004 /  
 PLOG / +1.0000000E-001  
 +3.3100000E+065 -1.7010000E+001 +4.8090000E+004 /  
 PLOG / +3.1600000E-001  
 +5.9800000E+051 -1.2620000E+001 +4.3000000E+004 /  
 PLOG / +1.0000000E+000  
 +1.4800000E+044 -1.0120000E+001 +4.0790000E+004 /  
 PLOG / +3.1600000E+000  
 +1.2600000E+059 -1.4330000E+001 +5.1390000E+004 /  
 PLOG / +1.0000000E+001  
 +4.9300000E+026 -4.6700000E+000 +3.4320000E+004 /  
 PLOG / +3.1600000E+001  
 +2.0600000E+033 -6.3800000E+000 +3.9520000E+004 /  
 PLOG / +1.0000000E+002  
 +1.3000000E+032 -5.9200000E+000 +4.0660000E+004 /  
 DUP  
 C2H3OO<=>CHOCHO+H  
 +4.7200000E+020 -2.6900000E+000 +3.2320000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +1.1900000E+028 -6.0100000E+000 +2.8740000E+004 /  
 PLOG / +1.0000000E-001  
 +1.4000000E+025 -4.8000000E+000 +2.8940000E+004 /  
 PLOG / +3.1600000E-001  
 +2.9100000E+020 -3.2900000E+000 +2.7550000E+004 /  
 PLOG / +1.0000000E+000  
 +1.5800000E+019 -2.8200000E+000 +2.7620000E+004 /  
 PLOG / +3.1600000E+000  
 +1.9300000E+022 -3.5400000E+000 +2.9980000E+004 /  
 PLOG / +1.0000000E+001  
 +7.5100000E+029 -5.7500000E+000 +3.4490000E+004 /  
 PLOG / +3.1600000E+001  
 +7.1400000E+061 -1.6160000E+001 +4.3280000E+004 /  
 PLOG / +1.0000000E+002  
 +1.1400000E+019 -2.5600000E+000 +2.9670000E+004 /  
 DUP  
 C2H3OO<=>CH2CO+OH  
 +1.5500000E+024 -3.8700000E+000 +4.9850000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +1.1500000E+047 -1.2280000E+001 +7.5330000E+004 /  
 PLOG / +1.0000000E-001  
 +8.4300000E+009 -2.0600000E+000 +3.3720000E+004 /  
 PLOG / +3.1600000E-001  
 +6.0600000E+004 +1.7000000E-001 +3.4220000E+004 /  
 PLOG / +1.0000000E+000  
 +1.5100000E+019 -3.6100000E+000 +4.3060000E+004 /

PLOG / +3.1600000E+000  
 +2.1300000E+033 -7.3900000E+000 +5.1610000E+004 /  
 PLOG / +1.0000000E+001  
 +4.4400000E+036 -7.9900000E+000 +5.4680000E+004 /  
 PLOG / +3.1600000E+001  
 +1.1900000E+037 -7.8000000E+000 +5.6460000E+004 /  
 PLOG / +1.0000000E+002  
 +9.0800000E+035 -7.2100000E+000 +5.7550000E+004 /  
 DUP  
 C2H3OO<=>CH2CO+OH  
 +1.5500000E+024 -3.8700000E+000 +4.9850000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +2.3100000E+002 -7.3000000E-001 +2.5710000E+004 /  
 PLOG / +1.0000000E-001 +1.8300000E-  
 023 +7.8400000E+000 +2.0190000E+004 /  
 PLOG / +3.1600000E-001  
 +3.8200000E+063 -2.0440000E+001 +4.3420000E+004 /  
 PLOG / +1.0000000E+000  
 +3.1800000E+027 -7.7600000E+000 +3.7230000E+004 /  
 PLOG / +3.1600000E+000 +2.3200000E-  
 005 +3.4700000E+000 +3.1560000E+004 /  
 PLOG / +1.0000000E+001 +1.0600000E-  
 001 +2.6400000E+000 +3.4160000E+004 /  
 PLOG / +3.1600000E+001  
 +5.6200000E+002 +1.7000000E+000 +3.6450000E+004 /  
 PLOG / +1.0000000E+002  
 +1.1100000E+007 +5.2000000E-001 +3.8670000E+004 /  
 DUP  
 C2H3OO<=>CH2O+HCO  
 +1.1900000E+020 -2.2900000E+000 +3.0170000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +1.6600000E+174 -5.5520000E+001 +6.0320000E+004 /  
 PLOG / +1.0000000E-001  
 +9.0300000E+066 -1.7250000E+001 +4.8120000E+004 /  
 PLOG / +3.1600000E-001  
 +1.8200000E+043 -9.8700000E+000 +3.7960000E+004 /  
 PLOG / +1.0000000E+000  
 +8.6400000E+033 -6.8800000E+000 +3.4370000E+004 /  
 PLOG / +3.1600000E+000  
 +7.2900000E+171 -4.3530000E+001 +1.9190000E+005 /  
 PLOG / +1.0000000E+001  
 +1.0300000E+032 -6.0600000E+000 +3.5500000E+004 /  
 PLOG / +3.1600000E+001  
 +1.8500000E+034 -6.5700000E+000 +3.8510000E+004 /  
 PLOG / +1.0000000E+002  
 +5.7000000E+029 -5.1900000E+000 +3.6800000E+004 /  
 DUP  
 C2H3OO<=>CH2O+HCO  
 +1.1900000E+020 -2.2900000E+000 +3.0170000E+004 !\AUTHOR: !\REF:  
 Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING  
 WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.  
 PLOG / +1.0000000E-002  
 +2.2700000E+035 -7.9700000E+000 +3.1280000E+004 /

```

PLOG / +1.0000000E-001
+2.0800000E+026 -4.9600000E+000 +2.8780000E+004 /
PLOG / +3.1600000E-001
+1.4500000E+020 -3.0800000E+000 +2.6630000E+004 /
PLOG / +1.0000000E+000
+1.0600000E+130 -3.9380000E+001 +5.4700000E+004 /
PLOG / +3.1600000E+000
+2.3500000E+034 -6.8700000E+000 +3.5700000E+004 /
PLOG / +1.0000000E+001
+2.1800000E+175 -5.3780000E+001 +6.8500000E+004 /
PLOG / +3.1600000E+001
+1.0700000E+185 -5.4220000E+001 +8.8990000E+004 /
PLOG / +1.0000000E+002
+4.6800000E+002 +1.8100000E+000 +1.8100000E+004 /
DUP
C2H3OO=>CH2O+H+CO
+1.1900000E+020 -2.2900000E+000 +3.0170000E+004 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002
+3.8800000E+174 -5.5520000E+001 +6.0320000E+004 /
PLOG / +1.0000000E-001
+2.1100000E+067 -1.7250000E+001 +4.8120000E+004 /
PLOG / +3.1600000E-001
+4.2600000E+043 -9.8700000E+000 +3.7960000E+004 /
PLOG / +1.0000000E+000
+2.0200000E+034 -6.8800000E+000 +3.4370000E+004 /
PLOG / +3.1600000E+000
+1.7000000E+172 -4.3530000E+001 +1.9190000E+005 /
PLOG / +1.0000000E+001
+2.4000000E+032 -6.0600000E+000 +3.5500000E+004 /
PLOG / +3.1600000E+001
+4.3200000E+034 -6.5700000E+000 +3.8510000E+004 /
PLOG / +1.0000000E+002
+1.3300000E+030 -5.1900000E+000 +3.6800000E+004 /
DUP
C2H3OO=>CH2O+H+CO
+1.1900000E+020 -2.2900000E+000 +3.0170000E+004 !\AUTHOR: !\REF:
Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS.
PLOG / +1.0000000E-002
+5.2900000E+035 -7.9700000E+000 +3.1280000E+004 /
PLOG / +1.0000000E-001
+4.8500000E+026 -4.9600000E+000 +2.8780000E+004 /
PLOG / +3.1600000E-001
+3.3700000E+020 -3.0800000E+000 +2.6630000E+004 /
PLOG / +1.0000000E+000
+2.4600000E+130 -3.9380000E+001 +5.4700000E+004 /
PLOG / +3.1600000E+000
+5.4900000E+034 -6.8700000E+000 +3.5700000E+004 /
PLOG / +1.0000000E+001
+5.0900000E+175 -5.3780000E+001 +6.8500000E+004 /
PLOG / +3.1600000E+001
+2.4900000E+185 -5.4220000E+001 +8.8990000E+004 /
PLOG / +1.0000000E+002
+1.0900000E+003 +1.8100000E+000 +1.8100000E+004 /
DUP

```

C2H3OO<=>CO+CH3O +1.1600000E-  
001 +3.1600000E+000 +1.8420000E+004 !\AUTHOR: !\REF: Goldsmith YEAR  
JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI  
HAS REFITTED SOME RATE CONSTANTS.

PLOG / +1.0000000E-002  
+5.2000000E+033 -7.9200000E+000 +3.1320000E+004 /  
PLOG / +1.0000000E-001  
+1.2600000E+098 -2.7090000E+001 +6.4060000E+004 /  
PLOG / +3.1600000E-001  
+1.8000000E+033 -7.2700000E+000 +3.3760000E+004 /  
PLOG / +1.0000000E+000  
+3.8300000E+033 -7.2000000E+000 +3.5100000E+004 /  
PLOG / +3.1600000E+000  
+1.2800000E+079 -1.9610000E+001 +7.4870000E+004 /  
PLOG / +1.0000000E+001  
+4.0700000E+032 -6.6200000E+000 +3.7210000E+004 /  
PLOG / +3.1600000E+001  
+6.8600000E+044 -1.0040000E+001 +4.7030000E+004 /  
PLOG / +1.0000000E+002 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
!PLOG/1.000E+02 -1.07E+04 1.33 15620.0/

DUP

C2H3OO<=>CO+CH3O +1.1600000E-  
001 +3.1600000E+000 +1.8420000E+004 !\AUTHOR: !\REF: Goldsmith YEAR  
JOURNAL ETC !\COMMENT: !Refitted by Yang from 500K to 2000K, maximum  
error is 18.13%

PLOG / +1.0000000E-002  
+2.3100000E+129 -4.1860000E+001 +4.5850000E+004 /  
PLOG / +1.0000000E-001  
+2.4200000E+028 -5.9900000E+000 +3.0540000E+004 /  
PLOG / +3.1600000E-001 +8.6900000E-  
050 +1.6630000E+001 -3.9000000E+003 /  
PLOG / +1.0000000E+000 +1.1900000E-  
039 +1.3610000E+001 -1.3170000E+003 /  
PLOG / +3.1600000E+000  
+8.8000000E+086 -2.3080000E+001 +6.1010000E+004 /  
PLOG / +1.0000000E+001  
+1.2700000E+003 +1.4400000E+000 +1.8660000E+004 /  
PLOG / +3.1600000E+001  
+1.9700000E+017 -2.2300000E+000 +2.8590000E+004 /  
PLOG / +1.0000000E+002  
+3.2500000E+004 +1.6940000E+000 +2.3327600E+004 /  
!PLOG/1.000E+02 1.16E-07 4.81 12010.0/

DUP

!C2H3OO<=>CO2+CH3 6.03E-03 3.46 17420 !\AUTHOR: !\REF: Goldsmith YEAR  
JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI  
HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

!PLOG/1.000E-02 5.09E+33 -7.95 31290.0/  
!PLOG/1.000E-01 1.21E+118 -33.13 73790.0/  
!PLOG/3.160E-01 8.56E+32 -7.21 33550.0/  
!PLOG/1.000E+00 3.27E+33 -7.22 34990.0/  
!PLOG/3.160E+00 3.49E-79 25.01 -21020.0/  
!PLOG/1.000E+01 8.16E+32 -6.76 37270.0/  
!PLOG/3.160E+01 7.01E+37 -8.06 42200.0/  
!PLOG/1.000E+02 -2.51E+03 1.41 14420.0/  
!DUP

!C2H3OO<=>CO2+CH3 6.03E-03 3.46 17420 !\AUTHOR: !\REF: Goldsmith YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

!PLOG/1.000E-02 4.20E+122 -39.75 43640.0/  
!PLOG/1.000E-01 1.96E+29 -6.29 30920.0/  
!PLOG/3.160E-01 5.10E-66 21.37 -11110.0/  
!PLOG/1.000E+00 1.76E-47 15.85 -5283.0/  
!PLOG/3.160E+00 3.82E+32 -6.8 35690.0/  
!PLOG/1.000E+01 4.62E+00 2.1 17170.0/  
!PLOG/3.160E+01 3.49E+14 -1.58 26470.0/  
!PLOG/1.000E+02 4.05E-09 5.14 10480.0/

!DUP

CHOCO+OH=>HCO+CO+H2O

+6.1329900E+004 +2.6500000E+000 -4.5864000E+003 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.

!\COMMENT:

!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION

\A

\N

\EA

!

---

C2H3+H<=>C2H2+H2

+1.7000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:86TSA/HAM !\COMMENT:

C2H3+H<=>H2CC+H2

+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:USC ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF USC MECH ESTIMATE?

C2H3+OH<=>C2H2+H2O

+3.0110000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:

C2H3+CH3<=>CH4+C2H2

+3.9200000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:Tsang, W.; Hampson, R.F., J. Phys. Chem. Ref. Data 15, 1087 (1986) !\COMMENT:

C2H3+C2H3<=>C2H2+C2H4

+9.6000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:

!=====

!\ENDSUBSPECIES: \C2H3

!=====

!-----

!\ENDSUBMECH: \C2H4

!-----

!-----

!\SUBMECH: \C2H2

!\MECHCOMMENTS:

!\MECHWARNINGS:

!-----

!

---

!\REACTIONCLASS: \UNIMOL

\A

\N

\EA

!  
-----  
C2H+H (+M) <=>C2H2 (+M)  
+1.0000000E+017 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: GRI  
3.0 !\COMMENT:  
LOW /  
+3.7500000E+033 -4.8000000E+000 +1.9000000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +6.4600000E-001  
+1.3200000E+002 +1.3150000E+003 +5.5660000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
C2H2 (+M) <=>H2CC (+M)  
+8.0000000E+014 -5.2000000E-001 +5.0750000E+004 !\AUTHOR: !\REF:99 LAS/  
WA !\COMMENT:  
LOW /  
+2.4500000E+015 -6.4000000E-001 +4.9700000E+004 / !LOW-PRESSURE-LIMIT  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / C2H2 / 2.500 / C2H4 / 2.500 / !3RD BODY COLLIDER EFFICIENCIES  
!

-----  
!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

-----  
C2H2+O<=>CH2+CO  
+7.3950000E+008 +1.2800000E+000 +2.4720000E+003 !\AUTHOR: !\REF:NGUYEN  
ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\COMMENT:  
C2H2+O<=>HCCO+H  
+2.9580000E+009 +1.2800000E+000 +2.4720000E+003 !\AUTHOR: !\REF:NGUYEN  
ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\COMMENT:  
C2H2+HO2<=>CH2CO+OH  
+6.0300000E+009 +0.0000000E+000 +7.9490000E+003 !\AUTHOR: !\REF:NGUYEN  
ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706 !\COMMENT:  
C2H2+HCO<=>C2H3+CO  
+1.0000000E+007 +2.0000000E+000 +6.0000000E+003 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
C2H2+CH2<=>C3H3+H  
+1.2000000E+013 +0.0000000E+000 +6.6200000E+003 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
C2H2+CH2 (S) <=>C3H3+H  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
C2H2+HCCO<=>C3H3+CO  
+1.0000000E+011 +0.0000000E+000 +3.0000000E+003 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
H2CC+H<=>C2H2+H  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
H2CC+OH<=>CH2CO+H  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
H2CC+O2<=>HCO+HCO  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI 3.0  
AND USC II !\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?  
!

-----  
!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA

!

---

C2H2+OH<=>C2H+H2O

+2.6320000E+006 +2.1400000E+000 +1.7060000E+004 !\AUTHOR: !\REF:SJK J.  
PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:

C2H2+OH<=>HCCOH+H

+2.8000000E+005 +2.2800000E+000 +1.2420000E+004 !\AUTHOR: !\REF:SJK J.  
PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:

PLOG / +1.0000000E-002

+2.8000000E+005 +2.2800000E+000 +1.2420000E+004 /

PLOG / +2.5000000E-002

+7.4670000E+005 +2.1600000E+000 +1.2550000E+004 /

PLOG / +1.0000000E-001

+1.7760000E+006 +2.0400000E+000 +1.2670000E+004 /

PLOG / +1.0000000E+000

+2.4150000E+006 +2.0000000E+000 +1.2710000E+004 /

PLOG / +1.0000000E+001

+3.2100000E+006 +1.9700000E+000 +1.2810000E+004 /

PLOG / +1.0000000E+002

+7.3470000E+006 +1.8900000E+000 +1.3600000E+004 /

C2H2+OH<=>CH2CO+H

+1.5780000E+003 +2.5600000E+000 -8.4450000E+002 !\AUTHOR: !\REF:SJK J.  
PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:

PLOG / +1.0000000E-002

+1.5780000E+003 +2.5600000E+000 -8.4450000E+002 /

PLOG / +2.5000000E-002

+1.5180000E+004 +2.2800000E+000 -2.9210000E+002 /

PLOG / +1.0000000E-001

+3.0170000E+005 +1.9200000E+000 +5.9810000E+002 /

PLOG / +1.0000000E+000

+7.5280000E+006 +1.5500000E+000 +2.1060000E+003 /

PLOG / +1.0000000E+001

+5.1010000E+006 +1.6500000E+000 +3.4000000E+003 /

PLOG / +1.0000000E+002

+1.4570000E+004 +2.4500000E+000 +4.4770000E+003 /

C2H2+OH<=>CH3+CO

+4.7570000E+005 +1.6800000E+000 -3.2980000E+002 !\AUTHOR: !\REF:SJK J.  
PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:

PLOG / +1.0000000E-002

+4.7570000E+005 +1.6800000E+000 -3.2980000E+002 /

PLOG / +2.5000000E-002

+4.3720000E+006 +1.4000000E+000 +2.2650000E+002 /

PLOG / +1.0000000E-001

+7.6480000E+007 +1.0500000E+000 +1.1150000E+003 /

PLOG / +1.0000000E+000

+1.2770000E+009 +7.3000000E-001 +2.5790000E+003 /

PLOG / +1.0000000E+001

+4.3120000E+008 +9.2000000E-001 +3.7360000E+003 /

PLOG / +1.0000000E+002

+8.2500000E+005 +1.7700000E+000 +4.6970000E+003 /

C2H2+OH<=>C2H2OH

+3.9130000E+032 -7.1260000E+000 +5.8240000E+003 !\AUTHOR: !\REF:SJK J.  
PHYS. CHEM A 2005, 109, 6045-6055 !\COMMENT:

PLOG / +1.0000000E-002

+3.9130000E+032 -7.1260000E+000 +5.8240000E+003 /

PLOG / +2.5000000E-002

+1.0670000E+032 -6.8470000E+000 +5.5080000E+003 /



```

PLOG / +1.0000000E-001
+1.6460000E+032 -6.7170000E+000 +5.8220000E+003 /
PLOG / +1.0000000E+000
+1.3870000E+031 -6.0870000E+000 +6.3480000E+003 /
PLOG / +1.0000000E+001
+2.8920000E+029 -5.2880000E+000 +7.0550000E+003 /
PLOG / +1.0000000E+002
+1.3670000E+025 -3.7540000E+000 +6.5430000E+003 /
H+HCCOH<=>H+CH2CO
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI
2.11 !\COMMENT:
!=====
!=====
!\SUBSPECIES: \C2H
!=====
!=====
C2H+O2<=>CO2+CHV
+2.1700000E+010 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:DEVRIENDT, VAN LOOK, CEURSTERS, AND PEETERS, CHEM PHYS LETT. 261
(1996) 450, C2H+O2 !\COMMENT:
C2H+O2<=>HCO+CO
+5.0000000E+013 +0.0000000E+000 +1.5000000E+003 !\AUTHOR: !\REF:GRI
!\COMMENT:
C2H+O<=>CO+CHV
+6.2000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:OHV
KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
C2H+O<=>CO+CH
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI
!\COMMENT:
C2H+H2<=>H+C2H2
+4.9000000E+005 +2.5000000E+000 +5.6000000E+002 !\AUTHOR: !\REF:GRI
!\COMMENT:
C2H+OH<=>H+HCCO
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI
!\COMMENT:
!=====
!=====
!\SUBSPECIES: \C2H
!=====
!=====
!-----
!-----
!\ENDSUBMECH: C2H2
!-----
!-----
!-----
!-----
!\SUBMECH: \CH3CHO
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!-----
!
!-----
!\REACTIONCLASS: \UNIMOL \A
\n \EA
!
```

CH3CHO (+M) <=> CH3+HCO (+M)  
+2.4500000E+022 -1.7400000E+000 +8.6355000E+004 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO. 2, 2010 !\COMMENT:  
LOW /  
+1.0300000E+059 -1.1300000E+001 +9.5912500E+004 / !LOW-PRESSURE-LIMIT  
TROE / +2.4900000E-003  
+7.1810000E+002 +6.0890000E+000 +3.7800000E+003 / !TROE PARAMETERS  
CH3CHO (+M) <=> CH4+CO (+M)  
+2.7200000E+021 -1.7400000E+000 +8.6355000E+004 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO. 2, 2010 !\COMMENT:  
LOW /  
+1.1440000E+058 -1.1300000E+001 +9.5912500E+004 / !LOW-PRESSURE-LIMIT  
TROE / +2.4900000E-003  
+7.1810000E+002 +6.0890000E+000 +3.7800000E+003 / !TROE PARAMETERS  
!

---

!\REACTIONCLASS: \RH\_ABSTRACTION \A  
\N \EA  
!

---

CH3CHO+O2<=>CH3CO+HO2  
+3.0100000E+013 +0.0000000E+000 +3.9150000E+004 !\AUTHOR: !\REF:BAULCH  
ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:  
CH3CHO+O<=>CH3CO+OH  
+5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR: !\REF:CURRAN,  
FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT IS SOURCE OF NIST DATA?  
CH3CHO+H<=>CH3CO+H2  
+1.3100000E+005 +2.5800000E+000 +1.2200000E+003 !\AUTHOR: !\REF:HARDING  
J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\COMMENT:  
CH3CHO+OH<=>CH3CO+H2O  
+3.3700000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: !\REF:JUAN  
LI'S PHD THESIS !\COMMENT: WARNING: UNPUBLISHED RESULTS?  
CH3CHO+HO2<=>CH3CO+H2O2  
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\AUTHOR:  
!\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:  
!\COMMENT:  
CH3CHO+CH3<=>CH3CO+CH4 +7.0800000E-  
004 +4.5800000E+000 +1.9660000E+003 !\AUTHOR: !\REF: GUPTE ET AL., PROC  
COMBUST INST 31 (2007) 167-174 !\COMMENT:  
CH3CHO+CH3O2<=>CH3CO+CH3O2H  
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:BAULCH  
ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT:  
CH3CHO+CH3CO3<=>CH3CO+CH3CO3H  
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:BAULCH  
ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992) !\COMMENT: WARNING: WHY IS  
THIS RATE CONSTANT SAME AS ABOVE?  
CH3CHO+H<=>CH2CHO+H2  
+2.7200000E+003 +3.1000000E+000 +5.2100000E+003 !\AUTHOR: !\REF:HARDING  
J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\COMMENT:  
CH3CHO+OH<=>CH2CHO+H2O  
+1.7200000E+005 +2.4000000E+000 +8.1500000E+002 !\AUTHOR: !\REF:TAYLOR  
ET AL. 1996 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

CH3CHO+OH<=>CH3+HOCHO  
+3.0000000E+015 -1.0760000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TAYLOR  
ET AL. 1996 !\COMMENT:

!=====  
=====

!\SUBSPECIES: \CH3CO

!=====  
=====

!

!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA

!

CH3CO(+M)<=>CH3+CO(+M)  
+1.0700000E+012 +6.3000000E-001 +1.6900000E+004 !\AUTHOR: !\REF:J.  
PHYS. CHEM. A 2006, 110, 5772-5781 !\COMMENT:

LOW /

+5.6500000E+018 -9.7000000E-001 +1.4600000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +6.2900000E-001

+8.7300000E+009 +5.5200000E+000 +7.6000000E+007 / !TROE PARAMETERS

CH3CO(+M)<=>CH2CO+H(+M)

+9.4130000E+007 +1.9170000E+000 +4.4987200E+004 !\AUTHOR: !\REF:J.  
PHYS. CHEM. A 2006, 110, 5772-5781

LOW /

+1.5160000E+051 -1.0270000E+001 +5.5390000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +6.0090000E-001

+8.1030000E+009 +6.6770000E+002 +5.0000000E+009 / !TROE PARAMETERS

!\COMMENT: DEFINED IN THE REVERSE FROM SJK, P DEPENDENCE FROM CHEMDIS,  
IMPORTANT FOR ACETONE FLAME SPEEDS WARNING: IF PRESSURE DEPENDENCIES FROM  
BOTH PATHWAYS ARE NOT FROM SINGLE CALCULATION THEN P-DEPENDENCY MAY BE  
WRONG

!

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA

!

CH3CO+H<=>CH2CO+H2  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE

CH3CO+O<=>CH2CO+OH

+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE

CH3CO+CH3<=>CH2CO+CH4

+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE

!

!\REACTIONCLASS: \R+O2 \A  
\N \EA

!

CH3CO+O2<=>CH3CO3  
+1.2000000E+011 +0.0000000E+000 -1.1000000E+003 !\AUTHOR: !\REF: CURRAN  
ESTIMATE !\COMMENT:

CH3CO3+HO2<=>CH3CO3H+O2  
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF: TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
H2O2+CH3CO3<=>HO2+CH3CO3H  
+2.4100000E+012 +0.0000000E+000 +9.9360000E+003 !\AUTHOR: !\REF: TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
CH4+CH3CO3<=>CH3+CH3CO3H  
+1.8100000E+011 +0.0000000E+000 +1.8480000E+004 !\AUTHOR: !\REF:BASED  
ON CH4+CH3O2 !\COMMENT: WARNING: HAS RATE CONSTANT BEEN ALTERED? BY OW  
MUCH?

!=====  
=====

!\ENDSUBSPECIES: \CH3CO

!=====  
=====

!=====  
=====

!\SUBSPECIES: \C2H3OH

!=====  
=====

!  
\_\_\_\_\_

!\REACTIONCLASS: \UNIMOL \A

\N \EA

!  
\_\_\_\_\_

C2H3OH<=>CH3CHO  
+7.4200000E+046 -1.0560000E+001 +6.7420000E+004 !\AUTHOR: !\REF:CHANGED  
PRODUCTS FROM CH3+HCO !\COMMENT:

PLOG / +1.0000000E-001

+7.4200000E+046 -1.0560000E+001 +6.7420000E+004 /

PLOG / +1.0000000E+000

+4.4200000E+042 -9.0900000E+000 +6.7069200E+004 /

PLOG / +1.0000000E+002

+2.9000000E+027 -4.3500000E+000 +6.1612900E+004 /

!  
\_\_\_\_\_

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!  
\_\_\_\_\_

C2H3OH+O2<=>CH2CHO+HO2  
+5.3100000E+011 +2.1000000E-001 +3.9830000E+004 !\AUTHOR: !\REF:ETHENOL  
CHEMISTRY FROM CURRAN/ YASUNAGA !\COMMENT: WARNING: WHAT IS SOURCE?

C2H3OH+O<=>CH2CHO+OH

+1.8750000E+006 +1.9000000E+000 -8.6000000E+002 !\AUTHOR: !\REF:ETHENOL  
CHEMISTRY FROM CURRAN/ YASUNAGA !\COMMENT: WARNING: WHAT IS SOURCE?

C2H3OH+H<=>CH2CHO+H2

+1.4800000E+003 +3.0770000E+000 +7.2200000E+003 !\AUTHOR: !\REF:ENOL+H  
RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608, !\COMMENT: WARNING: EXCEPT  
FOR SC2H4OH CHANNEL KEPT WKM CALCULATION

C2H3OH+OH<=>CH2CHO+H2O

+3.3300000E+009 +1.1000000E+000 +5.4050000E+002 !\AUTHOR: !\REF:ETHENOL  
CHEMISTRY FROM CURRAN/ YASUNAGA !\COMMENT: WARNING: WHAT IS SOURCE?

C2H3OH+CH3<=>CH2CHO+CH4

+2.0300000E-  
008 +5.9000000E+000 +1.0520000E+003 !\AUTHOR: !\REF:ETHENOL CHEMISTRY  
FROM CURRAN/ YASUNAGA !\COMMENT: WARNING: WHAT IS SOURCE?

C2H3OH+CH3O2<=>CH2CHO+CH3O2H  
+3.4000000E+003 +2.5000000E+000 +8.9220000E+003 !\AUTHOR: !\REF:ETHENOL  
CHEMISTRY FROM CURRAN/ YASUNAGA !\COMMENT: WARNING: WHAT IS SOURCE?  
C2H3OH+H<=>C2H2OH+H2  
+2.4700000E+007 +2.0300000E+000 +1.5200000E+004 !\AUTHOR: !\REF:ENOL+H  
RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608, !\COMMENT: WARNING: EXCEPT  
FOR SC2H4OH CHANNEL KEPT WKM CALCULATION  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

C2H3OH+H<=>PC2H4OH  
+3.0100000E+008 +1.5770000E+000 +3.6700000E+003 !\AUTHOR: !\REF:ENOL+H  
RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608, !\COMMENT: WARNING: EXCEPT  
FOR SC2H4OH CHANNEL KEPT WKM CALCULATION  
C2H3OH+HO2<=>CH3CHO+HO2  
+1.4900000E+005 +1.6700000E+000 +6.8100000E+003 !\AUTHOR: !\REF:DA  
SILVA BOZZELLI CHEMICAL PHYSICS LETTERS 483 (2009) 25-29 !\COMMENT:

!=====  
=====  
!\ENDSUBSPECIES: \C2H3OH  
!=====  
=====  
!=====  
=====  
!\SUBSPECIES: CH2CHO  
!=====  
=====  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

CH2CHO (+M) <=>CH2CO+H (+M)  
+1.4300000E+015 -1.5000000E-001 +4.5600000E+004 !\AUTHOR: !\REF:J.  
PHYS. CHEM. A 2006, 110, 5772-5781 !\COMMENT:  
LOW /  
+6.0000000E+029 -3.8000000E+000 +4.3423900E+004 / !LOW-PRESSURE-LIMIT  
TROE / +9.8500000E-001  
+3.9300000E+002 +9.8000000E+009 +5.0000000E+009 / !TROE PARAMETERS  
CH2CHO (+M) <=>CH3+CO (+M)  
+2.9300000E+012 +2.9000000E-001 +4.0300000E+004 !\AUTHOR: !\REF:J.  
PHYS. CHEM. A 2006, 110, 5772-5781 !\COMMENT:  
LOW /  
+9.5200000E+033 -5.0700000E+000 +4.1300000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +7.1300000E-017  
+1.1500000E+003 +4.9900000E+009 +1.7900000E+009 / !TROE PARAMETERS

!=====  
=====  
!\ENDSUBSPECIES: \CH2CHO  
!=====  
=====  
!=====  
=====  
!\SUBSPECIES: \CH3CO3H

!=====  
=====  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

CH3CO3H<=>CH3CO2+OH  
+5.0100000E+014 +0.0000000E+000 +4.0150000E+004 !\AUTHOR:  
!\REF:SAHETCHIAN ET AL. 1992 !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

CH3CO3+CH2O<=>CH3CO3H+HCO  
+1.9900000E+012 +0.0000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH3O2+CH2O !\COMMENT: WARNING: POORLY-DEFINED IN THIS DIRECTION?  
CH3CO3+C2H6<=>CH3CO3H+C2H5  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH3O2+CH2O !\COMMENT: WARNING: POORLY-DEFINED IN THIS DIRECTION?  
!

---

!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

---

CH3CO2+M<=>CH3+CO2+M  
+4.4000000E+015 +0.0000000E+000 +1.0500000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH3CO<=>CH3+CO !\COMMENT:  
!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

---

CH2CHO+O2<=>O2CH2CHO  
+1.5800000E+077 -2.1900000E+001 +1.9350000E+004 !\AUTHOR: !\REF:J. LEE,  
AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.5800000E+077 -2.1900000E+001 +1.9350000E+004 /  
PLOG / +1.0000000E-001  
+3.8800000E+069 -1.8840000E+001 +1.9240000E+004 /  
PLOG / +1.0000000E+000  
+7.8000000E+059 -1.5400000E+001 +1.7650000E+004 /  
PLOG / +1.0000000E+001  
+3.0500000E+050 -1.2200000E+001 +1.5630000E+004 /  
CH2CHO+O2<=>CH2CO+HO2  
+1.8800000E+005 +2.3700000E+000 +2.3730000E+004 !\AUTHOR: !\REF:J. LEE,  
AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.8800000E+005 +2.3700000E+000 +2.3730000E+004 /  
PLOG / +1.0000000E-001  
+1.8800000E+005 +2.3700000E+000 +2.7370000E+004 /  
PLOG / +1.0000000E+000  
+2.5100000E+005 +2.3300000E+000 +2.3800000E+004 /

PLOG / +1.0000000E+001  
 +7.0500000E+007 +1.6300000E+000 +2.5290000E+004 /  
 CH2CHO+O2=>CH2O+CO+OH  
 +2.6800000E+017 -1.8400000E+000 +6.5300000E+003 !\AUTHOR: !\REF:J. LEE,  
 AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +2.6800000E+017 -1.8400000E+000 +6.5300000E+003 /  
 PLOG / +1.0000000E-001  
 +1.5200000E+020 -2.5800000E+000 +8.9800000E+003 /  
 PLOG / +1.0000000E+000  
 +1.6500000E+019 -2.2200000E+000 +1.0340000E+004 /  
 PLOG / +1.0000000E+001  
 +8.9530000E+013 -6.0000000E-001 +1.0120000E+004 /  
 CH2CHO+O2<=>HO2CH2CO  
 +3.6400000E+065 -2.1870000E+001 +1.9020000E+004 !\AUTHOR: !\REF:J. LEE,  
 AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +3.6400000E+065 -2.1870000E+001 +1.9020000E+004 /  
 PLOG / +1.0000000E-001  
 +3.6400000E+058 -1.9000000E+001 +1.9090000E+004 /  
 PLOG / +1.0000000E+000  
 +6.6500000E+048 -1.5550000E+001 +1.7460000E+004 /  
 PLOG / +1.0000000E+001  
 +4.8000000E+038 -1.2140000E+001 +1.4960000E+004 /  
 O2CH2CHO<=>HO2CH2CO  
 +8.2700000E+030 -6.6500000E+000 +2.4500000E+004 !\AUTHOR: !\REF:J. LEE,  
 AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +8.2700000E+030 -6.6500000E+000 +2.4500000E+004 /  
 PLOG / +1.0000000E-001  
 +1.7300000E+026 -4.9900000E+000 +2.3760000E+004 /  
 PLOG / +1.0000000E+000  
 +9.0300000E+019 -2.9200000E+000 +2.2170000E+004 /  
 PLOG / +1.0000000E+001  
 +1.4300000E+016 -1.6700000E+000 +2.1210000E+004 /  
 O2CH2CHO<=>CH2CO+HO2  
 +2.0500000E+040 -1.3310000E+001 +5.2150000E+004 !\AUTHOR: !\REF:J. LEE,  
 AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +2.0500000E+040 -1.3310000E+001 +5.2150000E+004 /  
 PLOG / +1.0000000E-001  
 +5.7200000E+045 -1.4000000E+001 +5.2200000E+004 /  
 PLOG / +1.0000000E+000  
 +4.1600000E+055 -1.5760000E+001 +5.5080000E+004 /  
 PLOG / +1.0000000E+001  
 +1.1200000E+061 -1.6040000E+001 +6.0010000E+004 /  
 HO2CH2CO=>CO+CH2O+OH  
 +2.3600000E+017 -2.9500000E+000 +8.1000000E+003 !\AUTHOR: !\REF:J. LEE,  
 AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +2.3600000E+017 -2.9500000E+000 +8.1000000E+003 /  
 PLOG / +1.0000000E-001  
 +2.3800000E+018 -2.9500000E+000 +8.1000000E+003 /  
 PLOG / +1.0000000E+000  
 +2.5100000E+019 -2.9500000E+000 +8.1100000E+003 /  
 PLOG / +1.0000000E+001  
 +4.1600000E+020 -3.0200000E+000 +8.2400000E+003 /

HO2CH2CO<=>CH2CO+HO2  
+1.1200000E+007 -3.7600000E+000 +2.1680000E+004 !\AUTHOR: !\REF:J. LEE,  
AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.1200000E+007 -3.7600000E+000 +2.1680000E+004 /  
PLOG / +1.0000000E-001  
+1.1000000E+008 -3.7600000E+000 +2.1680000E+004 /  
PLOG / +1.0000000E+000  
+9.2000000E+008 -3.7300000E+000 +2.1630000E+004 /  
PLOG / +1.0000000E+001  
+2.0900000E+009 -3.5500000E+000 +2.1220000E+004 /

!=====  
=====

!\ENDSUBSPECIES: \CH3CO3H

!=====  
=====

!-----  
-----

!\ENDSUBMECH: \CH3CHO

!-----  
-----

!-----  
-----

!\SUBMECH: \CH2CO

!\MECHCOMMENTS:

!\MECHWARNINGS:

!-----  
-----

CH2+CO (+M) <=> CH2CO (+M)

+8.1000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

LOW /

+2.6900000E+033 -5.1100000E+000 +7.0950000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +5.9070000E-001

+2.7500000E+002 +1.2260000E+003 +5.1850000E+003 / !TROE PARAMETERS

H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES

!-----

!\REACTIONCLASS: \RH\_R\_ABSTRACTION

\A

\N \EA

!-----

CH2CO+H<=>HCCO+H2

+1.4010000E+015 -1.7100000E-001 +8.7832000E+003 !\AUTHOR: !\REF:WKM

(SEE COMMENTS AT BEGINNING OF FILE 15/ 09/ 2011 !\COMMENT: WARNING: SEE  
COMMENTS IN PREVIOUS VERSION OF MECHANISM

CH2CO+O<=>HCCO+OH

+1.0000000E+013 +0.0000000E+000 +8.0000000E+003 !\AUTHOR: !\REF:WKM

ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF ESTIMATE?

CH2CO+OH<=>HCCO+H2O

+1.0000000E+013 +0.0000000E+000 +2.0000000E+003 !\AUTHOR: !\REF:WKM

ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF ESTIMATE?

!-----

!\REACTIONCLASS: \RADICAL\_ADDITION

\A

\N \EA



!  
-----  
CH2CO+H<=>CH3+CO  
+7.7040000E+013 -1.7100000E-001 +4.1832000E+003 !\AUTHOR: !\REF:WKM  
(SEE COMMENTS AT BEGINNING OF FILE 15/ 09/ 2011 !\COMMENT: WARNING: SEE  
COMMENTS IN PREVIOUS VERSION OF MECHANISM  
CH+CH2O<=>H+CH2CO  
+9.4600000E+013 +0.0000000E+000 -5.1500000E+002 !\AUTHOR: !\REF:REG  
2.11 !\COMMENT: WARNING: SOURCE OF RATE CONSTANT UNCLEAR  
CH2CO+O<=>CH2+CO2  
+1.7500000E+012 +0.0000000E+000 +1.3500000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
CH2CO+OH<=>CH2OH+CO  
+2.0000000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR: !\REF:BROWN  
ET AL. CHEM. PHYS. LETT. 1989, 161, 491. !\COMMENT:  
CH2CO+CH2(S)<=>C2H4+CO  
+1.6000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WKM  
CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT  
CH2CO+CH3<=>C2H5+CO  
+4.7690000E+004 +2.3120000E+000 +9.4680000E+003 !\AUTHOR: !\REF:WKM  
CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT  
!

-----  
!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

-----  
HCCO+OH=>H2+CO+CO  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WKM  
CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT  
HCCO+O=>H+CO+CO  
+8.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WKM  
CALCULATION !\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT  
!=====

!\SUBSPECIES: \HCCO  
!=====

-----  
!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

-----  
CH+CO+M<=>HCCO+M  
+7.5700000E+022 -1.9000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:J.  
CHEM. PHYS. 108: 6709-6716 1998 !\COMMENT:  
!

-----  
!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

-----  
HCCO+H<=>CH2(S)+CO  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:GRI  
!\COMMENT:

HCCO+O2=>OH+CO+CO  
+1.9100000E+011 -2.0000000E-002 +1.0200000E+003 !\AUTHOR:  
!\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS JOURNAL/ISSUE?  
HCCO+O2=>CO2+CO+H  
+4.7800000E+012 -1.4200000E-001 +1.1500000E+003 !\AUTHOR:  
!\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS JOURNAL/ISSUE?  
CH+HCCO<=>CO+C2H2  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:REG  
2.11 !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
!=====  
=====  
!\ENDSUBSPECIES: \HCCO  
!=====  
=====  
!-----  
-----  
!\ENDSUBMECH: \CH2CO  
!-----  
-----  
!-----  
-----  
!\SUBMECH: \C2H5OH  
!\MECHCOMMENTS:  
!\MECHWARNINGS: KPS, 30/07/2015, LOW TEMPERATURE PATHWAYS FOR ETHANOL  
RADICALS+O2 ARE FROM VARYING SOURCES. ARE THERE ANY INCONSISTENCIES IN  
HPL/P-DEPENDENT KINETICS  
!-----  
-----  
!  
-----  
!\REACTIONCLASS: \UNIMOL \A  
\n \EA  
!

C2H5OH<=>C2H4+H2O  
+3.4100000E+059 -1.4200000E+001 +8.3672600E+004 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
PLOG / +1.0000000E-003  
+3.4100000E+059 -1.4200000E+001 +8.3672600E+004 /  
PLOG / +1.0000000E-002  
+2.6200000E+057 -1.3300000E+001 +8.5262200E+004 /  
PLOG / +1.0000000E-001  
+1.6500000E+052 -1.1500000E+001 +8.4745600E+004 /  
PLOG / +1.0000000E+000  
+5.2300000E+043 -8.9000000E+000 +8.1506700E+004 /  
PLOG / +1.0000000E+001  
+4.5900000E+032 -5.6000000E+000 +7.6062400E+004 /  
PLOG / +1.0000000E+002  
+3.8400000E+020 -2.0600000E+000 +6.9465500E+004 /  
C2H5OH<=>CH3+CH2OH  
+1.2000000E+054 -1.2900000E+001 +1.0000570E+005 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
PLOG / +1.0000000E-003  
+1.2000000E+054 -1.2900000E+001 +1.0000570E+005 /  
PLOG / +1.0000000E-002  
+5.1800000E+059 -1.4000000E+001 +9.9906400E+004 /

PLOG / +1.0000000E-001  
+1.6200000E+066 -1.5300000E+001 +1.0539050E+005 /  
PLOG / +1.0000000E+000  
+5.5500000E+064 -1.4500000E+001 +1.0618300E+005 /  
PLOG / +1.0000000E+001  
+1.5500000E+058 -1.2300000E+001 +1.0576800E+005 /  
PLOG / +1.0000000E+002  
+1.7800000E+047 -8.9600000E+000 +1.0105880E+005 /  
C2H5OH<=>C2H5+OH  
+8.1000000E+046 -1.1300000E+001 +1.1105340E+005 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
PLOG / +1.0000000E-003  
+8.1000000E+046 -1.1300000E+001 +1.1105340E+005 /  
PLOG / +1.0000000E-002  
+1.8600000E+056 -1.3500000E+001 +1.0723840E+005 /  
PLOG / +1.0000000E-001  
+4.6500000E+063 -1.5000000E+001 +1.0962280E+005 /  
PLOG / +1.0000000E+000  
+4.4600000E+065 -1.4900000E+001 +1.1234500E+005 /  
PLOG / +1.0000000E+001  
+2.7900000E+061 -1.3400000E+001 +1.1308020E+005 /  
PLOG / +1.0000000E+002  
+6.1700000E+051 -1.0300000E+001 +1.0994070E+005 /  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

C2H5OH+O<=>C2H5O+OH +1.4600000E-  
003 +4.7300000E+000 +1.7270000E+003 !\AUTHOR: !\REF:WU ET AL., J. PHYS.  
CHEM. A 2007, 111, 6693-6703 !\COMMENT:  
C2H5OH+OH<=>C2H5O+H2O +5.8100000E-  
003 +4.2800000E+000 -3.5600000E+003 !\AUTHOR: !\REF: SMB 04/ 09/ 2013  
!\COMMENT: Branching ratio changed for the underprediciotn of c2h4 in the  
JSR and flow reactor  
C2H5OH+H<=>C2H5O+H2  
+9.4500000E+002 +3.1400000E+000 +8.7011000E+003 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
C2H5OH+HO2<=>C2H5O+H2O2 +6.4700000E-  
007 +5.3000000E+000 +1.0533100E+004 !\AUTHOR: !\REF: Mittal 2013  
!\COMMENT: increased by 1.75 Zhou WARNING: WHAT IS SOURCE OF RATE  
CONSTANT?  
C2H5OH+CH3<=>C2H5O+CH4  
+2.0350000E+000 +3.5700000E+000 +7.7210000E+003 !\AUTHOR: !\REF:XU,  
Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004 !\COMMENT:  
C2H5OH+CH3O2<=>C2H5O+CH3O2H +3.2360000E-  
007 +5.3000000E+000 +1.0533100E+004 !\AUTHOR: !\REF:ANAOLGY WITH  
C2H5OH+HO2 !\COMMENT:  
C2H5OH+C2H5<=>PC2H4OH+C2H6  
+5.0000000E+010 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: !\REF:1/ 2 OF  
C4H10+C2H5 !\COMMENT: WARNING: POOR ANALOGY?  
C2H5OH+O2<=>SC2H4OH+HO2  
+1.5000000E+013 +0.0000000E+000 +5.0150000E+004 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:

C2H5OH+O<=>SC2H4OH+OH  
+1.4500000E+005 +2.4700000E+000 +8.7600000E+002 !\AUTHOR: !\REF:WU ET  
AL., J. PHYS. CHEM. A 2007, 111, 6693-6703 !\COMMENT:  
C2H5OH+H<=>SC2H4OH+H2  
+8.7900000E+004 +2.6800000E+000 +2.9100000E+003 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
C2H5OH+OH<=>SC2H4OH+H2O  
+7.5200000E+004 +2.4900000E+000 -1.4741000E+003 !\AUTHOR: !\REF: SMB  
04/ 09/ 2013 !\COMMENT: Branching ratio changed for the underprediciotn  
of c2h4 in the JSR and flow reactor  
C2H5OH+HO2<=>SC2H4OH+H2O2 +2.4500000E-  
005 +5.2600000E+000 +7.4751000E+003 !\AUTHOR: !\REF: Mittal 2013  
!\COMMENT: increased by 1.75 Zhou WARNING: WHAT IS SOURCE OF RATE  
CONSTANT?  
C2H5OH+CH3<=>SC2H4OH+CH4  
+1.9930000E+001 +3.3700000E+000 +7.6340000E+003 !\AUTHOR: !\REF:XU,  
Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004 !\COMMENT:  
C2H5OH+CH3O2<=>SC2H4OH+CH3O2H +1.2250000E-  
005 +5.2600000E+000 +7.4751000E+003 !\AUTHOR: !\REF:ANAOLGY WITH  
C2H5OH+HO2 !\COMMENT:  
C2H5OH+C2H5<=>SC2H4OH+C2H6  
+5.0000000E+010 +0.0000000E+000 +1.0400000E+004 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?  
C2H5OH+O2<=>PC2H4OH+HO2  
+2.0000000E+013 +0.0000000E+000 +5.2800000E+004 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
C2H5OH+O<=>PC2H4OH+OH  
+9.6900000E+002 +3.2300000E+000 +4.6580000E+003 !\AUTHOR: !\REF:WU ET  
AL., J. PHYS. CHEM. A 2007, 111, 6693-6703 !\COMMENT:  
C2H5OH+H<=>PC2H4OH+H2  
+5.3100000E+004 +2.8100000E+000 +7.4900000E+003 !\AUTHOR:  
!\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
!\COMMENT:  
C2H5OH+OH<=>PC2H4OH+H2O  
+3.7600000E+003 +2.7800000E+000 -1.8102000E+003 !\AUTHOR: !\AUTHOR:  
!\REF: SMB 04/ 09/ 2013 !\COMMENT: Branching ratio changed for the  
underprediciotn of c2h4 in the JSR and flow re  
C2H5OH+HO2<=>PC2H4OH+H2O2 +3.9860000E-  
002 +4.3000000E+000 +1.5333000E+004 !\AUTHOR: !\REF: Mittal 2013  
!\COMMENT: increased by 1.75 Zhou WARNING: WHAT IS SOURCE OF RATE  
CONSTANT?  
C2H5OH+CH3<=>PC2H4OH+CH4  
+3.3000000E+002 +3.3000000E+000 +1.2290000E+004 !\AUTHOR: !\REF:XU,  
Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004 !\COMMENT:  
C2H5OH+CH3O2<=>PC2H4OH+CH3O2H +1.9950000E-  
002 +4.3000000E+000 +1.5333000E+004 !\AUTHOR: !\REF:ANAOLGY WITH  
C2H5OH+HO2 !\COMMENT:  
!  


---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\n \EA  
!  


---

SC2H4OH<=>CH3CHO+H  
+5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF:WKM

CALCULATION. !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT? THEORY?  
PAPER?

PLOG / +1.0000000E-003  
+5.6900000E+052 -1.3380000E+001 +4.5049000E+004 /  
PLOG / +1.0000000E-002  
+3.2900000E+056 -1.4120000E+001 +4.8129000E+004 /  
PLOG / +1.0000000E-001  
+8.5800000E+057 -1.4160000E+001 +5.0743000E+004 /  
PLOG / +1.0000000E+000  
+5.3600000E+055 -1.3150000E+001 +5.1886000E+004 /  
PLOG / +1.0000000E+001  
+1.6600000E+048 -1.0640000E+001 +5.0297000E+004 /  
PLOG / +2.0000000E+001  
+8.2600000E+044 -9.5900000E+000 +4.9218000E+004 /  
PLOG / +5.0000000E+001  
+1.0100000E+040 -8.0600000E+000 +4.7439000E+004 /  
PLOG / +1.0000000E+002  
+1.1000000E+036 -6.8400000E+000 +4.5899000E+004 /

SC2H4OH<=>C2H3OH+H

+5.4000000E+046 -1.1630000E+001 +4.4323000E+004 !\AUTHOR: !\REF:WKM  
CALCULATION. !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT? THEORY?  
PAPER?

PLOG / +1.0000000E-003  
+5.4000000E+046 -1.1630000E+001 +4.4323000E+004 /  
PLOG / +1.0000000E-002  
+1.2100000E+051 -1.2550000E+001 +4.7240000E+004 /  
PLOG / +1.0000000E-001  
+2.8700000E+054 -1.3150000E+001 +5.0702000E+004 /  
PLOG / +1.0000000E+000  
+3.7900000E+053 -1.2510000E+001 +5.2560000E+004 /  
PLOG / +1.0000000E+001  
+6.3300000E+046 -1.0200000E+001 +5.1441000E+004 /  
PLOG / +2.0000000E+001  
+3.8700000E+043 -9.1700000E+000 +5.0440000E+004 /  
PLOG / +5.0000000E+001  
+5.0800000E+038 -7.6500000E+000 +4.8713000E+004 /  
PLOG / +1.0000000E+002  
+5.1200000E+034 -6.4100000E+000 +4.7182000E+004 /

SC2H4OH<=>C2H5O

+5.4800000E+045 -1.1630000E+001 +4.4328000E+004 !\AUTHOR: !\REF:WKM  
CALCULATION. !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT? THEORY?  
PAPER?

PLOG / +1.0000000E-003  
+5.4800000E+045 -1.1630000E+001 +4.4328000E+004 /  
PLOG / +1.0000000E-002  
+2.5400000E+049 -1.2370000E+001 +4.6445000E+004 /  
PLOG / +1.0000000E-001  
+1.6500000E+054 -1.3400000E+001 +5.0330000E+004 /  
PLOG / +1.0000000E+000  
+1.8100000E+055 -1.3310000E+001 +5.3132000E+004 /  
PLOG / +1.0000000E+001  
+4.5800000E+049 -1.1320000E+001 +5.2714000E+004 /  
PLOG / +2.0000000E+001  
+4.1100000E+046 -1.0330000E+001 +5.1834000E+004 /  
PLOG / +5.0000000E+001  
+6.6800000E+041 -8.8300000E+000 +5.0202000E+004 /  
PLOG / +1.0000000E+002  
+6.5400000E+037 -7.5800000E+000 +4.8697000E+004 /

SC2H4OH<=>PC2H4OH

+2.6500000E+036 -8.8600000E+000 +5.1019000E+004 !\AUTHOR: !\REF:WKM  
CALCULATION. !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT? THEORY?  
PAPER?

PLOG / +1.0000000E-003

+2.6500000E+036 -8.8600000E+000 +5.1019000E+004 /

PLOG / +1.0000000E-002

+3.5600000E+037 -8.8900000E+000 +5.1114000E+004 /

PLOG / +1.0000000E-001

+4.1400000E+039 -9.1900000E+000 +5.1912000E+004 /

PLOG / +1.0000000E+000

+5.8200000E+044 -1.0340000E+001 +5.5296000E+004 /

PLOG / +1.0000000E+001

+4.2600000E+048 -1.1060000E+001 +5.9458000E+004 /

PLOG / +2.0000000E+001

+8.8400000E+047 -1.0740000E+001 +5.9901000E+004 /

PLOG / +5.0000000E+001

+2.2300000E+045 -9.8400000E+000 +5.9604000E+004 /

PLOG / +1.0000000E+002

+1.7000000E+042 -8.8300000E+000 +5.8737000E+004 /

CH3+CH2O<=>C2H5O

+3.0000000E+011 +0.0000000E+000 +6.3360000E+003 !\AUTHOR: !\REF: CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?

CH3CHO+H<=>C2H5O

+4.6100000E+007 +1.7100000E+000 +7.0900000E+003 !\AUTHOR: !\REF:HARDING  
J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\COMMENT:

!

---

!\REACTIONCLASS: \R+O2

\A

\N \EA

!

---

C2H5O+O2<=>CH3CHO+HO2

+4.2800000E+010 +0.0000000E+000 +1.0970000E+003 !\AUTHOR: !\REF:  
HARTMANN ET AL. 1990 !\COMMENT:

O2C2H4OH<=>PC2H4OH+O2

+3.9000000E+016 -1.0000000E+000 +3.0000000E+004 !\AUTHOR: !\REF:BASED  
ON C3H6OH+O2 REACTION !\COMMENT:

O2C2H4OH=>OH+CH2O+CH2O

+1.2500000E+011 +0.0000000E+000 +1.8900000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?

SC2H4OH+O2<=>CH3CHO+HO2

+5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF:DA  
SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933 !\COMMENT:

PLOG / +1.0000000E-002

+5.2600000E+017 -1.6370000E+000 +8.3800000E+002 /

PLOG / +1.0000000E-001

+5.2600000E+017 -1.6370000E+000 +8.3800000E+002 /

PLOG / +1.0000000E+000

+5.2800000E+017 -1.6380000E+000 +8.3900000E+002 /

PLOG / +1.0000000E+001

+1.5400000E+018 -1.7710000E+000 +1.1200000E+003 /

PLOG / +1.0000000E+002

+3.7800000E+020 -2.4290000E+000 +3.0900000E+003 /

SC2H4OH+O2<=>C2H3OH+HO2

+5.5120000E+003 +2.4950000E+000 -4.1400000E+002 !\AUTHOR: !\REF:DA  
SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933 !\COMMENT:

PLOG / +1.0000000E-002  
+5.1200000E+002 +2.4960000E+000 -4.1400000E+002 /  
PLOG / +1.0000000E-001  
+5.3300000E+002 +2.4900000E+000 -4.0200000E+002 /  
PLOG / +1.0000000E+000  
+7.6200000E+002 +2.4460000E+000 -2.9600000E+002 /  
PLOG / +1.0000000E+001  
+8.9200000E+003 +2.1460000E+000 +4.7000000E+002 /  
PLOG / +1.0000000E+002  
+4.3800000E+005 +1.6990000E+000 +2.3300000E+003 /

!-----

!\ENDSUBMECH: C2H5OH

!-----

!-----

!\SUBMECH: \CH3OCH3

!\MECHCOMMENTS:

!\MECHWARNINGS:

!-----

!-----

!\REACTIONCLASS: \UNIMOL \A

\N \EA

!-----

CH3OCH3 (+M) <=> CH3+CH3O (+M)

+2.3300000E+019 -6.6100000E-001 +8.4139000E+004 !\AUTHOR: !\REF:R.  
SIVARAMAKRISHNAN, ET AL. COMBUSTION AND FLAME, 158 (2011) 61

LOW /

+1.7200000E+059 -1.1400000E+001 +9.3295600E+004 / !LOW-PRESSURE-LIMIT

TROE / +1.0000000E+000 +1.0000000E-

030 +8.8000000E+002 / !TROE PARAMETERS

H2 / 3.000 / CO / 2.250 / CO2 / 3.000 / N2 / 1.500 / H2O / 9.000 /

CH3OCH3 / 5.000 / CH4 / 3.000 / C2H6 / 4.500 / !3RD BODY COLLIDER

EFFICIENCIES

!-----

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!-----

CH3OCH3+OH<=>CH3OCH2+H2O

+9.3500000E+005 +2.2900000E+000 -7.8070000E+002 !\AUTHOR: !\REF:S.L.

FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL

KINETICS, 32 (2000) 713-740. !\COMMENT:

CH3OCH3+H<=>CH3OCH2+H2

+7.7210000E+006 +2.0900000E+000 +3.3840000E+003 !\AUTHOR: !\REF:CURRAN,

FIT TO NIST DATABASE !\COMMENT: WARNING: WHAT IS SOURCE?

CH3OCH3+O<=>CH3OCH2+OH

+7.7500000E+008 +1.3600000E+000 +2.2500000E+003 !\AUTHOR: !\REF:CURRAN

08 NIST FIT !\COMMENT: WARNING: WHAT IS SOURCE OF NIST DA

CH3OCH3+HO2<=>CH3OCH2+H2O2

+3.1700000E-

003 +4.6400000E+000 +1.0556000E+004 !\AUTHOR: !\REF:J. MENDES, C.-W.

ZHOU, H.J. CURRAN, THE JOURNAL OF PHYSICAL CHEMISTRY A, 118 (2014) 1300-

1308. !\COMMENT:

CH3OCH3+CH3O2<=>CH3OCH2+CH3O2H +1.2680000E-003 +4.6400000E+000 +1.0556000E+004 !\AUTHOR: !\REF:J. MENDES, C.-W. ZHOU, H.J. CURRAN, THE JOURNAL OF PHYSICAL CHEMISTRY A, 118 (2014) 1300-1308. !\COMMENT:  
CH3OCH3+CH3<=>CH3OCH2+CH4 +7.0200000E+000 +3.7800000E+000 +9.6871000E+003 !\AUTHOR: !\REF:R.S. TRANTER, P.T. LYNCH, C.J. ANNESLEY, THE JOURNAL OF PHYSICAL CHEMISTRY A, 116 (2012) 7287-7292. !\COMMENT: (A-FACTOR - 3.0)  
CH3OCH3+O2<=>CH3OCH2+HO2 +4.1000000E+013 +0.0000000E+000 +4.4910000E+004 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH3+CH3O<=>CH3OCH2+CH3OH +6.0200000E+011 +0.0000000E+000 +4.0740000E+003 !\AUTHOR: !\REF:ESTIMATE, S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH3+CH3OCH2O2<=>CH3OCH2+CH3OCH2O2H +5.0000000E+012 +0.0000000E+000 +1.7690000E+004 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH3+O2CHO<=>CH3OCH2+HO2CHO +4.4250000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH3+OCHO<=>CH3OCH2+HOCHO +1.0000000E+013 +0.0000000E+000 +1.7690000E+004 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA  
!

---

CH3OCH2+CH3O<=>CH3OCH3+CH2O +2.4100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH2+CH2O<=>CH3OCH3+HCO +5.4900000E+003 +2.8000000E+000 +5.8620000E+003 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH2+CH3CHO<=>CH3OCH3+CH3CO +1.2600000E+012 +0.0000000E+000 +8.4990000E+003 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

CH3OCH2<=>CH3+CH2O +8.0300000E+012 +4.4028400E-001 +2.6490700E+004 !\AUTHOR: !\REF:BURKE, CNF 2014 !\COMMENT: KPS: RKM/ME @ CBS-QB3.  
PLOG / +1.0000000E-002  
+7.4940000E+023 -4.5152000E+000 +2.5236100E+004 /



PLOG / +1.0000000E-001  
+6.9210000E+028 -5.7271000E+000 +2.7494900E+004 /  
PLOG / +1.0000000E+000  
+4.2290000E+029 -5.6103000E+000 +2.8898300E+004 /  
PLOG / +1.0000000E+001  
+6.6080000E+027 -4.7073000E+000 +2.9735200E+004 /  
PLOG / +1.0000000E+002  
+2.6590000E+029 -4.9358000E+000 +3.1785500E+004 /  
!

---

!\REACTIONCLASS: \R\_O2\_PRODUCTS \A  
\N \EA  
!

---

---

CH3OCH2+O2<=>CH3OCH2O2

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
PLOG / +1.0000000E-003  
+1.1200000E+018 -3.3700000E+000 -4.2940000E+003 /  
PLOG / +1.0000000E-002  
+1.3300000E+021 -3.9500000E+000 -2.6150000E+003 /  
PLOG / +1.0000000E+000  
+1.1300000E+028 -5.2400000E+000 +4.0880000E+003 /  
PLOG / +2.0000000E+000  
+3.9100000E+027 -5.0000000E+000 +4.5120000E+003 /  
PLOG / +1.0000000E+001  
+2.7500000E+024 -3.8700000E+000 +4.2900000E+003 /  
PLOG / +2.0000000E+001  
+2.9700000E+022 -3.2300000E+000 +3.7810000E+003 /  
PLOG / +5.0000000E+001  
+5.1900000E+019 -2.3500000E+000 +2.9080000E+003 /  
PLOG / +1.0000000E+002  
+5.4300000E+017 -1.7300000E+000 +2.2100000E+003 /

CH3OCH2+O2<=>CH2OCH2O2H

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
PLOG / +1.0000000E-003  
+5.0800000E+020 -4.3900000E+000 +4.6900000E+002 /  
PLOG / +1.0000000E-002  
+5.4700000E+023 -4.9600000E+000 +2.1830000E+003 /  
PLOG / +1.0000000E+000  
+2.8100000E+028 -5.6300000E+000 +7.8480000E+003 /  
PLOG / +2.0000000E+000  
+5.1900000E+027 -5.3300000E+000 +8.1440000E+003 /  
PLOG / +1.0000000E+001  
+9.6700000E+024 -4.3600000E+000 +8.4170000E+003 /  
PLOG / +2.0000000E+001  
+4.0800000E+023 -3.9000000E+000 +8.4940000E+003 /  
PLOG / +5.0000000E+001  
+5.0800000E+021 -3.2800000E+000 +8.5850000E+003 /  
PLOG / +1.0000000E+002  
+1.6200000E+020 -2.8100000E+000 +8.6190000E+003 /

CH3OCH2+O2=>CH2O+CH2O+OH

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452

PLOG / +1.0000000E-003  
 +8.0100000E+021 -3.1800000E+000 +3.0670000E+003 /  
 PLOG / +1.0000000E-002  
 +1.7300000E+023 -3.5500000E+000 +4.0500000E+003 /  
 PLOG / +1.0000000E+000  
 +2.0400000E+031 -5.7600000E+000 +1.1594000E+004 /  
 PLOG / +2.0000000E+000  
 +5.9900000E+031 -5.8700000E+000 +1.2710000E+004 /  
 PLOG / +1.0000000E+001  
 +9.3900000E+030 -5.5900000E+000 +1.4517000E+004 /  
 PLOG / +2.0000000E+001  
 +1.0900000E+030 -5.3000000E+000 +1.5051000E+004 /  
 PLOG / +5.0000000E+001  
 +3.5800000E+028 -4.8800000E+000 +1.5664000E+004 /  
 PLOG / +1.0000000E+002  
 +2.4100000E+027 -4.5500000E+000 +1.6107000E+004 /  
 CH3OCH2O2<=>CH2OCH2O2H  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
 CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
 PLOG / +1.0000000E-003  
 +1.9400000E+029 -6.9900000E+000 +2.2446000E+004 /  
 PLOG / +1.0000000E-002  
 +4.0700000E+027 -6.1600000E+000 +2.1619000E+004 /  
 PLOG / +1.0000000E+000  
 +2.5200000E+025 -4.7600000E+000 +2.2691000E+004 /  
 PLOG / +2.0000000E+000  
 +5.9700000E+024 -4.4800000E+000 +2.2868000E+004 /  
 PLOG / +1.0000000E+001  
 +4.4400000E+021 -3.3800000E+000 +2.2386000E+004 /  
 PLOG / +2.0000000E+001  
 +4.5200000E+019 -2.7400000E+000 +2.1803000E+004 /  
 PLOG / +5.0000000E+001  
 +5.7200000E+016 -1.8200000E+000 +2.0829000E+004 /  
 PLOG / +1.0000000E+002  
 +3.7000000E+014 -1.1300000E+000 +2.0034000E+004 /  
 CH3OCH2O2=>CH2O+CH2O+OH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
 CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
 PLOG / +1.0000000E-003  
 +2.0600000E+036 -8.3200000E+000 +3.3415000E+004 /  
 PLOG / +1.0000000E-002  
 +2.0700000E+039 -8.8600000E+000 +3.5842000E+004 /  
 PLOG / +1.0000000E+000  
 +1.1200000E+040 -8.4200000E+000 +3.9835000E+004 /  
 PLOG / +2.0000000E+000  
 +9.7200000E+038 -8.0400000E+000 +3.9923000E+004 /  
 PLOG / +1.0000000E+001  
 +6.2800000E+035 -6.9700000E+000 +3.9900000E+004 /  
 PLOG / +2.0000000E+001  
 +1.6000000E+034 -6.4600000E+000 +3.9850000E+004 /  
 PLOG / +5.0000000E+001  
 +8.3200000E+031 -5.7500000E+000 +3.9719000E+004 /  
 PLOG / +1.0000000E+002  
 +1.2200000E+030 -5.2000000E+000 +3.9549000E+004 /  
 CH2OCH2O2H=>CH2O+CH2O+OH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,

CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
PLOG / +1.0000000E-003  
+1.6600000E+023 -4.5300000E+000 +2.2243000E+004 /  
PLOG / +1.0000000E-002  
+5.3000000E+025 -4.9300000E+000 +2.4158000E+004 /  
PLOG / +1.0000000E+000  
+7.8100000E+022 -3.5000000E+000 +2.3156000E+004 /  
PLOG / +2.0000000E+000  
+4.9800000E+022 -3.3500000E+000 +2.3062000E+004 /  
PLOG / +1.0000000E+001  
+8.4600000E+022 -3.2200000E+000 +2.3559000E+004 /  
PLOG / +2.0000000E+001  
+9.0900000E+022 -3.1400000E+000 +2.3899000E+004 /  
PLOG / +5.0000000E+001  
+4.5900000E+022 -2.9400000E+000 +2.4262000E+004 /  
PLOG / +1.0000000E+002  
+1.4000000E+022 -2.7200000E+000 +2.4407000E+004 /  
!

---

!\REACTIONCLASS: \QOOH\_O2 \A  
\N \EA  
!

---

---

CH2OCH2O2H+O2<=>O2CH2OCH2O2H  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
PLOG / +1.0000000E-003  
+9.4200000E+012 -1.6800000E+000 -4.9980000E+003 /  
PLOG / +1.0000000E-002  
+8.1600000E+016 -2.5000000E+000 -2.7530000E+003 /  
PLOG / +1.0000000E+000  
+1.0600000E+022 -3.3000000E+000 +3.3890000E+003 /  
PLOG / +2.0000000E+000  
+3.4800000E+020 -2.7900000E+000 +3.1310000E+003 /  
PLOG / +1.0000000E+001  
+2.8600000E+016 -1.4800000E+000 +1.8730000E+003 /  
PLOG / +2.0000000E+001  
+8.5500000E+014 -1.0100000E+000 +1.3120000E+003 /  
PLOG / +5.0000000E+001  
+2.6800000E+013 -5.4000000E-001 +7.2700000E+002 /  
PLOG / +1.0000000E+002  
+4.8700000E+012 -3.2000000E-001 +4.2800000E+002 /  
CH2OCH2O2H+O2<=>HO2CH2OCHO+OH  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
PLOG / +1.0000000E-003  
+5.9000000E+020 -2.8800000E+000 +3.2340000E+003 /  
PLOG / +1.0000000E-002  
+2.0600000E+023 -3.5900000E+000 +5.1160000E+003 /  
PLOG / +1.0000000E+000  
+4.4500000E+029 -5.2900000E+000 +1.2791000E+004 /  
PLOG / +2.0000000E+000  
+2.4400000E+028 -4.9200000E+000 +1.2891000E+004 /  
PLOG / +1.0000000E+001  
+9.4200000E+023 -3.6800000E+000 +1.2049000E+004 /

PLOG / +2.0000000E+001  
+1.0400000E+022 -3.1600000E+000 +1.1505000E+004 /  
PLOG / +5.0000000E+001  
+6.9500000E+019 -2.6000000E+000 +1.0861000E+004 /  
PLOG / +1.0000000E+002  
+3.9600000E+018 -2.3100000E+000 +1.0500000E+004 /  
O2CH2OCH2O2H<=>HO2CH2OCHO+OH  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: BURKE,  
CNF 2014 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY,  
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452  
PLOG / +1.0000000E-003  
+9.0500000E+023 -4.8800000E+000 +1.8805000E+004 /  
PLOG / +1.0000000E-002  
+6.8400000E+026 -5.3200000E+000 +2.2533000E+004 /  
PLOG / +1.0000000E+000  
+5.0700000E+016 -1.8100000E+000 +2.1175000E+004 /  
PLOG / +2.0000000E+000  
+2.6600000E+014 -1.1100000E+000 +2.0310000E+004 /  
PLOG / +1.0000000E+001  
+1.6900000E+010 +1.8000000E-001 +1.8604000E+004 /  
PLOG / +2.0000000E+001  
+1.1100000E+009 +5.4000000E-001 +1.8100000E+004 /  
PLOG / +5.0000000E+001  
+1.0700000E+008 +8.4000000E-001 +1.7661000E+004 /  
PLOG / +1.0000000E+002  
+3.8600000E+007 +9.8000000E-001 +1.7467000E+004 /  
!

---

!\REACTIONCLASS: \RO2\_RO2\_PRODUCTS \A  
\N \EA  
!

---

CH3OCH2O2+CH3OCH2O2=>O2+CH3OCH2O+CH3OCH2O  
+1.5470000E+023 -4.5000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: NIST  
FIT !\COMMENT: 3 PARAMETER, A-FACTOR/3

!\SUBSPECIES: \CH3OCH2O2H

---

CH3OCH2O2+CH2O<=>CH3OCH2O2H+HCO  
+1.0000000E+012 +0.0000000E+000 +1.1660000E+004 !\AUTHOR:  
!\REF: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
!\COMMENT: 1/ 2 CH3O2+CH2O<=>CH3O2H+HCO  
CH3OCH2O2+CH3CHO<=>CH3OCH2O2H+CH3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF: S.L.  
FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL  
KINETICS, 32 (2000) 713-740. !\COMMENT:  
CH3OCH2O+OH<=>CH3OCH2O2H  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: S.L.  
FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL  
KINETICS, 32 (2000) 713-740. !\COMMENT:

!\ENDSUBSPECIES: \CH3OCH2O2H

```

!=====
=====
!\SUBSPECIES: \HO2CH2OCHO
!=====
=====
!
-----
!\REACTIONCLASS: \KHP_UNIMOL \A
\N \EA
!
-----
HO2CH2OCHO<=>OCH2OCHO+OH
+5.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:K.A.
SAHETCHIAN, ET AL., SYMPOSIUM (INTERNATIONAL) ON COMBUSTION, 24 (1992)
637-643.
!=====
=====
!\ENDSUBSPECIES: \HO2CH2OCHO
!=====
=====
!=====
=====
!\SUBSPECIES: \OCH2OCHO
!=====
=====
CH2O+OCHO<=>OCH2OCHO
+1.2500000E+011 +0.0000000E+000 +1.1900000E+004 !\AUTHOR: !\REF:
ESTIMATE WKM RECOMMENDATION 8/ 9/ 2010 !\COMMENT: WARNING: WHAT IS SOURCE
OF RATE CONSTANT?
OCH2OCHO<=>HOCH2OCO
+1.0000000E+011 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:
ESTIMATE WKM RECOMMENDATION 8/ 9/ 2010 !\COMMENT: WARNING: WHAT IS SOURCE
OF RATE CONSTANT?
HOCH2OCO<=>CH2OH+CO2
+1.1170000E+017 -1.5260000E+000 +2.0771900E+004 !\AUTHOR: !\REF:REVERSE
RATE CONSTANT OF S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL
JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
HOCH2OCO<=>HOCH2O+CO
+2.9200000E+018 -1.9650000E+000 +1.9619000E+004 !\AUTHOR: !\REF:REVERSE
RATE CONSTANT OF S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL
JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
!=====
=====
!\ENDSUBSPECIES: \OCH2OCHO
!=====
=====
!=====
=====
!\SUBSPECIES: \CH3OCH2O
!=====
=====
CH3O+CH2O<=>CH3OCH2O
+1.0000000E+011 +0.0000000E+000 +7.9600000E+003 !\AUTHOR: !\REF:S.L.
FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL
KINETICS, 32 (2000) 713-740. !\COMMENT:
CH3OCH2O+O2<=>CH3OCHO+HO2 +4.3800000E-
019 +9.5000000E+000 -5.5010000E+003 !\AUTHOR: !\REF:WANTUCK, P.J. E AL.
J. PHYS. CHEM. 91, 4653 (1987) !\COMMENT: ANALOGY TO CH3O+O2<=>CH2O+HO2

```

CH3OCH2O<=>CH3OCHO+H  
+3.3000000E+013 +4.0000000E-003 +2.6136300E+004 !\AUTHOR: !\REF:HIPPLER  
ET AL. PCCP. 3: 3450--2458 (2001). !\COMMENT: ANALOGY TO CH3O  
DECOMPOSITION HPL. DECREASED BY A FACTOR OF 2

!=====  
=====

!\ENDSUBSPECIES: \CH3OCH2O

!=====  
=====

!-----  
-----

!\ENDSUBMECH: \CH3OCH3

!-----  
-----

!-----  
-----

!\SUBMECH: \CH3OCHO

!\MECHCOMMENTS:

!\MECHWARNINGS: KPS, 30/07/2015, ANALOGIES SEEM DATED. SHOULD BE UPDATED  
AT SOME STAGE

!-----  
-----

!-----  
-----

!\REACTIONCLASS: \UNIMOL

\A

\N \EA

!-----  
-----

CH3O+HCO<=>CH3OCHO

+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:FISHER,  
E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000. !\COMMENT: Ultan removed  
21/08/15

CH3O+HCO<=>CH3OH+CO

+9.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:Friedrichs, G.; Davidson, D. F.; Hanson, R. K. Int J. Chem. Kinet.  
2004, 36, 157. !\COMMENT: Ultan added 21/08/15

CH3+OCHO<=>CH3OCHO

+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?

CH2OCHO+H<=>CH3OCHO

+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:FISHER,  
E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000. !\COMMENT:

CH3OCO+H<=>CH3OCHO

+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:FISHER,  
E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000. !\COMMENT:

!-----  
-----

!\REACTIONCLASS: \RH\_R\_ABSTRACTION

\A

\N \EA

!-----  
-----

CH3OCHO+O2<=>CH3OCO+HO2

+1.0000000E+013 +0.0000000E+000 +4.9700000E+004 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: HOW WERE THESE ESTIMATED?

CH3OCHO+O2<=>CH2OCHO+HO2

+2.0500000E+013 +0.0000000E+000 +5.2000000E+004 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: HOW WERE THESE ESTIMATED?

$\text{CH}_3\text{OCHO} + \text{OH} \rightleftharpoons \text{CH}_3\text{OCO} + \text{H}_2\text{O}$   
 +1.5800000E+007 +1.8000000E+000 +9.3400000E+002 !\AUTHOR: !\REF:ANOLOGY  
 TO PROPANE !\COMMENT: WARNING: POOR ANALOGY?  
 $\text{CH}_3\text{OCHO} + \text{OH} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{H}_2\text{O}$   
 +5.2700000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:ANOLOGY  
 TO PROPANE !\COMMENT: WARNING: POOR ANALOGY?  
 $\text{CH}_3\text{OCHO} + \text{HO}_2 \rightleftharpoons \text{CH}_3\text{OCO} + \text{H}_2\text{O}_2$   
 +4.8200000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE TSANG '88 PRIMARY H !\COMMENT: WARNING: POOR ANALOGY?  
 $\text{CH}_3\text{OCHO} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{OCHO} + \text{H}_2\text{O}_2$   
 +2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE TSANG '88 PRIMARY H !\COMMENT: WARNING: POOR ANALOGY?  
 $\text{CH}_3\text{OCHO} + \text{O} \rightleftharpoons \text{CH}_3\text{OCO} + \text{OH}$   
 +2.7550000E+005 +2.4500000E+000 +2.8300000E+003 !\AUTHOR: !\REF:TSANG,  
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:  
 $\text{CH}_3\text{OCHO} + \text{O} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{OH}$   
 +9.8000000E+005 +2.4300000E+000 +4.7500000E+003 !\AUTHOR: !\REF: FIT TO  
 COHEN/ WESTBERG '86 !\COMMENT: WARNING: IS THIS A DIRECT EXPERIMENT OR  
 ANALOGY?  
 $\text{CH}_3\text{OCHO} + \text{H} \rightleftharpoons \text{CH}_3\text{OCO} + \text{H}_2$   
 +6.5000000E+005 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:TSANG,  
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:  
 $\text{CH}_3\text{OCHO} + \text{H} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{H}_2$   
 +6.6500000E+005 +2.5400000E+000 +6.7560000E+003 !\AUTHOR: !\REF:TSANG,  
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:  
 $\text{CH}_3\text{OCHO} + \text{CH}_3 \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_4$  +7.5500000E-  
 001 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.  
 CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:  
 $\text{CH}_3\text{OCHO} + \text{CH}_3 \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_4$  +4.5200000E-  
 001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.  
 CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:  
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_3\text{OH}$   
 +5.4800000E+011 +0.0000000E+000 +5.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT: WARNING: HOW WERE THESE ESTIMATED  
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_3\text{OH}$   
 +2.1700000E+011 +0.0000000E+000 +6.4580000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT: WARNING: HOW WERE THESE ESTIMATED  
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O}_2 \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_3\text{O}_2\text{H}$   
 +4.8200000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:ANOLOGY  
 WITH HO2 !\COMMENT: WARNING: IS ANALOGY DATED?  
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O}_2 \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_3\text{O}_2\text{H}$   
 +2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:ANOLOGY  
 WITH HO2 !\COMMENT: WARNING: IS ANALOGY DATED?  
 $\text{CH}_3\text{OCHO} + \text{HCO} \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_2\text{O}$   
 +5.4000000E+006 +1.9000000E+000 +1.7010000E+004 !\AUTHOR: !\REF:TSANG,  
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
 $\text{CH}_3\text{OCHO} + \text{HCO} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_2\text{O}$   
 +1.0250000E+005 +2.5000000E+000 +1.8430000E+004 !\AUTHOR: !\REF:TSANG,  
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:  
 !

---

!\REACTIONCLASS: \RADICAL \A  
 \N \EA  
 !

---

$\text{CH}_3\text{OCO} \rightleftharpoons \text{CH}_2\text{OCHO}$   
 +1.6290000E+012 -1.8000000E-001 +4.0670000E+004 !\AUTHOR: !\REF:  
 !\COMMENT:

```

CH3OCO<=>CH3+CO2
+8.6910000E+017 -1.8100000E+000 +1.3656700E+004   !\AUTHOR: !\REF:
!\COMMENT:
PLOG /                                     +5.0000000E-002
+9.7200000E+012 -1.3100000E+000 +9.4167000E+003 /
PLOG /                                     +1.0000000E+000
+1.2500000E+016 -1.8300000E+000 +1.1340800E+004 /
PLOG /                                     +1.0000000E+001
+1.0400000E+018 -2.1000000E+000 +1.2826900E+004 /
PLOG /                                     +1.0000000E+002
+8.6900000E+017 -1.8100000E+000 +1.3656700E+004 /
CH3OCO<=>CH3O+CO
+8.6910000E+017 -1.8100000E+000 +1.3656700E+004   !\AUTHOR: !\REF:
!\COMMENT:
PLOG /                                     +5.0000000E-002
+1.0300000E+003 +1.2900000E+000 +2.5401000E+004 /
PLOG /                                     +1.0000000E+000
+4.0900000E+005 +8.1000000E-001 +2.1969100E+004 /
PLOG /                                     +1.0000000E+001
+9.0200000E+014 -1.7200000E+000 +2.1767500E+004 /
PLOG /                                     +1.0000000E+002
+2.8250000E+022 -3.4400000E+000 +2.3592400E+004 /
CH2O+HCO<=>CH2OCHO
+1.5000000E+011 +0.0000000E+000 +1.1900000E+004   !\AUTHOR: !\REF:
!\COMMENT:
!-----
!\ENDSUBMECH: \CH3OCHO
!-----
!+++++
!+++++
!+++++
!\END_KINETICS_MODULE: \C2
!+++++
!+++++
!+++++
!\KINETICS_MODULE: \C3
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
!+++++
!+++++
!+++++
!-----
!\SUBMECH: \C3H8
!\MECHCOMMENTS: THE REACTION NC3H7O2+H2<=>NC3H7O2H+H AND RELATED
ABSTRACTIONS ARE ILL-DEFINED IN THE REVERSE DIRECTION. WE SHOULD HAVE A
RATE RULE FOR ABSTRACTION FROM KHPS DEFINED IN THE OPPOSITE DIRECTION.
!\MECHWARNINGS:
!-----
!-----
!

```



!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

C3H8 (+M) <=> CH3+C2H5 (+M)  
+1.2900000E+037 -5.8400000E+000 +9.7380000E+004 !\AUTHOR:  
!\REF:OEHSCHLAEGER ET AL., PROC COMB INST 30 (2005) 1119-1127 !\COMMENT:  
LOW /  
+5.6400000E+074 -1.5740000E+001 +9.8714000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +3.1000000E-001  
+5.0000000E+001 +3.0000000E+003 +9.0000000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / AR / 0.700 / CO / 1.500 / CO2 / 2.000 / CH4 /  
2.000 / C2H6 / 3.000 / HE / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
NC3H7+H<=>C3H8  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING  
IC3H7+H<=>C3H8  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

C3H8+IC3H7<=>NC3H7+C3H8  
+3.0000000E+010 +0.0000000E+000 +1.2900000E+004 !\AUTHOR: !\REF:FROM  
HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE  
PUBLISHED. !\COMMENT: WARNING  
C3H8+O2<=>IC3H7+HO2  
+2.0000000E+013 +0.0000000E+000 +4.9640000E+004 !\AUTHOR: !\REF:  
Ingham, T.; Walker, R.W.; Woolford, R.E., Symp. Int. Combust. Proc. 25, 767-  
774 (1994) !\COMMENT:  
C3H8+H<=>IC3H7+H2  
+1.3000000E+006 +2.4000000E+000 +4.4710000E+003 !\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  
+5.4900000E+005 +2.5000000E+000 +3.1400000E+003 !\AUTHOR: !\REF:Tsang,  
W. Chemical kinetic data base for combustion chemistry. Part 3. Propane  
J. Phys. Chem. Ref. Data 17, 887 (1988) !\COMMENT:  
C3H8+OH<=>IC3H7+H2O  
+4.6700000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:  
Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by  
OH. 3. Propane, J. Phys. Chem., 90, 1949-1954 !\COMMENT:  
C3H8+HO2<=>IC3H7+H2O2  
+6.3200000E+001 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
C3H8+CH3<=>IC3H7+CH4  
+6.4000000E+004 +2.1700000E+000 +7.5200000E+003 !\AUTHOR: !\REF:FIT TO  
NIST DATABASE !\COMMENT:  
C3H8+C2H3<=>IC3H7+C2H4  
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:FROM  
HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE  
PUBLISHED. !\COMMENT: WARNING  
C3H8+C2H5<=>IC3H7+C2H6  
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:FROM

HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE  
PUBLISHED. !\COMMENT: WARNING  
C3H8+C3H5-A<=>IC3H7+C3H6  
+7.9400000E+011 +0.0000000E+000 +1.6200000E+004 !\AUTHOR: !\REF:DAGAUT  
ET AL., CST 71, 111(1990) !\COMMENT:  
C3H8+CH3O<=>IC3H7+CH3OH  
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:DRYER  
ESTIMATE !\COMMENT:  
C3H8+CH3O2<=>IC3H7+CH3O2H  
+1.0190000E+001 +3.5800000E+000 +1.4810000E+004 !\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  
+1.0190000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT: SCALED AS PER CARSTENSEN ET AL  
C3H8+NC3H7O2<=>IC3H7+NC3H7O2H  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975  
!\COMMENT:  
C3H8+CH3CO3<=>IC3H7+CH3CO3H  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975  
!\COMMENT:  
C3H8+O2CHO<=>IC3H7+HO2CHO  
+1.4750000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C3H8+IC3H7O2<=>IC3H7+IC3H7O2H  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975  
!\COMMENT:  
C3H8+O2<=>NC3H7+HO2  
+6.0000000E+013 +0.0000000E+000 +5.2290000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH C4H10+O2<=>PC4H9+HO2 !\COMMENT:  
C3H8+H<=>NC3H7+H2  
+3.4900000E+005 +2.6900000E+000 +6.4500000E+003 !\AUTHOR: !\REF:Curran  
estimate, 15% lower than Tsang, W. Chemical kinetic data base for  
combustion chemistry. Part 3. Propane J. Phys. Chem.  
C3H8+O<=>NC3H7+OH  
+3.7100000E+006 +2.4000000E+000 +5.5050000E+003 !\AUTHOR: !\REF:Tsang,  
W. Chemical kinetic data base for combustion chemistry. Part 3. Propane  
J. Phys. Chem. Ref. Data 17, 887 (1988) !\COMMENT:  
C3H8+OH<=>NC3H7+H2O  
+1.0540000E+010 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:  
Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by  
OH. 3. Propane, J. Phys. Chem., 90, 1949-1954 !\COMMENT:  
C3H8+HO2<=>NC3H7+H2O2  
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
C3H8+CH3<=>NC3H7+CH4 +9.0400000E-  
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.  
CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
C3H8+C2H3<=>NC3H7+C2H4  
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:FROM  
HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE  
PUBLISHED. !\COMMENT: WARNING

C3H8+C2H5<=>NC3H7+C2H6  
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:FROM  
HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE  
PUBLISHED. !\COMMENT: WARNING  
C3H8+C3H5-A<=>NC3H7+C3H6  
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 !\AUTHOR: !\REF:DAGAUT  
ET AL., CST 71, 111(1990) !\COMMENT:  
C3H8+CH3O<=>NC3H7+CH3OH  
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:DRYER  
ESTIMATE !\COMMENT:  
C3H8+CH3O2<=>NC3H7+CH3O2H  
+1.3860000E+000 +3.9700000E+000 +1.8280000E+004 !\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<=>NC3H7+C2H5O2H  
+1.3860000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT: SCALED AS PER CARSTENSEN ET AL  
C3H8+NC3H7O2<=>NC3H7+NC3H7O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C3H8+IC3H7O2<=>NC3H7+IC3H7O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C3H8+CH3CO3<=>NC3H7+CH3CO3H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C3H8+O2CHO<=>NC3H7+HO2CHO  
+5.5200000E+004 +2.5500000E+000 +1.6480000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_RECOMBIN \A  
\N \EA  
!

---

IC3H7+H<=>C2H5+CH3  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:GLAUDE,P.A. ET AL,PROC. COMBUST. INST !\COMMENT:  
IC3H7+OH<=>C3H6+H2O  
+2.4100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG,  
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
IC3H7+O<=>CH3COCH3+H  
+4.8180000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG,  
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
IC3H7+O<=>CH3CHO+CH3  
+4.8180000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG,  
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
!

---

!\REACTIONCLASS: \R+RO2 \A  
\N \EA  
!

---

NC3H7+HO2<=>NC3H7O+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE

NC3H7+CH3O2<=>NC3H7O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE  
IC3H7+HO2<=>IC3H7O+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE  
IC3H7+CH3O2<=>IC3H7O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE

!=====  
=====

!\SUBSPECIES: \NC3H7O  
!=====  
=====

!  
\_\_\_\_\_

!\REACTIONCLASS: \R\_BETA\_SCISSION \A  
\N \EA  
!  
\_\_\_\_\_

C2H5+CH2O<=>NC3H7O  
+1.0000000E+011 +0.0000000E+000 +3.4960000E+003 !\AUTHOR: !\REF: H.J.  
Curran, International Journal of Chemical Kinetics (2006) 38: 250-275.  
!\COMMENT:

C2H5CHO+H<=>NC3H7O  
+4.0000000E+012 +0.0000000E+000 +6.2600000E+003 !\AUTHOR: !\REF: H.J.  
Curran, International Journal of Chemical Kinetics (2006) 38: 250-275.  
!\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \NC3H7O  
!=====  
=====

!  
\_\_\_\_\_

!\SUBSPECIES: \IC3H7O  
!=====  
=====

!  
\_\_\_\_\_

!\REACTIONCLASS: \R\_BETA\_SCISSION \A  
\N \EA  
!  
\_\_\_\_\_

CH3+CH3CHO<=>IC3H7O  
+1.0000000E+011 +0.0000000E+000 +9.2560000E+003 !\AUTHOR: !\REF: H.J.  
Curran, International Journal of Chemical Kinetics (2006) 38: 250-275.  
!\COMMENT:

CH3COCH3+H<=>IC3H7O  
+2.0000000E+012 +0.0000000E+000 +7.2700000E+003 !\AUTHOR: !\REF: H.J.  
Curran, International Journal of Chemical Kinetics (2006) 38: 250-275.  
!\COMMENT:

!  
\_\_\_\_\_

!\REACTIONCLASS: \R\_O2\_PRODUCTS \A  
\N \EA  
!  
\_\_\_\_\_

IC3H7O+O2<=>CH3COCH3+HO2  
+9.0900000E+009 +0.0000000E+000 +3.9000000E+002 !\AUTHOR: !\REF:BALLA  
ET AL., CHEM. PHYSICS, 99, 323 (1985) !\COMMENT: WARNING: INCREDIBLY OLD  
RATE CONSTANT.

!=====  
=====

!\ENDSUBSPECIES: \IC3H7O

!=====  
=====

!

---

!\REACTIONCLASS: \R+O2 \A

\N \EA

!

---

NC3H7+O2<=>C3H6+HO2 +3.0000000E-  
019 +0.0000000E+000 +3.0000000E+003 !\AUTHOR: !\REF:REF:CURRAN INC. INT  
J CHEM KINET 38: 250-275, 2006 !\COMMENT:

NC3H7+O2<=>NC3H7O2

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\COMMENT:

!0512 ADD KWZ

PLOG / +1.0000000E-002

+9.2000000E+008 +4.0500000E-001 -4.3986500E+003 /

PLOG / +1.0000000E-001

+1.4500000E+014 -9.8400000E-001 -1.7108000E+003 /

PLOG / +1.0000000E+000

+2.0900000E+013 -4.9900000E-001 -9.3842300E+002 /

PLOG / +1.0000000E+001

+1.1500000E+020 -2.4200000E+000 +2.4512600E+003 /

PLOG / +1.0000000E+002

+2.0700000E+016 -1.3000000E+000 +8.0341900E+002 /

IC3H7+O2<=>IC3H7O2

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\COMMENT:

!0512 ADD KWZ

PLOG / +1.0000000E-002

+7.3300000E+005 +1.3300000E+000 -6.3456400E+003 /

PLOG / +1.0000000E-001

+2.2400000E+011 -1.0500000E-001 -3.6978700E+003 /

PLOG / +1.0000000E+000

+1.5400000E+018 -2.0200000E+000 -4.9856700E+002 /

PLOG / +1.0000000E+001

+6.7400000E+027 -4.8500000E+000 +3.7798200E+003 /

PLOG / +1.0000000E+002

+1.6700000E+029 -5.1500000E+000 +5.0364500E+003 /

!

---

!\REACTIONCLASS: \RO2\_ALKENE\_HO2 \A

\N \EA

!

---

IC3H7O2<=>C3H6+HO2

+1.2240000E+009 +1.2800000E+000 +3.0000000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING: CANNOT TELL WHAT REFERENCE IS  
NC3H7O2<=>C3H6+HO2

+6.2400000E+008 +1.2500000E+000 +2.9600000E+004 !\AUTHOR: !\REF: \VLN  
2011 !\COMMENT: WARNING: CANNOT TELL WHAT REFERENCE IS

!

!\REACTIONCLASS: \RO2\_QOOH \A  
\N \EA  
!

---

NC3H7O2<=>C3H6OOH1-2  
+4.0900000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:Sharma  
!\COMMENT: WARNING: KPS-NO CLUE AS TO SOURCE  
NC3H7O2<=>C3H6OOH1-3  
+3.5660000E+006 +1.6000000E+000 +2.1000000E+004 !\AUTHOR: !\REF  
!\COMMENT: WARNING: KPS-NO CLUE AS TO SOURCE  
IC3H7O2<=>C3H6OOH2-1  
+2.9170000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF  
!\COMMENT: WARNING: KPS-NO CLUE AS TO SOURCE  
!

---

!\REACTIONCLASS: \QOOH\_PRODUCTS \A  
\N \EA  
!

---

C3H6OOH1-2<=>C3H6O1-2+OH  
+1.2100000E+009 +1.0500000E+000 +1.1300000E+004 !\AUTHOR: !\REF:HIGH  
PRESSURE RATE RULES FOR ALKYL+O2 REACTIONS 2 VLN2012 !\COMMENT:  
C3H6OOH1-3<=>C3H6O1-3+OH  
+2.6400000E+009 +7.1000000E-001 +1.8500000E+004 !\AUTHOR: !\REF:HIGH  
PRESSURE RATE RULES FOR ALKYL+O2 REACTIONS 2 VLN2012 !\COMMENT:  
C3H6OOH1-2<=>C3H6+HO2  
+2.3400000E+010 +7.7000000E-001 +1.5300000E+004 !\AUTHOR: !\REF:Villano  
!\COMMENT:  
C3H6OOH1-3=>OH+CH2O+C2H4  
+2.8900000E+009 +1.3000000E+000 +2.6700000E+004 !\AUTHOR: !\REF:Villano  
!\COMMENT:  
C3H6OOH2-1<=>C2H3OOH+CH3  
+8.5600000E+010 +8.5000000E-001 +3.0700000E+004 !\AUTHOR: !\REF:Villano  
!\COMMENT:  
C3H6OOH1-2=>C2H4+CH2O+OH  
+1.3100000E+033 -7.0100000E+000 +4.8120000E+004 !\AUTHOR: !\REF:Villano  
!\COMMENT:  
!

---

!\REACTIONCLASS: \QOOH\_O2\_O2QOOH \A  
\N \EA  
!

---

C3H6OOH1-2+O2<=>C3H6OOH1-2O2  
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 !\ 080415A !\COMMENT:  
C3H6OOH1-3+O2<=>C3H6OOH1-3O2  
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 !\ 080415A !\COMMENT:  
C3H6OOH2-1+O2<=>C3H6OOH2-1O2  
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 !\ 080415A !\COMMENT:  
!

---

!\REACTIONCLASS: \O2QOOH\_ISOMERISATION \A  
\N \EA  
!

---

C3H6OOH1-2O2<=>C3H51-2,3OOH  
+2.9170000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:  
!\Analogy to 1st isomerisations !\COMMENT:  
C3H6OOH1-3O2<=>C3H52-1,3OOH  
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:  
!\Analogy to 1st isomerisations !\COMMENT:  
C3H6OOH2-1O2<=>C3H51-2,3OOH  
+3.5660000E+006 +1.6000000E+000 +2.1000000E+004 !\AUTHOR: !\REF:  
!\Analogy to 1st isomerisations !\COMMENT:  
C3H51-2,3OOH<=>AC3H5OOH+HO2  
+2.5600000E+013 -4.9000000E-001 +1.7770000E+004 !\AUTHOR: !\REF:  
BOZZELLI AND PITZ, 1993. SINEAD, MOD 0509 KWZ !\COMMENT:  
C3H52-1,3OOH<=>AC3H5OOH+HO2  
+1.1500000E+014 -6.3000000E-001 +1.7250000E+004 !\AUTHOR: !\REF:  
BOZZELLI AND PITZ, 1993. SINEAD, MOD 0509 KWZ !\COMMENT:  
C3H51-2,3OOH<=>C3H5O1-2OOH-3+OH  
+4.4500000E+009 +8.6000000E-001 +1.0800000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C3H51-2,3OOH<=>C3H5O1-3OOH-2+OH  
+2.6400000E+009 +7.1000000E-001 +1.8500000E+004 !\AUTHOR:  
!\REF:!\Hydroperoxy cyclic ether formation !\COMMENT: WARNING: KPS-CANNOT  
TELL WHAT IS HAPPENING.  
C3H52-1,3OOH<=>C3H5O1-2OOH-3+OH  
+1.2100000E+009 +1.0500000E+000 +1.1300000E+004 !\AUTHOR:  
!\REF:!\Hydroperoxy cyclic ether formation !\COMMENT: WARNING: KPS-CANNOT  
TELL WHAT IS HAPPENING.  
C3H5O1-2OOH-3=>CH2CHO+CH2O+OH  
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR:  
!\REF:!\Hydroperoxy cyclic ether formation !\COMMENT: WARNING: KPS-CANNOT  
TELL WHAT IS HAPPENING.  
C3H5O1-3OOH-2=>CH2CHO+CH2O+OH  
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR:  
!\REF:!\Hydroperoxy cyclic ether formation !\COMMENT: WARNING: KPS-CANNOT  
TELL WHAT IS HAPPENING.  
!

---

!\REACTIONCLASS: \O2QOOH\_KHP \A  
\N \EA  
!

---

C3H6OOH1-2O2<=>C3KET12+OH  
+6.0000000E+011 +0.0000000E+000 +2.6400000E+004 !\AUTHOR: !\REF:Sharma  
080415A !\COMMENT:  
C3H6OOH1-3O2<=>C3KET13+OH  
+7.5000000E+010 +0.0000000E+000 +2.1400000E+004 !\AUTHOR: !\REF:Sharma  
080415A !\COMMENT:  
C3H6OOH2-1O2<=>C3KET21+OH  
+3.0000000E+011 +0.0000000E+000 +2.3850000E+004 !\AUTHOR: !\REF:Sharma  
080415A !\COMMENT:  
!

---

!\REACTIONCLASS: \KHP\_DECOMP \A  
\N \EA  
!

---

C3KET12=>CH3CHO+HCO+OH  
+9.5000000E+015 +0.0000000E+000 +4.2540000E+004 !\AUTHOR: !\ C ZHOU

!REF: ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:  
C3KET13=>CH2O+CH2CHO+OH  
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:  
WARNING !\COMMENT:  
C3KET21=>CH2O+CH3CO+OH  
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:  
WARNING !\COMMENT:  
C3KET21=>OH+CH2O+CO+CH3  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF:  
WARNING !\COMMENT:  
C2H3OOH<=>CH2CHO+OH  
+8.4000000E+014 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT: WARNING  
C2H3OOH=>CH2CO+H+OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\ C ZHOU  
!REF: ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION

!\COMMENT:  
!ANALOGY TO IC4H7OOH DECOMPOSITION  
C3KET21<=>CH3COCH2O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:  
PLOG / +1.0000000E-002  
+1.4900000E+058 -1.3900000E+001 +5.4266900E+004 /  
PLOG / +1.0000000E-001  
+1.8000000E+054 -1.2400000E+001 +5.4193800E+004 /  
PLOG / +1.0000000E+000  
+3.3600000E+046 -9.8100000E+000 +5.2468500E+004 /  
PLOG / +1.0000000E+001  
+2.3900000E+036 -6.5400000E+000 +4.9429000E+004 /  
PLOG / +1.0000000E+002  
+1.2800000E+027 -3.6100000E+000 +4.6333100E+004 /

!=====  
=====  
!\SUBSPECIES: \NC3H7O2H  
!=====  
=====

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

NC3H7O2H<=>NC3H7O+OH  
+1.5000000E+016 +0.0000000E+000 +4.2500000E+004 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

NC3H7O2+H2<=>NC3H7O2H+H  
+3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
NC3H7O2+HO2<=>NC3H7O2H+O2  
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:TSANG,  
JPC REF. DATA, 16:471 (1987) !\COMMENT:



$\text{NC3H7O2} + \text{CH2O} \rightleftharpoons \text{NC3H7O2H} + \text{HCO}$   
 +5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO  $\text{CH2O} + \text{HO2}$  !\COMMENT:  
 $\text{NC3H7O2} + \text{CH4} \rightleftharpoons \text{NC3H7O2H} + \text{CH3}$   
 +1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO  $\text{CH4} + \text{HO2}$  !\COMMENT:  
 $\text{NC3H7O2} + \text{CH3OH} \rightleftharpoons \text{NC3H7O2H} + \text{CH2OH}$   
 +6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO  $\text{CH3OH} + \text{HO2}$  !\COMMENT:  
 $\text{NC3H7O2} + \text{CH3CHO} \rightleftharpoons \text{NC3H7O2H} + \text{CH3CO}$   
 +2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
 $\text{CH2O} + \text{HO2}$  !\COMMENT:  
 $\text{NC3H7O2} + \text{C2H4} \rightleftharpoons \text{NC3H7O2H} + \text{C2H3}$   
 +1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO  $\text{C2H4} + \text{HO2}$  !\COMMENT:  
 $\text{NC3H7O2} + \text{C2H6} \rightleftharpoons \text{NC3H7O2H} + \text{C2H5}$   
 +1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{C2H3CHO} \rightleftharpoons \text{NC3H7O2H} + \text{C2H3CO}$   
 +2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
 $\text{CH2O} + \text{HO2}$  !\COMMENT:  
 $\text{NC3H7O2} + \text{C2H5CHO} \rightleftharpoons \text{NC3H7O2H} + \text{C2H5CO}$   
 +2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE !\COMMENT:

!=====

!\ENDSUBSPECIES: \NC3H7O2H

!=====

!

---

!\REACTIONCLASS: \RO2\_R\_PRODUCTS \A  
 \N \EA  
 !

---

$\text{NC3H7O2} + \text{NC3H7O2} \rightleftharpoons \text{NC3H7O} + \text{NC3H7O} + \text{O2}$   
 +1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{CH3CO3} \rightleftharpoons \text{NC3H7O} + \text{CH3CO2} + \text{O2}$   
 +1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{C2H5O2} \rightleftharpoons \text{NC3H7O} + \text{C2H5O} + \text{O2}$   
 +1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{CH3} \rightleftharpoons \text{NC3H7O} + \text{CH3O}$   
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{C2H5} \rightleftharpoons \text{NC3H7O} + \text{C2H5O}$   
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{IC3H7} \rightleftharpoons \text{NC3H7O} + \text{IC3H7O}$   
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 $\text{NC3H7O2} + \text{NC3H7} \rightleftharpoons \text{NC3H7O} + \text{NC3H7O}$   
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:

NC3H7O2+C3H5-A<=>NC3H7O+C3H5O  
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 NC3H7O2+CH3O2=>NC3H7O+CH3O+O2  
 +1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 !=====

---

!\SUBSPECIES: \IC3H7O2H  
 !=====

---

!\REACTIONCLASS: \UNIMOL \A  
 \N \EA  
 !

---

IC3H7O+OH<=>IC3H7O2H  
 +1.0000000E+015 -8.0000000E-001 +0.0000000E+000 !\AUTHOR: !\REF:PITZ  
 ESTIMATE !\COMMENT: WARNING: HOW DOES REVERSE DECOMPOSITION RATE CONSTANT  
 COMPARE WITH CH3O+OH? ARE THERMODYNAMICS SENSIBLE?  
 !

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
 \N \EA  
 !

---

IC3H7O2+H2<=>IC3H7O2H+H  
 +3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG  
 AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:  
 IC3H7O2+HO2<=>IC3H7O2H+O2  
 +1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:TSANG,  
 JPC REF. DATA, 16:471 (1987) !\COMMENT:  
 IC3H7O2+CH2O<=>IC3H7O2H+HCO  
 +5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO CH2O+HO2 !\COMMENT:  
 IC3H7O2+CH4<=>IC3H7O2H+CH3  
 +1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO CH4+HO2 !\COMMENT:  
 IC3H7O2+CH3CHO<=>IC3H7O2H+CH3CO  
 +2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
 CH2O+HO2 !\COMMENT:  
 IC3H7O2+C2H4<=>IC3H7O2H+C2H3  
 +1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO C2H4+HO2 !\COMMENT:  
 IC3H7O2+CH3OH<=>IC3H7O2H+CH2OH  
 +6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:ANALOGY  
 TO CH3OH+HO2 !\COMMENT:  
 IC3H7O2+C2H6<=>IC3H7O2H+C2H5  
 +1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE !\COMMENT:  
 IC3H7O2+C2H3CHO<=>IC3H7O2H+C2H3CO  
 +2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
 CH2O+HO2 !\COMMENT:  
 IC3H7O2+C2H5CHO<=>IC3H7O2H+C2H5CO  
 +2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE !\COMMENT:

!  
-----  
!\REACTIONCLASS: \RO2\_R\_PRODUCTS \A  
\N \EA  
!

-----  
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+IC3H7O2=>O2+IC3H7O+IC3H7O  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+NC3H7O2=>IC3H7O+NC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+CH3<=>IC3H7O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+C2H5<=>IC3H7O+C2H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+IC3H7<=>IC3H7O+IC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+NC3H7<=>IC3H7O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+C3H5-A<=>IC3H7O+C3H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:

!=====

!\ENDSUBSPECIES: \IC3H7O2H

!=====

!=====

!\SUBSPECIES: C3H6O1-2/C3H6O1-3

!=====

!=====

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

-----  
C3H6O1-2<=>C2H4+CH2O  
+6.0000000E+014 +0.0000000E+000 +6.0000000E+004 !\AUTHOR:  
!\REF:!\FLOWERS, M. C., J. CHEM. SOC. FAR. TRANS. I 73, 1927 (1977)  
!\COMMENT: WARNING: REACTION IN WRONG CLASS  
C3H6O1-2+OH=>CH2O+C2H3+H2O  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT: WARNING: WHAT ARE SOURCES OF RATE  
CONSTANTS?

C3H6O1-2+H=>CH2O+C2H3+H2  
+2.6300000E+007 +2.0000000E+000 +5.0000000E+003 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT:

C3H6O1-2+O=>CH2O+C2H3+OH  
+8.4300000E+013 +0.0000000E+000 +5.2000000E+003 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT:

C3H6O1-2+HO2=>CH2O+C2H3+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT:

C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H  
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT:

C3H6O1-2+CH3=>CH2O+C2H3+CH4  
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT:

!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!

---

C3H6O1-3<=>C2H4+CH2O

+6.0000000E+014 +0.0000000E+000 +6.0000000E+004 !\AUTHOR:

!\REF:WESTBROOK AND PITZ ESTIMATE (1983) !\COMMENT: WARNING: REACTION IN  
WRONG CLASS

C3H6O1-3+OH=>CH2O+C2H3+H2O

+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT: WARNING: WHAT ARE SOURCES OF RATE CONSTANTS?

C3H6O1-3+O=>CH2O+C2H3+OH

+8.4300000E+013 +0.0000000E+000 +5.2000000E+003 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:

C3H6O1-3+H=>CH2O+C2H3+H2

+2.6300000E+007 +2.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:

C3H6O1-3+CH3O2=>CH2O+C2H3+CH3O2H

+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:

C3H6O1-3+HO2=>CH2O+C2H3+H2O2

+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:

C3H6O1-3+CH3=>CH2O+C2H3+CH4

+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:

!=====

=====

!\ENDSUBSPECIES: C3H6O1-2/C3H6O1-3

!=====

=====

!-----

-----

!\ENDSUBMECH: C3H8

!-----

-----

!-----

-----

!\SUBMECH: \C3H6

!\MECHCOMMENTS:

!\MECHWARNINGS:

!

---

!\REACTIONCLASS: \UNIMOL

\A

\N \EA

!

---

C2H3+CH3(+M)<=>C3H6(+M)

+2.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN

ET AL. IJCK 32 589-614 2000 !\COMMENT: WARNING

LOW /

+4.2700000E+058 -1.1940000E+001 +9.7698000E+003 / !LOW-PRESSURE-LIMIT

TROE / +1.7500000E-001

+1.3410000E+003 +6.0000000E+004 +1.0140000E+004 / !TROE PARAMETERS

CH2(S)+C2H4<=>CC3H6

+1.4400000E+051 -1.3100000E+001 +1.4200000E+004 !\AUTHOR: !\REF:

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002

+1.4400000E+051 -1.3100000E+001 +1.4200000E+004 /

PLOG / +1.0000000E-001

+3.3800000E+054 -1.3600000E+001 +1.6500000E+004 /

PLOG / +1.0000000E+000

+1.3500000E+054 -1.3000000E+001 +1.8900000E+004 /

PLOG / +1.0000000E+001

+2.7300000E+047 -1.0800000E+001 +1.4200000E+004 /

PLOG / +1.0000000E+002

+2.7100000E+050 -1.1200000E+001 +1.6700000E+004 /

DUP

CH2(S)+C2H4<=>CC3H6

+6.1600000E+040 -1.0500000E+001 +5.4281000E+003 !\AUTHOR: !\REF:

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002

+6.1600000E+040 -1.0500000E+001 +5.4281000E+003 /

PLOG / +1.0000000E-001

+6.9300000E+041 -1.0300000E+001 +6.1889000E+003 /

PLOG / +1.0000000E+000

+1.8100000E+037 -8.5500000E+000 +5.5210000E+003 /

PLOG / +1.0000000E+001

+4.2600000E+037 -8.3200000E+000 +4.7702000E+003 /

PLOG / +1.0000000E+002

+4.6800000E+035 -7.3700000E+000 +4.6891000E+003 /

DUP

CH2(S)+C2H4<=>C3H6

+4.8200000E+057 -1.4300000E+001 +1.7100000E+004 !\AUTHOR: !\REF:

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002

+4.8200000E+057 -1.4300000E+001 +1.7100000E+004 /

PLOG / +1.0000000E-001

+3.8400000E+059 -1.4400000E+001 +1.8400000E+004 /

PLOG / +1.0000000E+000

+2.1300000E+058 -1.3500000E+001 +2.0400000E+004 /

```

PLOG / +1.0000000E+001
+8.4800000E+052 -1.1600000E+001 +2.0700000E+004 /
PLOG / +1.0000000E+002
+6.0700000E+047 -9.8500000E+000 +2.2100000E+004 /
DUP
CH2(S)+C2H4<=>C3H6
+1.1500000E+045 -1.1100000E+001 +6.1452000E+003 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+1.1500000E+045 -1.1100000E+001 +6.1452000E+003 /
PLOG / +1.0000000E-001
+1.8300000E+045 -1.0700000E+001 +6.6385000E+003 /
PLOG / +1.0000000E+000
+1.3000000E+040 -8.7700000E+000 +5.8638000E+003 /
PLOG / +1.0000000E+001
+2.2700000E+032 -6.1400000E+000 +4.3179000E+003 /
PLOG / +1.0000000E+002
+1.2800000E+024 -3.4900000E+000 +2.5299000E+003 /
DUP
CH2(S)+C2H4<=>C3H5-A+H
+8.2000000E+019 -2.0600000E+000 +1.1500000E+003 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+8.2000000E+019 -2.0600000E+000 +1.1500000E+003 /
PLOG / +1.0000000E-001
+2.2700000E+021 -2.4400000E+000 +2.6500000E+003 /
PLOG / +1.0000000E+000
+4.4400000E+035 -6.5500000E+000 +1.3900000E+004 /
PLOG / +1.0000000E+001
+1.1800000E+028 -4.0900000E+000 +1.4000000E+004 /
PLOG / +1.0000000E+002
+6.5100000E+026 -3.5800000E+000 +1.8900000E+004 /
DUP
CH2(S)+C2H4<=>C3H5-A+H
+1.0800000E+007 +1.6200000E+000 -3.1746000E+003 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+1.0800000E+007 +1.6200000E+000 -3.1746000E+003 /
PLOG / +1.0000000E-001
+1.3700000E+005 +2.1500000E+000 -3.7992000E+003 /
PLOG / +1.0000000E+000
+3.8900000E+014 -4.2000000E-001 +1.2376000E+003 /
PLOG / +1.0000000E+001
+2.4500000E+010 +6.7000000E-001 +7.5093000E+002 /
PLOG / +1.0000000E+002
+1.8100000E+002 +2.9700000E+000 -7.4603000E+002 /
DUP
CH2(S)+C2H4<=>C2H3+CH3
+1.7700000E+019 -1.9400000E+000 +6.7900000E+003 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+1.7700000E+019 -1.9400000E+000 +6.7900000E+003 /
PLOG / +1.0000000E-001
+1.6800000E+019 -1.8000000E+000 +4.3100000E+003 /

```

PLOG / +1.0000000E+000  
+4.1600000E+024 -3.1900000E+000 +9.7600000E+003 /  
PLOG / +1.0000000E+001  
+7.8900000E+024 -3.0700000E+000 +1.3900000E+004 /  
PLOG / +1.0000000E+002  
+7.3600000E+029 -4.2800000E+000 +2.3800000E+004 /  
DUP  
CH2(S)+C2H4<=>C2H3+CH3  
+4.3000000E+012 +1.9000000E-001 -1.1041000E+002 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?  
PLOG / +1.0000000E-002  
+4.3000000E+012 +1.9000000E-001 -1.1041000E+002 /  
PLOG / +1.0000000E-001  
+2.2600000E+011 +5.4000000E-001 +4.7810000E+001 /  
PLOG / +1.0000000E+000  
+4.9200000E+009 +1.0200000E+000 +5.9977000E+002 /  
PLOG / +1.0000000E+001  
+1.4700000E+008 +1.3300000E+000 +1.2284000E+003 /  
PLOG / +1.0000000E+002  
+8.1100000E+010 +5.5000000E-001 +5.5065000E+003 /  
DUP  
C2H3+CH3<=>C3H5-A+H  
+4.1200000E+029 -4.9500000E+000 +8.0000000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?  
PLOG / +1.0000000E-002  
+4.1200000E+029 -4.9500000E+000 +8.0000000E+003 /  
PLOG / +1.0000000E-001  
+4.8600000E+030 -5.0300000E+000 +1.1300000E+004 /  
PLOG / +1.0000000E+000  
+5.3000000E+029 -4.5700000E+000 +1.4400000E+004 /  
PLOG / +1.0000000E+001  
+1.3200000E+030 -4.5400000E+000 +1.9300000E+004 /  
PLOG / +1.0000000E+002  
+5.1600000E+028 -4.0300000E+000 +2.3800000E+004 /  
DUP  
C2H3+CH3<=>C3H5-A+H  
+5.7300000E+015 -7.7000000E-001 +1.1959000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?  
PLOG / +1.0000000E-002  
+5.7300000E+015 -7.7000000E-001 +1.1959000E+003 /  
PLOG / +1.0000000E-001  
+2.0600000E+013 -7.4000000E-002 +1.4287000E+003 /  
PLOG / +1.0000000E+000  
+4.4800000E+010 +6.0000000E-001 +1.4216000E+003 /  
PLOG / +1.0000000E+001  
+4.1000000E+006 +1.7100000E+000 +1.0569000E+003 /  
PLOG / +1.0000000E+002 +1.3700000E-  
001 +3.9100000E+000 -3.5355000E+002 /  
DUP  
C3H6<=>C2H3+CH3  
+1.8800000E+078 -1.8700000E+001 +1.3000000E+005 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?  
PLOG / +1.0000000E-002  
+1.8800000E+078 -1.8700000E+001 +1.3000000E+005 /

```

PLOG / +1.0000000E-001
+8.7300000E+076 -1.7900000E+001 +1.3200000E+005 /
PLOG / +1.0000000E+000
+5.8000000E+075 -1.7200000E+001 +1.3400000E+005 /
PLOG / +1.0000000E+001
+8.1200000E+071 -1.5800000E+001 +1.3600000E+005 /
PLOG / +1.0000000E+002
+2.1500000E+064 -1.3400000E+001 +1.3500000E+005 /
DUP
C3H6<=>C2H3+CH3
+1.6900000E+059 -1.3600000E+001 +1.1329000E+005 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+1.6900000E+059 -1.3600000E+001 +1.1329000E+005 /
PLOG / +1.0000000E-001
+2.0000000E+060 -1.3700000E+001 +1.1489000E+005 /
PLOG / +1.0000000E+000
+6.7000000E+054 -1.1800000E+001 +1.1384000E+005 /
PLOG / +1.0000000E+001
+1.0600000E+047 -9.2700000E+000 +1.1151000E+005 /
PLOG / +1.0000000E+002
+7.2900000E+038 -6.7000000E+000 +1.0874000E+005 /
DUP
C3H6<=>C3H5-A+H
+9.1600000E+074 -1.7600000E+001 +1.2000000E+005 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+9.1600000E+074 -1.7600000E+001 +1.2000000E+005 /
PLOG / +1.0000000E-001
+1.7300000E+070 -1.6000000E+001 +1.2000000E+005 /
PLOG / +1.0000000E+000
+1.0800000E+071 -1.5900000E+001 +1.2486000E+005 /
PLOG / +1.0000000E+001
+6.4000000E+065 -1.4200000E+001 +1.2500000E+005 /
PLOG / +1.0000000E+002
+8.0500000E+056 -1.1500000E+001 +1.2200000E+005 /
DUP
C3H6<=>C3H5-A+H
+2.9800000E+054 -1.2300000E+001 +1.0120000E+005 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+2.9800000E+054 -1.2300000E+001 +1.0120000E+005 /
PLOG / +1.0000000E-001
+1.3700000E+043 -8.8700000E+000 +9.6365000E+004 /
PLOG / +1.0000000E+000
+6.2800000E+042 -8.5100000E+000 +9.8004000E+004 /
PLOG / +1.0000000E+001
+4.7300000E+035 -6.2600000E+000 +9.5644000E+004 /
PLOG / +1.0000000E+002
+4.3400000E+028 -4.0600000E+000 +9.3114000E+004 /
DUP
C3H6<=>CC3H6
+1.2600000E+064 -1.5600000E+001 +9.5000000E+004 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?

```



```

PLOG / +1.0000000E-002
+1.2600000E+064 -1.5600000E+001 +9.5000000E+004 /
PLOG / +1.0000000E-001
+3.9400000E+067 -1.6200000E+001 +1.0100000E+005 /
PLOG / +1.0000000E+000
+6.1400000E+068 -1.6200000E+001 +1.0600000E+005 /
PLOG / +1.0000000E+001
+9.7000000E+066 -1.5300000E+001 +1.0900000E+005 /
PLOG / +1.0000000E+002
+1.4500000E+062 -1.3600000E+001 +1.1000000E+005 /
DUP
C3H6<=>CC3H6
+4.8400000E+041 -9.6200000E+000 +7.9528000E+004 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+4.8400000E+041 -9.6200000E+000 +7.9528000E+004 /
PLOG / +1.0000000E-001
+8.0700000E+044 -1.0200000E+001 +8.2671000E+004 /
PLOG / +1.0000000E+000
+1.1500000E+047 -1.0600000E+001 +8.5502000E+004 /
PLOG / +1.0000000E+001
+1.3300000E+039 -7.9800000E+000 +8.3303000E+004 /
PLOG / +1.0000000E+002
+4.9700000E+031 -5.6000000E+000 +8.0987000E+004 /
DUP
CC3H6<=>C3H5-A+H
+2.3300000E+063 -1.4600000E+001 +1.0300000E+005 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+2.3300000E+063 -1.4600000E+001 +1.0300000E+005 /
PLOG / +1.0000000E-001
+7.0300000E+063 -1.4400000E+001 +1.0700000E+005 /
PLOG / +1.0000000E+000
+5.0700000E+064 -1.4300000E+001 +1.1200000E+005 /
PLOG / +1.0000000E+001
+4.9200000E+061 -1.3200000E+001 +1.1500000E+005 /
PLOG / +1.0000000E+002
+4.8200000E+057 -1.1700000E+001 +1.1800000E+005 /
DUP
CC3H6<=>C3H5-A+H
+1.1200000E+040 -8.3700000E+000 +8.5836000E+004 !\AUTHOR: !\REF:
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE
MECHANISM?
PLOG / +1.0000000E-002
+1.1200000E+040 -8.3700000E+000 +8.5836000E+004 /
PLOG / +1.0000000E-001
+1.0600000E+041 -8.3300000E+000 +8.8499000E+004 /
PLOG / +1.0000000E+000
+8.2300000E+043 -8.8800000E+000 +9.2907000E+004 /
PLOG / +1.0000000E+001
+1.2700000E+039 -7.3300000E+000 +9.3401000E+004 /
PLOG / +1.0000000E+002
+1.4500000E+028 -4.0200000E+000 +9.0995000E+004 /
DUP
CC3H6<=>C2H3+CH3
+8.3100000E+064 -1.5100000E+001 +1.1100000E+005 !\AUTHOR: !\REF:

```

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002  
+8.3100000E+064 -1.5100000E+001 +1.1100000E+005 /  
PLOG / +1.0000000E-001  
+8.2900000E+064 -1.4700000E+001 +1.1400000E+005 /  
PLOG / +1.0000000E+000  
+1.0000000E+070 -1.5700000E+001 +1.2200000E+005 /  
PLOG / +1.0000000E+001  
+1.6600000E+067 -1.4600000E+001 +1.2400000E+005 /  
PLOG / +1.0000000E+002  
+7.8700000E+062 -1.3100000E+001 +1.2700000E+005 /

DUP

CC3H6<=>C2H3+CH3

+1.5100000E+049 -1.1000000E+001 +9.9748000E+004 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002  
+1.5100000E+049 -1.1000000E+001 +9.9748000E+004 /  
PLOG / +1.0000000E-001  
+1.0500000E+045 -9.4600000E+000 +9.9275000E+004 /  
PLOG / +1.0000000E+000  
+3.3900000E+050 -1.0600000E+001 +1.0422000E+005 /  
PLOG / +1.0000000E+001  
+1.7600000E+047 -9.4300000E+000 +1.0493000E+005 /  
PLOG / +1.0000000E+002  
+1.8800000E+039 -6.9300000E+000 +1.0398000E+005 /

DUP

C3H5-T+H<=>C3H6

+4.9600000E+060 -1.5200000E+001 +1.8000000E+004 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002  
+4.9600000E+060 -1.5200000E+001 +1.8000000E+004 /  
PLOG / +1.0000000E-001  
+3.2000000E+062 -1.5100000E+001 +2.0100000E+004 /  
PLOG / +1.0000000E+000  
+2.3100000E+060 -1.4000000E+001 +2.1900000E+004 /  
PLOG / +1.0000000E+001  
+3.6900000E+054 -1.2000000E+001 +2.2100000E+004 /  
PLOG / +1.0000000E+002  
+1.1500000E+050 -1.0400000E+001 +2.3300000E+004 /

DUP

C3H5-T+H<=>C3H6

+1.4900000E+048 -1.2000000E+001 +7.2033000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

PLOG / +1.0000000E-002  
+1.4900000E+048 -1.2000000E+001 +7.2033000E+003 /  
PLOG / +1.0000000E-001  
+6.7600000E+046 -1.1100000E+001 +7.6299000E+003 /  
PLOG / +1.0000000E+000  
+1.0900000E+040 -8.6600000E+000 +6.4478000E+003 /  
PLOG / +1.0000000E+001  
+2.3800000E+031 -5.7300000E+000 +4.5060000E+003 /  
PLOG / +1.0000000E+002  
+5.6900000E+025 -3.8300000E+000 +3.2504000E+003 /

DUP

C3H5-T+H<=>C3H5-A+H

+2.1100000E+017 -1.0800000E+000 +1.2900000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?

PLOG / +1.0000000E-002  
+2.1100000E+017 -1.0800000E+000 +1.2900000E+003 /  
PLOG / +1.0000000E-001  
+9.0500000E+029 -4.9100000E+000 +8.5400000E+003 /  
PLOG / +1.0000000E+000  
+2.9800000E+030 -4.7900000E+000 +1.2000000E+004 /  
PLOG / +1.0000000E+001  
+8.2200000E+028 -4.1400000E+000 +1.5400000E+004 /  
PLOG / +1.0000000E+002  
+2.2800000E+029 -4.1200000E+000 +2.0900000E+004 /

DUP

C3H5-T+H<=>C3H5-A+H

+6.4100000E+003 +2.6100000E+000 -3.7784000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?

PLOG / +1.0000000E-002  
+6.4100000E+003 +2.6100000E+000 -3.7784000E+003 /  
PLOG / +1.0000000E-001  
+5.1900000E+014 -3.0000000E-001 +1.0904000E+003 /  
PLOG / +1.0000000E+000  
+8.1700000E+011 +4.9000000E-001 +1.1846000E+003 /  
PLOG / +1.0000000E+001  
+2.7900000E+009 +1.0900000E+000 +1.1875000E+003 /  
PLOG / +1.0000000E+002  
+6.7500000E+003 +2.7000000E+000 +3.7380000E+002 /

DUP

C3H5-T+H<=>C2H3+CH3

+3.3100000E+016 -6.9000000E-001 +5.2000000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?

PLOG / +1.0000000E-002  
+3.3100000E+016 -6.9000000E-001 +5.2000000E+003 /  
PLOG / +1.0000000E-001  
+9.0400000E+016 -8.1000000E-001 +4.8000000E+003 /  
PLOG / +1.0000000E+000  
+2.0100000E+024 -2.8600000E+000 +1.0900000E+004 /  
PLOG / +1.0000000E+001  
+2.7500000E+026 -3.3100000E+000 +1.5800000E+004 /  
PLOG / +1.0000000E+002  
+3.1500000E+032 -4.8300000E+000 +2.6000000E+004 /

DUP

C3H5-T+H<=>C2H3+CH3

+8.0400000E+013 -1.4000000E-001 +1.1500000E+003 !\AUTHOR: !\REF:  
WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
MECHANISM?

PLOG / +1.0000000E-002  
+8.0400000E+013 -1.4000000E-001 +1.1500000E+003 /  
PLOG / +1.0000000E-001  
+7.1700000E+010 +6.7000000E-001 +6.7380000E+002 /  
PLOG / +1.0000000E+000  
+9.9700000E+008 +1.3600000E+000 +1.5964000E+003 /  
PLOG / +1.0000000E+001  
+7.4100000E+007 +1.5700000E+000 +2.1088000E+003 /

PLOG / +1.0000000E+002  
 +2.7000000E+012 +3.2000000E-001 +6.7918000E+003 /  
 DUP  
 C3H6<=>C3H5-S+H  
 +7.7100000E+069 -1.6090000E+001 +1.4000000E+005 !\AUTHOR: !\REF:  
 !\COMMENT:  
 !  


---

 !\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
 \N \EA  
 !  


---

 C3H6+H<=>C3H5-A+H2  
 +3.6440000E+005 +2.4550000E+000 +4.3612000E+003 !\AUTHOR: !\REF:  
 WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE  
 MECHANISM?  
 C3H6+O2<=>C3H5-A+HO2  
 +5.9600000E+019 -1.6700000E+000 +4.6192100E+004 !\AUTHOR: !\REF:  
 ESTIMATE C3 NUIG S. M. BURKE !\COMMENT:  
 C3H6+O<=>C3H5-A+OH  
 +5.2400000E+011 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:  
 ANALOGY WITH C2H4 !\COMMENT: WARNING: HAS CAVALOTTI RELEASED UPDATED RATE  
 CONSTANTS FOR THIS?  
 C3H6+OH<=>C3H5-A+H2O  
 +4.4600000E+006 +2.0720000E+000 +1.0508000E+003 !\AUTHOR: !\REF:  
 WARNING: NO REFERENCE !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS  
 REACTION?  
 C3H6+HO2<=>C3H5-A+H2O2 +3.0700000E-  
 002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: WARNING: WHAT IS  
 REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?  
 C3H6+CH3<=>C3H5-A+CH4  
 +2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF: TSANG,  
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
 C3H6+CH3O<=>C3H5-A+CH3OH  
 +8.4000000E+010 +0.0000000E+000 +2.6000000E+003 !\AUTHOR: !\REF: BILL  
 !\COMMENT: !\REF: REDUCED EA BY DIFFERENCE BETWEEN BD FOR SECONDARY ALKYL  
 AND PRIMARY ALL  
 C3H6+CH3O2<=>C3H5-A+CH3O2H +7.6800000E-  
 002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: ANALOGY TO  
 C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM  
 C3H6+C2H5<=>C3H5-A+C2H6  
 +1.0000000E+011 +0.0000000E+000 +9.8000000E+003 !\AUTHOR: !\REF:  
 ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)  
 !\COMMENT:  
 C3H6+C2H5O2<=>C3H5-A+C2H5O2H +7.6800000E-  
 002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: ANALOGY TO  
 C3H6+HO2 !\COMMENT:  
 C3H6+CH3CO3<=>C3H5-A+CH3CO3H +7.6800000E-  
 002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: ANALOGY TO  
 C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM  
 C3H6+NC3H7O2<=>C3H5-A+NC3H7O2H +7.6800000E-  
 002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: ANALOGY TO  
 C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM  
 C3H6+IC3H7O2<=>C3H5-A+IC3H7O2H +7.6800000E-  
 002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: ANALOGY TO  
 C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM  
 C3H6+H<=>C3H5-T+H2  
 +1.4980000E+002 +3.3810000E+000 +8.9095000E+003 !\AUTHOR: !\REF:

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

C3H6+O<=>C3H5-T+OH

+6.0300000E+010 +7.0000000E-001 +7.6320000E+003 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT:

C3H6+OH<=>C3H5-T+H2O

+1.8000000E+006 +1.9790000E+000 +2.2352000E+003 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?

C3H6+HO2<=>C3H5-T+H2O2

+1.5600000E+004 +2.8200000E+000 +2.4427900E+004 !\AUTHOR: !\REF: C3

NUIG CALCULATION J.M !\COMMENT: WARNING: RESULTS ARE NOW PUBLISHED, UPDATED REFERENCE

C3H6+O2<=>C3H5-T+HO2

+1.0000000E+013 +0.0000000E+000 +5.8770000E+004 !\AUTHOR: !\REF:

ESTIMATE C3 NUIG S. M. BURKE !\COMMENT: WARNING: HOW WAS THIS ESTIMATED?

C3H6+CH3<=>C3H5-T+CH4 +8.4000000E-

001 +3.5000000E+000 +1.1660000E+004 !\AUTHOR: !\REF: TSANG, W. J. PHYS.

CHEM. REF. DATA 17, 887 (1988) !\COMMENT:

C3H6+H<=>C3H5-S+H2

+5.1010000E+002 +3.2340000E+000 +1.2357000E+004 !\AUTHOR: !\REF:

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

DUP

C3H6+H<=>C3H5-S+H2

+3.9690000E+002 +3.2520000E+000 +1.2007000E+004 !\AUTHOR: !\REF:

WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

DUP

C3H6+O2<=>C3H5-S+HO2

+2.0000000E+013 +0.0000000E+000 +6.2270000E+004 !\AUTHOR: !\REF:

ESTIMATE C3 NUIG S. M. BURKE !\COMMENT:

C3H6+O<=>C3H5-S+OH

+1.2000000E+011 +7.0000000E-001 +8.9591000E+003 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT:

C3H6+OH<=>C3H5-S+H2O

+1.8600000E+005 +2.3690000E+000 +2.5020000E+003 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?

C3H6+HO2<=>C3H5-S+H2O2

+9.5700000E+002 +3.0590000E+000 +2.0798600E+004 !\AUTHOR: !\REF: C3

NUIG CALCULATION J.M !\COMMENT: WARNING: RESULTS ARE NOW PUBLISHED, UPDATED REFERENCE

C3H6+CH3<=>C3H5-S+CH4

+1.3480000E+000 +3.5000000E+000 +1.2850000E+004 !\AUTHOR: !\REF: TSANG,

W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:

!

---

!\REACTIONCLASS: \R\_ADDITION\O

\A

\N

\EA

!

---

C3H6+O<=>C2H5+HCO

+7.4500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT: WARNING: THE PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.

C3H6+O=>CH2CO+CH3+H

+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT: WARNING: THE PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.

C3H6+O=>CH3CHCO+H+H

+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:

ANALOGY WITH C2H4 !\COMMENT: WARNING: THE PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.

!

---

!\REACTIONCLASS: \R\_ADDITION\H

\A

\N

\EA

!

---

C3H6+H<=>NC3H7

+1.0000000E+000 +1.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM

MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003

+7.9900000E+081 -2.3161000E+001 +2.2239000E+004 /

PLOG / +4.0000000E-002

+4.2400000E+068 -1.8427000E+001 +1.9665000E+004 /

PLOG / +1.0000000E+000

+1.0400000E+049 -1.1500000E+001 +1.5359000E+004 /

PLOG / +1.0000000E+001

+6.2000000E+041 -8.8920000E+000 +1.4637000E+004 /

PLOG / +1.0000000E+002 +1.0000000E-

010 +0.0000000E+000 +0.0000000E+000 /

!PLOG/ 100.0000 -6.450E+031 -5.851 8177.8/

DUP

C3H6+H<=>NC3H7

+1.0000000E+000 +1.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM

MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003

+1.8500000E+026 -5.8300000E+000 +3.8658000E+003 /

PLOG / +4.0000000E-002

+2.8200000E+030 -6.4900000E+000 +5.4708000E+003 /

PLOG / +1.0000000E+000

+3.7800000E+028 -5.5700000E+000 +5.6251000E+003 /

PLOG / +1.0000000E+001

+1.4600000E+025 -4.2800000E+000 +5.2478000E+003 /

PLOG / +1.0000000E+002

+4.2200000E+027 -4.3900000E+000 +9.3458000E+003 /

!PLOG/ 100.0000 7.240E+026 -4.210 6825.0/

DUP

C3H6+H<=>C2H4+CH3

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM

MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003

+1.5400000E+009 +1.3500000E+000 +2.5420000E+003 /

PLOG / +4.0000000E-002

+7.8800000E+010 +8.7000000E-001 +3.5996000E+003 /

PLOG / +1.0000000E+000

+2.6700000E+012 +4.7000000E-001 +5.4311000E+003 /

PLOG / +1.0000000E+001

+9.2500000E+022 -2.6000000E+000 +1.2898000E+004 /

PLOG / +1.0000000E+002

+1.3200000E+023 -2.4200000E+000 +1.6500000E+004 /

DUP

C3H6+H<=>C2H4+CH3

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: CURRAN  
EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM  
MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +4.0000000E-002 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +1.0000000E+000 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +1.0000000E+001  
+1.2400000E+005 +2.5200000E+000 +3.6791000E+003 /  
PLOG / +1.0000000E+002  
+2.5100000E+003 +2.9100000E+000 +3.9809000E+003 /

DUP

C3H6+H<=>IC3H7

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: CURRAN  
EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM  
MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003  
+1.3500000E+044 -1.0680000E+001 +8.1964000E+003 /  
PLOG / +4.0000000E-002  
+2.1100000E+057 -1.4230000E+001 +1.5147000E+004 /  
PLOG / +1.0000000E+000  
+3.2600000E+061 -1.4940000E+001 +2.0161000E+004 /  
PLOG / +1.0000000E+001  
+5.3000000E+056 -1.3120000E+001 +2.0667000E+004 /  
PLOG / +1.0000000E+002  
+1.1100000E+050 -1.0800000E+001 +2.0202000E+004 /

DUP

C3H6+H<=>IC3H7

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: CURRAN  
EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM  
MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003  
+2.1700000E+130 -3.2580000E+001 +1.3614000E+005 /  
PLOG / +4.0000000E-002  
+2.2500000E+029 -5.8400000E+000 +4.2419000E+003 /  
PLOG / +1.0000000E+000  
+1.0600000E+030 -5.6300000E+000 +5.6134000E+003 /  
PLOG / +1.0000000E+001  
+6.1100000E+026 -4.4400000E+000 +5.1823000E+003 /  
PLOG / +1.0000000E+002  
+2.7300000E+023 -3.2600000E+000 +4.5970000E+003 /

DUP

C2H4+CH3<=>NC3H7

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: CURRAN  
EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM  
MILLER/KLIPPENSTEIN??

PLOG / +1.3000000E-003  
+8.6700000E+048 -1.2540000E+001 +1.8206000E+004 /  
PLOG / +4.0000000E-002  
+1.0600000E+049 -1.2040000E+001 +2.0001000E+004 /  
PLOG / +1.0000000E+000  
+7.6700000E+047 -1.1170000E+001 +2.2366000E+004 /  
PLOG / +1.0000000E+001  
+1.8100000E+045 -1.0030000E+001 +2.3769000E+004 /

PLOG / +1.0000000E+002  
+2.0400000E+040 -8.2500000E+000 +2.4214000E+004 /  
DUP  
C2H4+CH3<=>NC3H7  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: CURRAN  
EST !\COMMENT: WARNING: ARE THESE RATE CONSTANTS NOT FROM  
MILLER/KLIPPENSTEIN??  
PLOG / +1.3000000E-003  
+1.1200000E+043 -1.1300000E+001 +1.3080000E+004 /  
PLOG / +4.0000000E-002  
+7.2800000E+039 -9.8800000E+000 +1.3164000E+004 /  
PLOG / +1.0000000E+000  
+2.6000000E+033 -7.4600000E+000 +1.2416000E+004 /  
PLOG / +1.0000000E+001  
+3.8500000E+027 -5.3800000E+000 +1.1455000E+004 /  
PLOG / +1.0000000E+002  
+1.6600000E+021 -3.1700000E+000 +1.0241000E+004 /  
DUP  
!

---

!\REACTIONCLASS: \R\_ADDITION\HO2 \A  
\N \EA  
!

---

C3H6+HO2<=>C3H6OOH2-1 +4.8500000E-  
021 +2.6500000E+000 +1.1201000E+004 !\AUTHOR: !\REF: WARNING !\COMMENT:  
WARNING: NO REFERENCE IN BASEMECH2907\_C7.inp  
PLOG / +1.3000000E-002  
+1.3100000E+013 -1.8400000E+000 +8.5610000E+003 /  
PLOG / +9.8690000E-001  
+5.9300000E+017 -2.6100000E+000 +1.1533000E+004 /  
PLOG / +9.8700000E+000  
+8.3400000E+024 -4.4000000E+000 +1.6440000E+004 /  
PLOG / +9.8690000E+001  
+3.7500000E+023 -3.6800000E+000 +1.7965000E+004 /  
C3H6+HO2<=>C3H6O1-2+OH  
+1.1300000E+019 -1.6800000E+000 +2.3587000E+004 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907\_C7.inp  
PLOG / +1.3000000E-002  
+3.7300000E+003 +2.6400000E+000 +1.1173000E+004 /  
PLOG / +9.8690000E-001  
+1.7800000E+012 +1.1000000E-001 +1.6137000E+004 /  
PLOG / +9.8700000E+000  
+3.9000000E+017 -1.4000000E+000 +2.0077000E+004 /  
PLOG / +9.8690000E+001  
+1.1300000E+019 -1.6800000E+000 +2.3587000E+004 /  
C3H6+HO2<=>IC3H7+O2  
+8.8700000E+022 -3.0900000E+000 +2.6586000E+004 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907\_C7.inp  
PLOG / +1.3000000E-002  
+1.0200000E+007 +1.1600000E+000 +1.0273000E+004 /  
PLOG / +9.8690000E-001  
+1.3100000E+020 -2.5800000E+000 +1.9078000E+004 /  
PLOG / +9.8700000E+000  
+4.1400000E+028 -4.9200000E+000 +2.6212000E+004 /  
PLOG / +9.8690000E+001  
+8.8700000E+022 -3.0900000E+000 +2.6586000E+004 /



C3H6OOH2-1<=>C3H6O1-2+OH  
+6.9100000E+007 +1.3700000E+000 +1.3373000E+004 !\AUTHOR: !\REF:  
WARNING !\COMMENT: WARNING: NO REFERENCE IN BASEMECH2907\_C7.inp  
PLOG / +1.3000000E-002  
+2.6600000E+035 -8.3600000E+000 +1.8056000E+004 /  
PLOG / +9.8690000E-001  
+1.9600000E+035 -7.6600000E+000 +2.0595000E+004 /  
PLOG / +9.8700000E+000  
+2.2400000E+033 -6.7500000E+000 +2.1619000E+004 /  
PLOG / +9.8690000E+001  
+8.4800000E+026 -4.5800000E+000 +2.0278000E+004 /  
!

---

!\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  
!

---

C3H5-A+H<=>C3H4-A+H2  
+1.2320000E+003 +3.0350000E+000 +2.5820000E+003 !\AUTHOR:  
!\REF:KLIPPENSTEIN & HARDING 2007 !\COMMENT:  
C3H5-A+OH<=>C3H4-A+H2O  
+6.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG,  
W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\COMMENT:  
C3H5-A+CH3<=>C3H4-A+CH4  
+3.0000000E+012 -3.2000000E-001 -1.3100000E+002 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-A+C2H5<=>C3H4-A+C2H6  
+4.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H5-A+C2H3<=>C3H4-A+C2H4  
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H4-A+C3H4-A<=>C3H5-A+C3H3  
+5.0000000E+014 +0.0000000E+000 +6.4746700E+004 !\AUTHOR: !\REF:ZIEGLER  
ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005) !\COMMENT:  
C3H5-S+H<=>C3H4-A+H2  
+3.3330000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H5-S+CH3<=>C3H4-A+CH4  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H5-S+H<=>C3H4-P+H2  
+3.3400000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-S+CH3<=>C3H4-P+CH4  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-T+H<=>C3H4-P+H2  
+3.3400000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H5-T+CH3<=>C3H4-P+CH4  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_RECOMB \A  
\N \EA  
!

---

C3H5-A+C3H5-A<=>C3H4-A+C3H6  
+9.5500000E+040 -9.3000000E+000 +1.2470000E+004 !\AUTHOR: !\REF:  
FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776 !\COMMENT:  
PLOG / +1.0000000E+000  
+4.7700000E+040 -9.3000000E+000 +1.2470000E+004 /  
PLOG / +4.0000000E+000  
+3.9700000E+032 -6.8000000E+000 +9.1800000E+003 /  
PLOG / +1.0000000E+001  
+1.4600000E+028 -5.5000000E+000 +7.4100000E+003 /  
C3H5-A+C2H5<=>C2H4+C3H6  
+4.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H5-A+HCO<=>C3H6+CO  
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-S+HCO<=>C3H6+CO  
+9.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-T+HCO<=>C3H6+CO  
+9.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-S+O<=>C2H4+HCO  
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-S+OH=>C2H4+HCO+H  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-S+HO2=>C2H4+HCO+OH  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-T+O<=>CH3+CH2CO  
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-T+OH=>CH3+CH2CO+H  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-T+HO2=>CH3+CH2CO+OH  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
!

---

!\REACTIONCLASS: \R+O \A  
\N \EA  
!

---

C3H5-A+O<=>C2H3CHO+H  
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG,  
W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\COMMENT:

!

---

!\REACTIONCLASS: \R+OH \A  
\N \EA

---

C3H5-A+OH=>C2H3CHO+H+H  
+5.3000000E+037 -6.7100000E+000 +2.9306000E+004 !\AUTHOR: !\REF:TSANG,  
W. J.PHYS.CHEM.REF.DATA 1991, 20, 221. !\COMMENT:  
PLOG / +1.0000000E-001  
+5.3000000E+037 -6.7100000E+000 +2.9306000E+004 /  
PLOG / +1.0000000E+000  
+4.2000000E+032 -5.1600000E+000 +3.0126000E+004 /  
PLOG / +1.0000000E+001  
+1.6000000E+020 -1.5600000E+000 +2.6330000E+004 /  
!

---

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA

---

C3H5-A+O2<=>C3H4-A+HO2  
+4.9900000E+015 -1.4000000E+000 +2.2428000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT: !\AUTHOR: !\REF:!\WANG, J. PHYS.  
CHEM. REF. DATA 20,  
PLOG / +1.0000000E+000  
+4.9900000E+015 -1.4000000E+000 +2.2428000E+004 /  
PLOG / +1.0000000E+001  
+2.1800000E+021 -2.8500000E+000 +3.0755000E+004 /  
C3H5-A+O2<=>CH3CO+CH2O  
+1.1900000E+015 -1.0100000E+000 +2.0128000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT: !\AUTHOR: !\REF:!\WANG, J. PHYS.  
CHEM. REF. DATA 20,  
PLOG / +1.0000000E+000  
+1.1900000E+015 -1.0100000E+000 +2.0128000E+004 /  
PLOG / +1.0000000E+001  
+7.1400000E+015 -1.2100000E+000 +2.1046000E+004 /  
C3H5-A+O2<=>C2H3CHO+OH  
+1.8200000E+013 -4.1000000E-001 +2.2859000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT: !\AUTHOR: !\REF:!\WANG, J. PHYS.  
CHEM. REF. DATA 20,  
PLOG / +1.0000000E+000  
+1.8200000E+013 -4.1000000E-001 +2.2859000E+004 /  
PLOG / +1.0000000E+001  
+2.4700000E+013 -4.5000000E-001 +2.3017000E+004 /  
C3H5-S+O2<=>CH3CHO+HCO  
+3.1000000E+031 -5.9440000E+000 +5.7484000E+003 !\AUTHOR: !\REF:  
ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:  
C3H5-S+O2<=>CH3CHCHO+O  
+5.3800000E+018 -2.1400000E+000 +5.1429000E+003 !\AUTHOR: !\REF:  
ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:  
C3H5-S+O2<=>C2H3CHO+OH  
+2.7000000E+019 -2.1400000E+000 +5.1429000E+003 !\AUTHOR: !\REF:  
ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:  
C3H5-T+O2<=>CH3COCH2+O  
+9.8600000E+025 -3.7510000E+000 +1.1255400E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H5-T+O2<=>CH3CO+CH2O  
+2.5500000E+020 -2.6080000E+000 +1.5657000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H5-T+O2<=>C3H4-A+HO2  
+3.5900000E+010 -2.7000000E-001 -4.1360000E+002 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_HO2 \A  
\N \EA  
!

---

---

C3H5-A+HO2<=>C3H5O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:

PLOG / +1.0000000E-002  
+1.0200000E+013 -1.5800000E-001 -1.4170000E+003 /  
PLOG / +1.0000000E-001  
+4.9800000E+014 -6.4200000E-001 -3.4910000E+002 /  
PLOG / +1.0000000E+000  
+7.7700000E+017 -1.5200000E+000 +2.3792000E+003 /  
PLOG / +1.0000000E+001  
+2.9300000E+015 -6.8400000E-001 +3.6153000E+003 /  
PLOG / +1.0000000E+002  
+1.6400000E+004 +2.7400000E+000 +1.1444000E+003 /

C3H5-A+HO2<=>AC3H5OOH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:

PLOG / +1.0000000E-002  
+1.9100000E+031 -7.2300000E+000 +1.3362000E+003 /  
PLOG / +1.0000000E-001  
+6.3100000E+042 -1.0300000E+001 +5.5689000E+003 /  
PLOG / +1.0000000E+000  
+1.0300000E+045 -1.0600000E+001 +7.8515000E+003 /  
PLOG / +1.0000000E+001  
+2.7900000E+037 -7.9200000E+000 +6.4979000E+003 /  
PLOG / +1.0000000E+002  
+1.4400000E+032 -6.0100000E+000 +6.0536000E+003 /

C3H5-A+HO2<=>C2H3CHO+H2O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:

PLOG / +1.0000000E-002  
+1.0900000E+000 +3.0100000E+000 -3.4211000E+003 /  
PLOG / +1.0000000E-001  
+6.3500000E+001 +2.5000000E+000 -2.3414000E+003 /  
PLOG / +1.0000000E+000  
+6.0500000E+005 +1.3900000E+000 +5.9510000E+002 /  
PLOG / +1.0000000E+001  
+3.1000000E+005 +1.5900000E+000 +2.6776000E+003 /  
PLOG / +1.0000000E+002 +5.0700000E-  
005 +4.5900000E+000 +9.2750000E+002 /

AC3H5OOH<=>C2H3CHO+H2O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:

PLOG / +1.0000000E-002  
+1.9900000E+050 -1.2700000E+001 +5.3531900E+004 /  
PLOG / +1.0000000E-001  
+4.7200000E+047 -1.1500000E+001 +5.4360900E+004 /  
PLOG / +1.0000000E+000  
+1.5000000E+040 -8.8400000E+000 +5.3179200E+004 /  
PLOG / +1.0000000E+001  
+2.5400000E+028 -5.0000000E+000 +4.9919400E+004 /  
PLOG / +1.0000000E+002  
+1.4800000E+016 -1.1200000E+000 +4.5949300E+004 /  
AC3H5OOH<=>C3H5O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-002  
+1.4900000E+058 -1.3900000E+001 +5.4266900E+004 /  
PLOG / +1.0000000E-001  
+1.8000000E+054 -1.2400000E+001 +5.4193800E+004 /  
PLOG / +1.0000000E+000  
+3.3600000E+046 -9.8100000E+000 +5.2468500E+004 /  
PLOG / +1.0000000E+001  
+2.3900000E+036 -6.5400000E+000 +4.9429000E+004 /  
PLOG / +1.0000000E+002  
+1.2800000E+027 -3.6100000E+000 +4.6333100E+004 /  
C3H5O<=>C2H3+CH2O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-003  
+7.2600000E+006 +1.8200000E-001 +1.7815500E+004 /  
PLOG / +1.0000000E-002  
+6.9700000E+016 -2.5000000E+000 +2.0878700E+004 /  
PLOG / +1.0000000E-001  
+6.6400000E+023 -4.2300000E+000 +2.3565000E+004 /  
PLOG / +1.0000000E+000  
+1.0700000E+026 -4.5600000E+000 +2.4622900E+004 /  
PLOG / +1.0000000E+001  
+6.5000000E+029 -5.3700000E+000 +2.6645000E+004 /  
PLOG / +1.0000000E+002  
+4.6300000E+031 -5.5900000E+000 +2.8915300E+004 /  
PLOG / +1.0000000E+003  
+8.5200000E+025 -3.6100000E+000 +2.7863400E+004 /  
C3H5O<=>CH2CHOCH2  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-003  
+3.1700000E+020 -4.1500000E+000 +1.2121300E+004 /  
PLOG / +1.0000000E-002  
+4.7900000E+024 -5.0300000E+000 +1.4606100E+004 /  
PLOG / +1.0000000E-001  
+1.9000000E+026 -5.1600000E+000 +1.6124400E+004 /  
PLOG / +1.0000000E+000  
+1.5100000E+028 -5.4000000E+000 +1.8165400E+004 /  
PLOG / +1.0000000E+001  
+2.4200000E+028 -5.1700000E+000 +1.9691200E+004 /  
PLOG / +1.0000000E+002  
+5.5700000E+024 -3.8600000E+000 +1.9395200E+004 /

PLOG / +1.0000000E+003  
 +1.3500000E+018 -1.7300000E+000 +1.7386500E+004 /  
 C3H5O<=>CH2CH2CHO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003 +5.2500000E-  
 049 +1.5500000E+001 -1.5639900E+004 /  
 PLOG / +1.0000000E-002 +1.4600000E-  
 088 +2.7600000E+001 -3.5995000E+004 /  
 PLOG / +1.0000000E-001 +4.4400000E-  
 022 +8.3800000E+000 -3.8190000E+003 /  
 PLOG / +1.0000000E+000  
 +6.2300000E+012 -1.4400000E+000 +1.0829200E+004 /  
 PLOG / +1.0000000E+001  
 +3.4800000E+042 -9.9100000E+000 +2.5297900E+004 /  
 PLOG / +1.0000000E+002  
 +1.8800000E+038 -8.1600000E+000 +2.5974500E+004 /  
 PLOG / +1.0000000E+003  
 +1.6700000E+021 -2.7400000E+000 +2.0337700E+004 /  
 C3H5O<=>C2H3CHO+H  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003  
 +3.0000000E+015 -2.3100000E+000 +1.4667900E+004 /  
 PLOG / +1.0000000E-002  
 +1.5000000E+022 -3.9600000E+000 +1.8283000E+004 /  
 PLOG / +1.0000000E-001  
 +1.9500000E+023 -3.9900000E+000 +1.9143300E+004 /  
 PLOG / +1.0000000E+000  
 +1.1500000E+025 -4.2400000E+000 +2.0311200E+004 /  
 PLOG / +1.0000000E+001  
 +1.7600000E+028 -4.8900000E+000 +2.2765200E+004 /  
 PLOG / +1.0000000E+002  
 +1.4100000E+027 -4.2800000E+000 +2.3770600E+004 /  
 PLOG / +1.0000000E+003  
 +2.5700000E+020 -2.0600000E+000 +2.2040100E+004 /  
 C3H5O<=>C2H4+HCO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003  
 +6.6200000E+016 -2.8400000E+000 +1.3197000E+004 /  
 PLOG / +1.0000000E-002  
 +1.2600000E+020 -3.5300000E+000 +1.5469200E+004 /  
 PLOG / +1.0000000E-001  
 +2.1300000E+021 -3.6400000E+000 +1.6584500E+004 /  
 PLOG / +1.0000000E+000  
 +1.0700000E+024 -4.1600000E+000 +1.8985000E+004 /  
 PLOG / +1.0000000E+001  
 +8.4200000E+025 -4.4000000E+000 +2.2382600E+004 /  
 PLOG / +1.0000000E+002  
 +1.8600000E+021 -2.7300000E+000 +2.3658800E+004 /  
 PLOG / +1.0000000E+003  
 +4.7500000E+008 +1.1400000E+000 +2.0922500E+004 /  
 CH2CHOCH2<=>C2H3+CH2O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:

!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-003  
+3.3000000E+009 -6.3800000E-001 +1.9747800E+004 /  
PLOG / +1.0000000E-002  
+3.3600000E+021 -3.9000000E+000 +2.3945200E+004 /  
PLOG / +1.0000000E-001  
+2.9100000E+029 -5.9000000E+000 +2.7249700E+004 /  
PLOG / +1.0000000E+000  
+1.8300000E+034 -6.9400000E+000 +3.0690400E+004 /  
PLOG / +1.0000000E+001  
+9.7200000E+033 -6.5000000E+000 +3.3002500E+004 /  
PLOG / +1.0000000E+002  
+2.6800000E+027 -4.2600000E+000 +3.3305600E+004 /  
PLOG / +1.0000000E+003  
+8.8100000E+014 -3.2600000E-001 +3.1553100E+004 /  
CH2CHOCH2<=>CH2CH2CHO  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-003 +8.0100000E-  
092 +2.7800000E+001 -3.7321200E+004 /  
PLOG / +1.0000000E-002 +7.7800000E-  
011 +3.7000000E+000 -2.7669000E+003 /  
PLOG / +1.0000000E-001  
+5.1100000E+015 -2.7600000E+000 +1.5937600E+004 /  
PLOG / +1.0000000E+000  
+4.4800000E+025 -5.2000000E+000 +2.1532200E+004 /  
PLOG / +1.0000000E+001  
+3.9700000E+034 -7.4100000E+000 +2.8116900E+004 /  
PLOG / +1.0000000E+002  
+5.6200000E+022 -3.5600000E+000 +2.5806700E+004 /  
PLOG / +1.0000000E+003  
+2.5100000E+020 -2.6300000E+000 +2.9288400E+004 /  
CH2CHOCH2<=>C2H3CHO+H  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-003  
+4.9300000E+024 -5.0500000E+000 +2.0108400E+004 /  
PLOG / +1.0000000E-002  
+2.1400000E+028 -5.8000000E+000 +2.2219400E+004 /  
PLOG / +1.0000000E-001  
+1.9300000E+032 -6.6400000E+000 +2.5108200E+004 /  
PLOG / +1.0000000E+000  
+8.6000000E+034 -7.1100000E+000 +2.8209100E+004 /  
PLOG / +1.0000000E+001  
+2.1700000E+034 -6.6400000E+000 +3.0647600E+004 /  
PLOG / +1.0000000E+002  
+4.1700000E+028 -4.7100000E+000 +3.1231900E+004 /  
PLOG / +1.0000000E+003  
+3.9800000E+018 -1.6200000E+000 +3.0129800E+004 /  
CH2CHOCH2<=>C2H4+HCO  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
\COMMENT:  
PLOG / +1.0000000E-003  
+8.2300000E+026 -5.8400000E+000 +1.9356900E+004 /

PLOG / +1.0000000E-002  
 +1.3200000E+029 -6.2100000E+000 +2.1293600E+004 /  
 PLOG / +1.0000000E-001  
 +3.4700000E+032 -6.9600000E+000 +2.4197300E+004 /  
 PLOG / +1.0000000E+000  
 +1.4400000E+036 -7.7600000E+000 +2.8007800E+004 /  
 PLOG / +1.0000000E+001  
 +9.7200000E+037 -8.0200000E+000 +3.2394600E+004 /  
 PLOG / +1.0000000E+002  
 +2.4300000E+031 -5.8100000E+000 +3.4295800E+004 /  
 PLOG / +1.0000000E+003  
 +3.7300000E+014 -7.2600000E-001 +3.2008300E+004 /  
 CH2CH2CHO<=>C2H3+CH2O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003 +6.8900000E-  
 069 +2.1500000E+001 +2.6380000E+003 /  
 PLOG / +1.0000000E-002 +5.3400000E-  
 033 +1.1100000E+001 +1.6749100E+004 /  
 PLOG / +1.0000000E-001  
 +6.1100000E+026 -6.0100000E+000 +4.4116700E+004 /  
 PLOG / +1.0000000E+000  
 +8.0400000E+035 -8.3100000E+000 +4.6919700E+004 /  
 PLOG / +1.0000000E+001  
 +5.5200000E+040 -9.1900000E+000 +5.0508700E+004 /  
 PLOG / +1.0000000E+002  
 +5.8500000E+035 -7.1800000E+000 +5.2038400E+004 /  
 PLOG / +1.0000000E+003  
 +1.9300000E+019 -1.9400000E+000 +4.8440000E+004 /  
 CH2CH2CHO<=>C2H3CHO+H  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003  
 +1.6100000E+010 -1.2400000E+000 +3.2371300E+004 /  
 PLOG / +1.0000000E-002  
 +5.8400000E+015 -2.6100000E+000 +3.2878400E+004 /  
 PLOG / +1.0000000E-001  
 +3.6400000E+023 -4.6000000E+000 +3.4275300E+004 /  
 PLOG / +1.0000000E+000  
 +7.5800000E+031 -6.6300000E+000 +3.7895400E+004 /  
 PLOG / +1.0000000E+001  
 +2.8600000E+032 -6.3000000E+000 +3.9990700E+004 /  
 PLOG / +1.0000000E+002  
 +1.5700000E+023 -3.1400000E+000 +3.8011700E+004 /  
 PLOG / +1.0000000E+003  
 +4.5200000E+012 +2.1400000E-001 +3.4570500E+004 /  
 CH2CH2CHO<=>C2H4+HCO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003  
 +2.9000000E+032 -7.2400000E+000 +2.5687500E+004 /  
 PLOG / +1.0000000E-002  
 +5.3000000E+033 -7.2800000E+000 +2.7100600E+004 /  
 PLOG / +1.0000000E-001  
 +2.0000000E+035 -7.4100000E+000 +2.9027300E+004 /



PLOG / +1.0000000E+000  
 +1.0100000E+034 -6.7000000E+000 +3.0018100E+004 /  
 PLOG / +1.0000000E+001  
 +9.7600000E+027 -4.6300000E+000 +2.8923900E+004 /  
 PLOG / +1.0000000E+002  
 +2.1100000E+019 -1.8500000E+000 +2.6239800E+004 /  
 PLOG / +1.0000000E+003  
 +1.5900000E+013 +6.3000000E-002 +2.4086300E+004 /  
 C2H3+CH2O<=>C2H3CHO+H  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003  
 +2.6000000E+004 +2.2600000E+000 +1.5103000E+003 /  
 PLOG / +1.0000000E-002  
 +5.1300000E+004 +2.1700000E+000 +1.6755000E+003 /  
 PLOG / +1.0000000E-001  
 +3.9900000E+005 +1.9100000E+000 +2.2183000E+003 /  
 PLOG / +1.0000000E+000  
 +1.7500000E+007 +1.4500000E+000 +3.4280000E+003 /  
 PLOG / +1.0000000E+001  
 +1.3500000E+009 +9.3300000E-001 +5.1730000E+003 /  
 PLOG / +1.0000000E+002  
 +2.2400000E+011 +3.5700000E-001 +8.0013000E+003 /  
 PLOG / +1.0000000E+003  
 +6.0100000E+005 +2.0900000E+000 +7.8956000E+003 /  
 C2H3+CH2O<=>C2H4+HCO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 \COMMENT:  
 PLOG / +1.0000000E-003  
 +1.1100000E+007 +1.0900000E+000 +1.8072000E+003 /  
 PLOG / +1.0000000E-002  
 +2.4700000E+007 +9.9300000E-001 +1.9949000E+003 /  
 PLOG / +1.0000000E-001  
 +2.4700000E+008 +7.0400000E-001 +2.5962000E+003 /  
 PLOG / +1.0000000E+000  
 +1.4200000E+010 +2.0900000E-001 +3.9342000E+003 /  
 PLOG / +1.0000000E+001  
 +3.4500000E+013 -7.2600000E-001 +6.9443000E+003 /  
 PLOG / +1.0000000E+002  
 +3.3100000E+014 -8.6600000E-001 +1.0965700E+004 /  
 PLOG / +1.0000000E+003  
 +1.6500000E+001 +3.1700000E+000 +9.3998000E+003 /  
 !

---

!\REACTIONCLASS: \R+CH3O2 \A  
 \N \EA  
 !

---

C3H5-A+CH3O2<=>C3H5O+CH3O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 ANOLOGY WITH C3H5-A+HO2 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +3.3300000E+012 -1.5800000E-001 -1.4170000E+003 /  
 PLOG / +1.0000000E-001  
 +1.6600000E+014 -6.4200000E-001 -3.4910000E+002 /

PLOG / +1.0000000E+000  
+2.5950000E+017 -1.5200000E+000 +2.3792000E+003 /  
PLOG / +1.0000000E+001  
+9.7800000E+014 -6.8400000E-001 +3.6153000E+003 /  
PLOG / +1.0000000E+002  
+5.4700000E+003 +2.7400000E+000 +1.1444000E+003 /  
C3H5-A+CH3O2<=>AC4H7OOH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ANOLOGY WITH C3H5-A+HO2 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.9100000E+031 -7.2300000E+000 +1.3362000E+003 /  
PLOG / +1.0000000E-001  
+6.3100000E+042 -1.0300000E+001 +5.5689000E+003 /  
PLOG / +1.0000000E+000  
+1.0300000E+045 -1.0600000E+001 +7.8515000E+003 /  
PLOG / +1.0000000E+001  
+2.7900000E+037 -7.9200000E+000 +6.4979000E+003 /  
PLOG / +1.0000000E+002  
+3.4000000E+029 -5.2800000E+000 +4.5398000E+003 /  
AC4H7OOH<=>C3H5O+CH3O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ANOLOGY WITH C3H5-A+HO2 !\COMMENT:  
PLOG / +1.0000000E-002  
+1.4900000E+058 -1.3900000E+001 +5.4266900E+004 /  
PLOG / +1.0000000E-001  
+1.8000000E+054 -1.2400000E+001 +5.4193800E+004 /  
PLOG / +1.0000000E+000  
+3.3600000E+046 -9.8100000E+000 +5.2468500E+004 /  
PLOG / +1.0000000E+001  
+2.3900000E+036 -6.5400000E+000 +4.9429000E+004 /  
PLOG / +1.0000000E+002  
+2.5600000E+027 -3.6100000E+000 +4.6333100E+004 /  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

C3H6+OH<=>C3H5OH+H  
+2.2900000E+013 +7.0000000E-002 +1.0580000E+004 !\AUTHOR: !\REF: ZADOR  
PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:  
PLOG / +1.3000000E-003  
+2.6700000E+013 +5.0000000E-002 +1.0611000E+004 /  
PLOG / +1.0000000E-002  
+2.7500000E+013 +5.0000000E-002 +1.0623000E+004 /  
PLOG / +1.3000000E-002  
+2.8700000E+013 +4.0000000E-002 +1.0634000E+004 /  
PLOG / +2.5000000E-002  
+1.5900000E+014 -1.6000000E-001 +1.1125000E+004 /  
PLOG / +1.0000000E-001  
+3.1000000E+014 -2.2000000E-001 +1.1407000E+004 /  
PLOG / +1.3150000E-001  
+3.7800000E+014 -2.4000000E-001 +1.1458000E+004 /  
PLOG / +1.0000000E+000  
+9.1500000E+007 +1.4200000E+000 +1.0087000E+004 /  
PLOG / +1.0000000E+001  
+3.6600000E+005 +2.1400000E+000 +1.0410000E+004 /

PLOG / +1.0000000E+002  
 +8.1900000E+002 +2.8400000E+000 +1.0481000E+004 /  
 C3H6+OH<=>C2H3OH+CH3  
 +1.2900000E+006 +1.6500000E+000 +1.2330000E+003 !\AUTHOR: !\REF: ZADOR  
 PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:  
 PLOG / +1.3000000E-003  
 +1.2900000E+006 +1.6500000E+000 +1.2330000E+003 /  
 PLOG / +1.0000000E-002  
 +1.8200000E+004 +2.1000000E+000 +1.1620000E+003 /  
 PLOG / +1.3000000E-002  
 +2.0400000E+003 +2.4800000E+000 +1.1280000E+003 /  
 PLOG / +2.5000000E-002  
 +2.8800000E+002 +2.8000000E+000 +1.1520000E+003 /  
 PLOG / +1.0000000E-001  
 +1.4000000E+001 +3.2100000E+000 +1.2080000E+003 /  
 PLOG / +1.3150000E-001  
 +7.7100000E+000 +3.2900000E+000 +1.2160000E+003 /  
 PLOG / +1.0000000E+000  
 +1.1300000E+004 +2.5000000E+000 +3.2380000E+003 /  
 PLOG / +1.0000000E+001  
 +2.4100000E+019 -1.7400000E+000 +1.3107000E+004 /  
 PLOG / +1.0000000E+002 +3.3000000E-  
 001 +3.7000000E+000 +3.6650000E+003 /  
 C3H6+OH<=>IC3H5OH+H  
 +2.8700000E+000 +2.9200000E+000 +6.2500000E+002 !\AUTHOR: !\REF: ZADOR  
 PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:  
 PLOG / +1.3000000E-003  
 +2.8700000E+000 +2.9200000E+000 +6.2500000E+002 /  
 PLOG / +1.0000000E-002 +4.8400000E-  
 001 +2.9800000E+000 +7.0400000E+002 /  
 PLOG / +1.3000000E-002 +3.1300000E-  
 001 +3.0400000E+000 +7.2100000E+002 /  
 PLOG / +2.5000000E-002 +9.3300000E-  
 003 +3.6200000E+000 +6.7700000E+002 /  
 PLOG / +1.0000000E-001 +4.6400000E-  
 005 +4.4800000E+000 +6.8700000E+002 /  
 PLOG / +1.3150000E-001 +2.7100000E-  
 005 +4.5600000E+000 +7.0700000E+002 /  
 PLOG / +1.0000000E+000 +7.6500000E-  
 007 +5.0500000E+000 +8.7400000E+002 /  
 PLOG / +1.0000000E+001  
 +2.6400000E+015 -8.0000000E-001 +1.2728000E+004 /  
 PLOG / +1.0000000E+002 +4.8700000E-  
 004 +4.3200000E+000 +4.0200000E+003 /  
 C3H6+OH<=>SC3H5OH+H  
 +2.8700000E+000 +2.9200000E+000 +6.2500000E+002 !\AUTHOR: !\REF: ZADOR  
 PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT: SINEAD, MOD  
 0509 KWZ  
 PLOG / +1.3000000E-003  
 +3.4700000E+006 +1.5300000E+000 +4.2880000E+003 /  
 PLOG / +1.0000000E-002  
 +1.0800000E+007 +1.3400000E+000 +4.5760000E+003 /  
 PLOG / +1.3000000E-002  
 +9.7600000E+006 +1.3300000E+000 +4.5890000E+003 /  
 PLOG / +2.5000000E-002  
 +5.1400000E+006 +1.3600000E+000 +4.5940000E+003 /  
 PLOG / +1.0000000E-001  
 +3.1300000E+005 +1.6900000E+000 +4.6030000E+003 /

PLOG / +1.3150000E-001  
 +1.3900000E+005 +1.8000000E+000 +4.6030000E+003 /  
 PLOG / +1.0000000E+000  
 +1.0300000E+002 +2.8300000E+000 +4.5300000E+003 /  
 PLOG / +1.0000000E+001 +3.4000000E-  
 002 +3.8900000E+000 +4.3900000E+003 /  
 PLOG / +1.0000000E+002 +4.4600000E-  
 006 +5.0300000E+000 +4.1320000E+003 /  
 C3H6+OH<=>CH3CHO+CH3  
 +6.9300000E+005 +1.4900000E+000 -5.3600000E+002 !\AUTHOR: !\REF: ZADOR  
 PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:  
 PLOG / +1.3000000E-003  
 +6.9300000E+005 +1.4900000E+000 -5.3600000E+002 /  
 PLOG / +1.0000000E-002  
 +5.9400000E+003 +2.0100000E+000 -5.6000000E+002 /  
 PLOG / +1.3000000E-002  
 +1.1000000E+003 +2.2200000E+000 -6.8000000E+002 /  
 PLOG / +2.5000000E-002  
 +1.0700000E+002 +2.5000000E+000 -7.5900000E+002 /  
 PLOG / +1.0000000E-001 +7.8300000E-  
 001 +3.1000000E+000 -9.1900000E+002 /  
 PLOG / +1.3150000E-001 +3.0700000E-  
 001 +3.2200000E+000 -9.4600000E+002 /  
 PLOG / +1.0000000E+000 +3.1600000E-  
 004 +4.0500000E+000 -1.1440000E+003 /  
 PLOG / +1.0000000E+001 +7.5900000E-  
 006 +4.4900000E+000 -6.8000000E+002 /  
 PLOG / +1.0000000E+002 +5.4500000E-  
 005 +4.2200000E+000 +1.1410000E+003 /  
 C3H6+OH<=>C3H6OH1-2  
 +5.1000000E+054 -2.0700000E+001 +3.2402000E+004 !\AUTHOR: !\REF: ZADOR  
 PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:  
 PLOG / +1.3000000E-003  
 +2.3000000E+078 -2.0700000E+001 +3.2402000E+004 /  
 PLOG / +1.0000000E-002  
 +2.7400000E+077 -2.0000000E+001 +3.3874000E+004 /  
 PLOG / +1.3000000E-002  
 +1.0700000E+076 -1.9580000E+001 +3.2874000E+004 /  
 PLOG / +2.5000000E-002  
 +3.6800000E+073 -1.8790000E+001 +3.1361000E+004 /  
 PLOG / +1.0000000E-001  
 +1.0400000E+068 -1.7010000E+001 +2.7909000E+004 /  
 PLOG / +1.3150000E-001  
 +7.2300000E+066 -1.6640000E+001 +2.7162000E+004 /  
 PLOG / +1.0000000E+000  
 +1.9500000E+059 -1.4170000E+001 +2.3079000E+004 /  
 PLOG / +1.0000000E+001  
 +7.5800000E+053 -1.2230000E+001 +2.2976000E+004 /  
 PLOG / +1.0000000E+002  
 +1.4300000E+048 -1.0230000E+001 +2.3772000E+004 /  
 DUP  
 C3H6+OH<=>C3H6OH1-2  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !\AUTHOR: !\REF: ZADOR  
 PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:  
 PLOG / +1.3000000E-003  
 +6.4100000E+059 -1.5840000E+001 +1.1594000E+004 /  
 PLOG / +1.0000000E-002  
 +7.2800000E+059 -1.5510000E+001 +1.2898000E+004 /

PLOG / +1.3000000E-002  
+2.7900000E+059 -1.5340000E+001 +1.2913000E+004 /  
PLOG / +2.5000000E-002  
+2.6500000E+058 -1.4930000E+001 +1.2936000E+004 /  
PLOG / +1.0000000E-001  
+1.3500000E+056 -1.4040000E+001 +1.2945000E+004 /  
PLOG / +1.3150000E-001  
+3.9800000E+055 -1.3850000E+001 +1.2887000E+004 /  
PLOG / +1.0000000E+000  
+1.5500000E+050 -1.2040000E+001 +1.1493000E+004 /  
PLOG / +1.0000000E+001  
+6.4100000E+041 -9.3500000E+000 +8.9210000E+003 /  
PLOG / +1.0000000E+002  
+2.3000000E+032 -6.3100000E+000 +6.0880000E+003 /

DUP

C3H6+OH<=>C3H6OH2-1

+5.1000000E+054 -2.0700000E+001 +3.2402000E+004 !\AUTHOR: !\REF: ZADOR  
PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:

PLOG / +1.3000000E-003  
+2.1400000E+059 -1.5840000E+001 +1.1594000E+004 /  
PLOG / +1.0000000E-002  
+2.4300000E+059 -1.5510000E+001 +1.2898000E+004 /  
PLOG / +1.3000000E-002  
+9.3000000E+058 -1.5340000E+001 +1.2913000E+004 /  
PLOG / +2.5000000E-002  
+8.8300000E+057 -1.4930000E+001 +1.2936000E+004 /  
PLOG / +1.0000000E-001  
+4.5000000E+055 -1.4040000E+001 +1.2945000E+004 /  
PLOG / +1.3150000E-001  
+1.3300000E+055 -1.3850000E+001 +1.2887000E+004 /  
PLOG / +1.0000000E+000  
+5.1800000E+049 -1.2040000E+001 +1.1493000E+004 /  
PLOG / +1.0000000E+001  
+2.1400000E+041 -9.3500000E+000 +8.9210000E+003 /  
PLOG / +1.0000000E+002  
+7.6500000E+031 -6.3100000E+000 +6.0880000E+003 /

DUP

C3H6+OH<=>C3H6OH2-1

+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !\AUTHOR: !\REF: ZADOR  
PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053 !\COMMENT:

PLOG / +1.3000000E-003  
+7.6800000E+077 -2.0700000E+001 +3.2402000E+004 /  
PLOG / +1.0000000E-002  
+9.1300000E+076 -2.0000000E+001 +3.3874000E+004 /  
PLOG / +1.3000000E-002  
+3.5500000E+075 -1.9580000E+001 +3.2874000E+004 /  
PLOG / +2.5000000E-002  
+1.2300000E+073 -1.8790000E+001 +3.1361000E+004 /  
PLOG / +1.0000000E-001  
+3.4500000E+067 -1.7010000E+001 +2.7909000E+004 /  
PLOG / +1.3150000E-001  
+2.4100000E+066 -1.6640000E+001 +2.7162000E+004 /  
PLOG / +1.0000000E+000  
+6.5000000E+058 -1.4170000E+001 +2.3079000E+004 /  
PLOG / +1.0000000E+001  
+2.5300000E+053 -1.2230000E+001 +2.2976000E+004 /  
PLOG / +1.0000000E+002  
+4.7800000E+047 -1.0230000E+001 +2.3772000E+004 /

DUP

!=====

!\SUBSPECIES: \C3H5OH

!=====

!

!\REACTIONCLASS: \UNIMOL \A  
\N \EA

!

CH2CCH2OH+H<=>C3H5OH  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA

!

C3H5OH+H<=>CH2CCH2OH+H2  
+3.9000000E+005 +2.5000000E+000 +5.8210000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

C3H5OH+O2<=>CH2CCH2OH+HO2  
+4.0000000E+013 +0.0000000E+000 +6.0690000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

C3H5OH+OH<=>CH2CCH2OH+H2O  
+5.0600000E+012 +0.0000000E+000 +5.9600000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

C3H5OH+CH3<=>CH2CCH2OH+CH4  
+2.4000000E+011 +0.0000000E+000 +8.0300000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

CH2CCH2OH+H2O2<=>C3H5OH+HO2  
+3.0100000E+009 +0.0000000E+000 +2.5830000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

!

!\REACTIONCLASS: \R\_DECOMPOSITION \A  
\N \EA

!

CH2CCH2OH<=>C2H2+CH2OH  
+2.1630000E+040 -8.3100000E+000 +4.5110000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT: WARNING: ARE ALL DECOMPOSITION RATE CONSTANTS FROM A  
RELIABLE/CONSISTENT SOURCE?

CH2CCH2OH<=>CH2O+C2H3  
+9.2400000E+010 +8.7000000E-001 +3.0460000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:

CH2CCH2OH<=>C2H3CHO+H  
+1.1100000E+011 +4.8000000E-001 +3.6770000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:

CH2CCH2OH<=>HCO+C2H4  
+9.2400000E+010 +8.7000000E-001 +3.0460000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:

!

!\REACTIONCLASS: \R\_O2\_PRODUCTS \A  
\N \EA  
!

---

CH2CCH2OH+O2=>CH2OH+CO+CH2O  
+4.3350000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
C3H5O+O2<=>C2H3CHO+HO2  
+1.0000000E+012 +0.0000000E+000 +6.0000000E+003 !\AUTHOR:  
!\REF:ACETALDEHYDE ANALOG !\COMMENT:

!=====  
!=====  
!\ENDSUBSPECIES: \C3H5OH  
!=====  
!=====  
!

!=====  
!\SUBSPECIES: \C3H6OH2-1/C3H6OH2-1  
!=====  
!=====  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

CH3COCH3+H<=>C3H6OH2-1  
+8.0000000E+012 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:  
!\REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13 !\COMMENT: WARNING: THIS  
REFERENCE ALSO PRESENT: ANALOGY WITH CH3CHOH -->CH3CHO+H.  
IC3H5OH+H<=>C3H6OH2-1  
+6.2500000E+011 +5.1000000E-001 +4.0200000E+003 !\AUTHOR: !\REF:BASED  
ON IC4H8+H<=>IC4H9 !\COMMENT:  
C2H5CHO+H<=>C3H6OH1-2  
+8.0000000E+012 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:  
!\REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13 !\COMMENT: WARNING: THIS  
REFERENCE ALSO PRESENT: ANALOGY WITH CH3CHOH -->CH3CHO+H.  
C3H5-T+OH<=>IC3H5OH  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:REVERSE  
BY ANALOGY HCO+OH -->PRODUCTS !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_O2\_ALKENE\_HO2 \A  
\N \EA  
!

---

C3H6OH2-1+O2<=>CH3COCH3+HO2  
+1.5000000E+012 +0.0000000E+000 +5.0000000E+003 !\AUTHOR:  
!\REF:!\MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS. CHEM. 1990, 94, 3016  
!\COMMENT:  
C3H6OH1-2+O2<=>C2H5CHO+HO2  
+1.5000000E+012 +0.0000000E+000 +5.0000000E+003 !\AUTHOR:  
!\REF:!\MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS. CHEM. 1990, 94, 3016  
!\COMMENT:  
!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA

!

---

C3H6OH1-2+O2<=>HOC3H6O2  
+1.2000000E+011 +0.0000000E+000 -1.1000000E+003 !\AUTHOR: !\ WILK,  
CERNANSKY, PITZ, AND WESTBROOK, C&F 1988. !\COMMENT:  
C3H6OH2-1+O2<=>HOC3H6O2  
+1.2000000E+011 +0.0000000E+000 -1.1000000E+003 !\AUTHOR: !\ WILK,  
CERNANSKY, PITZ, AND WESTBROOK, C&F 1988. !\COMMENT: !not existing in  
Aramco 1.3, lumped for now.  
HOC3H6O2=>CH3CHO+CH2O+OH  
+1.2500000E+010 +0.0000000E+000 +1.8900000E+004 !\AUTHOR: !\ !\COMMENT:  
ESTIMATED  
!C3H6OH1-2+O2<=>TQJC3H6OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.05E+114 -33.81 24741/  
!PLOG/ 0.01 2.13E+114 -33.44 26448/  
!PLOG/ 0.1 1.62E+110 -31.75 26612/  
!PLOG/ 1 6.00E+101 -28.79 25197/  
!PLOG/ 10 5.36E+89 -24.76 22402/  
!PLOG/ 40 1.55E+81 -21.95 20197/  
!PLOG/ 100 1.51E+75 -20 18578/  
!PLOG/ 200 3.16E+70 -18.48 17287/  
!  
!C3H6OH1-2+O2<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.21E+26 -5.09 5755/  
!PLOG/ 0.01 1.41E+31 -6.55 8781/  
!PLOG/ 0.1 5.08E+34 -7.53 11702/  
!PLOG/ 1 1.67E+34 -7.27 13418/  
!PLOG/ 10 2.82E+28 -5.41 13318/  
!PLOG/ 40 2.50E+22 -3.52 12314/  
!PLOG/ 100 2.82E+17 -1.99 11286/  
!PLOG/ 200 1.93E+13 -0.71 10340/  
!DUP  
!C3H6OH1-2+O2<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 2.45E+21 -4.19 6837/  
!PLOG/ 0.01 1.40E+30 -6.75 11554/  
!PLOG/ 0.1 9.11E+39 -9.56 17834/  
!PLOG/ 1 5.16E+42 -10.17 22412/  
!PLOG/ 10 6.07E+32 -6.94 22738/  
!PLOG/ 40 3.88E+20 -3.14 20677/  
!PLOG/ 100 3.32E+10 -0.03 18552/  
!PLOG/ 200 1.22E+02 2.57 16623/  
!DUP  
!C3H6OH1-2+O2<=>SC3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.26E+25 -4.69 5755/  
!PLOG/ 0.01 1.44E+30 -6.15 8785/  
!PLOG/ 0.1 4.78E+33 -7.11 11695/  
!PLOG/ 1 1.40E+33 -6.84 13395/  
!PLOG/ 10 2.12E+27 -4.96 13277/  
!PLOG/ 40 1.78E+21 -3.07 12265/  
!PLOG/ 100 1.97E+16 -1.53 11234/  
!PLOG/ 200 1.32E+12 -0.25 10285/  
!DUP  
!C3H6OH1-2+O2<=>SC3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:



!PLOG/ 0.001 3.22E+23 -4.69 5341/  
!PLOG/ 0.01 4.80E+28 -6.18 8461/  
!PLOG/ 0.1 1.71E+32 -7.16 11410/  
!PLOG/ 1 1.53E+32 -7.02 13378/  
!PLOG/ 10 5.55E+29 -6.14 15100/  
!PLOG/ 40 1.72E+26 -4.97 15849/  
!PLOG/ 100 4.46E+21 -3.51 15644/  
!PLOG/ 200 5.06E+16 -1.96 14979/  
!DUP  
!C3H6OH1-2+O2<=>TQC3H6OI 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 6.36E+104 -33.74 22390/  
!PLOG/ 0.01 7.96E+103 -33.01 22966/  
!PLOG/ 0.1 6.99E+96 -30.48 20584/  
!PLOG/ 1 1.04E+88 -27.47 16629/  
!PLOG/ 10 3.13E+96 -29.62 20346/  
!PLOG/ 40 2.79E+105 -32.04 24971/  
!PLOG/ 100 4.64E+109 -33.12 27657/  
!PLOG/ 200 2.06E+111 -33.48 29197/  
!C3H6OH1-2+O2<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 3.03E+37 -8.35 6940/  
!PLOG/ 0.01 1.07E+42 -9.64 9965/  
!PLOG/ 0.1 9.22E+43 -10.12 12427/  
!PLOG/ 1 1.14E+42 -9.42 13806/  
!PLOG/ 10 1.80E+38 -8.13 15131/  
!PLOG/ 40 1.61E+34 -6.8 15691/  
!PLOG/ 100 7.00E+29 -5.41 15552/  
!PLOG/ 200 3.74E+25 -4.06 15118/  
!C3H6OH1-2+O2<=>QC3H5OHP 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.18E+118 -37.6 26229 /  
!PLOG/ 0.01 1.91E+131 -40.73 34079/  
!PLOG/ 0.1 5.81E+138 -42.17 40750/  
!PLOG/ 1 5.05E+134 -40.19 43580/  
!PLOG/ 10 2.07E+117 -34.26 41516/  
!PLOG/ 40 1.71E+101 -29.04 38094/  
!PLOG/ 100 1.25E+89 -25.15 35203/  
!PLOG/ 200 2.98E+79 -22.09 32802/  
!C3H6OH1-2+O2<=>CY(COC)COH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 2.11E+18 -2.87 6870/  
!PLOG/ 0.01 3.02E+27 -5.54 11842/  
!PLOG/ 0.1 1.36E+37 -8.29 18165/  
!PLOG/ 1 1.21E+39 -8.66 22517/  
!PLOG/ 10 1.53E+28 -5.13 22530/  
!PLOG/ 40 2.72E+15 -1.16 20283/  
!PLOG/ 100 1.06E+05 2.06 18044/  
!PLOG/ 200 2.30E-04 4.73 16037/  
!C3H6OH1-2+O2<=>TQC3H5OHI 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.76E+53 -19.87 9019/  
!PLOG/ 0.01 4.68E+67 -23.92 11892/  
!PLOG/ 0.1 2.07E+91 -30.58 17347/  
!PLOG/ 1 2.84E+100 -32.4 20041/  
!PLOG/ 10 1.16E+115 -35.81 27656/  
!PLOG/ 40 4.87E+123 -37.83 33314/  
!PLOG/ 100 7.95E+124 -37.82 35683/

!PLOG/ 200 4.58E+122 -36.86 36374/  
!C3H6OH1-2+O2<=>CCY(COC)OH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.42E+32 -6.95 6210/  
!PLOG/ 0.01 5.19E+36 -8.24 9233/  
!PLOG/ 0.1 5.77E+38 -8.76 11715/  
!PLOG/ 1 2.86E+36 -7.95 12823/  
!PLOG/ 10 1.37E+32 -6.51 13646/  
!PLOG/ 40 2.15E+29 -5.56 14541/  
!PLOG/ 100 1.20E+26 -4.51 14778/  
!PLOG/ 200 3.31E+22 -3.37 14606/  
!TQJC3H6OH<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 9.73E+65 -18.5 42975/  
!PLOG/ 0.01 1.04E+64 -17.25 44419/  
!PLOG/ 0.1 7.90E+59 -15.59 44504/  
!PLOG/ 1 9.35E+53 -13.49 43566/  
!PLOG/ 10 4.13E+44 -10.39 41279/  
!PLOG/ 40 6.57E+38 -8.49 39745/  
!PLOG/ 100 8.32E+34 -7.23 38675/  
!PLOG/ 200 9.46E+31 -6.28 37849/  
!DUP  
!TQJC3H6OH<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 5.27E+64 -18 42872/  
!PLOG/ 0.01 4.82E+62 -16.74 44284/  
!PLOG/ 0.1 3.42E+58 -15.07 44348/  
!PLOG/ 1 4.05E+52 -12.97 43402/  
!PLOG/ 10 1.93E+43 -9.88 41120/  
!PLOG/ 40 3.28E+37 -7.99 39593/  
!PLOG/ 100 4.35E+33 -6.74 38527/  
!PLOG/ 200 5.13E+30 -5.79 37706/  
!DUP  
!TQJC3H6OH<=>TQC3H6OI 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 3.78E+50 -12.91 31539/  
!PLOG/ 0.01 1.42E+45 -10.94 30864/  
!PLOG/ 0.1 1.50E+40 -9.21 29932/  
!PLOG/ 1 3.12E+35 -7.64 28864/  
!PLOG/ 10 2.73E+29 -5.67 27243/  
!PLOG/ 40 8.88E+25 -4.54 26272/  
!PLOG/ 100 4.60E+23 -3.8 25622/  
!PLOG/ 200 9.08E+21 -3.25 25131/  
!TQJC3H6OH<=>QC3H5OHP 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 9.16E+62 -18.02 45297/  
!PLOG/ 0.01 2.56E+62 -17.1 47393/  
!PLOG/ 0.1 1.25E+59 -15.61 47984/  
!PLOG/ 1 1.97E+53 -13.49 47281/  
!PLOG/ 10 1.91E+43 -10.15 44926/  
!PLOG/ 40 7.68E+36 -8.05 43267/  
!PLOG/ 100 3.49E+32 -6.64 42089/  
!PLOG/ 200 1.77E+29 -5.57 41173/  
!TQJC3H6OH<=>TQC3H5OHI 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 9.57E+58 -15.99 38293/  
!PLOG/ 0.01 7.27E+54 -14.25 38593/  
!PLOG/ 0.1 8.30E+49 -12.44 38031/

!PLOG/ 1 1.90E+44 -10.51 36905/  
!PLOG/ 10 2.18E+36 -7.9 34865/  
!PLOG/ 40 4.10E+31 -6.36 33581/  
!PLOG/ 100 3.00E+28 -5.35 32704/  
!PLOG/ 200 1.34E+26 -4.59 32035/  
!TQC3H6OI<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 8.09E+38 -9.91 19096/  
!PLOG/ 0.01 9.09E+39 -9.93 19135/  
!PLOG/ 0.1 1.89E+41 -10.02 19407/  
!PLOG/ 1 7.47E+23 -4.1 14658/  
!PLOG/ 10 2.95E+33 -6.75 18685/  
!PLOG/ 40 4.24E+36 -7.56 20307/  
!PLOG/ 100 7.83E+36 -7.54 20747/  
!PLOG/ 200 7.63E+35 -7.17 20641/  
!QC3H5OHP<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 3.29E+57 -15.64 28576/  
!PLOG/ 0.01 9.65E+58 -15.75 29927/  
!PLOG/ 0.1 2.19E+50 -12.66 28547/  
!PLOG/ 1 1.67E+49 -12.05 29204/  
!PLOG/ 10 7.08E+40 -9.26 27188/  
!PLOG/ 40 1.32E+30 -5.82 24071/  
!PLOG/ 100 1.15E+30 -5.8 24053/  
!PLOG/ 200 1.12E+30 -5.8 24050/  
!QC3H5OHP<=>CY(COC)COH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.11E+51 -12.97 28497/  
!PLOG/ 0.01 5.58E+51 -12.87 29529/  
!PLOG/ 0.1 3.03E+44 -10.28 28326/  
!PLOG/ 1 1.42E+44 -9.98 28986/  
!PLOG/ 10 9.69E+37 -7.93 27491/  
!PLOG/ 40 5.90E+29 -5.3 25095/  
!PLOG/ 100 5.27E+29 -5.29 25081/  
!PLOG/ 200 5.15E+29 -5.28 25078/  
!TQC3H5OHI<=>CCY(COC)OH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.10E+31 -7.21 14640/  
!PLOG/ 0.01 1.37E+32 -7.24 14716/  
!PLOG/ 0.1 3.34E+33 -7.35 15127/  
!PLOG/ 1 1.86E+23 -3.68 12864/  
!PLOG/ 10 9.88E+31 -6.23 16040/  
!PLOG/ 40 1.25E+34 -6.78 17056/  
!PLOG/ 100 7.73E+33 -6.67 17176/  
!PLOG/ 200 2.13E+33 -6.45 17170/  
!TQC3H5OHI<=>SC3H5OH+HO2 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 6.01E+27 -7.27 14658/  
!PLOG/ 0.01 7.78E+28 -7.3 14733/  
!PLOG/ 0.1 3.27E+30 -7.48 15191/  
!PLOG/ 1 2.81E+17 -2.82 12336/  
!PLOG/ 10 1.92E+26 -5.22 16146/  
!PLOG/ 40 7.61E+27 -5.49 17483/  
!PLOG/ 100 1.91E+26 -4.86 17429/  
!PLOG/ 200 2.94E+24 -4.18 17285/  
!  
!C3H6OH2-1+O2<=>IQJC3H6OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:

!PLOG/ 0.001 3.34E+111 -32.67 25143/  
!PLOG/ 0.01 4.84E+107 -31.05 25460/  
!PLOG/ 0.1 2.41E+100 -28.42 24474/  
!PLOG/ 1 4.55E+89 -24.78 22176/  
!PLOG/ 10 1.14E+76 -20.31 18721/  
!PLOG/ 40 9.25E+66 -17.35 16238/  
!PLOG/ 100 6.20E+60 -15.36 14499/  
!PLOG/ 200 1.30E+56 -13.86 13159/  
!  
!C3H6OH2-1+O2<=>CHOCOCH3+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.59E+15 -1.63 8947/  
!PLOG/ 0.01 5.07E+20 -3.24 11938/  
!PLOG/ 0.1 5.00E+25 -4.66 15251/  
!PLOG/ 1 3.18E+26 -4.79 17388/  
!PLOG/ 10 6.00E+20 -2.95 17297/  
!PLOG/ 40 1.70E+14 -0.91 16099/  
!PLOG/ 100 7.91E+08 0.73 14913/  
!PLOG/ 200 3.03E+04 2.08 13854/  
!  
!C3H6OH2-1+O2<=>IQC3H6OT 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.12E+102 -32.4 23496/  
!PLOG/ 0.01 4.23E+95 -30.04 22067/  
!PLOG/ 0.1 3.45E+83 -26.08 17114/  
!PLOG/ 1 8.16E+82 -25.61 16198/  
!PLOG/ 10 1.04E+97 -29.54 22648/  
!PLOG/ 40 7.25E+103 -31.42 26487/  
!PLOG/ 100 2.48E+106 -32.06 28397/  
!PLOG/ 200 1.39E+107 -32.2 29446/  
!  
!C3H6OH2-1+O2<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 4.39E+48 -11.88 11603/  
!PLOG/ 0.01 9.82E+50 -12.49 14143/  
!PLOG/ 0.1 3.43E+49 -11.94 15561/  
!PLOG/ 1 2.43E+45 -10.56 16415/  
!PLOG/ 10 4.98E+39 -8.68 17473/  
!PLOG/ 40 7.99E+33 -6.83 17502/  
!PLOG/ 100 1.02E+29 -5.28 17165/  
!PLOG/ 200 7.18E+24 -3.99 16747/  
!  
!C3H6OH2-1+O2<=>CH3+HO2CH2CHO 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 2.91E+40 -9.23 10830/  
!PLOG/ 0.01 9.66E+43 -10.2 13698/  
!PLOG/ 0.1 1.34E+44 -10.13 15661/  
!PLOG/ 1 2.57E+41 -9.18 17047/  
!PLOG/ 10 1.82E+36 -7.46 18330/  
!PLOG/ 40 8.82E+29 -5.44 18205/  
!PLOG/ 100 1.74E+24 -3.65 17600/  
!PLOG/ 200 2.16E+19 -2.12 16925/  
!  
!C3H6OH2-1+O2<=>IQC3H5OHPJ 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.03E+115 -35.13 25407/  
!PLOG/ 0.01 1.10E+129 -38.89 32891/  
!PLOG/ 0.1 5.15E+135 -40.38 38573/

!PLOG/ 1 7.27E+129 -38.13 39933/  
!PLOG/ 10 4.50E+112 -32.49 37045/  
!PLOG/ 40 7.72E+97 -27.79 33612/  
!PLOG/ 100 5.17E+86 -24.26 30799/  
!PLOG/ 200 4.70E+77 -21.41 28440/  
!  
!C3H6OH2-1+O2<=>C2H3OH+CH2O+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 5.10E+24 -4.31 13009/  
!PLOG/ 0.01 6.91E+33 -6.97 17935/  
!PLOG/ 0.1 1.74E+41 -9.03 23613/  
!PLOG/ 1 2.26E+36 -7.32 25633/  
!PLOG/ 10 3.15E+17 -1.4 22782/  
!PLOG/ 40 9.35E+00 3.71 19114/  
!PLOG/ 100 5.59E-12 7.46 16156/  
!PLOG/ 200 1.27E-21 10.41 13733/  
!  
!C3H6OH2-1+O2<=>CY(CCOC)OH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\  
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 3.06E+33 -7.24 11476/  
!PLOG/ 0.01 6.56E+42 -9.92 17197/  
!PLOG/ 0.1 8.24E+46 -10.95 22090/  
!PLOG/ 1 4.48E+38 -8.22 23019/  
!PLOG/ 10 1.01E+18 -1.77 19496/  
!PLOG/ 40 1.16E+01 3.44 15637/  
!PLOG/ 100 4.85E-12 7.23 12599/  
!PLOG/ 200 8.64E-22 10.21 10126/  
!!  
!IQJC3H6OH<=>CHOCOCH3+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 3.58E+71 -20.62 52656/  
!PLOG/ 0.01 9.67E+71 -20.08 54935/  
!PLOG/ 0.1 3.39E+67 -18.18 55330/  
!PLOG/ 1 7.26E+58 -15.09 54016/  
!PLOG/ 10 4.57E+46 -11.01 51172/  
!PLOG/ 40 4.31E+38 -8.38 49054/  
!PLOG/ 100 2.12E+33 -6.66 47587/  
!PLOG/ 200 2.72E+29 -5.41 46486/  
!!  
!IQJC3H6OH<=>IQC3H6OT 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.04E+45 -11.2 31755/  
!PLOG/ 0.01 2.90E+40 -9.62 30945/  
!PLOG/ 0.1 4.85E+35 -8.01 29850/  
!PLOG/ 1 2.62E+30 -6.28 28498/  
!PLOG/ 10 3.37E+24 -4.37 26873/  
!PLOG/ 40 9.75E+20 -3.23 25861/  
!PLOG/ 100 5.61E+18 -2.52 25208/  
!PLOG/ 200 1.44E+17 -2.01 24740/  
!  
!IQJC3H6OH<=>IQC3H5OHPJ 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.36E+50 -12.93 36743/  
!PLOG/ 0.01 3.36E+45 -11.27 36143/  
!PLOG/ 0.1 1.13E+40 -9.41 34990/  
!PLOG/ 1 5.93E+33 -7.33 33438/  
!PLOG/ 10 4.24E+26 -5 31502/  
!PLOG/ 40 1.97E+22 -3.61 30275/

!PLOG/ 100 3.43E+19 -2.72 29477/  
!PLOG/ 200 3.69E+17 -2.09 28900/  
!  
!IQC3H6OT<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 9.82E+39 -9.95 20737/  
!PLOG/ 0.01 1.19E+41 -9.97 20814/  
!PLOG/ 0.1 2.60E+42 -10.07 21229/  
!PLOG/ 1 2.63E+32 -6.47 19139/  
!PLOG/ 10 1.32E+40 -8.68 22120/  
!PLOG/ 40 4.04E+41 -9.03 23000/  
!PLOG/ 100 9.07E+40 -8.77 23008/  
!PLOG/ 200 6.70E+39 -8.38 22782/  
!  
!IQC3H6OT<=>CH3+HO2CH2CHO 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 2.04E+37 -9.27 20741/  
!PLOG/ 0.01 2.54E+38 -9.29 20821/  
!PLOG/ 0.1 7.13E+39 -9.42 21267/  
!PLOG/ 1 2.95E+28 -5.34 18891/  
!PLOG/ 10 1.31E+36 -7.46 22106/  
!PLOG/ 40 2.19E+37 -7.68 23084/  
!PLOG/ 100 1.39E+36 -7.22 23018/  
!PLOG/ 200 2.67E+34 -6.63 22672/  
!  
!IQC3H5OHPJ<=>C2H3OH+CH2O+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 4.25E+16 -3.66 19364/  
!PLOG/ 0.01 2.98E+33 -8.01 27106/  
!PLOG/ 0.1 3.46E+38 -8.83 31412/  
!PLOG/ 1 7.07E+28 -5.46 29633/  
!PLOG/ 10 2.01E+13 -0.43 25278/  
!PLOG/ 40 1.43E+13 -0.38 25238/  
!PLOG/ 100 1.38E+13 -0.38 25234/  
!PLOG/ 200 1.37E+13 -0.37 25233/  
!  
!IQC3H5OHPJ<=>CY(CCOC)OH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF:  
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 1.12E+25 -5.59 19349/  
!PLOG/ 0.01 7.20E+32 -7.6 23093/  
!PLOG/ 0.1 2.22E+34 -7.65 25130/  
!PLOG/ 1 2.40E+27 -5.28 23663/  
!PLOG/ 10 2.24E+17 -2.04 20810/  
!PLOG/ 40 1.82E+17 -2.01 20786/  
!PLOG/ 100 1.78E+17 -2.01 20783/  
!PLOG/ 200 1.77E+17 -2.01 20782/  
!  
!IQC3H5OHPJ<=>AC3H5OOH+OH 1.420E+036 -15.840 11594.0 !\AUTHOR: !\ REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT:  
!PLOG/ 0.001 6.07E+13 -4.21 22478/  
!PLOG/ 0.01 9.74E+39 -10.89 33616/  
!PLOG/ 0.1 2.18E+49 -12.65 40359/  
!PLOG/ 1 3.32E+37 -8.42 38539/  
!PLOG/ 10 2.34E+16 -1.56 32712/  
!PLOG/ 40 1.44E+16 -1.49 32656/  
!PLOG/ 100 1.38E+16 -1.48 32651/  
!PLOG/ 200 1.37E+16 -1.48 32649/  
!

```

!!TQJC3H6OH=>CH3CHO+CH2O+OH 1.250E+011 0.000 18900.0 !\AUTHOR:
!\REF:CURRAN ESTIMATE
!=====
!!\ENDSUBSPECIES: \C3H6OH2-1/C3H6OH2-1
!=====
!!=====
!!\SUBSPECIES: \CY(COC)COH\CCY(COC)OH\CY(CCOC)OH\CHOCOCH3
!!=====
!CY(COC)COH+OH=>C2H2OH+CH2O+H2O 1.26E3 2.97 -2660.6 !\AUTHOR: !\ C-W
ZHOU, J. M. SIMMIE, AND H. J. CURRAN, COMBUST AND FLAME, 2011, 158, 726-
731 !\COMMENT:
!CY(COC)COH+OH=>C2H3CHO+OH+H2O 5.66E2 2.93 -4039.4 !\AUTHOR: !\ C-W ZHOU,
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:
!CY(COC)COH+OH=>CH2CO+CH2OH+H2O 2.26E3 2.73 -4688 !\AUTHOR: !\ C-W ZHOU,
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:
!CY(COC)COH+HO2=>C2H2OH+CH2O+H2O2 1.4E-5 5.26 8267.9 !\AUTHOR: !\ C-W
ZHOU, J. M. SIMMIE, AND H. J. CURRAN, IJCK, 2012, 44, 155-164 !\COMMENT:
!CY(COC)COH+HO2=>C2H3CHO+OH+H2O2 1.81E-1 3.98 9056.7 !\AUTHOR: !\ J.
MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:
!CY(COC)COH+HO2=>CH2CO+CH2OH+H2O2 8.6 3.46 9732.326 !\AUTHOR: !\ J.
MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:
!
!CCY(COC)OH+OH=>CH3CHCO+OH+H2O 2.26E3 2.73 -4688 !\AUTHOR: !\ C-W ZHOU,
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:
!CCY(COC)OH+HO2=>CH3CHCO+OH+H2O2 8.6 3.46 9732.326 !\AUTHOR: !\ J.
MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:
!
!CY(CCOC)OH+OH=>CH2O+CH2CO+H+H2O 2.26E3 2.73 -4688 !\AUTHOR: !\ C-W ZHOU,
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:
!CY(CCOC)OH+OH=>CH2O+C2H2OH+H2O 5.66E2 2.93 -4039.4 !\AUTHOR: !\ C-W
ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233
!\COMMENT:
!CY(CCOC)OH+HO2=>CH2O+CH2CO+H+H2O2 8.6 3.46 9732.326 !\AUTHOR: !\ J.
MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:
!CY(CCOC)OH+HO2=>CH2O+C2H2OH+H2O2 1.81E-1 3.98 9056.7 !\AUTHOR: !\ J.
MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:
!
!CHOCOCH3+OH=>CH3CHCO+OH+H2O 61329.9 2.65 -4586.4 !\AUTHOR: !\REF:J.
MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.
!\COMMENT:
!!=====
!!\ENDSUBSPECIES: \CY(COC)COH\CCY(COC)OH\CY(CCOC)OH\CHOCOCH3
!!=====
!!=====
!!\SUBSPECIES: \SC3H5OH
!!=====
!

```

---

```

!\REACTIONCLASS: \UNIMOL \A
\n \EA

```

!  
-----  
SC3H5OH<=>C2H5CHO  
+8.5900000E+011 +3.1800000E-001 +5.5900000E+004 !\AUTHOR: !\REF:SARATHY  
ET AL. CNF2012 !\COMMENT:  
!

-----  
!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

-----  
SC3H5OH+O2=>C2H3CHO+H+HO2  
+3.0000000E+013 +0.0000000E+000 +3.9100000E+004 !\AUTHOR: !\REF:BILL  
SEPT 2013 !\COMMENT: FOR SC3H5OH, ASSUME THAT THE ALLYL HYDROGEN IS  
ABSTRACTED AND THEN C2H3CHO+H ARE F  
SC3H5OH+OH=>C2H3CHO+H+H2O  
+3.1000000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF: TSANG  
1991 !\COMMENT:  
SC3H5OH+H=>C2H3CHO+H+H2  
+1.7300000E+005 +2.5000000E+000 +2.4920000E+003 !\AUTHOR: !\REF: TSANG  
1991 !\COMMENT:  
SC3H5OH+O=>C2H3CHO+H+OH  
+1.7500000E+012 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF: TSANG  
1991 !\COMMENT:  
SC3H5OH+HO2=>C2H3CHO+H+H2O2  
+9.6000000E+003 +2.6000000E+000 +1.3900000E+004 !\AUTHOR: !\REF: TSANG  
1991 !\COMMENT:  
SC3H5OH+CH3=>C2H3CHO+H+CH4  
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF: TSANG  
1991 !\COMMENT:  
SC3H5OH+CH3O2=>C2H3CHO+H+CH3O2H  
+9.6000000E+003 +2.6000000E+000 +1.3900000E+004 !\AUTHOR: !\REF: USE  
HO2 ABSTRACTION RATE CONSTANT !\COMMENT:  
SC3H5OH+CH3O=>C2H3CHO+H+CH3OH  
+8.3000000E+010 +0.0000000E+000 +2.6000000E+003 !\AUTHOR: !\REF:  
LITERATURE SOURCE UNKNOWN !\COMMENT: USED SECONDARY ALKYL H RATE FOR N-  
ALKANE+CH3O, REDUCED EA BY DIFFERENCE BETWEEN BD  
SC3H5OH+HO2<=>C2H5CHO+HO2  
+1.4900000E+005 +1.6700000E+000 +6.8100000E+003 !\AUTHOR: !\REF:  
DASILVA, BOZZELLI, CHEM. PHYS. LETT. 483 (2009) 25-29. !\COMMENT: !\REF:  
FROM PROPANOL, MAN ET AL. CNF2013:  
SC3H5OH+HOCHO<=>C2H5CHO+HOCHO +2.8100000E-  
002 +3.2860000E+000 -4.5090000E+003 !\AUTHOR: !\REF: DASILVA, ANGEW.  
CHEM. 122 (2010) 7685-7687 !\COMMENT:

=====  
!\ENDSUBSPECIES: \SC3H5OH  
=====

!!\SUBSPECIES: \TQC3H5OHI  
=====

!!  
-----  
!!\REACTIONCLASS: \R+O2 \A \N \EA



!!

---

!TQC3H5OHI+O2<=>TQC3H5OHIO2 5.05E+12 -0.1 -695.45 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT: !\  
ANALOGY TO O2+QOOH\_2

!TQC3H5OHIO2<=>TQC3H5OHIO-I 2.56E+12 -0.13 34360 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!TQC3H5OHIO-I<=>HO2CHO+CH3CHO+OH 5.819E+05 2.40 22790 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!TQC3H5OHIO-I<=>C3KET12+HO2 1.829E+10 0.790 15100 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!TQC3H5OHIO2<=>TQC3H5OHIO-P 5.69E+08 7.80E-01 21850 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!TQC3H5OHIO-P<=>C2H3COHOOH+HO2 1.83E+10 7.90E-01 15100 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!TQC3H5OHIO-P<=>C2H3OOH+HOCHO+OH 5.38E+11 0.070 24800 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!TQC3H5OHIO-P<=>COHOHCY(COC)+OH 2.28E+08 1.29E+00 9890 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!TQC3H5OHIO-P<=>OHCY(COCC)OOH+OH 4.58E+15 -1.08E+00 18440 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!C2H3COHOOH=>HOCHO+C2H3+OH 1.59E+20 -1.5 42879.46 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!COHOHCY(COC)=>HOCHO+CH2CHO+OH 1.59E+20 -1.5 42879.46 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!OHCY(COCC)OOH=>HOCHO+CH2CHO+OH 1.59E+20 -1.5 42879.46 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!

!TQC3H5OHIO2<=>TQC3H5OHTO2 2.956E+09 0.04 16350 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!TQC3H5OHTO2<=>OHCOCOHCY(COC)+OH 1.2E+10 0.35 15700 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!OHCOCOHCY(COC)=>CO+CH3CHO+2OH 1.59E+20 -1.5 42879.46 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!

!IQC3H5OHPJ+O2<=>IQC3H5OHPJO2 9.35626E+11 0.1 -1072.98 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!IQC3H5OHPJO2<=>IQC3H5OTQ-I 4.13E+07 1.0 21070 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!IQC3H5OTQ-I=>OH+CH2O+HO2CH2CHO 1.20E+10 0.35 15700 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!HO2CH2CHO=>OH+CH2O+HCO 1.59E+20 -1.5 42879.46 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!

!IQC3H5OHPJO2<=>IQC3H5OHQ-SJ 8.204E10 0.13 19470 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!IQC3H5OHQ-SJ<=>CHOCOHCY(COC)+OH 1.2E+10 0.35 15700 !\AUTHOR: !\ C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:  
!CHOCOHCY(COC)=>OH+CH2O+H+CHOCHO 1.59E+20 -1.5 42879.46 !\AUTHOR: !\ C  
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION  
!\COMMENT:

!

!!=====
=====
!!\ENDSUBSPECIES: \TQC3H5OHI
!!=====
=====

!
-----
!\REACTIONCLASS: \AROMATIC\_GROWTH \A
\N \EA
!

C3H5-A+C2H2<=>CVCCVCCJ
+1.0000000E+012 +0.0000000E+000 +6.8834000E+003 !\AUTHOR: !\REF:CURRAN
ESTIMATE !\COMMENT:
C3H5-A+C2H3=>C5H6+H+H
+1.6000000E+035 -1.4000000E+001 +6.1137700E+004 !\AUTHOR: !\REF:CURRAN
ESTIMATE !\COMMENT:

!-----
!-----
!\ENDSUBMECH: C3H6
!-----
!-----
!-----

!\SUBMECH: \C3H4-A\C3H4-P
!\MECHCOMMENTS: KPS, 22/07/2015 REACTION CH3CHCHO+H2<=>C2H5CHO+H MOVED
FROM JOHN BUGLERS C5 MECHANISM TO THIS MECHANISM AS THIS IS FIRST
!\MECHCOMMENTS: INSTANCE OF CH3CHCHO APPEARING IN MASTER MECHANISM. THE
ABOVE CROSS REACTION DOES NOT MEAN THAT A C2H5CHO MECHANISM IS REQUIRED
TO SIMULATE THE
!\MECHCOMMENTS: PYROLYSIS OF C3H4-A/C3H4-P AS CH3CHCHO IS ONLY FORMED IN
THE OXIDATION OF C3H4-A/C3H4-P DUE TO AN OH ADDITION REACTION
!\MECHWARNINGS: THERE APPEAR TO BE SOME POORLY DOCUMENTED RATE CONSTANTS
IN THE C3H2 AND AROMATIC GROWTH SUB-MODULES. THE C3H3 RECOMBINATION RATE
CONSTANTS ARE A MESS. KPS 31/07/2015

!-----
!-----
!

!\REACTIONCLASS: \UNIMOL \A
\N \EA
!

C2H+CH3<=>C3H4-P
+8.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:PITZ
ESTIMATE !\COMMENT:
C3H4-A<=>C3H4-P
+4.7860000E+048 -1.0000000E+001 +8.8685000E+004 !\AUTHOR: !\REF:
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN
BASEMECH2907\_C7.INP
PLOG / +1.0000000E+000
+7.7620000E+039 -7.8000000E+000 +7.8446000E+004 /
PLOG / +1.0000000E+001
+4.7860000E+048 -1.0000000E+001 +8.8685000E+004 /
CC3H4<=>C3H4-P
+1.6600000E+037 -7.2400000E+000 +4.8013000E+004 !\AUTHOR: !\REF:
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN
BASEMECH2907\_C7.INP

PLOG / +3.9500000E-002  
+2.5120000E+050 -1.1820000E+001 +5.0914000E+004 /  
PLOG / +1.0000000E+000  
+1.2300000E+037 -7.5100000E+000 +4.5551000E+004 /  
PLOG / +1.0000000E+001  
+1.6600000E+037 -7.2400000E+000 +4.8013000E+004 /  
CC3H4<=>C3H4-A  
+5.0120000E+035 -6.8700000E+000 +5.1298000E+004 !\AUTHOR: !\REF:  
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN  
BASEMECH2907\_C7.INP  
PLOG / +3.9500000E-002  
+9.7720000E+043 -9.9700000E+000 +5.6007000E+004 /  
PLOG / +1.0000000E+000  
+2.5120000E+026 -4.5600000E+000 +4.3922000E+004 /  
PLOG / +1.0000000E+001  
+5.0120000E+035 -6.8700000E+000 +5.1298000E+004 /  
C3H4-P<=>C3H3+H  
+6.4800000E+030 -4.6550000E+000 +9.3925200E+004 !\AUTHOR: !\REF:  
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN  
BASEMECH2907\_C7.INP  
PLOG / +1.0000000E+000  
+6.4800000E+030 -4.6550000E+000 +9.3925200E+004 /  
PLOG / +1.0000000E+001  
+1.2100000E+025 -2.7870000E+000 +9.2376100E+004 /  
C3H4-A<=>C3H3+H  
+1.3200000E+031 -4.7490000E+000 +9.2079500E+004 !\AUTHOR: !\REF:  
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN  
BASEMECH2907\_C7.INP  
PLOG / +1.0000000E+000  
+1.3200000E+031 -4.7490000E+000 +9.2079500E+004 /  
PLOG / +1.0000000E+001  
+3.6500000E+025 -2.9500000E+000 +9.0624900E+004 /  
C3H3+H<=>CC3H4  
+3.2360000E+018 -2.0500000E+000 +2.0530000E+003 !\AUTHOR: !\REF:  
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN  
BASEMECH2907\_C7.INP  
PLOG / +3.9500000E-002  
+8.9130000E+112 -2.8260000E+001 +8.3611000E+004 /  
PLOG / +1.0000000E+000  
+1.0720000E+021 -2.9500000E+000 +2.6870000E+003 /  
PLOG / +1.0000000E+001  
+3.2360000E+018 -2.0500000E+000 +2.0530000E+003 /  
!

---

!\REACTIONCLASS: \R\_CAT\_ISO \A  
\N \EA  
!

---

C3H4-P+C3H3<=>C3H4-A+C3H3  
+6.1400000E+006 +1.7400000E+000 +1.0450000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

C3H4-P+O2<=>C3H3+HO2  
+3.0000000E+013 +0.0000000E+000 +4.2630000E+004 !\AUTHOR: !\REF:  
WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO REFERENCE IN  
BASEMECH2907\_C7.INP  
C3H4-P+O<=>C3H3+OH  
+7.6500000E+008 +1.5000000E+000 +8.6000000E+003 !\AUTHOR:  
\REF:GLAUDE,P.A. ET AL,PROC. COMBUST. INST !\COMMENT:  
C3H4-P+H<=>C3H3+H2  
+3.5720000E+004 +2.8250000E+000 +4.8210000E+003 !\AUTHOR: !\REF:  
ANALOGIES WITH C3H6 A AND S !\COMMENT:  
C3H4-P+OH<=>C3H3+H2O  
+4.9400000E+006 +2.0270000E+000 +1.0596000E+003 !\AUTHOR: !\REF:  
ANALOGIES WITH C3H6 A AND S !\COMMENT:  
C3H4-P+HO2<=>C3H3+H2O2 +9.5500000E-  
002 +4.1700000E+000 +9.6328000E+003 !\AUTHOR: !\REF:DAGAUT, P. ET AL.,  
CST 71, 111(1990). !\COMMENT:  
C3H4-P+CH3<=>C3H3+CH4  
+1.8000000E+012 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H4-P+CH3O2<=>C3H3+CH3O2H +9.5500000E-  
002 +4.1700000E+000 +9.6328000E+003 !\AUTHOR: !\REF:DAGAUT, P. ET AL.,  
CST 71, 111(1990). !\COMMENT:  
C3H4-P+C2H<=>C2H2+C3H3  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H4-P+C2H3<=>C3H3+C2H4  
+1.0000000E+012 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H4-P+C3H5-A<=>C3H3+C3H6  
+3.0000000E+012 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H4-A+H<=>C3H3+H2  
+6.6250000E+003 +3.0950000E+000 +5.5220000E+003 !\AUTHOR: !\REF:  
ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:  
C3H4-A+O2<=>C3H3+HO2  
+4.0000000E+013 +0.0000000E+000 +4.1320000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:  
C3H4-A+OH<=>C3H3+H2O  
+1.4820000E+005 +2.4920000E+000 +1.8072000E+003 !\AUTHOR: !\REF:  
ANALOGIES WITH C3H6 A AND S !\COMMENT:  
C3H4-A+CH3<=>C3H3+CH4  
+1.3000000E+012 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C3H4-A+HO2<=>C3H3+H2O2 +3.5800000E-  
002 +4.1700000E+000 +9.6328000E+003 !\AUTHOR: !\REF:DAGAUT, P. ET AL.,  
CST 71, 111(1990). !\COMMENT:  
C3H4-A+CH3O2<=>C3H3+CH3O2H +7.1610000E-  
002 +4.1700000E+000 +9.6328000E+003 !\AUTHOR: !\REF:DAGAUT, P. ET AL.,  
CST 71, 111(1990). !\COMMENT:  
C3H4-A+C3H5-A<=>C3H3+C3H6  
+2.0000000E+011 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_ADDITION\H  
\N \EA

\A

---

C3H4-A+H<=>C3H4-P+H

+2.4400000E+010 +1.0400000E+000 +2.1590000E+003 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT:

PLOG / +1.0000000E-003

+8.4900000E+010 +8.9000000E-001 +2.5030000E+003 /

PLOG / +3.9000000E-002

+1.4800000E+013 +2.6000000E-001 +4.1030000E+003 /

PLOG / +1.0000000E+000

+2.4800000E+015 -3.3000000E-001 +6.4360000E+003 /

PLOG / +1.0000000E+001

+2.3500000E+025 -3.2300000E+000 +1.3165000E+004 /

PLOG / +1.0000000E+002

+1.0200000E+024 -2.6700000E+000 +1.5552000E+004 /

DUP

C3H4-A+H<=>C3H4-P+H

+2.4400000E+010 +1.0400000E+000 +2.1590000E+003 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE

PLOG / +1.0000000E-003 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /

PLOG / +3.9000000E-002 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /

PLOG / +1.0000000E+000 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /

PLOG / +1.0000000E+001  
+1.7900000E+007 +1.9800000E+000 +4.5210000E+003 /

PLOG / +1.0000000E+002  
+4.6300000E+004 +2.6200000E+000 +4.4660000E+003 /

DUP

C3H4-A+H<=>C3H5-A

+2.2100000E+061 -1.5250000E+001 +2.0076000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE

PLOG / +1.0000000E-003  
+2.2100000E+061 -1.5250000E+001 +2.0076000E+004 /

PLOG / +3.9000000E-002  
+1.2400000E+052 -1.2020000E+001 +1.7839000E+004 /

PLOG / +1.0000000E+000  
+4.6700000E+051 -1.1450000E+001 +2.1340000E+004 /

PLOG / +1.0000000E+001  
+3.7500000E+048 -1.0270000E+001 +2.2511000E+004 /

PLOG / +1.0000000E+002  
+4.2300000E+043 -8.6100000E+000 +2.2522000E+004 /

DUP

C3H4-A+H<=>C3H5-A

+2.2100000E+061 -1.5250000E+001 +2.0076000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE

PLOG / +1.0000000E-003  
+2.8000000E+038 -8.6700000E+000 +8.0350000E+003 /

PLOG / +3.9000000E-002  
+9.3300000E+036 -8.1900000E+000 +7.4620000E+003 /

PLOG / +1.0000000E+000  
+3.3200000E+030 -5.7800000E+000 +6.9130000E+003 /

PLOG / +1.0000000E+001  
+2.2900000E+026 -4.3200000E+000 +6.1630000E+003 /

PLOG / +1.0000000E+002  
+4.3800000E+021 -2.7100000E+000 +5.1870000E+003 /

DUP

C3H4-A+H<=>C3H5-S

+1.1000000E+030 -6.5200000E+000 +1.5200000E+004 !\AUTHOR: !\REF:DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT:

PLOG / +1.0000000E-001

+1.1000000E+030 -6.5200000E+000 +1.5200000E+004 /

PLOG / +1.0000000E+000

+5.4000000E+029 -6.0900000E+000 +1.6300000E+004 /

PLOG / +1.0000000E+001

+2.6000000E+031 -6.2300000E+000 +1.8700000E+004 /

PLOG / +1.0000000E+002

+3.2000000E+031 -5.8800000E+000 +2.1500000E+004 /

C3H4-A+H<=>C3H5-T

+6.4400000E+102 -2.7510000E+001 +5.1768000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE

IF CORRECT REFERENCE

PLOG / +1.0000000E-003

+6.4400000E+102 -2.7510000E+001 +5.1768000E+004 /

PLOG / +3.9000000E-002

+1.5500000E+053 -1.3100000E+001 +1.4472000E+004 /

PLOG / +1.0000000E+000

+1.9000000E+053 -1.2590000E+001 +1.6726000E+004 /

PLOG / +1.0000000E+001

+7.9500000E+051 -1.1820000E+001 +1.8286000E+004 /

PLOG / +1.0000000E+002

+4.2100000E+052 -1.1640000E+001 +2.2262000E+004 /

DUP

C3H4-A+H<=>C3H5-T

+6.4400000E+102 -2.7510000E+001 +5.1768000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE

IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003

+1.1000000E+054 -1.4290000E+001 +1.0809000E+004 /

PLOG / +3.9000000E-002

+9.8800000E+044 -1.1210000E+001 +8.2120000E+003 /

PLOG / +1.0000000E+000

+2.8100000E+040 -9.4200000E+000 +7.8500000E+003 /

PLOG / +1.0000000E+001

+2.6000000E+035 -7.5700000E+000 +7.1470000E+003 /

PLOG / +1.0000000E+002

+9.8800000E+029 -5.5300000E+000 +6.5810000E+003 /

DUP

C3H4-A+H<=>CH3+C2H2

+3.7400000E+001 +3.3500000E+000 +5.7800000E+001 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE

IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003

+1.2300000E+008 +1.5300000E+000 +4.7370000E+003 /

PLOG / +3.9000000E-002

+2.7200000E+009 +1.2000000E+000 +6.8340000E+003 /

PLOG / +1.0000000E+000

+1.2600000E+020 -1.8300000E+000 +1.5003000E+004 /

PLOG / +1.0000000E+001

+1.6800000E+016 -6.0000000E-001 +1.4754000E+004 /

PLOG / +1.0000000E+002

+1.3700000E+017 -7.9000000E-001 +1.7603000E+004 /

DUP

C3H4-A+H<=>CH3+C2H2

+3.7400000E+001 +3.3500000E+000 +5.7800000E+001 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +3.9000000E-002 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +1.0000000E+000  
+1.2300000E+004 +2.6800000E+000 +6.3350000E+003 /  
PLOG / +1.0000000E+001  
+3.3100000E+008 +1.1400000E+000 +8.8860000E+003 /  
PLOG / +1.0000000E+002  
+1.2800000E+006 +1.7100000E+000 +9.7740000E+003 /

DUP

C3H4-P+H<=>C3H5-T

+8.8500000E+051 -1.3040000E+001 +1.2325000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003  
+8.8500000E+051 -1.3040000E+001 +1.2325000E+004 /  
PLOG / +3.9000000E-002  
+3.1700000E+052 -1.2690000E+001 +1.4226000E+004 /  
PLOG / +1.0000000E+000  
+2.8700000E+053 -1.2510000E+001 +1.6853000E+004 /  
PLOG / +1.0000000E+001  
+9.5100000E+051 -1.1740000E+001 +1.8331000E+004 /  
PLOG / +1.0000000E+002  
+4.5100000E+052 -1.1580000E+001 +2.2207000E+004 /

DUP

C3H4-P+H<=>C3H5-T

+8.8500000E+051 -1.3040000E+001 +1.2325000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003  
+1.9700000E+046 -1.1910000E+001 +7.4560000E+003 /  
PLOG / +3.9000000E-002  
+2.5900000E+045 -1.1230000E+001 +8.0460000E+003 /  
PLOG / +1.0000000E+000  
+6.9300000E+039 -9.1100000E+000 +7.4580000E+003 /  
PLOG / +1.0000000E+001  
+6.8000000E+034 -7.2900000E+000 +6.7220000E+003 /  
PLOG / +1.0000000E+002  
+5.6500000E+029 -5.3900000E+000 +6.1500000E+003 /

DUP

C3H4-P+H<=>C3H5-S

+3.3800000E+049 -1.2750000E+001 +1.4072000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +3.9000000E-002  
+3.3800000E+049 -1.2750000E+001 +1.4072000E+004 /  
PLOG / +1.0000000E+000  
+1.3700000E+051 -1.2550000E+001 +1.5428000E+004 /  
PLOG / +1.0000000E+001  
+3.8800000E+050 -1.1900000E+001 +1.6915000E+004 /

PLOG / +1.0000000E+002  
+2.1700000E+049 -1.1100000E+001 +1.8746000E+004 /  
DUP  
C3H4-P+H<=>C3H5-S  
+3.3800000E+049 -1.2750000E+001 +1.4072000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.  
PLOG / +1.0000000E-003  
+1.4900000E+038 -1.0110000E+001 +7.4580000E+003 /  
PLOG / +3.9000000E-002  
+2.9800000E+043 -1.1430000E+001 +8.7360000E+003 /  
PLOG / +1.0000000E+000  
+5.7500000E+039 -9.5100000E+000 +8.7720000E+003 /  
PLOG / +1.0000000E+001  
+4.3300000E+040 -9.6000000E+000 +9.4010000E+003 /  
PLOG / +1.0000000E+002  
+3.4400000E+034 -7.3600000E+000 +8.5580000E+003 /  
DUP  
C3H4-P+H<=>CH3+C2H2  
+2.1200000E+010 +1.0600000E+000 +3.9450000E+003 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.  
PLOG / +1.0000000E-003  
+2.4400000E+010 +1.0400000E+000 +3.9800000E+003 /  
PLOG / +3.9000000E-002  
+3.8900000E+010 +9.8900000E-001 +4.1140000E+003 /  
PLOG / +1.0000000E+000  
+3.4600000E+012 +4.4200000E-001 +5.4630000E+003 /  
PLOG / +1.0000000E+001  
+1.7200000E+014 -1.0000000E-002 +7.1340000E+003 /  
PLOG / +1.0000000E+002  
+1.9000000E+015 -2.9000000E-001 +8.3060000E+003 /  
C3H4-P+H<=>C3H5-A  
+1.1000000E+060 -1.4560000E+001 +2.8100000E+004 !\AUTHOR: !\REF: DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT:  
PLOG / +1.0000000E-001  
+1.1000000E+060 -1.4560000E+001 +2.8100000E+004 /  
PLOG / +1.0000000E+000  
+4.9100000E+060 -1.4370000E+001 +3.1644000E+004 /  
PLOG / +2.0000000E+000  
+3.0400000E+060 -1.4190000E+001 +3.2642000E+004 /  
PLOG / +5.0000000E+000  
+9.0200000E+059 -1.3890000E+001 +3.3953000E+004 /  
PLOG / +1.0000000E+001  
+2.2000000E+059 -1.3610000E+001 +3.4900000E+004 /  
PLOG / +1.0000000E+002  
+1.6000000E+055 -1.2070000E+001 +3.7500000E+004 /  
C3H5-A<=>C3H5-T  
+3.9000000E+059 -1.5420000E+001 +7.5400000E+004 !\AUTHOR: !\REF: DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:  
PLOG / +1.0000000E-001  
+3.9000000E+059 -1.5420000E+001 +7.5400000E+004 /  
PLOG / +1.0000000E+000  
+7.0600000E+056 -1.4080000E+001 +7.5868000E+004 /  
PLOG / +2.0000000E+000  
+4.8000000E+055 -1.3590000E+001 +7.5949000E+004 /  
PLOG / +5.0000000E+000  
+4.8600000E+053 -1.2810000E+001 +7.5883000E+004 /



PLOG / +1.0000000E+001  
+6.4000000E+051 -1.2120000E+001 +7.5700000E+004 /  
PLOG / +1.0000000E+002  
+2.8000000E+043 -9.2700000E+000 +7.4000000E+004 /  
C3H5-A<=>C3H5-S  
+1.3000000E+055 -1.4530000E+001 +7.3800000E+004 !\AUTHOR: !\REF:DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:  
PLOG / +1.0000000E-001  
+1.3000000E+055 -1.4530000E+001 +7.3800000E+004 /  
PLOG / +1.0000000E+000  
+5.0000000E+051 -1.3020000E+001 +7.3300000E+004 /  
PLOG / +1.0000000E+001  
+9.7000000E+048 -1.1730000E+001 +7.3700000E+004 /  
PLOG / +1.0000000E+002  
+4.8600000E+044 -9.8400000E+000 +7.3400000E+004 /  
C2H2+CH3<=>C3H5-T  
+6.8000000E+020 -4.1600000E+000 +1.8000000E+004 !\AUTHOR: !\REF:DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:  
PLOG / +1.0000000E-001  
+6.8000000E+020 -4.1600000E+000 +1.8000000E+004 /  
PLOG / +1.0000000E+000  
+4.9900000E+022 -4.3900000E+000 +1.8850000E+004 /  
PLOG / +2.0000000E+000  
+6.0000000E+023 -4.6000000E+000 +1.9571000E+004 /  
PLOG / +5.0000000E+000  
+7.3100000E+025 -5.0600000E+000 +2.1150000E+004 /  
PLOG / +1.0000000E+001  
+9.3000000E+027 -5.5500000E+000 +2.2900000E+004 /  
PLOG / +1.0000000E+002  
+3.8000000E+036 -7.5800000E+000 +3.1300000E+004 /  
C3H5-T<=>C3H5-S  
+1.6000000E+044 -1.2160000E+001 +5.2200000E+004 !\AUTHOR: !\REF:DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:  
PLOG / +1.0000000E-001  
+1.6000000E+044 -1.2160000E+001 +5.2200000E+004 /  
PLOG / +1.0000000E+000  
+1.5000000E+048 -1.2710000E+001 +5.3900000E+004 /  
PLOG / +1.0000000E+001  
+5.1000000E+052 -1.3370000E+001 +5.7200000E+004 /  
PLOG / +1.0000000E+002  
+5.8000000E+051 -1.2430000E+001 +5.9200000E+004 /  
C2H2+CH3<=>C3H5-A  
+8.2000000E+053 -1.3320000E+001 +3.3200000E+004 !\AUTHOR: !\REF:DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT: WARNING:  
PLOG / +1.0000000E-001  
+8.2000000E+053 -1.3320000E+001 +3.3200000E+004 /  
PLOG / +1.0000000E+000  
+2.6800000E+053 -1.2820000E+001 +3.5730000E+004 /  
PLOG / +2.0000000E+000  
+3.6400000E+052 -1.2460000E+001 +3.6127000E+004 /  
PLOG / +5.0000000E+000  
+1.0400000E+051 -1.1890000E+001 +3.6476000E+004 /  
PLOG / +1.0000000E+001  
+4.4000000E+049 -1.1400000E+001 +3.6700000E+004 /  
PLOG / +1.0000000E+002  
+3.8000000E+044 -9.6300000E+000 +3.7600000E+004 /  
CH3+C2H2<=>C3H5-S  
+1.7800000E+042 -1.0400000E+001 +1.3647000E+004 !\AUTHOR: !\REF: MILLER

ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003  
+1.7800000E+042 -1.0400000E+001 +1.3647000E+004 /  
PLOG / +3.9000000E-002  
+1.5200000E+044 -1.0730000E+001 +1.5256000E+004 /  
PLOG / +1.0000000E+000  
+1.1900000E+044 -1.0190000E+001 +1.8728000E+004 /  
PLOG / +1.0000000E+001  
+6.0200000E+043 -9.7400000E+000 +2.0561000E+004 /  
PLOG / +1.0000000E+002  
+1.4200000E+042 -8.9100000E+000 +2.2235000E+004 /

DUP

CH3+C2H2<=>C3H5-S

+1.7800000E+042 -1.0400000E+001 +1.3647000E+004 !\AUTHOR: !\REF: MILLER  
ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438 !\COMMENT: WARNING: UNSURE  
IF CORRECT REFERENCE BASED ON INFO.

PLOG / +1.0000000E-003 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +3.9000000E-002 +1.0000000E-  
010 +0.0000000E+000 +0.0000000E+000 /  
PLOG / +1.0000000E+000  
+8.4900000E+035 -8.4300000E+000 +1.2356000E+004 /  
PLOG / +1.0000000E+001  
+3.0400000E+032 -7.0100000E+000 +1.2357000E+004 /  
PLOG / +1.0000000E+002  
+1.6900000E+027 -5.0700000E+000 +1.1690000E+004 /

DUP

!

---

!\REACTIONCLASS: \R\_ADDITION\O \A  
\N \EA  
!

---

C3H4-P+O<=>HCCO+CH3

+7.3000000E+012 +0.0000000E+000 +2.2500000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H4-P+O<=>C2H4+CO

+1.0000000E+013 +0.0000000E+000 +2.2500000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H4-P+O<=>C2H3+HCO

+3.2000000E+012 +0.0000000E+000 +2.0100000E+003 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:

C3H4-A+O<=>C2H4+CO

+2.0000000E+007 +1.8000000E+000 +1.0000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H4-A+O<=>C2H2+CH2O

+3.0000000E-  
003 +4.6100000E+000 -4.2430000E+003 !\AUTHOR: !\REF:DAGAUT, P. ET AL.,  
CST 71, 111(1990). !\COMMENT:

!

---

!\REACTIONCLASS: \R\_ADDITION\OH \A  
\N \EA  
!

---

C3H4-A+OH<=>CH2CCH2OH

+1.1100000E+012 +0.0000000E+000 -3.0400000E+002 !\AUTHOR: !\REF:  
ESTIMATE ATKINSON 1984 C3 NUIG S.M.B !\COMMENT:

C3H4-A+OH<=>SC3H4OH  
+2.2200000E+012 +0.0000000E+000 -3.0400000E+002 !\AUTHOR: !\REF:  
ESTIMATE ATKINSON 1984 C3 NUIG S.M.B !\COMMENT:  
SC3H4OH<=>CH2CO+CH3  
+9.2400000E+010 +8.7000000E-001 +3.0460000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH CURRAN 2006 ALKYL DECOMP !\COMMENT:  
C3H4-P+OH<=>PC3H4OH-2  
+3.9300000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984 !\COMMENT:  
C3H4-P+OH<=>SC3H4OH  
+2.3600000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984 !\COMMENT:  
PC3H4OH-2<=>CH3CHCHO  
+3.5600000E+010 +8.8000000E-001 +2.3238000E+004 !\AUTHOR: !\REF: MATHEU  
ET AL. IJCK, 2003, 35, 95--119 !\COMMENT:  
!CH3CHCHO<=>C2H3CHO+H 4.164E+012 -0.020 32410.0 !\AUTHOR: !\REF: PELUCCHI  
ECM 2013 !\COMMENT:  
CH3CHCHO<=>C2H3CHO+H  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !IC3H7<=>C3H6+H 1.0 1.0  
1.0  
PLOG / +1.0000000E-002  
+1.7400000E+050 -1.1730000E+001 +5.2870000E+004 /  
PLOG / +1.0000000E-001  
+1.1300000E+047 -1.0570000E+001 +5.0479000E+004 /  
PLOG / +1.0000000E+000  
+2.9400000E+043 -9.2900000E+000 +4.8810000E+004 /  
PLOG / +2.5000000E+000  
+1.1600000E+042 -8.7800000E+000 +4.8382000E+004 /  
PLOG / +5.0000000E+000  
+9.4800000E+040 -8.4000000E+000 +4.8095000E+004 /  
PLOG / +1.0000000E+001  
+7.1900000E+039 -8.0100000E+000 +4.7818000E+004 /  
PLOG / +2.5000000E+001  
+2.1300000E+038 -7.4900000E+000 +4.7438000E+004 /  
PLOG / +5.0000000E+001  
+1.4200000E+037 -7.0900000E+000 +4.7128000E+004 /  
CH3CHCHO<=>CH3CHCO+H  
+8.3280000E+012 -2.0000000E-002 +3.2410000E+004 !\AUTHOR: !\REF:  
PELUCCHI ECM 2013 !\COMMENT:  
!\MISC  
CH3CHCHO+H2<=>C2H5CHO+H  
+2.1600000E+005 +2.3800000E+000 +1.8990000E+004 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: THIS REACTION WAS MOVED FROM  
C5 MECHANISM WHEN MASTER MECHANISM WAS CONSTRUCTED.  
!

---

!\REACTIONCLASS: \R\_ADDITION\HO2

\A

\N

\EA

!

---

C3H4-P+HO2=>C2H4+CO+OH  
+3.0000000E+012 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
C3H4-A+HO2=>C2H4+CO+OH  
+1.0000000E+011 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:

C3H4-A+HO2=>CH2CO+CH2+OH  
+4.0000000E+012 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_ADDITION\CH2 \A  
\N \EA  
!

---

C3H4-A+C2H<=>C2H2+C3H3  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

!=====  
=====  
!\SUBSPECIES: \C3H3  
!=====  
=====  
!

---

!\REACTIONCLASS: \R\_R\_PRODUCTS \A  
\N \EA  
!

---

C3H3+O<=>CH2O+C2H  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H3+HO2=>OH+CO+C2H3  
+8.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H3+HCO<=>C3H4-A+CO  
+2.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C3H3+HCO<=>C3H4-P+CO  
+2.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C2H5+C2H<=>C3H3+CH3  
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:Tsang,  
W.; Hampson, R.F., J. Phys. Chem. Ref. Data 15, 1087 (1986) !\COMMENT:

C3H3+O2<=>CH2CO+HCO  
+1.7000000E+005 +1.7000000E+000 +1.5000000E+003 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE

C3H3+CH<=>C4H3-N+H  
+7.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: JAM  
!\COMMENT: WARNING: PRESUMABLY JAM STANDS FOR JAMES A. MILLER?  
!

---

!\REACTIONCLASS: \R+HO2 \A  
\N \EA  
!

---

C3H3+HO2<=>C3H3O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS.  
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT:

PLOG / +1.0000000E-002  
+1.0200000E+013 -1.5800000E-001 -1.4170000E+003 /  
PLOG / +1.0000000E-001  
+4.9800000E+014 -6.4200000E-001 -3.4910000E+002 /

PLOG / +1.0000000E+000  
 +7.7700000E+017 -1.5200000E+000 +2.3792000E+003 /  
 PLOG / +1.0000000E+001  
 +2.9300000E+015 -6.8400000E-001 +3.6153000E+003 /  
 PLOG / +1.0000000E+002  
 +1.6400000E+004 +2.7400000E+000 +1.1444000E+003 /  
 C3H3+HO2<=>C3H3O2H  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS.  
 CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +1.9100000E+031 -7.2300000E+000 +1.3362000E+003 /  
 PLOG / +1.0000000E-001  
 +6.3100000E+042 -1.0300000E+001 +5.5689000E+003 /  
 PLOG / +1.0000000E+000  
 +1.0300000E+045 -1.0600000E+001 +7.8515000E+003 /  
 PLOG / +1.0000000E+001  
 +2.7900000E+037 -7.9200000E+000 +6.4979000E+003 /  
 PLOG / +1.0000000E+002  
 +4.7300000E+025 -4.1300000E+000 +2.9238000E+003 /  
 C3H3+HO2<=>C2HCHO+H2O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS.  
 CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +1.0900000E+000 +3.0100000E+000 -3.4211000E+003 /  
 PLOG / +1.0000000E-001  
 +6.3500000E+001 +2.5000000E+000 -2.3414000E+003 /  
 PLOG / +1.0000000E+000  
 +6.0500000E+005 +1.3900000E+000 +5.9510000E+002 /  
 PLOG / +1.0000000E+001  
 +3.1000000E+005 +1.5900000E+000 +2.6776000E+003 /  
 PLOG / +1.0000000E+002 +5.0700000E-  
 005 +4.5900000E+000 +9.2750000E+002 /  
 C3H3O2H<=>C2HCHO+H2O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS.  
 CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +1.9900000E+050 -1.2700000E+001 +5.3531900E+004 /  
 PLOG / +1.0000000E-001  
 +4.7200000E+047 -1.1500000E+001 +5.4360900E+004 /  
 PLOG / +1.0000000E+000  
 +1.5000000E+040 -8.8400000E+000 +5.3179200E+004 /  
 PLOG / +1.0000000E+001  
 +2.5400000E+028 -5.0000000E+000 +4.9919400E+004 /  
 PLOG / +1.0000000E+002  
 +1.4800000E+016 -1.1200000E+000 +4.5949300E+004 /  
 C2H+CH2O<=>C3H3O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 !\COMMENT:  
 PLOG / +1.0000000E-003 +5.9250000E-  
 004 +2.6090000E+000 -4.2973000E+003 /  
 PLOG / +1.0000000E-002  
 +5.6880000E+006 -7.3000000E-002 -1.2341000E+003 /  
 PLOG / +1.0000000E-001  
 +5.3900000E+013 -1.8030000E+000 +1.4522000E+003 /

PLOG / +1.0000000E+000  
+8.7330000E+015 -2.0740000E+000 +2.5101000E+003 /  
PLOG / +1.0000000E+001  
+5.3050000E+019 -2.9430000E+000 +4.5322000E+003 /  
PLOG / +1.0000000E+002  
+3.7790000E+021 -3.1630000E+000 +6.8025000E+003 /  
!\C2HCHO  
C2HCHO<=>C2H2+CO  
+2.5100000E+014 +0.0000000E+000 +6.8000000E+004 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
C2H+HCO<=>C2HCHO  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
!

---

!\REACTIONCLASS: \R\_R\_RECOMB\H \A  
\N \EA  
!

---

C3H3+H<=>C3H2+H2  
+2.1400000E+005 +2.5200000E+000 +7.4530000E+003 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
C3H3+H<=>C3H2(S)+H2  
+3.3110000E+013 +1.9500000E-001 +1.7579000E+004 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
PLOG / +3.9500000E-002  
+2.9510000E+009 +1.2800000E+000 +1.3474000E+004 /  
PLOG / +1.0000000E+000  
+1.0970000E+010 +1.1300000E+000 +1.3929000E+004 /  
PLOG / +1.0000000E+001  
+3.3110000E+013 +1.9500000E-001 +1.7579000E+004 /  
C3H3+H<=>H2CCC(S)+H2  
+1.0000000E+018 -1.2300000E+000 +1.5111000E+004 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
PLOG / +3.9500000E-002  
+2.6920000E+009 +1.0500000E+000 +5.3710000E+003 /  
PLOG / +1.0000000E+000  
+2.8840000E+013 -3.0000000E-002 +9.4480000E+003 /  
PLOG / +1.0000000E+001  
+1.0000000E+018 -1.2300000E+000 +1.5111000E+004 /  
C3H3+H<=>C3H2C+H2  
+7.2440000E+009 +6.0600000E-001 +1.8356000E+004 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
PLOG / +3.9500000E-002  
+1.0720000E+007 +1.3700000E+000 +1.5557000E+004 /  
PLOG / +1.0000000E+000  
+1.3490000E+007 +1.3400000E+000 +1.5560000E+004 /  
PLOG / +1.0000000E+001  
+7.2440000E+009 +6.0600000E-001 +1.8356000E+004 /  
C3H2C+O2<=>C2H2+CO2  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
!

---

!\REACTIONCLASS: \R\_R\_RECOMB\OH \A  
\N \EA  
!

---

C3H3+OH<=>C3H2+H2O  
 +2.0000000E+013 +0.0000000E+000 +8.0000000E+003 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 C3H3+OH<=>CH2O+C2H2  
 +2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 C3H3+OH<=>C2H3+HCO  
 +1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 C3H3+OH<=>C2H4+CO  
 +1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 C3H3+OH<=>C3H2(S)+H2O  
 +1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 C3H3+OH<=>H2CCC(S)+H2O  
 +1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 !=====

!\SUBSPECIES: \C3H2  
 !=====

C3H2(S)+M<=>C3H2+M  
 +1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 C3H2(S)+H<=>H2CCC(S)+H  
 +1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 H2CCC(S)+O2<=>CO2+C2H2  
 +1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
 WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN SOURCE  
 !=====

!\ENDSUBSPECIES: \C3H2  
 !=====

!

---

!\REACTIONCLASS: \AROMATIC\_GROWTH \A  
 \N \EA  
 !

---

C3H3+C3H3<=>C6H5+H  
 +1.0467000E+054 -1.1880000E+001 +2.8757000E+004 !\AUTHOR: !\REF: FROM  
 MILLER, BUT SLIGHTLY DIFFERENT THAN IN PUBLISHED PAPER (WARNING: WHAT IS  
 LITERATURE REFERENCE??) !\COMMENT:  
 PLOG / +3.9470000E-002  
 +1.0467000E+054 -1.1880000E+001 +2.8757000E+004 /  
 PLOG / +1.0000000E+000  
 +1.6975000E+048 -9.9770000E+000 +3.6755000E+004 /  
 PLOG / +1.0000000E+001  
 +3.6712000E+026 -3.8790000E+000 +2.8963000E+004 /  
 C3H3+C3H3<=>C6H6  
 +1.8189000E+074 -1.8140000E+001 +3.1896000E+004 !\AUTHOR: !\REF: FROM  
 SCOTT SKEEN 2011 WHO GOT IT FROM MILLER: (SLIGHTLY DIFFERENT THAN IN  
 MILLER AND KLIPPENSTEIN 2003 PUBLICATION)

```

PLOG / +3.9470000E-002
+1.6400000E+066 -1.5902000E+001 +2.7529000E+004 /
PLOG / +1.0000000E+000
+3.1609000E+055 -1.2550000E+001 +2.2264000E+004 /
PLOG / +1.0000000E+001
+3.8888000E+050 -1.1010000E+001 +2.0320000E+004 /
C3H3+C3H3<=>FULVENE
+6.3069000E+076 -1.9070000E+001 +3.1542000E+004 !\AUTHOR: !\REF: FROM
SCOTT SKEEN 2011 WHO GOT IT FROM MILLER: (SLIGHTLY DIFFERENT THAN IN
MILLER AND KLIPPENSTEIN 2003 PUBLICATION)
PLOG / +3.9470000E-002
+7.2500000E+065 -1.6015000E+001 +2.5035000E+004 /
PLOG / +1.0000000E+000
+1.3798000E+066 -1.5660000E+001 +2.8260000E+004 /
PLOG / +1.0000000E+001
+1.2584000E+056 -1.2610000E+001 +2.3515000E+004 /
C3H3+C3H5-A=>FULVENE+H+H
+3.2600000E+029 -5.3970000E+000 +3.3900000E+003 !\AUTHOR: !\ JAM, YG,
ET AL 2007 !\COMMENT: WARNING: WHAT IS ORIGINAL LITERATURE SOURCE?
C3H3+C3H4-A<=>C6H6+H
+1.4000000E+012 +0.0000000E+000 +9.9904000E+003 !\AUTHOR: !\REF: CURRAN
ESTIMATE !\COMMENT: WARNING: THIS IS A STRANGE REFERENCE-HAS HENRY WORKED
ON AROMATIC CHEMISTRY?
!-----
!\ENDSUBMECH: C3H4-A/C3H4-P
!-----
!=====
!\SUBSPECIES: \CH3CHCO
!=====
!-----
!\REACTIONCLASS: \RH_R_LUMPED \A
\N \EA
!-----
CH3CHCO+OH<=>C2H5+CO2
+1.7300000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR:
!\REF: ESTIMATE !\COMMENT: WARNING: METHYL KETENE CHEMISTRY NOT DETAILED.
CH3CHCO+OH<=>SC2H4OH+CO
+2.0000000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR:
!\REF: ESTIMATE !\COMMENT: WARNING: METHYL KETENE CHEMISTRY NOT DETAILED.
CH3CHCO+H<=>C2H5+CO
+4.4000000E+012 +0.0000000E+000 +1.4590000E+003 !\AUTHOR:
!\REF: ESTIMATE !\COMMENT: WARNING: METHYL KETENE CHEMISTRY NOT DETAILED.
CH3CHCO+O<=>CH3CHO+CO
+3.2000000E+012 +0.0000000E+000 -4.3700000E+002 !\AUTHOR:
!\REF: ESTIMATE !\COMMENT: WARNING: METHYL KETENE CHEMISTRY NOT DETAILED.
!=====
!\SUBSPECIES: \CH3CHCO
!=====
!-----

```



!\SUBMECH: \CH3COCH3  
!\MECHCOMMENTS:  
!\MECHWARNINGS:

!-----  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

---

CH3COCH3<=>CH3CO+CH3  
+2.0500000E+058 -1.2796000E+001 +1.0003010E+005 !\AUTHOR: !\REF: SAXENA  
ET AL. PROCEEDINGS. 32 123-130 (2009) !\COMMENT:  
PLOG / +1.0000000E-002  
+2.0500000E+058 -1.2796000E+001 +1.0003010E+005 /  
PLOG / +1.0000000E-001  
+3.3000000E+051 -1.0574000E+001 +9.8221200E+004 /  
PLOG / +1.0000000E+000  
+1.3100000E+042 -7.6570000E+000 +9.4660600E+004 /  
PLOG / +1.0000000E+001  
+2.1600000E+033 -4.9890000E+000 +9.0916500E+004 /  
PLOG / +1.0000000E+002  
+9.4000000E+028 -3.6690000E+000 +8.9022800E+004 /  
CH3COCH2+H<=>CH3COCH3  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WJP:  
BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006 !\COMMENT:  
!

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

CH3COCH3+OH<=>CH3COCH2+H2O  
+1.2500000E+005 +2.4830000E+000 +4.4500000E+002 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT: WARNING: CORRECT REFERENCE?  
CH3COCH3+H<=>CH3COCH2+H2  
+9.8000000E+005 +2.4300000E+000 +5.1600000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
CH3COCH3+O<=>CH3COCH2+OH  
+5.1300000E+011 +2.1100000E-001 +4.8900000E+003 !\AUTHOR: !\REF:FIT TO  
DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98 !\COMMENT:  
CH3COCH3+CH3<=>CH3COCH2+CH4  
+3.9600000E+011 +0.0000000E+000 +9.7840000E+003 !\AUTHOR: !\REF:S.  
Pichon, Combustion and Flame (2009) 156(2) 494-504. !\COMMENT:  
CH3COCH3+CH3O<=>CH3COCH2+CH3OH  
+4.3400000E+011 +0.0000000E+000 +6.4600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
CH3COCH3+O2<=>CH3COCH2+HO2  
+6.0300000E+013 +0.0000000E+000 +4.8500000E+004 !\AUTHOR: !\REF:A-  
FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM DHRXN !\COMMENT:  
CH3COCH3+HO2<=>CH3COCH2+H2O2  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO ETHANE !\COMMENT: WARNING: BAD ANALOGY?  
CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO ETHANE !\COMMENT: WARNING: BAD ANALOGY?

CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21  
+1.0000000E+011 +0.0000000E+000 +5.0000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \R+HO2 \A  
\N \EA  
!

---

CH3COCH2+HO2<=>CH3COCH2O+OH  
+2.4100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WJP:  
BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006 !\COMMENT: WARNING:  
DEFINITELY WRONG REFERENCE  
CH3COCH2+CH3O2<=>CH3COCH2O+CH3O  
+1.2050000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WJP:  
BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006 !\COMMENT: WARNING:  
DEFINITELY WRONG REFERENCE  
CH3COCH2O<=>CH3CO+CH2O  
+5.8720000E+020 -2.4218000E+000 +1.0535800E+004 !\AUTHOR: !\REF: A-  
FACTOR BY ANALOGY WITH C2H5+CH2O<=>NC3H7O AND EA FROM DHRXN AND IP., H.  
J. CURRAN, INT. J. CHEM. KINET. 38 (4) (2006) 250-275.  
!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA  
!

---

CH3COCH2+O2<=>CH3COCH2O2  
+1.2000000E+011 +0.0000000E+000 -1.1000000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
CH2CO+CH3<=>CH3COCH2  
+1.7600000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:WJP:  
BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006 !\COMMENT:  
CH2O+CH3COCH2O2<=>HCO+C3KET21  
+1.2880000E+011 +0.0000000E+000 +9.0000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
HO2+CH3COCH2O2<=>C3KET21+O2  
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
!

!\ENDSUBMECH: \CH3COCH3  
!-----  
!-----  
!-----  
!-----

!\SUBMECH: \C2H3CHO  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----  
!-----

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

C2H3+HCO<=>C2H3CHO  
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

C2H3CHO+H<=>C2H3CO+H2  
+1.3400000E+013 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:BASED  
ON CH3CHO+H !\COMMENT:  
C2H3CHO+O<=>C2H3CO+OH  
+5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR: !\REF:BASED  
ON CH3CHO+H !\COMMENT:  
C2H3CHO+OH<=>C2H3CO+H2O  
+9.2400000E+006 +1.5000000E+000 -9.6200000E+002 !\AUTHOR: !\REF:TAYLOR  
ET AL. 1996 !\COMMENT:  
C2H3CHO+O2<=>C2H3CO+HO2  
+1.0050000E+013 +0.0000000E+000 +4.0700000E+004 !\AUTHOR: !\REF:TAYLOR  
ET AL. 1996 !\COMMENT:  
C2H3CHO+HO2<=>C2H3CO+H2O2  
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:BASED  
ON CH3CHO+HO2 !\COMMENT:  
C2H3CHO+CH3<=>C2H3CO+CH4  
+2.6080000E+006 +1.7800000E+000 +5.9110000E+003 !\AUTHOR: !\REF:BASED  
ON CH3CHO+HO2 !\COMMENT:  
C2H3CHO+C2H3<=>C2H3CO+C2H4  
+1.7400000E+012 +0.0000000E+000 +8.4400000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH ACETALDEHYDE. !\COMMENT:  
C2H3CHO+CH3O<=>C2H3CO+CH3OH  
+1.0000000E+012 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH CH3CHO+CH3O !\COMMENT:  
C2H3CHO+CH3O2<=>C2H3CO+CH3O2H  
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:BASED  
ON CH3CHO+HO2 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

---

C2H3+CO<=>C2H3CO  
+1.5100000E+011 +0.0000000E+000 +4.8100000E+003 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT: WARNING:  
WOULD THIS BE BETTER DEFINED IN OTHER DIRECTION?  
!-----

!\ENDSUBMECH: CH3COCH3  
!-----

!\SUBMECH: \C2H5CHO  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----

```

!
-----
!\REACTIONCLASS:  \UNIMOL                \A
\N                \EA
!
-----
C2H5+HCO<=>C2H5CHO
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000  !\AUTHOR: !\REF:CURRAN
ESTIMATE !\COMMENT:
!
-----
!\REACTIONCLASS:  \RH_R_ABSTRACTION      \A
\N                \EA
!
-----
C2H5CHO+H<=>C2H5CO+H2
+4.0000000E+013 +0.0000000E+000 +4.2000000E+003  !\AUTHOR: !\REF:ANALOGY
WITH CH3CHO+H !\COMMENT:
C2H5CHO+O<=>C2H5CO+OH
+5.0000000E+012 +0.0000000E+000 +1.7900000E+003  !\AUTHOR: !\REF:ANALOGY
WITH CH3CHO+O !\COMMENT:
C2H5CHO+OH<=>C2H5CO+H2O
+2.6900000E+010 +7.6000000E-001 -3.4000000E+002  !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
C2H5CHO+CH3<=>C2H5CO+CH4
+2.6080000E+006 +1.7800000E+000 +5.9110000E+003  !\AUTHOR: !\REF:FIT TO
DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98 !\COMMENT:
C2H5CHO+HO2<=>C2H5CO+H2O2
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004  !\AUTHOR: !\REF:ANALOGY
WITH CH3CHO+HO2 !\COMMENT:
C2H5CHO+CH3O<=>C2H5CO+CH3OH
+1.0000000E+012 +0.0000000E+000 +3.3000000E+003  !\AUTHOR: !\REF:
ANALOGY WITH CH3CHO+CH3O !\COMMENT:
C2H5CHO+CH3O2<=>C2H5CO+CH3O2H
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004  !\AUTHOR: !\REF:ANALOGY
WITH CH3CHO+HO2 !\COMMENT:
C2H5CHO+C2H5<=>C2H5CO+C2H6
+1.0000000E+012 +0.0000000E+000 +8.0000000E+003  !\AUTHOR:
!\REF:ACETALDEHYDE ANALOG !\COMMENT:
C2H5CHO+C2H5O<=>C2H5CO+C2H5OH
+6.0260000E+011 +0.0000000E+000 +3.3000000E+003  !\AUTHOR:
!\REF:ACETALDEHYDE ANALOG !\COMMENT:
C2H5CHO+C2H5O2<=>C2H5CO+C2H5O2H
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004  !\AUTHOR: !\REF:BASED
ON CH3CHO+HO2 !\COMMENT:
C2H5CHO+O2<=>C2H5CO+HO2
+1.0050000E+013 +0.0000000E+000 +4.0700000E+004  !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
C2H5CHO+CH3CO3<=>C2H5CO+CH3CO3H
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004  !\AUTHOR: !\REF:BASED
ON CH3CHO+HO2 !\COMMENT:
C2H5CHO+C2H3<=>C2H5CO+C2H4
+1.7000000E+012 +0.0000000E+000 +8.4400000E+003  !\AUTHOR: !\REF:
ANALOGY WITH ACETALDEHYDE !\COMMENT:
C2H5CHO+NC3H7<=>C2H5CO+C3H8
+1.7000000E+012 +0.0000000E+000 +8.4400000E+003  !\AUTHOR: !\REF:ANALOGY
WITH ACETALDEHYDE !\COMMENT:

```

C2H5CHO+IC3H7<=>C2H5CO+C3H8  
+1.7000000E+012 +0.0000000E+000 +8.4400000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH ACETALDEHYDE !\COMMENT:  
C2H5CHO+C3H5-A<=>C2H5CO+C3H6  
+1.7000000E+012 +0.0000000E+000 +8.4400000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH ACETALDEHYDE !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ALPHA\_SCISSION \A  
\N \EA  
!

---

C2H5+CO<=>C2H5CO  
+1.5100000E+011 +0.0000000E+000 +4.8100000E+003 !\AUTHOR: !\REF:TSANG  
AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT: WARNING:  
WOULD THIS BE BETTER DEFINED IN OTHER DIRECTION?

!\ENDSUBMECH: C2H5CHO  
!

!\END\_KINETICS\_MODULE: \C3

!\KINETICS\_MODULE: \C4  
!\MODCOMMENTS: THERE IS LOTS OF CROSSOVER BETWEEN C4H7/C4H9 RADICALS AND  
THEIR RO2/RO PRODUCTS. A FULL C4 MECHANISM IS LIKELY REQUIRED AT ALL  
TIMES IF SIMULATING ANY OF THE ALKANE/ALKENE ISOMERS  
!\MODWARNINGS: KPS, 22/07/2015 REATIONS OF C4H7O12-4\C4H7O13-4\C4H7O23-1  
FROM KUIWENS "OTHER DECOMPOSITIONS" IN C6/C7 MECHANISM HAVE BEEN MOVED TO  
THE \C4\_CYC\_ETH PART OF THIS MECAHNISM. KUIWEN AND I NEED TO TALK ABOUT  
THIS

!\KINETICS\_MODULE: \C4

!\MODCOMMENTS: THERE IS LOTS OF CROSSOVER BETWEEN C4H7/C4H9 RADICALS AND  
THEIR RO2/RO PRODUCTS. A FULL C4 MECHANISM IS LIKELY REQUIRED AT ALL  
TIMES IF SIMULATING ANY OF THE ALKANE/ALKENE ISOMERS

!\MODWARNINGS: KPS, 22/07/2015 REATIONS OF C4H7O12-4\C4H7O13-4\C4H7O23-1  
FROM KUIWENS "OTHER DECOMPOSITIONS" IN C6/C7 MECHANISM HAVE BEEN MOVED TO  
THE \C4\_CYC\_ETH PART OF THIS MECAHNISM. KUIWEN AND I NEED TO TALK ABOUT  
THIS

!\MODSUBMECHS:

!\MECHWARNINGS: SOMEONE HAS UPDATED PC4H9 AND SC4H9 THERMAL  
DECOMPOSITIONS SINCE MECHANISM ASSEMBLY BEGAN. THIS ALTERATION MUST BE  
ADDRESSED BEFORE MECHANISM IS FINALISED. KPS 31/07/2015  
!\MECHWARNINGS: SOMEONE HAS REMOVED THE REACTIONS C4H8OOH1-2<=>C4H8-1+HO2  
C4H8OOH2-1<=>C4H8-1+HO2 C4H8OOH2-3<=>C4H8-2+HO2 OUT OF BASEMECH2907 MUST  
BE ADDRESSED BEFORE FINALISATION

!\SUBMECH: \C4H10

!\MECHCOMMENTS:

!\MECHWARNINGS: SOMEONE HAS UPDATED PC4H9 AND SC4H9 THERMAL  
DECOMPOSITIONS SINCE MECHANISM ASSEMBLY BEGAN. THIS ALTERATION MUST BE  
ADDRESSED BEFORE MECHANISM IS FINALISED. KPS 31/07/2015

!\MECHWARNINGS: SOMEONE HAS REMOVED THE REACTIONS C4H8OOH1-2<=>C4H8-1+HO2  
C4H8OOH2-1<=>C4H8-1+HO2 C4H8OOH2-3<=>C4H8-2+HO2 OUT OF BASEMECH2907 MUST  
BE ADDRESSED BEFORE FINALISATION

!\MECHWARNINGS: COMMENTS ON RATE CONSTANTS IN USE IN C4 LTC ARE NOT VERY  
DETAILED. CAN WE IMPROVE UPON THIS?

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA

!

---

C4H10(+M)<=>C2H5+C2H5(+M)  
+1.3550000E+037 -6.0360000E+000 +9.2929000E+004 !\AUTHOR: !\REF:BASED  
ON OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253 !\COMMENT:  
LOW /  
+4.7200000E+018 +0.0000000E+000 +4.9578000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +7.9980000E-002 +1.0000000E-  
020 +3.2430000E+004 +4.8580000E+003 / !TROE PARAMETERS  
C4H10(+M)<=>NC3H7+CH3(+M)  
+6.6000000E+052 -1.0626000E+001 +1.0033000E+005 !\AUTHOR: !\REF:BASED  
ON OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253 !\COMMENT:  
LOW /  
+5.3400000E+017 +0.0000000E+000 +4.2959000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +9.5020000E-002 +1.0000000E-  
020 +5.3480000E+003 +4.3260000E+003 / !TROE PARAMETERS  
C4H10<=>PC4H9+H  
+4.8000000E+040 -7.0600000E+000 +1.1530200E+005 !\AUTHOR:  
!\REF:ESTIMATE FROM RECOMBINATION (1E14 0 0) !\COMMENT: WARNING: WHAT IS  
SOURCE OF P-DEPENDENCE?  
PLOG / +1.0000000E-002  
+4.4500000E+090 -2.1910000E+001 +1.4056400E+005 /  
PLOG / +1.0000000E-001  
+4.6300000E+076 -1.7640000E+001 +1.3466900E+005 /  
PLOG / +1.0000000E+000  
+4.9400000E+058 -1.2320000E+001 +1.2543500E+005 /  
PLOG / +1.0000000E+001  
+4.8000000E+040 -7.0600000E+000 +1.1530200E+005 /  
PLOG / +1.0000000E+002  
+1.4900000E+027 -3.1500000E+000 +1.0732300E+005 /  
C4H10<=>SC4H9+H  
+8.5200000E+038 -6.5800000E+000 +1.1055600E+005 !\AUTHOR:  
!\REF:ESTIMATE FROM RECOMBINATION (1E14 0 0) !\COMMENT: WARNING: WHAT IS  
SOURCE OF P-DEPENDENCE?  
PLOG / +1.0000000E-002  
+3.1000000E+088 -2.1240000E+001 +1.3635500E+005 /  
PLOG / +1.0000000E-001  
+4.3400000E+073 -1.6760000E+001 +1.2959000E+005 /  
PLOG / +1.0000000E+000  
+7.3900000E+055 -1.1520000E+001 +1.2019900E+005 /  
PLOG / +1.0000000E+001  
+8.5200000E+038 -6.5800000E+000 +1.1055600E+005 /  
PLOG / +1.0000000E+002  
+5.4000000E+026 -3.0500000E+000 +1.0331300E+005 /  
!\WARNING: THESE REACTIONS CHANGED WHEN ASSEMBLING MASTER MECHANISM.  
ABOVE P-DEPENDENT RATE CONSTANTS NOW IN BASMECH2907\_C7.INP. CLARIFY WITH  
KZ  
!\WARNING:PC4H9+H<=>C4H10 3.610E+013 0.000 0.0  
!\WARNING:SC4H9+H<=>C4H10 3.610E+013 0.000 0.0  
!

---

!\REACTIONCLASS: \RH\_H\_ABSTRACTION \A  
\N \EA  
!

---

C4H10+H<=>PC4H9+H2  
+3.4900000E+005 +2.6900000E+000 +6.4500000E+003 !\AUTHOR: !\REF:TSANG,  
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:

C4H10+O2<=>PC4H9+HO2  
+6.0000000E+013 +0.0000000E+000 +5.2340000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH C4H10+O2<=>PC4H9+HO2 !\COMMENT: WARNING: SOURCE IS UNCLEAR  
C4H10+O<=>PC4H9+OH  
+1.1300000E+014 +0.0000000E+000 +7.8500000E+003 !\AUTHOR:  
!\REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705 (1983)  
!\COMMENT:  
C4H10+OH<=>PC4H9+H2O  
+1.0540000E+010 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:  
Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by  
OH. 3. Propane, J. Phys. Chem., 90, 1949-1955 !\COMMENT:  
C4H10+HO2<=>PC4H9+H2O2  
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
C4H10+CH3<=>PC4H9+CH4 +9.0400000E-  
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.  
CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
C4H10+CH3O<=>PC4H9+CH3OH  
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:DRYER  
ESTIMATE !\COMMENT:  
C4H10+CH3O2<=>PC4H9+CH3O2H  
+1.3860000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.,  
!\COMMENT: SCALED AS PER CARSTENSEN ET AL  
C4H10+O2CHO<=>PC4H9+HO2CHO  
+1.6800000E+013 +0.0000000E+000 +2.0440000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH RH+RO2 -->R+RO2H !\COMMENT:  
C4H10+C2H5<=>PC4H9+C2H6  
+1.5800000E+011 +0.0000000E+000 +1.2300000E+004 !\AUTHOR: !\REF:ALLARA,  
D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980) !\COMMENT:  
C4H10+C2H3<=>PC4H9+C2H4  
+1.0000000E+012 +0.0000000E+000 +1.8000000E+004 !\AUTHOR:  
!\REF:SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17,  
174 (1978) !\COMMENT:  
C4H10+C2H5O<=>PC4H9+C2H5OH  
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:ANOLOGY  
TO CH3O !\COMMENT:  
C4H10+C2H5O2<=>PC4H9+C2H5O2H  
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.,  
!\COMMENT: SCALED AS PER CARSTENSEN ET AL  
C4H10+CH3CO3<=>PC4H9+CH3CO3H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+C3H5-A<=>PC4H9+C3H6  
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 !\AUTHOR: !\REF:ALLARA,  
D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980) !\COMMENT:  
C4H10+NC3H7O2<=>PC4H9+NC3H7O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+IC3H7O2<=>PC4H9+IC3H7O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+PC4H9<=>SC4H9+C4H10  
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:  
WESTBROOK AND PITZ ESTIMATE (1983) !\COMMENT:

C4H10+PC4H9O2<=>PC4H9+PC4H9O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+SC4H9O2<=>PC4H9+SC4H9O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+IC4H9O2<=>PC4H9+IC4H9O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+TC4H9O2<=>PC4H9+TC4H9O2H  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+H<=>SC4H9+H2  
+2.6000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:TSANG,  
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
C4H10+O2<=>SC4H9+HO2  
+4.0000000E+013 +0.0000000E+000 +4.9800000E+004 !\AUTHOR: !\REF:  
Ingham,T.; Walker,R.W.; Woolford,R.E., Symp. Int. Combust. Proc. 25, 767-  
774 (1994) !\COMMENT:  
C4H10+O<=>SC4H9+OH  
+5.6200000E+013 +0.0000000E+000 +5.2000000E+003 !\AUTHOR:  
!\REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705 (1983)  
!\COMMENT:  
C4H10+OH<=>SC4H9+H2O  
+9.3400000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:  
Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by  
OH. 3. Propane, J. Phys. Chem., 90, 1949-1955 !\COMMENT:  
C4H10+HO2<=>SC4H9+H2O2  
+1.2640000E+002 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
C4H10+CH3<=>SC4H9+CH4  
+3.0200000E+000 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:TSANG,  
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
C4H10+CH3O<=>SC4H9+CH3OH  
+6.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:DRYER  
ESTIMATE !\COMMENT:  
C4H10+CH3O2<=>SC4H9+CH3O2H  
+2.0370000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.,  
!\COMMENT: SCALED AS PER CARSTENSEN ET AL  
C4H10+O2CHO<=>SC4H9+HO2CHO  
+1.1200000E+013 +0.0000000E+000 +1.7690000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH RH+RO2 -->R+RO2H !\COMMENT:  
C4H10+C2H5<=>SC4H9+C2H6  
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:ALLARA,  
D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980) !\COMMENT:  
C4H10+C2H3<=>SC4H9+C2H4  
+8.0000000E+011 +0.0000000E+000 +1.6800000E+004 !\AUTHOR:  
!\REF:SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17,  
174 (1978) !\COMMENT:  
C4H10+C2H5O<=>SC4H9+C2H5OH  
+6.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:ANOLOGY  
TO CH3O !\COMMENT:  
C4H10+C2H5O2<=>SC4H9+C2H5O2H  
+1.2640000E+002 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:



C4H10+CH3CO3<=>SC4H9+CH3CO3H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR:  
!\REF:!\WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION  
SEATTLE AUGUST 1988 !\COMMENT:  
C4H10+C3H5-A<=>SC4H9+C3H6  
+3.1600000E+011 +0.0000000E+000 +1.6400000E+004 !\AUTHOR: !\REF:ALLARA,  
D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980) !\COMMENT:  
C4H10+NC3H7O2<=>SC4H9+NC3H7O2H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+IC3H7O2<=>SC4H9+IC3H7O2H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+PC4H9O2<=>SC4H9+PC4H9O2H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+SC4H9O2<=>SC4H9+SC4H9O2H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+IC4H9O2<=>SC4H9+IC4H9O2H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
C4H10+TC4H9O2<=>SC4H9+TC4H9O2H  
+1.1200000E+013 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:

!

---

!\REACTIONCLASS: \RADICAL\_UNIMOL \A  
\N \EA

!

---

!\REACTIONCLASS: \R+HO2 \A  
\N \EA

!

---

PC4H9+HO2<=>PC4H9O+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
CH3O2+PC4H9<=>CH3O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9+HO2<=>SC4H9O+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9+CH3O2<=>CH3O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:

!

---

!\REACTIONCLASS: \R\_BETA\_SCISSION \A  
\N \EA

!

---

C2H5+CH3CHO<=>SC4H9O  
+3.3300000E+010 +0.0000000E+000 +6.3970000E+003 !\AUTHOR: !\REF:Henry

!\COMMENT:

!

---

!\REACTIONCLASS: \R+O2 \A  
\N \EA

---

PC4H9+O2<=>C4H8-1+HO2 +8.3700000E-001 +3.5900000E+000 +1.1960000E+004 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:

PC4H9+O2<=>PC4H9O2 +6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi !\COMMENT:

SC4H9+O2<=>C4H8-1+HO2 +5.3500000E-001 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:

SC4H9+O2<=>C4H8-2+HO2 +1.0700000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:

SC4H9+O2<=>SC4H9O2 +3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi !\COMMENT:

!=====

=====

!\SUBSPECIES: \PC4H9O2

!=====

=====

!

---

!\REACTIONCLASS: \RO2+RH\_RO2H\_R \A  
\N \EA

---

PC4H9O2+H2<=>PC4H9O2H+H +3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:

PC4H9O2+HO2<=>PC4H9O2H+O2 +1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:

PC4H9O2+H2O2<=>PC4H9O2H+HO2 +2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:ANALOGY TO H2O2+CH3O2<=>HO2+CH3O2H !\COMMENT:

PC4H9O2+CH4<=>PC4H9O2H+CH3 +1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:ANALOGY TO CH4+HO2 !\COMMENT:

PC4H9O2+CH3OH<=>PC4H9O2H+CH2OH +6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:ANALOGY TO CH3OH+HO2 !\COMMENT:

PC4H9O2+CH2O<=>PC4H9O2H+HCO +5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2 !\COMMENT:

PC4H9O2+C2H6<=>PC4H9O2H+C2H5 +1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:

PC4H9O2+CH3CHO<=>PC4H9O2H+CH3CO +2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF CH2O+HO2 !\COMMENT:

PC4H9O2+C2H4<=>PC4H9O2H+C2H3  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H4+HO2 !\COMMENT:  
PC4H9O2+C3H6<=>PC4H9O2H+C3H5-A +5.3500000E-  
002 +4.2070000E+000 +1.3288100E+004 !\AUTHOR: !\REF:ANALOGY TO C3H6+HO2  
!\COMMENT:  
PC4H9O2+C2H5CHO<=>PC4H9O2H+C2H5CO  
+2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
PC4H9O2+C2H3CHO<=>PC4H9O2H+C2H3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
PC4H9O2+C3H8<=>PC4H9O2H+NC3H7  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
PC4H9O2+C3H8<=>PC4H9O2H+IC3H7  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975  
!\COMMENT:  
!

---

!\REACTIONCLASS: \RO2+R\_PRODUCTS \A  
\N \EA  
!

---

PC4H9O2+CH3<=>PC4H9O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+C2H5<=>PC4H9O+C2H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+IC3H7<=>PC4H9O+IC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+NC3H7<=>PC4H9O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+C3H5-A<=>PC4H9O+C3H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+PC4H9<=>PC4H9O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+SC4H9<=>PC4H9O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
PC4H9O2+C4H71-3<=>PC4H9O+C4H71-O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \KHP\_DECOMP \A  
\N \EA  
!

---

PC4H9O2H<=>PC4H9O+OH  
+1.5000000E+016 +0.0000000E+000 +4.2500000E+004 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:

!  
-----  
!\REACTIONCLASS: \RO2+RO2\_PRODUCTS \A  
\N \EA  
!

PC4H9O2+CH3O2=>PC4H9O+CH3O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
PC4H9O2+CH3CO3=>PC4H9O+CH3CO2+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
PC4H9O2+C2H5O2=>PC4H9O+C2H5O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
PC4H9O2+NC3H7O2=>PC4H9O+NC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
PC4H9O2+IC3H7O2=>PC4H9O+IC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
PC4H9O2+PC4H9O2=>PC4H9O+PC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
PC4H9O2+SC4H9O2=>PC4H9O+SC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO CLEAR REFERENCE PROVIDED  
!

!\REACTIONCLASS: \RO2\_QOOH \A  
\N \EA  
!

PC4H9O2<=>C4H8OOH1-2  
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:Sharma  
!\COMMENT: A factor revalued 20140425 KWZ 2.005E+008 1.100 30100.0  
PC4H9O2<=>C4H8OOH1-3  
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:Sharma  
!\COMMENT: A factor revalued 20140425 KWZ 6.798E+006 1.300 18200.0  
PC4H9O2<=>C4H8OOH1-4  
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:Sharma  
!\COMMENT: A factor revalued 20140425 KWZ 4.111E+005 1.500 20000.0  
!

!\REACTIONCLASS: \RO2\_ALKENE\_HO2 \A  
\N \EA  
!

PC4H9O2<=>C4H8-1+HO2  
+1.2580000E+008 +1.3800000E+000 +2.8900000E+004 !\AUTHOR: !\REF:Villano  
!\COMMENT:  
!=====  
=====  
!\SUBSPECIES: \SC4H9O2  
!=====  
=====

IC3H7O2+PC4H9<=>IC3H7O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
NC3H7O2+PC4H9<=>NC3H7O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+PC4H9<=>SC4H9O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC3H7O2+SC4H9<=>IC3H7O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
NC3H7O2+SC4H9<=>NC3H7O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RO2+RH\_RO2H\_R \A  
\N \EA  
!

---

SC4H9O2+H2<=>SC4H9O2H+H  
+3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG &  
HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:  
SC4H9O2+HO2<=>SC4H9O2H+O2  
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+CH2O<=>SC4H9O2H+HCO  
+5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH2O+HO2 !\COMMENT:  
SC4H9O2+CH3CHO<=>SC4H9O2H+CH3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH2O+HO2 !\COMMENT:  
SC4H9O2+C2H6<=>SC4H9O2H+C2H5  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
SC4H9O2+C2H5CHO<=>SC4H9O2H+C2H5CO  
+2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
SC4H9O2+C3H6<=>SC4H9O2H+C3H5-A +5.3500000E-  
002 +4.2070000E+000 +1.3288100E+004 !\AUTHOR: !\REF:ANALOGY TO C3H6+HO2  
!\COMMENT:  
SC4H9O2+C2H4<=>SC4H9O2H+C2H3  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H4+HO2 !\COMMENT:  
SC4H9O2+CH3OH<=>SC4H9O2H+CH2OH  
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH3OH+HO2 !\COMMENT:  
SC4H9O2+C2H3CHO<=>SC4H9O2H+C2H3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
SC4H9O2+CH4<=>SC4H9O2H+CH3  
+1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:ANALOGY  
TO CH4+HO2 !\COMMENT:  
SC4H9O2+H2O2<=>SC4H9O2H+HO2  
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:ANALOGY  
TO H2O2+CH3O2<=>HO2+CH3O2H !\COMMENT:

SC4H9O2+C3H8<=>SC4H9O2H+NC3H7  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
SC4H9O2+C3H8<=>SC4H9O2H+IC3H7  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975  
!\COMMENT:  
!

---

!\REACTIONCLASS: \RO2+RO2\_PRODUCTS \A  
\N \EA  
!

---

SC4H9O2+CH3O2=>SC4H9O+CH3O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+SC4H9O2=>SC4H9O+SC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RO2+R\_PRODUCTS \A  
\N \EA  
!

---

SC4H9O2+CH3<=>SC4H9O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+C2H5<=>SC4H9O+C2H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+IC3H7<=>SC4H9O+IC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+NC3H7<=>SC4H9O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+SC4H9<=>SC4H9O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+C3H5-A<=>SC4H9O+C3H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
SC4H9O2+C4H71-3<=>SC4H9O+C4H71-O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:

```

!
-----
!\REACTIONCLASS:  \KHP_DECOMP                \A
\N                \EA
!
-----
SC4H9O+OH<=>SC4H9O2H
+1.0000000E+015 -8.0000000E-001 +0.0000000E+000    !\AUTHOR: !\REF:PITZ
ESTIMATE !\COMMENT:
!
-----
!\REACTIONCLASS:  \RO2+QOOH                \A
\N                \EA
!
-----
SC4H9O2<=>C4H8OOH2-1
+1.4580000E+009 +1.1000000E+000 +3.3500000E+004    !\AUTHOR: !\REF:Sharma
!\COMMENT: A factor revalued 20140425 KWZ 4.862E+008 1.100 33500.0
SC4H9O2<=>C4H8OOH2-3
+1.7160000E+009 +9.0000000E-001 +2.9500000E+004    !\AUTHOR: !\REF:Sharma
!\COMMENT: A factor revalued 20140425 KWZ 8.580E+008 0.900 29500.0
SC4H9O2<=>C4H8OOH2-4
+1.4390000E+007 +1.4000000E+000 +2.0800000E+004    !\AUTHOR: !\REF:Sharma
!\COMMENT: A factor revalued 20140425 KWZ 4.795E+006 1.400 20800.0
!
-----
!\REACTIONCLASS:  \RO2+ALKENE_HO2          \A
\N                \EA
!
-----
SC4H9O2<=>C4H8-1+HO2
+5.1300000E+009 +1.0000000E+000 +3.0400000E+004    !\AUTHOR: !\REF:Villano
!\COMMENT:
!
-----
!\REACTIONCLASS:  \QOOH_ALKENE_HO2        \A
\N                \EA
!
-----
!\REACTIONCLASS:  \QOOH_CYC_ETH_OH        \A
\N                \EA
!
-----
C4H8OOH1-2<=>C4H8O1-2+OH
+1.7100000E+009 +1.0600000E+000 +1.0900000E+004    !\AUTHOR: !\REF:Villano
(From Kuiwen's Mech) !\COMMENT:
C4H8OOH1-3<=>C4H8O1-3+OH
+2.5900000E+009 +6.9000000E-001 +1.6000000E+004    !\AUTHOR: !\REF:Villano
(From Kuiwen's Mech) !\COMMENT:
C4H8OOH1-4<=>C4H8O1-4+OH
+1.7200000E+008 +7.6000000E-001 +1.1100000E+004    !\AUTHOR: !\REF:Villano
(From Kuiwen's Mech) !\COMMENT:
C4H8OOH2-4<=>C4H8O1-3+OH
+2.4400000E+009 +7.8000000E-001 +1.8000000E+004    !\AUTHOR: !\REF:Villano
(From Kuiwen's Mech) !\COMMENT:

```

!=====  
=====  
!\SUBSPECIES: \C4\_CYC\_ETH  
!=====  
=====  
!

---

!\REACTIONCLASS: \LUMPED\_ABSTRACTION \A  
\N \EA  
!

---

---

C4H8O1-2+H=>CH2O+C3H5-A+H2  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-2+O=>CH2O+C3H5-A+OH  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-2+OH=>CH2O+C3H5-A+H2O  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-2+HO2=>CH2O+C3H5-A+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-2+CH3=>CH2O+C3H5-A+CH4  
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-2+CH3O2=>CH2O+C3H5-A+CH3O2H  
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-3+H=>CH2O+C3H5-A+H2  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-3+O=>CH2O+C3H5-A+OH  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-3+OH=>CH2O+C3H5-A+H2O  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-3+CH3=>CH2O+C3H5-A+CH4  
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H  
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-4+H=>CH2O+C3H5-A+H2  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-4+O=>CH2O+C3H5-A+OH  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-4+OH=>CH2O+C3H5-A+H2O  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:



C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-4+CH3=>CH2O+C3H5-A+CH4  
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H  
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O2-3+H=>CH2O+C3H5-A+H2  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O2-3+OH=>CH2O+C3H5-A+H2O  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O2-3+O=>CH2O+C3H5-A+OH  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O2-3+HO2=>CH2O+C3H5-A+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O2-3+CH3O2=>CH2O+C3H5-A+CH3O2H  
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
C4H8O2-3+CH3=>CH2O+C3H5-A+CH4  
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:

!=====  
!=====  
!\ENDSUBSPECIES: \C4\_CYC\_ETH  
!=====  
!=====  
!

---

!\REACTIONCLASS: \QOOH\_DECOMP \A  
\N \EA  
!

---

C4H8OOH1-3=>OH+CH2O+C3H6  
+1.2300000E+009 +1.3000000E+000 +2.4900000E+004 !\AUTHOR: !\REF:Villano  
(From Kuiwen's Mech) !\COMMENT:  
C4H8OOH2-4=>OH+CH3CHO+C2H4  
+3.0800000E+008 +1.5000000E+000 +2.3500000E+004 !\AUTHOR: !\REF:Villano  
(From Kuiwen's Mech) !\COMMENT:  
!

---

!\REACTIONCLASS: \QOOH+O2\_PRODUCTS \A  
\N \EA  
!

---

C4H8OOH1-2+O2<=>C4H8OOH1-2O2  
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-3+O2<=>C4H8OOH1-3O2  
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:

C4H8OOH1-4+O2<=>C4H8OOH1-4O2  
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH2-1+O2<=>C4H8OOH2-1O2  
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH2-3+O2<=>C4H8OOH2-3O2  
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH2-4+O2<=>C4H8OOH2-4O2  
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!

---

!\REACTIONCLASS: \O2QOOH\_ALKENEKHP\_HO2 \A  
\N \EA  
!

---

C4H8OOH1-2O2<=>C4H72-1OOH+HO2  
+2.5400000E+010 +8.0400000E-001 +3.0098500E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-3O2<=>C4H71-4OOH+HO2  
+5.1300000E+009 +1.0000000E+000 +3.0400000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-3O2<=>C4H72-1OOH+HO2  
+2.5400000E+010 +8.0400000E-001 +3.0098500E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-4O2<=>C4H71-4OOH+HO2  
+1.4400000E+007 +1.3800000E+000 +2.8900000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH2-3O2<=>C4H71-3OOH+HO2  
+5.1300000E+009 +1.0000000E+000 +3.0400000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH2-4O2<=>C4H71-3OOH+HO2  
+1.4400000E+007 +1.3800000E+000 +2.8900000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!

---

!\REACTIONCLASS: \O2QOOH\_POOH \A  
\N \EA  
!

---

C4H8OOH1-2O2<=>C4H71-3,4OOH  
+1.4400000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-2O2<=>C4H72-3,4OOH  
+1.7200000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-2O2<=>NC4KET12+OH  
+2.4400000E+007 +1.6000000E+000 +2.7900000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-3O2<=>C4H71-2,4OOH  
+1.4600000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H8OOH1-3O2<=>C4H72-1,3OOH  
+1.7200000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:

C4H8OOH1-3O2<=>NC4KET13+OH  
 +1.0900000E+004 +2.4000000E+000 +1.9900000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH1-4O2<=>C4H72-1,4OOH  
 +1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 DUP  
 C4H8OOH1-4O2<=>C4H72-1,4OOH  
 +4.0100000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 DUP  
 C4H8OOH1-4O2<=>NC4KET14+OH  
 +4.8000000E+003 +1.7000000E+000 +1.6600000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-1O2<=>C4H72-3,4OOH  
 +1.7200000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-1O2<=>C4H71-3,4OOH  
 +1.2300000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-1O2<=>NC4KET21+OH  
 +2.7600000E+008 +1.2000000E+000 +2.5700000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-3O2<=>C4H71-2,3OOH  
 +1.4600000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 DUP  
 C4H8OOH2-3O2<=>C4H71-2,3OOH  
 +1.4400000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 DUP  
 C4H8OOH2-3O2<=>NC4KET23+OH  
 +1.7500000E+006 +1.7000000E+000 +2.6000000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-4O2<=>C4H71-2,4OOH  
 +1.2300000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-4O2<=>C4H72-1,3OOH  
 +4.0100000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H8OOH2-4O2<=>NC4KET24+OH  
 +5.7900000E+001 +2.9000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 !

---

!\REACTIONCLASS: \POOH\_PRODUCTS1

\A

\N

\EA

!

---

C4H71-3,4OOH<=>C4H7O1-3OOH-4+OH  
 +2.4400000E+009 +7.8000000E-001 +1.8000000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H71-3,4OOH<=>C4H7O1-4OOH-2+OH  
 +1.7200000E+009 +7.6000000E-001 +1.1100000E+004 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:  
 C4H72-3,4OOH<=>C4H7O2-3OOH-1+OH  
 +6.9900000E+009 +8.1500000E-001 +9.7883000E+003 !\AUTHOR: !\REF:Miyoshi  
 A/2 compared to R+O2 080415A !\COMMENT:

C4H72-3,4OOH<=>C4H7O1-3OOH-2+OH  
+2.5900000E+009 +6.9000000E-001 +1.6000000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-2,4OOH<=>C4H7O1-2OOH-4+OH  
+2.3500000E+010 +6.8000000E-001 +1.0800000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-2,4OOH<=>C4H7O1-4OOH-2+OH  
+1.7200000E+009 +7.6000000E-001 +1.1100000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,3OOH<=>C4H7O1-2OOH-3+OH  
+1.7100000E+009 +1.0600000E+000 +1.0900000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,3OOH<=>C4H7O2-3OOH-1+OH  
+6.9900000E+009 +8.1500000E-001 +9.7883000E+003 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,4OOH<=>C4H7O1-2OOH-4+OH  
+1.7100000E+009 +1.0600000E+000 +1.0900000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,4OOH<=>C4H7O1-3OOH-4+OH  
+2.5900000E+009 +6.9000000E-001 +1.6000000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-2,3OOH<=>C4H7O1-2OOH-3+OH  
+2.3500000E+010 +6.8000000E-001 +1.0800000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-2,3OOH<=>C4H7O1-3OOH-2+OH  
+2.4400000E+009 +7.8000000E-001 +1.8000000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-3,4OOH=>C2H4+OH+HO2CH2CHO  
+1.2300000E+009 +1.3000000E+000 +2.4900000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!  
!

---

!\REACTIONCLASS: \POOH\_PRODUCTS2 \A  
\N \EA  
!

---

C4H72-3,4OOH<=>C4H72-1OOH+HO2  
+2.5680000E+011 +5.3800000E-001 +1.5324700E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!C4H71-1,2OOH<=>NC4KET12+OH 9.000E+014 0.000 1500.0 !\AUTHOR:  
!\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-2,4OOH<=>C4H71-4OOH+HO2  
+2.6700000E+011 +5.0000000E-001 +1.5800000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,3OOH<=>C4H72-1OOH+HO2  
+2.5680000E+011 +5.3800000E-001 +1.5324700E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,3OOH<=>C4H71-3OOH+HO2  
+6.0300000E+009 +9.5000000E-001 +1.5200000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!C4H71-1,3OOH<=>NC4KET13+OH 9.000E+014 0.000 1500.0 !\AUTHOR:  
!\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,4OOH<=>C4H71-4OOH+HO2  
+2.5680000E+011 +5.3800000E-001 +1.5324700E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!C4H72-1,2OOH<=>NC4KET21+OH 9.000E+014 0.000 1500.0 !\AUTHOR:  
!\REF:Miyoshi A/2 compared to R+O2 080415A !\COMMENT:

C4H71-2,3OOH<=>C4H71-3OOH+HO2  
+6.0300000E+009 +9.5000000E-001 +1.5200000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H72-1,4OOH<=>C4H72-1OOH+HO2  
+2.6700000E+011 +5.0000000E-001 +1.5800000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!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  
!

---

C4H72-1OOH=>CH2O+C3H5-S+OH  
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!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:  
C4H71-3OOH=>C2H3CHO+CH3+OH  
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
C4H71-3OOH=>CH3CHO+C2H3+OH  
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:Miyoshi  
A/2 compared to R+O2 080415A !\COMMENT:  
!

---

!\REACTIONCLASS: \KHP\_DECOMP \A  
\N \EA  
!

---

NC4KET12=>C2H5CHO+HCO+OH  
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT:  
NC4KET13=>CH3CHO+CH2CHO+OH  
+1.0500000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT: EA+1.4K,20140430  
KWZ  
NC4KET14=>CH2CH2CHO+CH2O+OH  
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT:  
NC4KET21=>CH2O+C2H5CO+OH  
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT:  
NC4KET23=>CH3CHO+CH3CO+OH  
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT:  
NC4KET24=>CH2O+CH3COCH2+OH  
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT: EA+1K,20140430 KWZ  
HO2CH2CHO=>CH2O+HCO+OH  
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:  
WARNING: NO ORIGINAL REFERENCE IN MECHANISM !\COMMENT:

!-----  
!-----  
!\ENDSUBMECH: \C4H10  
!-----  
!-----  
!\SUBMECH: \IC4H10  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

---

IC4H10 (+M) <=> CH3+IC3H7 (+M)  
+2.5200000E+031 -4.1020000E+000 +9.1495000E+004 !\AUTHOR:  
!\REF:OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253  
!\COMMENT:  
LOW /  
+2.4100000E+019 +0.0000000E+000 +5.2576000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +3.6620000E-001  
+8.1530000E+002 +6.0790000E+001 +1.0000000E+020 / !TROE PARAMETERS  
IC4H10 <=> TC4H9+H  
+2.5100000E+098 -2.3810000E+001 +1.4530000E+005 !\AUTHOR:  
!\REF:OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253.  
!\COMMENT:  
IC4H10 <=> IC4H9+H  
+9.8500000E+095 -2.3110000E+001 +1.4760000E+005 !\AUTHOR:  
!\REF:OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253.  
!\COMMENT:  
!

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

IC4H10+CH3 <=> IC4H9+CH4  
+1.3600000E+000 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:TSANG,  
J. PHYS. CHEM. REF. DATA 19, 1-68 (1990) !\COMMENT:  
IC4H10+H <=> IC4H9+H2  
+1.8100000E+006 +2.5400000E+000 +6.7560000E+003 !\AUTHOR: !\REF:TSANG,  
J. PHYS. CHEM. REF. DATA 19, 1-68 (1990) !\COMMENT:  
IC4H10+OH <=> IC4H9+H2O  
+6.6540000E+004 +2.6650000E+000 -1.6890000E+002 !\AUTHOR: !\REF:JOE  
MICHAELS SYMP. PAPER 2008. !\COMMENT:  
IC4H10+C2H5 <=> IC4H9+C2H6  
+1.5100000E+012 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:ALLARA  
AND SHAW ANALOG !\COMMENT:  
IC4H10+HO2 <=> IC4H9+H2O2  
+6.1200000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:

$\text{IC4H10+O} \rightleftharpoons \text{IC4H9+OH}$   
+4.0460000E+007 +2.0340000E+000 +5.1360000E+003 !\AUTHOR: !\REF:NIST  
STANDARD REFERENCE DATABASE 17 -2Q98 !\COMMENT:  
 $\text{IC4H10+CH3O} \rightleftharpoons \text{IC4H9+CH3OH}$   
+4.8000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+CH3O !\COMMENT:  
 $\text{IC4H10+O2} \rightleftharpoons \text{IC4H9+HO2}$   
+9.0000000E+013 +0.0000000E+000 +5.2290000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH C4H10+O2 $\rightleftharpoons$ PC4H9+HO2 !\COMMENT:  
 $\text{IC4H10+CH3O2} \rightleftharpoons \text{IC4H9+CH3O2H}$   
+2.0790000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
 $\text{IC4H10+C2H5O2} \rightleftharpoons \text{IC4H9+C2H5O2H}$   
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:SCOTT  
AND WALKER C&F 129(4) 365--377 2002 (\*1.5) !\COMMENT:  
 $\text{IC4H10+CH3CO3} \rightleftharpoons \text{IC4H9+CH3CO3H}$   
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+NC3H7O2} \rightleftharpoons \text{IC4H9+NC3H7O2H}$   
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+IC3H7O2} \rightleftharpoons \text{IC4H9+IC3H7O2H}$   
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+IC4H9O2} \rightleftharpoons \text{IC4H9+IC4H9O2H}$   
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+TC4H9O2} \rightleftharpoons \text{IC4H9+TC4H9O2H}$   
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+O2CHO} \rightleftharpoons \text{IC4H9+HO2CHO}$   
+2.5200000E+013 +0.0000000E+000 +2.0440000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+SC4H9O2} \rightleftharpoons \text{IC4H9+SC4H9O2H}$   
+2.2500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+SC4H9O2} \rightleftharpoons \text{TC4H9+SC4H9O2H}$   
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
 $\text{IC4H10+PC4H9O2} \rightleftharpoons \text{IC4H9+PC4H9O2H}$   
+2.2500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H6+HO2 !\COMMENT:  
 $\text{IC4H10+H} \rightleftharpoons \text{TC4H9+H2}$   
+6.0200000E+005 +2.4000000E+000 +2.5830000E+003 !\AUTHOR: !\REF:TSANG,  
J. PHYS. CHEM. REF. DATA 19, 1-68 (1990) !\COMMENT:  
 $\text{IC4H10+CH3} \rightleftharpoons \text{TC4H9+CH4}$  +9.0400000E-  
001 +3.4600000E+000 +4.5980000E+003 !\AUTHOR: !\REF:TSANG, J. PHYS.  
CHEM. REF. DATA 19, 1-68 (1990) !\COMMENT:  
 $\text{IC4H10+OH} \rightleftharpoons \text{TC4H9+H2O}$   
+2.9250000E+004 +2.5310000E+000 -1.6590000E+003 !\AUTHOR: !\REF:JOE  
MICHAELS SYMP. PAPER 2008. !\COMMENT:  
 $\text{IC4H10+C2H5} \rightleftharpoons \text{TC4H9+C2H6}$   
+1.0000000E+011 +0.0000000E+000 +7.9000000E+003 !\AUTHOR: !\REF:FROM  
ISOBUTYL RATE !\COMMENT:

IC4H10+HO2<=>TC4H9+H2O2  
+4.3320000E+002 +3.0100000E+000 +1.2090000E+004 !\AUTHOR: !\REF: X0.666  
!\COMMENT: WARNING. SOURCE UNCLEAR  
IC4H10+O<=>TC4H9+OH  
+1.9680000E+005 +2.4020000E+000 +1.1500000E+003 !\AUTHOR: !\REF:NIST  
STANDARD REFERENCE DATABASE 17 -2Q98 !\COMMENT:  
IC4H10+CH3O<=>TC4H9+CH3OH  
+1.9000000E+010 +0.0000000E+000 +2.8000000E+003 !\AUTHOR: !\REF:TAMURA  
ESTIMATE !\COMMENT:  
IC4H10+O2<=>TC4H9+HO2  
+1.0000000E+013 +0.0000000E+000 +4.8200000E+004 !\AUTHOR: !\REF:  
Ingham,T.; Walker,R.W.; Woolford,R.E., Symp. Int. Combust. Proc. 25, 767-  
774 (1994) !\COMMENT:  
IC4H10+O2CHO<=>TC4H9+HO2CHO  
+2.8000000E+012 +0.0000000E+000 +1.6010000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH RH+RO2 -->R+RO2H !\COMMENT:  
IC4H10+PC4H9O2<=>TC4H9+PC4H9O2H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+CH3O2<=>TC4H9+CH3O2H  
+1.3660000E+002 +3.1200000E+000 +1.3190000E+004 !\AUTHOR: !\REF:J.  
AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.  
!\COMMENT:  
IC4H10+C2H5O2<=>TC4H9+C2H5O2H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+CH3CO3<=>TC4H9+CH3CO3H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+NC3H7O2<=>TC4H9+NC3H7O2H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+IC3H7O2<=>TC4H9+IC3H7O2H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+IC4H9O2<=>TC4H9+IC4H9O2H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+TC4H9O2<=>TC4H9+TC4H9O2H  
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,  
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988  
!\COMMENT:  
IC4H10+IC4H9<=>TC4H9+IC4H10  
+2.5000000E+010 +0.0000000E+000 +7.9000000E+003 !\AUTHOR:  
!\REF:WESTBROOK AND PITZ ESTIMATE (1983) !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_ISOMERISATION

\A

\N

\EA

!

---



IC4H9<=>TC4H9  
+3.5600000E+010 +8.8000000E-001 +3.4600000E+004 !\AUTHOR: !\REF:D.M.  
Matheu, W.H. Green, J.M. Grenda, Int. J. Chem. Kin. 2003 Volume 35, Issue  
3, 2003, Pages: 95-119 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_BETA\_SCISSION \A  
\N \EA  
!

---

IC4H9<=>C3H6+CH3  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\ FROM K.  
ZHANG ESTIMATED !\COMMENT:  
PLOG / +1.0000000E-001  
+3.1500000E+041 -9.5000000E+000 +3.3486000E+004 /  
PLOG / +1.0000000E+000  
+6.7500000E+044 -1.0070000E+001 +3.7209000E+004 /  
PLOG / +1.0000000E+001  
+7.7900000E+044 -9.7000000E+000 +3.9751000E+004 /  
PLOG / +1.0000000E+002  
+3.6100000E+039 -7.7800000E+000 +3.9583000E+004 /  
!

---

!\REACTIONCLASS: \R\_RO2 \A  
\N \EA  
!

---

TC4H9+HO2<=>TC4H9O+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
TC4H9+CH3O2<=>TC4H9O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
TC4H9+NC3H7O2<=>TC4H9O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
TC4H9+SC4H9O2<=>TC4H9O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
TC4H9+PC4H9O2<=>TC4H9O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
TC4H9+IC3H7O2<=>TC4H9O+IC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC4H9+HO2<=>IC4H9O+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC4H9+CH3O2<=>IC4H9O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC4H9+NC3H7O2<=>IC4H9O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
IC4H9+SC4H9O2<=>IC4H9O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:

```

IC4H9+PC4H9O2<=>IC4H9O+PC4H9O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003    !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
IC4H9+IC3H7O2<=>IC4H9O+IC3H7O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003    !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
!=====
=====
!\SUBSPECIES: \TC4H9O
!=====
=====
!
!
!
!\REACTIONCLASS: \R_BETA_SCISSION                \A
\N                \EA
!
!
!
CH3COCH3+CH3<=>TC4H9O
+1.5000000E+011 +0.0000000E+000 +1.1900000E+004    !\AUTHOR: !\REF:CURRAN
INC. INT J CHEM KINET 38: 250?275, 2006 !\COMMENT:
!
!
!\REACTIONCLASS: \R_O2                            \A
\N                \EA
!
!
!
TC4H9O+O2<=>IC4H8O+HO2
+8.1000000E+011 +0.0000000E+000 +4.7000000E+003    !\AUTHOR: !\REF:PITZ
ESTIMATE !\COMMENT:
!=====
=====
!\ENDSUBSPECIES: \TC4H9O
!=====
=====
!
!\SUBSPECIES: \IC4H9O
!=====
=====
!
!
!\REACTIONCLASS: \R_R_ABSTRACTION                \A
\N                \EA
!
!
!
IC4H9O+H<=>IC3H7CHO+H2
+1.9900000E+013 +0.0000000E+000 +0.0000000E+000    !\AUTHOR: !\REF:ANALOGY
CH3O+X -->CH2O+HX TSANG/ HAMPSON 86 !\COMMENT:
IC4H9O+O2<=>IC3H7CHO+HO2
+1.9300000E+011 +0.0000000E+000 +1.6600000E+003    !\AUTHOR:
!\REF:!\ZABARNICK, S. AND HEICKLEN, J., IJCK, 17, 503 (1985). !\COMMENT:
IC4H9O+O<=>IC3H7CHO+OH
+6.0000000E+012 +0.0000000E+000 +0.0000000E+000    !\AUTHOR: !\REF:ANALOGY
CH3O+X -->CH2O+HX TSANG/ HAMPSON 86 !\COMMENT:
IC4H9O+OH<=>IC3H7CHO+H2O
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000    !\AUTHOR: !\REF:ANALOGY
CH3O+X -->CH2O+HX TSANG/ HAMPSON 86 !\COMMENT:

```

IC4H9O+HO2<=>IC3H7CHO+H2O2  
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX TSANG/ HAMPSON 86 !\COMMENT:  
IC4H9O+CH3<=>IC3H7CHO+CH4  
+2.4000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX TSANG/ HAMPSON 86 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_BETA\_SCISSION \A  
\N \EA  
!

---

IC3H7CHO+H<=>IC4H9O  
+1.0000000E+012 +0.0000000E+000 +5.8600000E+003 !\AUTHOR: !\REF:CURRAN  
INC. INT J CHEM KINET 38: 250?275, 2006 !\COMMENT:  
CH2O+IC3H7<=>IC4H9O  
+5.0000000E+010 +0.0000000E+000 +2.3300000E+003 !\AUTHOR: !\REF:CURRAN  
INC. INT J CHEM KINET 38: 250?275, 2006 !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \IC4H9O

!=====  
=====

!=====  
=====

!\SUBSPECIES: \IC3H7CHO\IC4H8O\SC4H7OH-I

!=====  
=====

!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

TC3H6CHO+H<=>IC3H7CHO  
+2.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES !\COMMENT:  
SC4H7OH-I<=>IC3H7CHO  
+8.5900000E+011 +3.1800000E-001 +5.5900000E+004 !\AUTHOR: !\REF:  
AUTOMERIZATION OF 1-PROPENOL (CH3CHCHOH) TO PROPANAL (C2H5CHO) !\COMMENT:  
IC3H7+HCO<=>IC3H7CHO  
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:TSANG  
J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
IC4H8O<=>IC3H7CHO  
+4.1800000E+013 +0.0000000E+000 +5.2720000E+004 !\AUTHOR: !\REF: X 2.0  
!\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

IC3H7CHO+HO2<=>IC3H7CO+H2O2  
+3.0000000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:BASED  
ON CH3CHO+HO2 !\COMMENT:  
IC3H7CHO+CH3<=>IC3H7CO+CH4  
+3.9800000E+012 +0.0000000E+000 +8.7000000E+003 !\AUTHOR:

!\REF: BIRRELL, R.N.; TROTMAN-DICKENSON, A.F. J. CHEM. SOC. 1960, 2059  
 !\COMMENT:  
 IC3H7CHO+O<=>IC3H7CO+OH  
 +7.1800000E+012 +0.0000000E+000 +1.3890000E+003 !\AUTHOR:  
 !\REF: SINGLETON, D.L. ET AL. CAN. J. CHEM. 1977, 55, 3321. !\COMMENT:  
 IC3H7CHO+O2<=>IC3H7CO+HO2  
 +4.0000000E+013 +0.0000000E+000 +3.7600000E+004 !\AUTHOR:  
 !\REF: !\BALDWIN, R.R. ET AL. J. CHEM. SOC. FAR. TRANS. 1979, 75, 1433  
 !\COMMENT:  
 IC3H7CHO+OH<=>IC3H7CO+H2O  
 +2.6900000E+010 +7.6000000E-001 -3.4000000E+002 !\AUTHOR: !\REF: SEMMES  
 ET AL. INTL. J. CHEM. KINET. 1985, 17, 303. !\COMMENT:  
 IC3H7CHO+H<=>IC3H7CO+H2  
 +2.6000000E+012 +0.0000000E+000 +2.6000000E+003 !\AUTHOR: !\REF: CURRAN  
 ESTIMATE !\COMMENT:  
 IC3H7CHO+OH<=>IC3H6CHO+H2O  
 +3.1200000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF: CURRAN  
 ESTIMATE !\COMMENT:  
 IC3H7CHO+HO2<=>IC3H6CHO+H2O2  
 +2.7400000E+004 +2.5500000E+000 +1.5500000E+004 !\AUTHOR: !\REF: CURRAN  
 ESTIMATE !\COMMENT:  
 IC3H7CHO+CH3O2<=>IC3H6CHO+CH3O2H  
 +4.7600000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF: CURRAN  
 ESTIMATE !\COMMENT:  
 TC3H6CHO+H2<=>IC3H7CHO+H  
 +2.1600000E+005 +2.3800000E+000 +1.8990000E+004 !\AUTHOR: !\REF: ANALOGY  
 WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES !\COMMENT:  
 IC3H7CHO+HO2<=>TC3H6CHO+H2O2  
 +8.0000000E+010 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF: SYMP.  
 INTL. COMB. PROC. 1979, 17, 525. !\COMMENT:  
 IC3H7CHO+OH<=>TC3H6CHO+H2O  
 +1.6840000E+012 +0.0000000E+000 -7.8100000E+002 !\AUTHOR: !\REF: SEMMES  
 ET AL. INTL. J. CHEM. KINET. 1985, 17, 303. !\COMMENT:  
 IC4H8O+OH<=>IC3H6CHO+H2O  
 +7.5200000E+004 +2.4900000E+000 -1.4741000E+003 !\AUTHOR: !\REF: ANALOGY  
 TO C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 IC4H8O+H<=>IC3H6CHO+H2  
 +8.7900000E+004 +2.6800000E+000 +2.9100000E+003 !\AUTHOR: !\REF: ANALOGY  
 TO C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 IC4H8O+HO2<=>IC3H6CHO+H2O2 +2.4500000E-  
 005 +5.2600000E+000 +7.4751000E+003 !\AUTHOR: !\REF: ANALOGY TO  
 C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 IC4H8O+CH3O2<=>IC3H6CHO+CH3O2H +1.2250000E-  
 005 +5.2600000E+000 +7.4751000E+003 !\AUTHOR: !\REF: ANALOGY TO  
 C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 IC4H8O+CH3<=>IC3H6CHO+CH4  
 +1.9930000E+001 +3.3700000E+000 +7.6340000E+003 !\AUTHOR: !\REF: ANALOGY  
 TO C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 IC4H8O+O<=>IC3H6CHO+OH  
 +1.4500000E+005 +2.4700000E+000 +8.7600000E+002 !\AUTHOR: !\REF: ANALOGY  
 TO C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 IC4H8O+O2<=>IC3H6CHO+HO2  
 +1.5000000E+013 +0.0000000E+000 +5.0150000E+004 !\AUTHOR: !\REF: ANALOGY  
 TO C2H5OH+R=SC2H4OH+RH !\COMMENT:  
 !=====  
 =====  
 !\SUBSPECIES: \TC3H6CHO

!=====  
=====  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

IC3H5CHO+H<=>TC3H6CHO  
+1.3000000E+013 +0.0000000E+000 +1.2000000E+003 !\AUTHOR: !\REF:H.J.  
Curran, International Journal of Chemical Kinetics (2006) 38: 250-275.  
!\COMMENT:  
IC3H6CO+H<=>TC3H6CHO  
+1.3000000E+013 +0.0000000E+000 +4.8000000E+003 !\AUTHOR: !\REF:H.J.  
Curran, International Journal of Chemical Kinetics (2006) 38: 250-275.  
!\COMMENT:  
IC3H6CO+OH<=>IC3H7+CO2  
+1.7300000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR: !\REF:ANALOGY  
TO 1C4H8+OH !\COMMENT:  
IC3H6CO+OH<=>C3H6OH2-1+CO  
+2.0000000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
!

---

---

!\REACTIONCLASS: \R\_RH\_ABSTRACTION \A  
\N \EA  
!

---

TC3H6CHO+HO2<=>IC3H7CHO+O2  
+3.6750000E+012 +0.0000000E+000 +1.3100000E+003 !\AUTHOR:  
!\REF:!\LOHDI, Z.H.; WALKER, R.W.; J. CHEM. SOC. FARAD. 1991 87, 2361  
(C3H5-A+HO2) (X 0.5) !\COMMENT:  
TC3H6CHO+CH3<=>IC3H5CHO+CH4  
+3.0100000E+012 -3.2000000E-001 -1.3100000E+002 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
TC3H6CHO+CH2O<=>IC3H7CHO+HCO  
+2.5200000E+008 +1.9000000E+000 +1.8190000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES !\COMMENT:  
TC3H6CHO+IC4H8<=>IC3H7CHO+IC4H7  
+4.7000000E+002 +3.3000000E+000 +1.9840000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES !\COMMENT:  
!

---

---

!\REACTIONCLASS: \R\_O2\_RO2 \A  
\N \EA  
!

---

TC3H6CHO+O2<=>TC3H6O2CHO  
+1.9900000E+017 -2.1000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
TO NEOPENTYL, Xi, Z.; Han, W-J.; Bayes, K.D., J. Phys. Chem. 92, 3450  
(1988) !\COMMENT:  
TC3H6O2CHO<=>IC3H5O2HCHO  
+6.0000000E+011 +0.0000000E+000 +2.9880000E+004 !\AUTHOR: !\REF:ANALOGY  
TO NEOPENTYL, Xi, Z.; Han, W-J.; Bayes, K.D., J. Phys. Chem. 92, 3450  
(1988) !\COMMENT:  
TC3H6O2CHO<=>TC3H6O2HCO  
+1.0000000E+011 +0.0000000E+000 +2.5750000E+004 !\AUTHOR: !\REF:ANALOGY

TO NEOPENTYL, Xi, Z.; Han, W-J.; Bayes, K.D., J. Phys. Chem. 92, 3450 (1988) !\COMMENT:

IC3H5CHO+HO2<=>IC3H5O2HCHO  
+2.2300000E+011 +0.0000000E+000 +1.0600000E+004 !\AUTHOR: !\REF:SLAGLE ET AL. J. PHYS. CHEM. 1991, 95 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_HO2\_PRODUCTS \A  
\N \EA  
!

---

TC3H6OCHO+OH<=>TC3H6CHO+HO2  
+2.0180000E+017 -1.2000000E+000 +2.1010000E+004 !\AUTHOR: !\REF:ANALOGY WITH C3H5-A+CH3 -->1-C4H8 TSANG 91 (PROPENE). !\COMMENT:  
TC3H6OCHO<=>CH3COCH3+HCO  
+3.9800000E+013 +0.0000000E+000 +9.7000000E+003 !\AUTHOR: !\REF:CURRAN AND GAFFURI, 1995. !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_OH\_TERMINATION \A  
\N \EA  
!

---

TC3H6CHO+OH<=>IC3H6OHCHO  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:  
C3H6OH2-1+HCO<=>IC3H6OHCHO  
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:!\TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:  
!=====

!\SUBSPECIES: \IC3H5CHO  
!=====

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

IC3H5CHO+H<=>IC3H5CO+H2  
+7.1474036E+005 +2.3567400E+000 +1.5771627E+003 !\AUTHOR:  
!\REF:ANALOGOUS TO ISOBUTERALDEHYDE+X !\COMMENT:  
IC3H5CHO+O2<=>IC3H5CO+HO2  
+2.0000000E+013 +0.0000000E+000 +4.0700000E+004 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
IC3H5CHO+O<=>IC3H5CO+OH  
+7.1800000E+012 +0.0000000E+000 +1.3890000E+003 !\AUTHOR:  
!\REF:ANALOGOUS TO ISOBUTERALDEHYDE+X !\COMMENT:  
IC3H5CHO+OH<=>IC3H5CO+H2O  
+6.1329900E+004 +2.6500000E+000 -4.5864000E+003 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.  
!\COMMENT:  
IC3H5CHO+HO2<=>IC3H5CO+H2O +1.1773000E-004 +4.9196600E+000 +3.6842744E+003 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104. !\COMMENT:  
IC3H5CHO+CH3<=>IC3H5CO+CH4  
+1.2487900E+000 +3.6338600E+000 +4.3289348E+003 !\AUTHOR: !\REF:J.

MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.  
!\COMMENT:  
IC3H5CHO+H<=>IC3H4CHO-A+H2  
+3.6400000E+005 +2.4550000E+000 +4.3612000E+003 !\AUTHOR: !\REF:  
ANALOGY TO ALLYL RADICAL IN C3H6 !\COMMENT:  
IC3H5CHO+O2<=>IC3H4CHO-A+HO2  
+5.9600000E+019 -1.6700000E+000 +4.6192100E+004 !\AUTHOR: !\REF:  
ANALOGY TO ALLYL RADICAL IN C3H6 !\COMMENT:  
IC3H5CHO+OH<=>IC3H4CHO-A+H2O  
+4.4600000E+006 +2.0720000E+000 +1.0508000E+003 !\AUTHOR: !\REF:  
ANALOGY TO ALLYL RADICAL IN C3H6 !\COMMENT:  
IC3H5CHO+O<=>IC3H4CHO-A+OH  
+5.2400000E+011 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:  
ANALOGY TO ALLYL RADICAL IN C3H6 !\COMMENT:  
IC3H5CHO+HO2<=>IC3H4CHO-A+H2O2 +3.0700000E-  
002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: ANALOGY TO ALLYL  
RADICAL IN C3H6 !\COMMENT:  
IC3H5CHO+CH3<=>IC3H4CHO-A+CH4  
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
ANALOGY TO ALLYL RADICAL IN C3H6 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

IC3H5CO<=>C3H5-T+CO  
+1.2780000E+020 -1.8900000E+000 +3.4460000E+004 !\AUTHOR:  
!\REF:ANALOGOUS TO ISOBUTERALDEHYDE+X !\COMMENT:  
C3H4-A+HCO<=>IC3H4CHO-A  
+4.0209730E+004 +2.5181500E+000 +8.8475357E+003 !\AUTHOR: !\ REF:  
ANALOGY TO C3H4-A+CH3-->IC4H7 ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-  
311++G(D,P) LEVEL OF THEORY !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

IC3H7+CO<=>IC3H7CO  
+1.5000000E+011 +0.0000000E+000 +4.8100000E+003 !\AUTHOR:  
!\REF:NAROZNIK, M; NIEDZIELSKI, J. J. PHOTOCHEM. 1986, 32, 281 !\COMMENT:  
C2H3CHO+CH3<=>IC3H6CHO  
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \IC3H5CHO

!=====  
=====

!=====  
=====

!\ENDSUBSPECIES: \TC3H6CHO

!=====  
=====

!=====  
=====

!\SUBSPECIES: \SC4H7OH-I

!=====  
=====  
!

---

!\REACTIONCLASS: \R\_CAT\_ISO \A  
\N \EA  
!

---

SC4H7OH-I+HO2<=>IC3H7CHO+HO2  
+1.4900000E+005 +1.6700000E+000 +6.8100000E+003 !\AUTHOR: !\ KETO-ENOL  
ISOMERIZATIONS !\COMMENT: WARNING: SOURCE OF RATE CONSTANT UNKNOWN  
SC4H7OH-I+HOCHO<=>IC3H7CHO+HOCHO +2.8100000E-  
002 +3.2860000E+000 -4.5090000E+003 !\AUTHOR: !\ KETO-ENOL  
ISOMERIZATIONS !\COMMENT: WARNING: SOURCE OF RATE CONSTANT UNKNOWN  
!

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

SC4H7OH-I+H<=>IC4H6OH+H2  
+7.2900000E+005 +2.4550000E+000 +4.3612000E+003 !\AUTHOR: !\REF:  
ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION !\COMMENT:  
SC4H7OH-I+O<=>IC4H6OH+OH  
+1.0500000E+012 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:  
ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION !\COMMENT:  
SC4H7OH-I+OH<=>IC4H6OH+H2O  
+4.3950169E+004 +2.6784100E+000 -8.2710300E+002 !\AUTHOR: !\REF:  
ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION !\COMMENT:  
SC4H7OH-I+HO2<=>IC4H6OH+H2O +2.9200000E-  
001 +4.1200000E+000 +1.2802000E+004 !\AUTHOR: !\REF: ANALOGY TO IC4H8  
IN ALLYL RADICAL FORMATION !\COMMENT:  
SC4H7OH-I+CH3<=>IC4H6OH+CH4  
+4.4200000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION !\COMMENT:  
SC4H7OH-I+CH3O<=>IC4H6OH+CH3OH  
+1.6800000E+011 +0.0000000E+000 +2.6000000E+003 !\AUTHOR: !\REF:  
ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION !\COMMENT:  
SC4H7OH-I+CH3O2<=>IC4H6OH+CH3O2H  
+1.9280000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION !\COMMENT:  
!

---

---

!\REACTIONCLASS: \R\_R\_PRODUCTS \A  
\N \EA  
!

---

IC4H6OH+H=>CH3+C3H4-A+OH  
+4.0209730E+004 +2.5181500E+000 +8.8475357E+003 !\AUTHOR: !\ BUTENOL  
RADICAL DECOMPOSITION !\COMMENT:

!=====  
=====  
!

!\ENDSUBSPECIES: \SC4H7OH-I

!=====  
=====  
!

!=====  
=====  
!

!\ENDSUBSPECIES: \IC3H7CHO\IC4H8O



!=====  
=====  
!

---

!\REACTIONCLASS: \R\_O2\_ALKENE\_HO2 \A  
\N \EA  
!

---

TC4H9+O2<=>IC4H8+HO2 +8.3700000E-001 +3.5900000E+000 +1.1960000E+004 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:  
IC4H9+O2<=>IC4H8+HO2  
+1.0700000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N,IC3H7+O2) !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_O2\_RO2 \A  
\N \EA  
!

---

IC4H9+O2<=>IC4H9O2  
+6.6946000E+013 -3.0000000E-001 -1.8720000E+002 !\AUTHOR: !\REF: F. GOLDSMITH JPCA, 2012 !\COMMENT:  
TC4H9+O2<=>TC4H9O2  
+6.6946000E+013 -3.0000000E-001 -1.8720000E+002 !\AUTHOR: !\REF: F. GOLDSMITH JPCA, 2012 !\COMMENT:  
!

---

!\REACTIONCLASS: \RO2\_ALKENE\_HO2 \A  
\N \EA  
!

---

IC4H9O2<=>IC4H8+HO2  
+1.9400000E+008 +1.2700000E+000 +2.9600000E+004 !\AUTHOR: !\ ALL USE DEAN'S DATA FIRST TWO 2011, SECOND TWO 2013 !\COMMENT:  
!

---

!\REACTIONCLASS: \RO2\_QOOH \A  
\N \EA  
!

---

IC4H9O2<=>IC4H8O2H-I  
+9.8200000E+007 +1.3000000E+000 +2.1500000E+004 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701 !\COMMENT:  
IC4H9O2<=>IC4H8O2H-T  
+2.3100000E+009 +8.0000000E-001 +2.7100000E+004 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701 !\COMMENT:  
TC4H9O2<=>TC4H8O2H-I  
+4.5210000E+009 +1.2000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701 !\COMMENT:  
!

---

!\REACTIONCLASS: \QOOH\_DECOMP \A  
\N \EA

!  
-----  
IC4H8O2H-I<=>CC4H8O+OH  
+4.4700000E+011 +0.0000000E+000 +2.1900000E+004 !\AUTHOR: !\REF:GREEN  
2003 !\COMMENT:  
IC4H8O2H-I=>OH+CH2O+C3H6  
+8.4510000E+015 -6.8000000E-001 +2.9170000E+004 !\AUTHOR: !\REF:GREEN  
2003 !\COMMENT:  
!=====  
=====  
!\SUBSPECIES: \CC4H8O  
!=====  
=====  
!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

-----  
CC4H8O+OH=>CH2O+C3H5-A+H2O  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
CC4H8O+H=>CH2O+C3H5-A+H2  
+3.5100000E+007 +2.0000000E+000 +5.0000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
CC4H8O+O=>CH2O+C3H5-A+OH  
+1.1240000E+014 +0.0000000E+000 +5.2000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
CC4H8O+HO2=>CH2O+C3H5-A+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
CC4H8O+CH3O2=>CH2O+C3H5-A+CH3O2H  
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
CC4H8O+CH3=>CH2O+C3H5-A+CH4  
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
!=====  
=====  
!\ENDSUBSPECIES: \CC4H8O  
!=====  
=====  
!

!\REACTIONCLASS: \QOOH\_O2 \A  
\N \EA  
!

-----  
IC4H8O2H-I+O2<=>IC4H8OOH-IO2  
+9.3531600E+011 +1.0000000E-001 -1.0108800E+003 !\AUTHOR:  
!\REF:GOLDSMITH, JPCA, 2012 !\COMMENT:  
IC4H8O2H-T+O2<=>IC4H8OOH-TO2  
+5.0448200E+012 -1.0000000E-001 -6.5520000E+002 !\AUTHOR:  
!\REF:GOLDSMITH, JPCA, 2012 !\COMMENT:  
TC4H8O2H-I+O2<=>TC4H8OOH-IO2  
+2.2844294E+010 +5.0000000E-001 -7.8624000E+002 !\AUTHOR:  
!\REF:GOLDSMITH, JPCA, 2012 !\COMMENT:

!

---

!\REACTIONCLASS: \O2QOOH\_PRODUCTS \A  
\N \EA  
!

---

IC4H8OOH-IO2<=>IC4KETII+OH  
+5.0000000E+010 +0.0000000E+000 +2.1400000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM  
IC4H8OOH-TO2<=>IC4KETIT+OH  
+4.0000000E+011 +0.0000000E+000 +3.1500000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM  
IC4H8OOH-TO2<=>TIC4H7Q2-I  
+6.0000000E+011 +0.0000000E+000 +3.4500000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM  
IC4H8OOH-IO2<=>IIC4H7Q2-I  
+3.7500000E+010 +0.0000000E+000 +2.4400000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM  
IC4H8OOH-IO2<=>IIC4H7Q2-T  
+1.0000000E+011 +0.0000000E+000 +2.9200000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM  
TC4H8OOH-IO2<=>TIC4H7Q2-I  
+9.8200000E+007 +1.3000000E+000 +2.1500000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM  
IC4H8O2H-T<=>IC4H8O+OH  
+1.5500000E+012 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: !\REF: GREEN  
2003 WARNING: IS THIS CORRECT? !\COMMENT: WARNING: NO REFERENCES IN  
MECHANISM

!

---

!\REACTIONCLASS: \POOH\_DECOMP \A  
\N \EA  
!

---

AC3H5OOH+CH2O2H<=>IIC4H7Q2-I  
+8.5000000E+010 +0.0000000E+000 +1.0600000E+004 !\AUTHOR: !\REF: CURRAN  
ESTIMATED !\COMMENT:  
IC4H7OOH+HO2<=>IIC4H7Q2-T  
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF: CURRAN  
ESTIMATED !\COMMENT:  
TIC4H7Q2-I<=>IC4H7OOH+HO2  
+1.6000000E+012 +2.3000000E-001 +1.5200000E+004 !\AUTHOR: !\REF: GREEN  
2003 !\COMMENT:

!

!\SUBSPECIES: \IC4KETII\IC4KETIT

!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA

!  
-----  
IC4KETII=>CH2O+C2H5CO+OH  
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF: CURRAN  
ESTIMATED !\COMMENT:  
!=====

!-----  
!\ENDSUBSPECIES: IC4KETII\IC4KETIT  
!=====

!  
-----  
!\REACTIONCLASS: \RO2\_RO2 \A  
\N \EA  
!  
-----  
IC4H9O2+CH3O2=>IC4H9O+CH3O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+C2H5O2=>IC4H9O+C2H5O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+CH3CO3=>IC4H9O+CH3CO2+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+IC4H9O2=>O2+IC4H9O+IC4H9O  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+TC4H9O2=>IC4H9O+TC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+PC4H9O2=>IC4H9O+PC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+SC4H9O2=>IC4H9O+SC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+NC3H7O2=>IC4H9O+NC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+HO2=>IC4H9O+OH+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+CH3O2=>TC4H9O+CH3O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+C2H5O2=>TC4H9O+C2H5O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+CH3CO3=>TC4H9O+CH3CO2+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+TC4H9O2=>O2+TC4H9O+TC4H9O  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.

TC4H9O2+PC4H9O2=>TC4H9O+PC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+SC4H9O2=>TC4H9O+SC4H9O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+HO2=>TC4H9O+OH+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
!

---

!\REACTIONCLASS: \RO2\_R \A  
\N \EA  
!

---

IC4H9O2+CH3<=>IC4H9O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+C2H5<=>IC4H9O+C2H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+IC3H7<=>IC4H9O+IC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+NC3H7<=>IC4H9O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+PC4H9<=>IC4H9O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+SC4H9<=>IC4H9O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+IC4H9<=>IC4H9O+IC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+TC4H9<=>IC4H9O+TC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+C3H5-A<=>IC4H9O+C3H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+C4H71-3<=>IC4H9O+C4H71-O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
IC4H9O2+IC4H7<=>IC4H9O+IC4H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+CH3<=>TC4H9O+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.

TC4H9O2+C2H5<=>TC4H9O+C2H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+IC3H7<=>TC4H9O+IC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+NC3H7<=>TC4H9O+NC3H7O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+PC4H9<=>TC4H9O+PC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+SC4H9<=>TC4H9O+SC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+IC4H9<=>TC4H9O+IC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+TC4H9<=>TC4H9O+TC4H9O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+C3H5-A<=>TC4H9O+C3H5O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.  
TC4H9O2+C4H71-3<=>TC4H9O+C4H71-O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT: WARNING: NO REFERENCE IN MECHANISM.

!=====

=====

!\SUBSPECIES: \IC4H9O2H

!=====

=====

!

---

!\REACTIONCLASS: \UNIMOL \A

\N \EA

!

---

IC4H9O2H<=>IC4H9O+OH

+1.5000000E+016 +0.0000000E+000 +4.2500000E+004 !\AUTHOR:

!\REF:ESTIMATE !\COMMENT:

!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!

---

IC4H9O2+HO2<=>IC4H9O2H+O2

+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR:

!\REF:ESTIMATE? !\COMMENT:

IC4H9O2+H2O2<=>IC4H9O2H+HO2

+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:

!\REF:WESTBROOK ESTIMATE !\COMMENT:

IC4H9O2+H2<=>IC4H9O2H+H

+3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG &  
HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:

IC4H9O2+CH4<=>IC4H9O2H+CH3  
+1.1300000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+CH3OH<=>IC4H9O2H+CH2OH  
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+CH2O<=>IC4H9O2H+HCO  
+1.3000000E+011 +0.0000000E+000 +9.0000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+C2H6<=>IC4H9O2H+C2H5  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+C2H4<=>IC4H9O2H+C2H3  
+8.5900000E+000 +3.7540000E+000 +2.7132000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE: ANALOGY WITH C2H4+CH3O2 !\COMMENT:  
IC4H9O2+C2H5OH<=>IC4H9O2H+PC2H4OH  
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+C2H5OH<=>IC4H9O2H+SC2H4OH  
+4.2000000E+012 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+CH3CHO<=>IC4H9O2H+CH3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
IC4H9O2+C3H8<=>IC4H9O2H+IC3H7  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+C3H8<=>IC4H9O2H+NC3H7  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
IC4H9O2+C2H3CHO<=>IC4H9O2H+C2H3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
IC4H9O2+C2H5CHO<=>IC4H9O2H+C2H5CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
IC4H9O2+C3H6<=>IC4H9O2H+C3H5-A +5.3500000E-  
002 +4.2070000E+000 +1.3288100E+004 !\AUTHOR: !\REF: ANALOGY TO  
C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM

!=====  
=====

!\SUBSPECIES: \TC4H9O2H

!=====  
=====

!

---

!\REACTIONCLASS: \UNIMOL \A

\N \EA

!

---

TC4H9O2H<=>TC4H9O+OH  
+5.9500000E+015 +0.0000000E+000 +4.2540000E+004 !\AUTHOR:  
!\REF:ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!

---

TC4H9O2+CH4<=>TC4H9O2H+CH3  
+1.1300000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+C2H6<=>TC4H9O2H+C2H5  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+C3H8<=>TC4H9O2H+IC3H7  
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+C3H8<=>TC4H9O2H+NC3H7  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+CH3OH<=>TC4H9O2H+CH2OH  
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+C2H5OH<=>TC4H9O2H+PC2H4OH  
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+C2H5OH<=>TC4H9O2H+SC2H4OH  
+4.2000000E+012 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+CH3CHO<=>TC4H9O2H+CH3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
TC4H9O2+C2H3CHO<=>TC4H9O2H+C2H3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
TC4H9O2+C2H5CHO<=>TC4H9O2H+C2H5CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF  
CH2O+HO2 !\COMMENT:  
TC4H9O2+HO2<=>TC4H9O2H+O2  
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR:  
!\REF:ESTIMATE? !\COMMENT:  
TC4H9O2+H2O2<=>TC4H9O2H+HO2  
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+CH2O<=>TC4H9O2H+HCO  
+1.3000000E+011 +0.0000000E+000 +9.0000000E+003 !\AUTHOR:  
!\REF:WESTBROOK ESTIMATE !\COMMENT:  
TC4H9O2+C2H4<=>TC4H9O2H+C2H3  
+8.5900000E+000 +3.7540000E+000 +2.7132000E+004 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:  
TC4H9O2+H2<=>TC4H9O2H+H  
+3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:TSANG &  
HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986 !\COMMENT:  
TC4H9O2+C3H6<=>TC4H9O2H+C3H5-A +5.3500000E-  
002 +4.2070000E+000 +1.3288100E+004 !\AUTHOR: !\REF: ANALOGY TO  
C3H6+HO2 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM  
!-----  
-----  
!\ENDSUBMECH: \IC4H10  
!-----  
-----  
!-----  
-----  
!\SUBMECH: \IC4H8



!\MECHCOMMENTS:

!\MECHWARNINGS:

!-----  
-----  
!

---

!\REACTIONCLASS: \UNIMOL \A

\N \EA

!

---

IC4H8<=>IC4H7-I1+H

+7.7100000E+069 -1.6090000E+001 +1.4000000E+005 ! AUTHOR: !REF:USING  
HPL FROM C3H5-A+H(+M)<=>C3H6(+M) AND QRRK TO GET PRESSURE DEPENDENT WITH  
A FACTOR OF 3 ADJUSTMENT TO GIVE BETTER FR PREDICTION

IC4H8<=>C3H5-T+CH3

+1.4200000E+093 -2.2790000E+001 +1.3382500E+005 ! AUTHOR: !REF:USING  
HPL FROM C3H5-A+H(+M)<=>C3H6(+M) AND QRRK TO GET PRESSURE DEPENDENT WITH  
A FACTOR OF 3 ADJUSTMENT TO GIVE BETTER FR PREDICTION

PLOG / +1.0000000E-001

+1.2600000E+094 -2.2990000E+001 +1.3402400E+005 /

PLOG / +1.0000000E+000

+6.7600000E+093 -2.2510000E+001 +1.3793300E+005 /

PLOG / +3.5000000E+000

+3.1400000E+090 -2.1370000E+001 +1.3786600E+005 /

PLOG / +1.0000000E+001

+9.2000000E+085 -1.9940000E+001 +1.3649800E+005 /

PLOG / +3.5000000E+001

+6.0500000E+078 -1.7760000E+001 +1.3343700E+005 /

PLOG / +1.0000000E+002

+4.8700000E+071 -1.5650000E+001 +1.2991900E+005 /

IC4H8<=>IC4H7+H

+4.6600000E+092 -2.2450000E+001 +1.2905900E+005 ! AUTHOR: !REF:USING  
HPL FROM C3H5-A+H(+M)<=>C3H6(+M) AND QRRK TO GET PRESSURE DEPENDENT WITH  
A FACTOR OF 3 ADJUSTMENT TO GIVE BETTER FR PREDICTION

PLOG / +1.0000000E-001

+7.5100000E+095 -2.3380000E+001 +1.2921400E+005 /

PLOG / +1.0000000E+000

+3.5900000E+088 -2.0990000E+001 +1.2781300E+005 /

PLOG / +3.5000000E+000

+2.9600000E+082 -1.9120000E+001 +1.2545600E+005 /

PLOG / +1.0000000E+001

+2.1300000E+076 -1.7270000E+001 +1.2262900E+005 /

PLOG / +3.5000000E+001

+1.1300000E+068 -1.4820000E+001 +1.1841600E+005 /

PLOG / +1.0000000E+002

+4.7300000E+060 -1.2660000E+001 +1.1440400E+005 /

!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!

---

IC4H8+OH<=>IC4H7+H2O

+4.3950169E+004 +2.6784100E+000 -8.2710300E+002 !\AUTHOR: !\REF:

!\COMMENT:

IC4H8+OH<=>IC4H7-I1+H2O

+1.0930095E+004 +2.8147700E+000 +1.1141999E+003 !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+O2<=>IC4H7+HO2  
+3.1200000E+013 +0.0000000E+000 +3.7450000E+004 !AUTHOR: !REF:  
YASUNAGA, PROC. COMBUST INST., 2009, 32, 453-460. INCREASED BY 40% AT  
800-1000 K.  
IC4H8+O2<=>IC4H7-I1+HO2  
+2.0000000E+013 +0.0000000E+000 +6.2270000E+004 !AUTHOR: !REF: C-J CHEN  
AND J. W. BOZZELLI J. PHYS. CHEM. A, 2000, 104, 9715-9732.  
IC4H8+H<=>IC4H7+H2  
+7.2900000E+005 +2.4550000E+000 +4.3612000E+003 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727  
IC4H8+H<=>IC4H7-I1+H2  
+8.6210000E+002 +3.2500000E+000 +1.2166980E+004 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727  
IC4H8+O<=>IC4H7+OH  
+1.0500000E+012 +7.0000000E-001 +5.8840000E+003 !AUTHOR: !REF: ANALOGY  
WITH C2H4  
IC4H8+O<=>IC4H7-I1+OH  
+1.2000000E+011 +7.0000000E-001 +8.9591000E+003 !AUTHOR: !REF: ANALOGY  
WITH C2H4  
IC4H8+HO2<=>IC4H7+H2O2 +2.9200000E-  
001 +4.1200000E+000 +1.2802000E+004 !AUTHOR: !REF: ZADOR (J. PHYS.  
CHEM. A., 2011,115,10218)  
IC4H8+HO2<=>IC4H7-I1+H2O2  
+9.7038941E+004 +2.5489200E+000 +2.4733172E+004 !AUTHOR: !REF: C3 NUIG  
CALCULATION J.MENDES  
IC4H8+CH3<=>IC4H7+CH4  
+3.2000000E+012 +0.0000000E+000 +1.0000000E+004 !AUTHOR: !REF:  
YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.  
IC4H8+CH3<=>IC4H7-I1+CH4  
+2.0000000E+012 +0.0000000E+000 +1.5000000E+004 !AUTHOR: !REF:  
YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.  
IC4H8+CH3O<=>IC4H7+CH3OH  
+1.6800000E+011 +0.0000000E+000 +2.6000000E+003 !AUTHOR: !REF: ANALOGY  
TO C3H6+CH3O  
IC4H8+C3H5-A<=>IC4H7+C3H6  
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 ! AUTHOR:  
!REF:WESTBROOK AND PITZ ESTIMATE 1983  
IC4H8+C3H5-S<=>IC4H7+C3H6  
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 ! AUTHOR:  
!REF:WESTBROOK AND PITZ ESTIMATE 1983  
IC4H8+C3H5-T<=>IC4H7+C3H6  
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 ! AUTHOR:  
!REF:WESTBROOK AND PITZ ESTIMATE 1983  
IC4H8+CH3O2<=>IC4H7+CH3O2H +1.5400000E-  
001 +4.4030000E+000 +1.3547200E+004 !AUTHOR: !REF:ANALOGY TO C3H6+CH3O2  
IC4H8+CH3CO3<=>IC4H7+CH3CO3H +1.5400000E-  
001 +4.4030000E+000 +1.3547200E+004 !AUTHOR: !REF:ANALOGY TO C3H6+CH3O2  
IC4H8+O2CHO<=>IC4H7+HO2CHO  
+1.9280000E+004 +2.6000000E+000 +1.3910000E+004 !AUTHOR: !REF:ANALOGY  
WITH RH+RO2 --> R+RO2H  
IC4H9O2+IC4H8<=>TC4H9O2H+IC4H7  
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !AUTHOR: !REF:WESTBROOK  
ESTIMATE  
TC4H9O2+IC4H8<=>TC4H9O2H+IC4H7  
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !AUTHOR: !REF:WESTBROOK  
ESTIMATE

PC4H9O2+IC4H8<=>PC4H9O2H+IC4H7  
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !AUTHOR: !REF:WESTBROOK  
ESTIMATE  
SC4H9O2+IC4H8<=>SC4H9O2H+IC4H7  
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !AUTHOR: !REF:WESTBROOK  
ESTIMATE  
IC3H7O2+IC4H8<=>IC3H7O2H+IC4H7  
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !AUTHOR: !REF:WESTBROOK  
ESTIMATE  
NC3H7O2+IC4H8<=>NC3H7O2H+IC4H7  
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !AUTHOR: !REF:WESTBROOK  
ESTIMATE  
IC4H7O+IC4H8<=>IC4H7OH+IC4H7  
+2.7000000E+011 +0.0000000E+000 +4.0000000E+003 !AUTHOR: !REF:PITZ  
ESTIMATE  
IC4H8+CH2CCH2OH<=>IC4H7+C3H5OH  
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 !AUTHOR: !REF:CURRAN  
ESTIMATE

!

---

!\REACTIONCLASS: \RA\_DECOMPOSITION \A  
\N \EA

!

---

IC4H7<=>IC4H7-I1  
+1.3000000E+055 -1.4530000E+001 +7.3800000E+004 !\AUTHOR: !\REF:DAVIS  
AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589 !\COMMENT:  
PLOG / +1.0000000E-001  
+1.3000000E+055 -1.4530000E+001 +7.3800000E+004 /  
PLOG / +1.0000000E+000  
+5.0000000E+051 -1.3020000E+001 +7.3300000E+004 /  
PLOG / +1.0000000E+001  
+9.7000000E+048 -1.1730000E+001 +7.3700000E+004 /  
PLOG / +1.0000000E+002  
+4.8600000E+044 -9.8400000E+000 +7.3400000E+004 /  
C3H4-A+CH3<=>IC4H7  
+4.0209700E+004 +2.5000000E+000 +8.8475000E+003 !\AUTHOR: !\REF: C ZHOU  
CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY  
!\COMMENT:

!

---

!\REACTIONCLASS: \RA\_HO2\_PRODUCTS \A  
\N \EA

!

---

IC4H7+HO2<=>IC4H7O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-002  
+1.0200000E+013 -1.5800000E-001 -1.4170000E+003 /  
PLOG / +1.0000000E-001  
+4.9800000E+014 -6.4200000E-001 -3.4910000E+002 /  
PLOG / +1.0000000E+000  
+7.7700000E+017 -1.5200000E+000 +2.3792000E+003 /  
PLOG / +1.0000000E+001  
+2.9300000E+015 -6.8400000E-001 +3.6153000E+003 /  
PLOG / +1.0000000E+002  
+1.6400000E+004 +2.7400000E+000 +1.1444000E+003 /

IC4H7+HO2<=>IC4H7OOH

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-002  
+1.9100000E+031 -7.2300000E+000 +1.3362000E+003 /  
PLOG / +1.0000000E-001  
+6.3100000E+042 -1.0300000E+001 +5.5689000E+003 /  
PLOG / +1.0000000E+000  
+1.0300000E+045 -1.0600000E+001 +7.8515000E+003 /  
PLOG / +1.0000000E+001  
+2.7900000E+037 -7.9200000E+000 +6.4979000E+003 /  
PLOG / +1.0000000E+002  
+1.4400000E+032 -6.0100000E+000 +6.0536000E+003 /

IC4H7+HO2<=>IC3H5CHO+H2O

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-002  
+1.0900000E+000 +3.0100000E+000 -3.4211000E+003 /  
PLOG / +1.0000000E-001  
+6.3500000E+001 +2.5000000E+000 -2.3414000E+003 /  
PLOG / +1.0000000E+000  
+6.0500000E+005 +1.3900000E+000 +5.9510000E+002 /  
PLOG / +1.0000000E+001  
+3.1000000E+005 +1.5900000E+000 +2.6776000E+003 /  
PLOG / +1.0000000E+002 +5.0700000E-  
005 +4.5900000E+000 +9.2750000E+002 /

IC4H7OOH<=>IC3H5CHO+H2O

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-002  
+1.9900000E+050 -1.2700000E+001 +5.3531900E+004 /  
PLOG / +1.0000000E-001  
+4.7200000E+047 -1.1500000E+001 +5.4360900E+004 /  
PLOG / +1.0000000E+000  
+1.5000000E+040 -8.8400000E+000 +5.3179200E+004 /  
PLOG / +1.0000000E+001  
+2.5400000E+028 -5.0000000E+000 +4.9919400E+004 /  
PLOG / +1.0000000E+002  
+1.4800000E+016 -1.1200000E+000 +4.5949300E+004 /

IC4H7OOH<=>IC4H7O+OH

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-002  
+1.4900000E+058 -1.3900000E+001 +5.4266900E+004 /  
PLOG / +1.0000000E-001  
+1.8000000E+054 -1.2400000E+001 +5.4193800E+004 /  
PLOG / +1.0000000E+000  
+3.3600000E+046 -9.8100000E+000 +5.2468500E+004 /  
PLOG / +1.0000000E+001  
+2.3900000E+036 -6.5400000E+000 +4.9429000E+004 /  
PLOG / +1.0000000E+002  
+1.2800000E+027 -3.6100000E+000 +4.6333100E+004 /

IC4H7O<=>C3H5-T+CH2O

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-003  
+7.2600000E+006 +1.8200000E-001 +1.7815500E+004 /

PLOG / +1.0000000E-002  
 +6.9700000E+016 -2.5000000E+000 +2.0878700E+004 /  
 PLOG / +1.0000000E-001  
 +6.6400000E+023 -4.2300000E+000 +2.3565000E+004 /  
 PLOG / +1.0000000E+000  
 +1.0700000E+026 -4.5600000E+000 +2.4622900E+004 /  
 PLOG / +1.0000000E+001  
 +6.5000000E+029 -5.3700000E+000 +2.6645000E+004 /  
 PLOG / +1.0000000E+002  
 +4.6300000E+031 -5.5900000E+000 +2.8915300E+004 /  
 PLOG / +1.0000000E+003  
 +8.5200000E+025 -3.6100000E+000 +2.7863400E+004 /  
 IC4H7O<=>IC3H5OCH2  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +3.1700000E+020 -4.1500000E+000 +1.2121300E+004 /  
 PLOG / +1.0000000E-002  
 +4.7900000E+024 -5.0300000E+000 +1.4606100E+004 /  
 PLOG / +1.0000000E-001  
 +1.9000000E+026 -5.1600000E+000 +1.6124400E+004 /  
 PLOG / +1.0000000E+000  
 +1.5100000E+028 -5.4000000E+000 +1.8165400E+004 /  
 PLOG / +1.0000000E+001  
 +2.4200000E+028 -5.1700000E+000 +1.9691200E+004 /  
 PLOG / +1.0000000E+002  
 +5.5700000E+024 -3.8600000E+000 +1.9395200E+004 /  
 PLOG / +1.0000000E+003  
 +1.3500000E+018 -1.7300000E+000 +1.7386500E+004 /  
 IC4H7O<=>IC3H6CHO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003 +5.2500000E-  
 049 +1.5500000E+001 -1.5639900E+004 /  
 PLOG / +1.0000000E-002 +1.4600000E-  
 088 +2.7600000E+001 -3.5995000E+004 /  
 PLOG / +1.0000000E-001 +4.4400000E-  
 022 +8.3800000E+000 -3.8190000E+003 /  
 PLOG / +1.0000000E+000  
 +6.2300000E+012 -1.4400000E+000 +1.0829200E+004 /  
 PLOG / +1.0000000E+001  
 +3.4800000E+042 -9.9100000E+000 +2.5297900E+004 /  
 PLOG / +1.0000000E+002  
 +1.8800000E+038 -8.1600000E+000 +2.5974500E+004 /  
 PLOG / +1.0000000E+003  
 +1.6700000E+021 -2.7400000E+000 +2.0337700E+004 /  
 IC4H7O<=>IC3H5CHO+H  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +3.0000000E+015 -2.3100000E+000 +1.4667900E+004 /  
 PLOG / +1.0000000E-002  
 +1.5000000E+022 -3.9600000E+000 +1.8283000E+004 /  
 PLOG / +1.0000000E-001  
 +1.9500000E+023 -3.9900000E+000 +1.9143300E+004 /  
 PLOG / +1.0000000E+000  
 +1.1500000E+025 -4.2400000E+000 +2.0311200E+004 /

PLOG / +1.0000000E+001  
 +1.7600000E+028 -4.8900000E+000 +2.2765200E+004 /  
 PLOG / +1.0000000E+002  
 +1.4100000E+027 -4.2800000E+000 +2.3770600E+004 /  
 PLOG / +1.0000000E+003  
 +2.5700000E+020 -2.0600000E+000 +2.2040100E+004 /  
 IC4H7O<=>C3H6+HCO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +6.6200000E+016 -2.8400000E+000 +1.3197000E+004 /  
 PLOG / +1.0000000E-002  
 +1.2600000E+020 -3.5300000E+000 +1.5469200E+004 /  
 PLOG / +1.0000000E-001  
 +2.1300000E+021 -3.6400000E+000 +1.6584500E+004 /  
 PLOG / +1.0000000E+000  
 +1.0700000E+024 -4.1600000E+000 +1.8985000E+004 /  
 PLOG / +1.0000000E+001  
 +8.4200000E+025 -4.4000000E+000 +2.2382600E+004 /  
 PLOG / +1.0000000E+002  
 +1.8600000E+021 -2.7300000E+000 +2.3658800E+004 /  
 PLOG / +1.0000000E+003  
 +4.7500000E+008 +1.1400000E+000 +2.0922500E+004 /  
 IC3H5OCH2<=>C3H5-T+CH2O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +3.3000000E+009 -6.3800000E-001 +1.9747800E+004 /  
 PLOG / +1.0000000E-002  
 +3.3600000E+021 -3.9000000E+000 +2.3945200E+004 /  
 PLOG / +1.0000000E-001  
 +2.9100000E+029 -5.9000000E+000 +2.7249700E+004 /  
 PLOG / +1.0000000E+000  
 +1.8300000E+034 -6.9400000E+000 +3.0690400E+004 /  
 PLOG / +1.0000000E+001  
 +9.7200000E+033 -6.5000000E+000 +3.3002500E+004 /  
 PLOG / +1.0000000E+002  
 +2.6800000E+027 -4.2600000E+000 +3.3305600E+004 /  
 PLOG / +1.0000000E+003  
 +8.8100000E+014 -3.2600000E-001 +3.1553100E+004 /  
 IC3H5OCH2<=>IC3H6CHO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003 +8.0100000E-  
 092 +2.7800000E+001 -3.7321200E+004 /  
 PLOG / +1.0000000E-002 +7.7800000E-  
 011 +3.7000000E+000 -2.7669000E+003 /  
 PLOG / +1.0000000E-001  
 +5.1100000E+015 -2.7600000E+000 +1.5937600E+004 /  
 PLOG / +1.0000000E+000  
 +4.4800000E+025 -5.2000000E+000 +2.1532200E+004 /  
 PLOG / +1.0000000E+001  
 +3.9700000E+034 -7.4100000E+000 +2.8116900E+004 /  
 PLOG / +1.0000000E+002  
 +5.6200000E+022 -3.5600000E+000 +2.5806700E+004 /  
 PLOG / +1.0000000E+003  
 +2.5100000E+020 -2.6300000E+000 +2.9288400E+004 /

IC3H5OCH2<=>IC3H5CHO+H

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-003  
+4.9300000E+024 -5.0500000E+000 +2.0108400E+004 /  
PLOG / +1.0000000E-002  
+2.1400000E+028 -5.8000000E+000 +2.2219400E+004 /  
PLOG / +1.0000000E-001  
+1.9300000E+032 -6.6400000E+000 +2.5108200E+004 /  
PLOG / +1.0000000E+000  
+8.6000000E+034 -7.1100000E+000 +2.8209100E+004 /  
PLOG / +1.0000000E+001  
+2.1700000E+034 -6.6400000E+000 +3.0647600E+004 /  
PLOG / +1.0000000E+002  
+4.1700000E+028 -4.7100000E+000 +3.1231900E+004 /  
PLOG / +1.0000000E+003  
+3.9800000E+018 -1.6200000E+000 +3.0129800E+004 /

IC3H5OCH2<=>C3H6+HCO

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-003  
+8.2300000E+026 -5.8400000E+000 +1.9356900E+004 /  
PLOG / +1.0000000E-002  
+1.3200000E+029 -6.2100000E+000 +2.1293600E+004 /  
PLOG / +1.0000000E-001  
+3.4700000E+032 -6.9600000E+000 +2.4197300E+004 /  
PLOG / +1.0000000E+000  
+1.4400000E+036 -7.7600000E+000 +2.8007800E+004 /  
PLOG / +1.0000000E+001  
+9.7200000E+037 -8.0200000E+000 +3.2394600E+004 /  
PLOG / +1.0000000E+002  
+2.4300000E+031 -5.8100000E+000 +3.4295800E+004 /  
PLOG / +1.0000000E+003  
+3.7300000E+014 -7.2600000E-001 +3.2008300E+004 /

IC3H6CHO<=>C3H5-T+CH2O

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-003 +6.8900000E-  
069 +2.1500000E+001 +2.6380000E+003 /  
PLOG / +1.0000000E-002 +5.3400000E-  
033 +1.1100000E+001 +1.6749100E+004 /  
PLOG / +1.0000000E-001  
+6.1100000E+026 -6.0100000E+000 +4.4116700E+004 /  
PLOG / +1.0000000E+000  
+8.0400000E+035 -8.3100000E+000 +4.6919700E+004 /  
PLOG / +1.0000000E+001  
+5.5200000E+040 -9.1900000E+000 +5.0508700E+004 /  
PLOG / +1.0000000E+002  
+5.8500000E+035 -7.1800000E+000 +5.2038400E+004 /  
PLOG / +1.0000000E+003  
+1.9300000E+019 -1.9400000E+000 +4.8440000E+004 /

IC3H6CHO<=>IC3H5CHO+H

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
PLOG / +1.0000000E-003  
+1.6100000E+010 -1.2400000E+000 +3.2371300E+004 /  
PLOG / +1.0000000E-002  
+5.8400000E+015 -2.6100000E+000 +3.2878400E+004 /

PLOG / +1.0000000E-001  
 +3.6400000E+023 -4.6000000E+000 +3.4275300E+004 /  
 PLOG / +1.0000000E+000  
 +7.5800000E+031 -6.6300000E+000 +3.7895400E+004 /  
 PLOG / +1.0000000E+001  
 +2.8600000E+032 -6.3000000E+000 +3.9990700E+004 /  
 PLOG / +1.0000000E+002  
 +1.5700000E+023 -3.1400000E+000 +3.8011700E+004 /  
 PLOG / +1.0000000E+003  
 +4.5200000E+012 +2.1400000E-001 +3.4570500E+004 /  
 IC3H6CHO<=>C3H6+HCO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +2.9000000E+032 -7.2400000E+000 +2.5687500E+004 /  
 PLOG / +1.0000000E-002  
 +5.3000000E+033 -7.2800000E+000 +2.7100600E+004 /  
 PLOG / +1.0000000E-001  
 +2.0000000E+035 -7.4100000E+000 +2.9027300E+004 /  
 PLOG / +1.0000000E+000  
 +1.0100000E+034 -6.7000000E+000 +3.0018100E+004 /  
 PLOG / +1.0000000E+001  
 +9.7600000E+027 -4.6300000E+000 +2.8923900E+004 /  
 PLOG / +1.0000000E+002  
 +2.1100000E+019 -1.8500000E+000 +2.6239800E+004 /  
 PLOG / +1.0000000E+003  
 +1.5900000E+013 +6.3000000E-002 +2.4086300E+004 /  
 C3H5-T+CH2O<=>IC3H5CHO+H  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +2.6000000E+004 +2.2600000E+000 +1.5103000E+003 /  
 PLOG / +1.0000000E-002  
 +5.1300000E+004 +2.1700000E+000 +1.6755000E+003 /  
 PLOG / +1.0000000E-001  
 +3.9900000E+005 +1.9100000E+000 +2.2183000E+003 /  
 PLOG / +1.0000000E+000  
 +1.7500000E+007 +1.4500000E+000 +3.4280000E+003 /  
 PLOG / +1.0000000E+001  
 +1.3500000E+009 +9.3300000E-001 +5.1730000E+003 /  
 PLOG / +1.0000000E+002  
 +2.2400000E+011 +3.5700000E-001 +8.0013000E+003 /  
 PLOG / +1.0000000E+003  
 +6.0100000E+005 +2.0900000E+000 +7.8956000E+003 /  
 C3H5-T+CH2O<=>C3H6+HCO  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: KINETICS  
 FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346  
 PLOG / +1.0000000E-003  
 +1.1100000E+007 +1.0900000E+000 +1.8072000E+003 /  
 PLOG / +1.0000000E-002  
 +2.4700000E+007 +9.9300000E-001 +1.9949000E+003 /  
 PLOG / +1.0000000E-001  
 +2.4700000E+008 +7.0400000E-001 +2.5962000E+003 /  
 PLOG / +1.0000000E+000  
 +1.4200000E+010 +2.0900000E-001 +3.9342000E+003 /  
 PLOG / +1.0000000E+001  
 +3.4500000E+013 -7.2600000E-001 +6.9443000E+003 /



PLOG / +1.0000000E+002  
+3.3100000E+014 -8.6600000E-001 +1.0965700E+004 /  
PLOG / +1.0000000E+003  
+1.6500000E+001 +3.1700000E+000 +9.3998000E+003 /  
!

---

!\REACTIONCLASS: \R\_CH3O2\_PRODUCTS \A  
\N \EA  
!

---

IC4H7+CH3O2<=>IC4H7O+CH3O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ANALOGY WITH C3H5-A+HO2 !\COMMENT:

PLOG / +1.0000000E-002  
+3.3300000E+012 -1.5800000E-001 -1.4170000E+003 /  
PLOG / +1.0000000E-001  
+1.6600000E+014 -6.4200000E-001 -3.4910000E+002 /  
PLOG / +1.0000000E+000  
+2.5950000E+017 -1.5200000E+000 +2.3792000E+003 /  
PLOG / +1.0000000E+001  
+9.7800000E+014 -6.8400000E-001 +3.6153000E+003 /  
PLOG / +1.0000000E+002  
+5.4700000E+003 +2.7400000E+000 +1.1444000E+003 /

IC4H7+CH3O2<=>IC4H7OCH3  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ANALOGY WITH C3H5-A+HO2 !\COMMENT:

PLOG / +1.0000000E-002  
+1.9100000E+031 -7.2300000E+000 +1.3362000E+003 /  
PLOG / +1.0000000E-001  
+6.3100000E+042 -1.0300000E+001 +5.5689000E+003 /  
PLOG / +1.0000000E+000  
+1.0300000E+045 -1.0600000E+001 +7.8515000E+003 /  
PLOG / +1.0000000E+001  
+2.7900000E+037 -7.9200000E+000 +6.4979000E+003 /  
PLOG / +1.0000000E+002  
+3.4000000E+029 -5.2800000E+000 +4.5398000E+003 /

IC4H7OCH3<=>IC4H7O+CH3O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
ANALOGY WITH C3H5-A+HO2 !\COMMENT:

PLOG / +1.0000000E-002  
+1.4900000E+058 -1.3900000E+001 +5.4266900E+004 /  
PLOG / +1.0000000E-001  
+1.8000000E+054 -1.2400000E+001 +5.4193800E+004 /  
PLOG / +1.0000000E+000  
+3.3600000E+046 -9.8100000E+000 +5.2468500E+004 /  
PLOG / +1.0000000E+001  
+2.3900000E+036 -6.5400000E+000 +4.9429000E+004 /  
PLOG / +1.0000000E+002  
+2.5600000E+027 -3.6100000E+000 +4.6333100E+004 /  
!

---

!\REACTIONCLASS: \R\_IC4H7O2\_PRODUCCTS \A  
\N \EA  
!

---

IC4H7O2+IC4H7<=>IC4H7O+IC4H7O  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\ ANALOGY TO  
IC4H7+HO2 DIVIDED 4 !\COMMENT:

PLOG / +1.0000000E-002  
 +2.5500000E+012 -1.5800000E-001 -1.4170000E+003 /  
 PLOG / +1.0000000E-001  
 +1.2500000E+014 -6.4200000E-001 -3.4910000E+002 /  
 PLOG / +1.0000000E+000  
 +1.9400000E+017 -1.5200000E+000 +2.3792000E+003 /  
 PLOG / +1.0000000E+001  
 +7.3300000E+014 -6.8400000E-001 +3.6153000E+003 /  
 PLOG / +1.0000000E+002  
 +4.1000000E+003 +2.7400000E+000 +1.1444000E+003 /  
 IC4H7O2+IC4H7<=>IC4H7OOIC4H7  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\ ANALOGY TO  
 IC4H7+HO2 DIVIDED 4 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +4.7800000E+030 -7.2300000E+000 +1.3362000E+003 /  
 PLOG / +1.0000000E-001  
 +1.5800000E+042 -1.0300000E+001 +5.5689000E+003 /  
 PLOG / +1.0000000E+000  
 +2.5800000E+044 -1.0600000E+001 +7.8515000E+003 /  
 PLOG / +1.0000000E+001  
 +6.9800000E+036 -7.9200000E+000 +6.4979000E+003 /  
 PLOG / +1.0000000E+002  
 +3.6000000E+031 -6.0100000E+000 +6.0536000E+003 /  
 IC4H7OOIC4H7<=>IC4H7O+IC4H7O  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\ ANALOGY TO  
 IC4H7+HO2 DIVIDED 4 !\COMMENT:  
 PLOG / +1.0000000E-002  
 +3.7300000E+057 -1.3900000E+001 +5.4266900E+004 /  
 PLOG / +1.0000000E-001  
 +4.5000000E+053 -1.2400000E+001 +5.4193800E+004 /  
 PLOG / +1.0000000E+000  
 +8.4000000E+045 -9.8100000E+000 +5.2468500E+004 /  
 PLOG / +1.0000000E+001  
 +5.9800000E+035 -6.5400000E+000 +4.9429000E+004 /  
 PLOG / +1.0000000E+002  
 +3.2000000E+026 -3.6100000E+000 +4.6333100E+004 /  
 !

---

!\REACTIONCLASS: \R\_RO2 \A  
 \N \EA  
 !

---

IC4H7+NC3H7O2<=>IC4H7O+NC3H7O  
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 IC4H7+PC4H9O2<=>IC4H7O+PC4H9O  
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 IC4H7+SC4H9O2<=>IC4H7O+SC4H9O  
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 IC4H7+IC3H7O2<=>IC4H7O+IC3H7O  
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:  
 IC4H7+TC4H9O2<=>IC4H7O+TC4H9O  
 +7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:  
 !\REF:ESTIMATE !\COMMENT:

!

---

!\REACTIONCLASS: \RA\_RA\_RECOMBINATION \A  
\N \EA

---

IC4H7+IC4H7<=>C3H4-A+AC5H10  
+9.5500000E+040 -9.3000000E+000 +1.2470000E+004 !\AUTHOR: \REF:  
FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4750-4761 !\COMMENT:  
PLOG / +1.0000000E+000  
+4.1000000E+040 -9.3000000E+000 +1.2470000E+004 /  
PLOG / +4.0000000E+000  
+3.4100000E+032 -6.8000000E+000 +9.1800000E+003 /  
PLOG / +1.0000000E+001  
+1.2600000E+028 -5.5000000E+000 +7.4100000E+003 /  
IC4H7+IC4H7<=>H15DE25DM  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !AUTHOR: ! ANALOGY FROM  
PROPENE, DEVIDED BY 2.3  
PLOG / +3.9000000E-002  
+3.2700000E+064 -1.5935000E+001 +2.0230000E+004 /  
PLOG / +7.8000000E-002  
+7.5000000E+059 -1.4490000E+001 +1.8600000E+004 /  
PLOG / +1.5600000E-001  
+1.1400000E+055 -1.2995000E+001 +1.6700000E+004 /  
H15DE25DM+H<=>H15DE25DM-S+H2  
+1.4200000E+006 +2.3151654E+000 +2.0759558E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+O2<=>H15DE25DM-S+HO2  
+4.0000000E+014 +0.0000000E+000 +3.8890000E+004 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+O<=>H15DE25DM-S+OH  
+1.5924300E+011 +7.0000000E-001 +1.3000000E+001 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+OH<=>H15DE25DM-S+H2O  
+8.9500000E+004 +2.6369657E+000 -6.0000000E+000 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+HO2<=>H15DE25DM-S+H2O2  
+1.0000000E+000 +3.8873669E+000 +9.3863572E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+CH3<=>H15DE25DM-S+CH4  
+1.0000000E+000 +3.6490200E+000 +3.3740520E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+H<=>H15DE25DM-A+H2  
+7.2900000E+005 +2.4550000E+000 +4.3612000E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+O2<=>H15DE25DM-A+HO2  
+1.8600000E+009 +1.3010000E+000 +4.0939000E+004 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+O<=>H15DE25DM-A+OH  
+1.0500000E+012 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+OH<=>H15DE25DM-A+H2O  
+2.5300000E+005 +2.4600000E+000 +7.2944000E+002 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM+HO2<=>H15DE25DM-A+H2O2 +2.9200000E-  
001 +4.1200000E+000 +1.2802000E+004 !\AUTHOR: !\REF: WARNING CAN YOU  
REFERENCE CW? !\COMMENT: WARNING

H15DE25DM+CH3<=>H15DE25DM-A+CH4  
+4.4200000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
C3H5-T+B13DE2M<=>H15DE25DM-S  
+7.0700000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:C ZHOU  
ESTIMATEDG  
C3H4-A+AC5H9-D<=>H15DE25DM-A  
+2.8400000E+004 +2.5000000E+000 +8.8475000E+003 !\AUTHOR: !\REF: C ZHOU  
CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY  
H15DE25DM-S+HO2<=>H15DE25DM-SO+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
IC3H5CHO+IC4H7<=>H15DE25DM-SO  
+2.5000000E+010 +0.0000000E+000 +6.3297400E+003 !\AUTHOR: !\REF: H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275  
C3H5-T+IC4H7CHO<=>H15DE25DM-SO  
+2.5000000E+010 +0.0000000E+000 +1.5526420E+004 !\AUTHOR: !\REF: H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275  
IC4H7CHO+OH=>CH2CHO+C3H4-A+H2O  
+5.0640000E+007 +2.4600000E+000 +7.2944000E+002 !\AUTHOR: !\REF:  
WARNING CAN YOU REFERENCE CW? !\COMMENT: WARNING  
H15DE25DM-A+HO2<=>H15DE25DM-AO+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF: THE  
SAME AS ALLYL+HO2  
H15DE2M-T+CH2O<=>H15DE25DM-AO  
+2.5000000E+010 +0.0000000E+000 +4.7865800E+003 !\AUTHOR: !\REF:  
ESTIMATE BASED ON CURRAN IJCK 2006, 38, 250  
IC4H7+C3H4-A<=>H15DE2M-T  
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:  
ESTIMATE BASED ON CURRAN IJCK 2006, 38, 250  
!

---

!\REACTIONCLASS: \RS\_R\_PRODUCTS \A  
\N \EA  
!

---

IC4H7-I1+H<=>C3H4-A+CH4  
+3.3330000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DAGAUT,  
P. ET AL., CST 71, 111(1990). !\COMMENT:  
IC4H7-I1+H<=>C3H4-P+CH4  
+3.3400000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
IC4H7-I1+O<=>C3H6+HCO  
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
IC4H7-I1+OH=>C3H6+HCO+H  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
IC4H7-I1+HO2=>C3H6+HCO+OH  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
IC4H7-I1+HCO<=>IC4H8+CO  
+9.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
IC4H7-I1+CH3<=>C3H4-P+C2H6  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

---

!\REACTIONCLASS: \RS\_O2\_PRODUCTS \A  
 \N \EA  
 !

---

IC4H7-I1+O2<=>CH3COCH3+HCO  
 +3.1000000E+031 -5.9440000E+000 +5.7484000E+003 !\AUTHOR: !\REF:  
 ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:  
 IC4H7-I1+O2<=>TC3H6CHO+O  
 +5.3800000E+018 -2.1400000E+000 +5.1429000E+003 !\AUTHOR: !\REF:  
 ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:  
 IC4H7-I1+O2<=>IC3H5CHO+OH  
 +2.7000000E+019 -2.1400000E+000 +5.1429000E+003 !\AUTHOR: !\REF:  
 ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:  
 !

---

!\REACTIONCLASS: \RA\_O2 \A  
 \N \EA  
 !

---

IC4H7+O2<=>IC4H7O2  
 +1.0900000E+010 +5.6725000E-001 +2.2900000E+003 !\AUTHOR: !\REF:  
 CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-  
 9732. !\COMMENT: HPL ONLY  
 IC4H7+O<=>IC3H5CHO+H  
 +6.0300000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: CURRAN  
 ESTIMATE !\COMMENT: HPL ONLY  
 !

---

!\REACTIONCLASS: \RAO2\_ISOMERISATION \A  
 \N \EA  
 !

---

IC4H7O2<=>IC4H6OOH-I  
 +1.4100000E+005 +1.8358600E+000 +1.9820000E+004 !\AUTHOR: !\REF:  
 CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-  
 9732. !\COMMENT:  
 IC4H7O2<=>CCYCCOOC-T1  
 +1.1900000E+008 +8.0412000E-001 +2.8020000E+004 !\AUTHOR: !\REF:  
 CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-  
 9732. !\COMMENT:  
 IC4H7O2<=>C2CYCOOC-I1  
 +1.0700000E+008 +8.9161000E-001 +2.9720000E+004 !\AUTHOR: !\REF:  
 CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-  
 9732. !\COMMENT:  
 !

---

!\REACTIONCLASS: \RAO2\_DECOMPOSITION \A  
 \N \EA  
 !

---

IC4H7O2<=>IC4H7O+O  
 +1.8200000E+014 +0.0000000E+000 +6.0620000E+004 !\AUTHOR: !\REF:  
 CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-  
 9732. !\COMMENT:  
 IC4H7O2<=>IC3H5CHO+OH  
 +1.5200000E+009 +1.0252400E+000 +3.9460000E+004 !\AUTHOR: !\REF:

CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

!

---

!\REACTIONCLASS: \RAO2\_ISOMERISATION\_PRODUCTS\_DECOMP \A  
\N \EA

!

---

IC4H6OOH-I<=>CVCYCCOC+OH  
+6.8200000E+012 -3.4545000E-001 +4.2140000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

IC4H6OOH-I<=>C3H4-A+CH2O2H  
+1.1800000E+012 +9.1203000E-001 +5.1390000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

IC4H6OOH-I<=>IC3H5CHO+OH  
+2.4200000E+009 +8.7390000E-001 +5.4090000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

CCYCCOOC-T1<=>CCYC2OCO  
+4.5600000E+011 +9.2729000E-001 +1.7470000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

CCYCCOOC-T1<=>CCYCCOOC-I2  
+3.5600000E+013 +0.0000000E+000 +3.8820000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

CCYCCOOC-I2<=>CHOIC3H6O  
+3.1900000E+014 +0.0000000E+000 +3.0000000E+003 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

C2CYCOOC-I1<=>IC3H5OOCH2  
+4.4100000E+013 -2.2618000E-001 +1.8500000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

IC3H5OOCH2<=>CH3COCH2+CH2O  
+1.4100000E+010 +0.0000000E+000 +1.0000000E+003 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

CHOIC3H6O<=>CH3CHCHO+CH2O  
+4.3000000E+012 +0.0000000E+000 +9.7800000E+003 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

CCYC2OCO<=>CCYCCO-T1+CH2O  
+1.7400000E+013 +0.0000000E+000 +1.8150000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

C2CYCOOC-I1<=>CCYC2OCO  
+1.2100000E+013 +1.0180000E-001 +2.0320000E+004 !\AUTHOR: !\REF:  
CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM. A., 2000, 104, 9715-9732. !\COMMENT:

!

---

!\REACTIONCLASS: \RAO2\_RAO2 \A  
\N \EA

!

IC4H7O2+IC4H7O2=>IC4H7O+IC4H7O+O2  
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
ALKANES ESTIMATED !\COMMENT: WHAT IS SOURCE OF RATE CONSTANT?  
! IC4H8+HO2<=>IC4H7+H2O2 DIVIDED BY 2  
IC4H7O2+IC4H8<=>IC4H7+IC4H7OOH +1.4600000E-  
001 +4.1200000E+000 +1.2802000E+004 !\AUTHOR: !\REF: !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA  
!

---

---

IC4H8+H<=>IC4H9  
+1.0000000E+000 +1.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727  
PLOG / +1.3000000E-003  
+7.9900000E+081 -2.3161000E+001 +2.2239000E+004 /  
PLOG / +4.0000000E-002  
+4.2400000E+068 -1.8427000E+001 +1.9665000E+004 /  
PLOG / +1.0000000E+000  
+1.0400000E+049 -1.1500000E+001 +1.5359000E+004 /  
PLOG / +1.0000000E+001  
+6.2000000E+041 -8.8920000E+000 +1.4637000E+004 /  
!PLOG/ 100.0000 -6.450E+031 -5.851 8177.8/  
DUP

IC4H8+H<=>IC4H9  
+1.0000000E+000 +1.0000000E+000 +0.0000000E+000 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727  
PLOG / +1.3000000E-003  
+1.8500000E+026 -5.8300000E+000 +3.8658000E+003 /  
PLOG / +4.0000000E-002  
+2.8200000E+030 -6.4900000E+000 +5.4708000E+003 /  
PLOG / +1.0000000E+000  
+3.7800000E+028 -5.5700000E+000 +5.6251000E+003 /  
PLOG / +1.0000000E+001  
+1.4600000E+025 -4.2800000E+000 +5.2478000E+003 /  
!REF: REFIT TO ONE PARAMETER TO AVOID PROBLEMS WITH NEGATIVE K  
PLOG / +1.0000000E+002  
+4.2200000E+027 -4.3900000E+000 +9.3458000E+003 /  
DUP

IC4H8+H<=>TC4H9  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727  
PLOG / +1.3000000E-003  
+1.3500000E+044 -1.0680000E+001 +8.1964000E+003 /  
PLOG / +4.0000000E-002  
+2.1100000E+057 -1.4230000E+001 +1.5147000E+004 /  
PLOG / +1.0000000E+000  
+3.2600000E+061 -1.4940000E+001 +2.0161000E+004 /  
PLOG / +1.0000000E+001  
+5.3000000E+056 -1.3120000E+001 +2.0667000E+004 /  
PLOG / +1.0000000E+002  
+1.1100000E+050 -1.0800000E+001 +2.0202000E+004 /  
DUP

IC4H8+H<=>TC4H9  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727

PLOG / +1.3000000E-003  
+2.1700000E+130 -3.2580000E+001 +1.3614000E+005 /  
PLOG / +4.0000000E-002  
+2.2500000E+029 -5.8400000E+000 +4.2419000E+003 /  
PLOG / +1.0000000E+000  
+1.0600000E+030 -5.6300000E+000 +5.6134000E+003 /  
PLOG / +1.0000000E+001  
+6.1100000E+026 -4.4400000E+000 +5.1823000E+003 /  
PLOG / +1.0000000E+002  
+2.7300000E+023 -3.2600000E+000 +4.5970000E+003 /

DUP

!DIVIDED BY 3 TO HAVE BETTER PREDICTION OF PROPENE IN FR

IC4H8+H<=>C3H6+CH3

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727

PLOG / +1.3000000E-003  
+5.1300000E+008 +1.3500000E+000 +2.5420000E+003 /  
PLOG / +4.0000000E-002  
+2.6300000E+010 +8.7000000E-001 +3.5996000E+003 /  
PLOG / +1.0000000E+000  
+8.9000000E+011 +4.7000000E-001 +5.4311000E+003 /  
PLOG / +1.0000000E+001  
+3.0800000E+022 -2.6000000E+000 +1.2898000E+004 /  
PLOG / +1.0000000E+002  
+4.4000000E+022 -2.4200000E+000 +1.6500000E+004 /

DUP

IC4H8+H<=>C3H6+CH3

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !AUTHOR: !REF: MILLER  
AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117, 2718-2727

PLOG / +1.3000000E-003  
+7.7000000E+002 +1.3500000E+000 +2.5420000E+003 /  
PLOG / +4.0000000E-002  
+3.9400000E+004 +8.7000000E-001 +3.5996000E+003 /  
PLOG / +1.0000000E+000  
+1.3400000E+006 +4.7000000E-001 +5.4311000E+003 /  
PLOG / +1.0000000E+001  
+4.1300000E+004 +2.5200000E+000 +3.6791000E+003 /  
PLOG / +1.0000000E+002  
+8.3700000E+002 +2.9100000E+000 +3.9809000E+003 /

DUP

!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\HO2 \A

\N \EA

!

---

IC4H8+HO2<=>TC4H9O2 +1.0400000E-  
001 +3.4500000E+000 +4.3380000E+003 !\AUTHOR: !\REF: ZADOR (J. PHYS.  
CHEM. A., 2011,115,10218) !\COMMENT:

IC4H8+HO2<=>IC4H8O2H-T

+1.6400000E+004 +2.4300000E+000 +8.3000000E+003 !\AUTHOR: !\ REF:  
VILLANO, S, M.; CARSTENSEN, H-H.; DEAN, A. M. J. PHYS. CHEM. A., 2013,  
117, 6458. !\COMMENT:

IC4H8+HO2<=>TC4H8O2H-I

+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: ZADOR  
(J. PHYS. CHEM. A., 2011,115,10218) !\COMMENT:

PLOG / +1.3000000E-002  
+6.6700000E+014 -2.1400000E+000 +1.4188000E+004 /



PLOG / +9.8690000E-001  
+6.2500000E+006 +6.4000000E-001 +9.0730000E+003 /  
PLOG / +9.8690000E+000  
+7.9600000E+006 +8.2000000E-001 +8.7710000E+003 /  
PLOG / +9.8690000E+001  
+2.0500000E+013 -8.2000000E-001 +1.2919000E+004 /  
IC4H8+HO2<=>IC4H8O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: ZADOR  
(J. PHYS. CHEM. A., 2011,115,10218) !\COMMENT:  
PLOG / +1.3000000E-002  
+1.1800000E+004 +2.2900000E+000 +1.1321000E+004 /  
PLOG / +9.8690000E-001  
+5.3000000E+004 +2.1000000E+000 +1.1797000E+004 /  
PLOG / +9.8690000E+000  
+1.4700000E+009 +8.3000000E-001 +1.4808000E+004 /  
PLOG / +9.8690000E+001  
+1.9600000E+017 -1.4500000E+000 +2.1195000E+004 /  
TC4H8O2H-I<=>IC4H8O+OH  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: ZADOR  
(J. PHYS. CHEM. A., 2011,115,10218) !\COMMENT:  
PLOG / +1.3000000E-002  
+5.2300000E+017 -2.9700000E+000 +8.2150000E+003 /  
PLOG / +9.8690000E-001  
+4.3900000E+022 -3.9000000E+000 +1.1424000E+004 /  
PLOG / +9.8690000E+000  
+4.0000000E+025 -4.5000000E+000 +1.3952000E+004 /  
PLOG / +9.8690000E+001  
+1.2100000E+027 -4.6600000E+000 +1.6324000E+004 /  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\O \A  
\N \EA  
!

---

IC4H8+O<=>IC3H7+HCO  
+7.4500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:  
ANALOGY WITH C2H4 !\COMMENT:  
IC4H8+O=>CH2CO+CH3+CH3  
+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:  
ANALOGY WITH C2H4 !\COMMENT:  
IC4H8+O=>IC3H6CO+H+H  
+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:  
ANALOGY WITH C2H4 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

IC4H8+OH<=>IC4H7OH+H  
+2.2900000E+013 +7.0000000E-002 +1.0580000E+004 !AUTHOR: ! ANALOGY TO  
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25  
PLOG / +1.3000000E-003  
+2.6700000E+013 +5.0000000E-002 +1.0611000E+004 /  
PLOG / +1.0000000E-002  
+2.7500000E+013 +5.0000000E-002 +1.0623000E+004 /  
PLOG / +1.3000000E-002  
+2.8700000E+013 +4.0000000E-002 +1.0634000E+004 /

PLOG / +2.5000000E-002  
+1.5900000E+014 -1.6000000E-001 +1.1125000E+004 /  
PLOG / +1.0000000E-001  
+3.1000000E+014 -2.2000000E-001 +1.1407000E+004 /  
PLOG / +1.3150000E-001  
+3.7800000E+014 -2.4000000E-001 +1.1458000E+004 /  
PLOG / +1.0000000E+000  
+9.1500000E+007 +1.4200000E+000 +1.0087000E+004 /  
PLOG / +1.0000000E+001  
+3.6600000E+005 +2.1400000E+000 +1.0410000E+004 /  
PLOG / +1.0000000E+002  
+8.1900000E+002 +2.8400000E+000 +1.0481000E+004 /  
IC4H8+OH<=>SC3H5OH+CH3  
+1.2900000E+006 +1.6500000E+000 +1.2330000E+003 !AUTHOR: ! ANALOGY TO  
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25  
PLOG / +1.3000000E-003  
+5.1600000E+005 +1.6500000E+000 +1.2330000E+003 /  
PLOG / +1.0000000E-002  
+7.2800000E+003 +2.1000000E+000 +1.1620000E+003 /  
PLOG / +1.3000000E-002  
+8.1600000E+002 +2.4800000E+000 +1.1280000E+003 /  
PLOG / +2.5000000E-002  
+1.1500000E+002 +2.8000000E+000 +1.1520000E+003 /  
PLOG / +1.0000000E-001  
+5.6000000E+000 +3.2100000E+000 +1.2080000E+003 /  
PLOG / +1.3150000E-001  
+3.0800000E+000 +3.2900000E+000 +1.2160000E+003 /  
PLOG / +1.0000000E+000  
+4.5200000E+003 +2.5000000E+000 +3.2380000E+003 /  
PLOG / +1.0000000E+001  
+9.6400000E+018 -1.7400000E+000 +1.3107000E+004 /  
PLOG / +1.0000000E+002 +1.3200000E-  
001 +3.7000000E+000 +3.6650000E+003 /  
IC4H8+OH<=>IC3H5OH+CH3  
+1.2900000E+006 +1.6500000E+000 +1.2330000E+003 !AUTHOR: ! ANALOGY TO  
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25  
PLOG / +1.3000000E-003  
+2.0600000E+006 +1.6500000E+000 +1.2330000E+003 /  
PLOG / +1.0000000E-002  
+2.9100000E+004 +2.1000000E+000 +1.1620000E+003 /  
PLOG / +1.3000000E-002  
+3.2600000E+003 +2.4800000E+000 +1.1280000E+003 /  
PLOG / +2.5000000E-002  
+4.6100000E+002 +2.8000000E+000 +1.1520000E+003 /  
PLOG / +1.0000000E-001  
+2.2400000E+001 +3.2100000E+000 +1.2080000E+003 /  
PLOG / +1.3150000E-001  
+1.2300000E+001 +3.2900000E+000 +1.2160000E+003 /  
PLOG / +1.0000000E+000  
+1.8100000E+004 +2.5000000E+000 +3.2380000E+003 /  
PLOG / +1.0000000E+001  
+3.8600000E+019 -1.7400000E+000 +1.3107000E+004 /  
PLOG / +1.0000000E+002 +5.2800000E-  
001 +3.7000000E+000 +3.6650000E+003 /  
IC4H8+OH<=>SC4H7OH-I+H  
+2.8700000E+000 +2.9200000E+000 +6.2500000E+002 !AUTHOR: ! ANALOGY TO  
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25

PLOG / +1.3000000E-003  
 +2.8700000E+000 +2.9200000E+000 +6.2500000E+002 /  
 PLOG / +1.0000000E-002 +4.8400000E-  
 001 +2.9800000E+000 +7.0400000E+002 /  
 PLOG / +1.3000000E-002 +3.1300000E-  
 001 +3.0400000E+000 +7.2100000E+002 /  
 PLOG / +2.5000000E-002 +9.3300000E-  
 003 +3.6200000E+000 +6.7700000E+002 /  
 PLOG / +1.0000000E-001 +4.6400000E-  
 005 +4.4800000E+000 +6.8700000E+002 /  
 PLOG / +1.3150000E-001 +2.7100000E-  
 005 +4.5600000E+000 +7.0700000E+002 /  
 PLOG / +1.0000000E+000 +7.6500000E-  
 007 +5.0500000E+000 +8.7400000E+002 /  
 PLOG / +1.0000000E+001  
 +2.6400000E+015 -8.0000000E-001 +1.2728000E+004 /  
 PLOG / +1.0000000E+002 +4.8700000E-  
 004 +4.3200000E+000 +4.0200000E+003 /  
 IC4H8+OH<=>CH3COCH3+CH3  
 +6.9300000E+005 +1.4900000E+000 -5.3600000E+002 !AUTHOR: ! ANALOGY TO  
 C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25  
 PLOG / +1.3000000E-003  
 +6.9300000E+005 +1.4900000E+000 -5.3600000E+002 /  
 PLOG / +1.0000000E-002  
 +5.9400000E+003 +2.0100000E+000 -5.6000000E+002 /  
 PLOG / +1.3000000E-002  
 +1.1000000E+003 +2.2200000E+000 -6.8000000E+002 /  
 PLOG / +2.5000000E-002  
 +1.0700000E+002 +2.5000000E+000 -7.5900000E+002 /  
 PLOG / +1.0000000E-001 +7.8300000E-  
 001 +3.1000000E+000 -9.1900000E+002 /  
 PLOG / +1.3150000E-001 +3.0700000E-  
 001 +3.2200000E+000 -9.4600000E+002 /  
 PLOG / +1.0000000E+000 +3.1600000E-  
 004 +4.0500000E+000 -1.1440000E+003 /  
 PLOG / +1.0000000E+001 +7.5900000E-  
 006 +4.4900000E+000 -6.8000000E+002 /  
 PLOG / +1.0000000E+002 +5.4500000E-  
 005 +4.2200000E+000 +1.1410000E+003 /  
 IC4H8+OH<=>IC4H8OH-IT  
 +5.1000000E+054 -2.0700000E+001 +3.2402000E+004 !AUTHOR: ! ANALOGY TO  
 C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25  
 PLOG / +1.3000000E-003  
 +2.3000000E+078 -2.0700000E+001 +3.2402000E+004 /  
 PLOG / +1.0000000E-002  
 +2.7400000E+077 -2.0000000E+001 +3.3874000E+004 /  
 PLOG / +1.3000000E-002  
 +1.0700000E+076 -1.9580000E+001 +3.2874000E+004 /  
 PLOG / +2.5000000E-002  
 +3.6800000E+073 -1.8790000E+001 +3.1361000E+004 /  
 PLOG / +1.0000000E-001  
 +1.0400000E+068 -1.7010000E+001 +2.7909000E+004 /  
 PLOG / +1.3150000E-001  
 +7.2300000E+066 -1.6640000E+001 +2.7162000E+004 /  
 PLOG / +1.0000000E+000  
 +1.9500000E+059 -1.4170000E+001 +2.3079000E+004 /  
 PLOG / +1.0000000E+001  
 +7.5800000E+053 -1.2230000E+001 +2.2976000E+004 /

```

PLOG / +1.0000000E+002
+1.4300000E+048 -1.0230000E+001 +2.3772000E+004 /
DUP
IC4H8+OH<=>IC4H8OH-IT
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! ANALOGY TO
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25
PLOG / +1.3000000E-003
+6.4100000E+059 -1.5840000E+001 +1.1594000E+004 /
PLOG / +1.0000000E-002
+7.2800000E+059 -1.5510000E+001 +1.2898000E+004 /
PLOG / +1.3000000E-002
+2.7900000E+059 -1.5340000E+001 +1.2913000E+004 /
PLOG / +2.5000000E-002
+2.6500000E+058 -1.4930000E+001 +1.2936000E+004 /
PLOG / +1.0000000E-001
+1.3500000E+056 -1.4040000E+001 +1.2945000E+004 /
PLOG / +1.3150000E-001
+3.9800000E+055 -1.3850000E+001 +1.2887000E+004 /
PLOG / +1.0000000E+000
+1.5500000E+050 -1.2040000E+001 +1.1493000E+004 /
PLOG / +1.0000000E+001
+6.4100000E+041 -9.3500000E+000 +8.9210000E+003 /
PLOG / +1.0000000E+002
+2.3000000E+032 -6.3100000E+000 +6.0880000E+003 /
DUP
IC4H8+OH<=>IC4H8OH-TI
+5.1000000E+054 -2.0700000E+001 +3.2402000E+004 !AUTHOR: ! ANALOGY TO
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25
PLOG / +1.3000000E-003
+2.1400000E+059 -1.5840000E+001 +1.1594000E+004 /
PLOG / +1.0000000E-002
+2.4300000E+059 -1.5510000E+001 +1.2898000E+004 /
PLOG / +1.3000000E-002
+9.3000000E+058 -1.5340000E+001 +1.2913000E+004 /
PLOG / +2.5000000E-002
+8.8300000E+057 -1.4930000E+001 +1.2936000E+004 /
PLOG / +1.0000000E-001
+4.5000000E+055 -1.4040000E+001 +1.2945000E+004 /
PLOG / +1.3150000E-001
+1.3300000E+055 -1.3850000E+001 +1.2887000E+004 /
PLOG / +1.0000000E+000
+5.1800000E+049 -1.2040000E+001 +1.1493000E+004 /
PLOG / +1.0000000E+001
+2.1400000E+041 -9.3500000E+000 +8.9210000E+003 /
PLOG / +1.0000000E+002
+7.6500000E+031 -6.3100000E+000 +6.0880000E+003 /
DUP
IC4H8+OH<=>IC4H8OH-TI
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! ANALOGY TO
C3H6+OH !\COMMENT: ! KEEP TOTAL THE SAME, BRANCHING RATIO 75:25
PLOG / +1.3000000E-003
+7.6800000E+077 -2.0700000E+001 +3.2402000E+004 /
PLOG / +1.0000000E-002
+9.1300000E+076 -2.0000000E+001 +3.3874000E+004 /
PLOG / +1.3000000E-002
+3.5500000E+075 -1.9580000E+001 +3.2874000E+004 /
PLOG / +2.5000000E-002
+1.2300000E+073 -1.8790000E+001 +3.1361000E+004 /

```

PLOG / +1.0000000E-001  
+3.4500000E+067 -1.7010000E+001 +2.7909000E+004 /  
PLOG / +1.3150000E-001  
+2.4100000E+066 -1.6640000E+001 +2.7162000E+004 /  
PLOG / +1.0000000E+000  
+6.5000000E+058 -1.4170000E+001 +2.3079000E+004 /  
PLOG / +1.0000000E+001  
+2.5300000E+053 -1.2230000E+001 +2.2976000E+004 /  
PLOG / +1.0000000E+002  
+4.7800000E+047 -1.0230000E+001 +2.3772000E+004 /  
DUP  
!

---

!\REACTIONCLASS: \ROH\_O2 \A  
\N \EA  
!

---

---

IC4H8OH-IT+O2<=>TQJC4H8OH  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+1.0500000E+114 -3.3810000E+001 +2.4741000E+004 /  
PLOG / +1.0000000E-002  
+2.1300000E+114 -3.3440000E+001 +2.6448000E+004 /  
PLOG / +1.0000000E-001  
+1.6200000E+110 -3.1750000E+001 +2.6612000E+004 /  
PLOG / +1.0000000E+000  
+6.0000000E+101 -2.8790000E+001 +2.5197000E+004 /  
PLOG / +1.0000000E+001  
+5.3600000E+089 -2.4760000E+001 +2.2402000E+004 /  
PLOG / +4.0000000E+001  
+1.5500000E+081 -2.1950000E+001 +2.0197000E+004 /  
PLOG / +1.0000000E+002  
+1.5100000E+075 -2.0000000E+001 +1.8578000E+004 /  
PLOG / +2.0000000E+002  
+3.1600000E+070 -1.8480000E+001 +1.7287000E+004 /  
IC4H8OH-IT+O2<=>IC4H7OH+HO2  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+1.2100000E+026 -5.0900000E+000 +5.7550000E+003 /  
PLOG / +1.0000000E-002  
+1.4100000E+031 -6.5500000E+000 +8.7810000E+003 /  
PLOG / +1.0000000E-001  
+5.0800000E+034 -7.5300000E+000 +1.1702000E+004 /  
PLOG / +1.0000000E+000  
+1.6700000E+034 -7.2700000E+000 +1.3418000E+004 /  
PLOG / +1.0000000E+001  
+2.8200000E+028 -5.4100000E+000 +1.3318000E+004 /  
PLOG / +4.0000000E+001  
+2.5000000E+022 -3.5200000E+000 +1.2314000E+004 /  
PLOG / +1.0000000E+002  
+2.8200000E+017 -1.9900000E+000 +1.1286000E+004 /  
PLOG / +2.0000000E+002  
+1.9300000E+013 -7.1000000E-001 +1.0340000E+004 /  
DUP

IC4H8OH-IT+O2<=>IC4H7OH+HO2  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +2.4500000E+021 -4.1900000E+000 +6.8370000E+003 /  
 PLOG / +1.0000000E-002  
 +1.4000000E+030 -6.7500000E+000 +1.1554000E+004 /  
 PLOG / +1.0000000E-001  
 +9.1100000E+039 -9.5600000E+000 +1.7834000E+004 /  
 PLOG / +1.0000000E+000  
 +5.1600000E+042 -1.0170000E+001 +2.2412000E+004 /  
 PLOG / +1.0000000E+001  
 +6.0700000E+032 -6.9400000E+000 +2.2738000E+004 /  
 PLOG / +4.0000000E+001  
 +3.8800000E+020 -3.1400000E+000 +2.0677000E+004 /  
 PLOG / +1.0000000E+002  
 +3.3200000E+010 -3.0000000E-002 +1.8552000E+004 /  
 PLOG / +2.0000000E+002  
 +1.2200000E+002 +2.5700000E+000 +1.6623000E+004 /  
 DUP  
 IC4H8OH-IT+O2<=>SC4H7OH-I+HO2  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.2600000E+025 -4.6900000E+000 +5.7550000E+003 /  
 PLOG / +1.0000000E-002  
 +1.4400000E+030 -6.1500000E+000 +8.7850000E+003 /  
 PLOG / +1.0000000E-001  
 +4.7800000E+033 -7.1100000E+000 +1.1695000E+004 /  
 PLOG / +1.0000000E+000  
 +1.4000000E+033 -6.8400000E+000 +1.3395000E+004 /  
 PLOG / +1.0000000E+001  
 +2.1200000E+027 -4.9600000E+000 +1.3277000E+004 /  
 PLOG / +4.0000000E+001  
 +1.7800000E+021 -3.0700000E+000 +1.2265000E+004 /  
 PLOG / +1.0000000E+002  
 +1.9700000E+016 -1.5300000E+000 +1.1234000E+004 /  
 PLOG / +2.0000000E+002  
 +1.3200000E+012 -2.5000000E-001 +1.0285000E+004 /  
 DUP  
 IC4H8OH-IT+O2<=>SC4H7OH-I+HO2  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +3.2200000E+023 -4.6900000E+000 +5.3410000E+003 /  
 PLOG / +1.0000000E-002  
 +4.8000000E+028 -6.1800000E+000 +8.4610000E+003 /  
 PLOG / +1.0000000E-001  
 +1.7100000E+032 -7.1600000E+000 +1.1410000E+004 /  
 PLOG / +1.0000000E+000  
 +1.5300000E+032 -7.0200000E+000 +1.3378000E+004 /  
 PLOG / +1.0000000E+001  
 +5.5500000E+029 -6.1400000E+000 +1.5100000E+004 /  
 PLOG / +4.0000000E+001  
 +1.7200000E+026 -4.9700000E+000 +1.5849000E+004 /  
 PLOG / +1.0000000E+002  
 +4.4600000E+021 -3.5100000E+000 +1.5644000E+004 /

PLOG / +2.0000000E+002  
 +5.0600000E+016 -1.9600000E+000 +1.4979000E+004 /  
 DUP  
 IC4H8OH-IT+O2<=>TQC4H8OI  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +6.3600000E+104 -3.3740000E+001 +2.2390000E+004 /  
 PLOG / +1.0000000E-002  
 +7.9600000E+103 -3.3010000E+001 +2.2966000E+004 /  
 PLOG / +1.0000000E-001  
 +6.9900000E+096 -3.0480000E+001 +2.0584000E+004 /  
 PLOG / +1.0000000E+000  
 +1.0400000E+088 -2.7470000E+001 +1.6629000E+004 /  
 PLOG / +1.0000000E+001  
 +3.1300000E+096 -2.9620000E+001 +2.0346000E+004 /  
 PLOG / +4.0000000E+001  
 +2.7900000E+105 -3.2040000E+001 +2.4971000E+004 /  
 PLOG / +1.0000000E+002  
 +4.6400000E+109 -3.3120000E+001 +2.7657000E+004 /  
 PLOG / +2.0000000E+002  
 +2.0600000E+111 -3.3480000E+001 +2.9197000E+004 /  
 IC4H8OH-IT+O2=>CH3COCH3+CH2O+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +3.0300000E+037 -8.3500000E+000 +6.9400000E+003 /  
 PLOG / +1.0000000E-002  
 +1.0700000E+042 -9.6400000E+000 +9.9650000E+003 /  
 PLOG / +1.0000000E-001  
 +9.2200000E+043 -1.0120000E+001 +1.2427000E+004 /  
 PLOG / +1.0000000E+000  
 +1.1400000E+042 -9.4200000E+000 +1.3806000E+004 /  
 PLOG / +1.0000000E+001  
 +1.8000000E+038 -8.1300000E+000 +1.5131000E+004 /  
 PLOG / +4.0000000E+001  
 +1.6100000E+034 -6.8000000E+000 +1.5691000E+004 /  
 PLOG / +1.0000000E+002  
 +7.0000000E+029 -5.4100000E+000 +1.5552000E+004 /  
 PLOG / +2.0000000E+002  
 +3.7400000E+025 -4.0600000E+000 +1.5118000E+004 /  
 IC4H8OH-IT+O2<=>QC4H7OHP  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.1800000E+118 -3.7600000E+001 +2.6229000E+004 /  
 PLOG / +1.0000000E-002  
 +1.9100000E+131 -4.0730000E+001 +3.4079000E+004 /  
 PLOG / +1.0000000E-001  
 +5.8100000E+138 -4.2170000E+001 +4.0750000E+004 /  
 PLOG / +1.0000000E+000  
 +5.0500000E+134 -4.0190000E+001 +4.3580000E+004 /  
 PLOG / +1.0000000E+001  
 +2.0700000E+117 -3.4260000E+001 +4.1516000E+004 /  
 PLOG / +4.0000000E+001  
 +1.7100000E+101 -2.9040000E+001 +3.8094000E+004 /  
 PLOG / +1.0000000E+002  
 +1.2500000E+089 -2.5150000E+001 +3.5203000E+004 /

PLOG / +2.0000000E+002  
 +2.9800000E+079 -2.2090000E+001 +3.2802000E+004 /  
 IC4H8OH-IT+O2<=>CCY(CCO)COH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +2.1100000E+018 -2.8700000E+000 +6.8700000E+003 /  
 PLOG / +1.0000000E-002  
 +3.0200000E+027 -5.5400000E+000 +1.1842000E+004 /  
 PLOG / +1.0000000E-001  
 +1.3600000E+037 -8.2900000E+000 +1.8165000E+004 /  
 PLOG / +1.0000000E+000  
 +1.2100000E+039 -8.6600000E+000 +2.2517000E+004 /  
 PLOG / +1.0000000E+001  
 +1.5300000E+028 -5.1300000E+000 +2.2530000E+004 /  
 PLOG / +4.0000000E+001  
 +2.7200000E+015 -1.1600000E+000 +2.0283000E+004 /  
 PLOG / +1.0000000E+002  
 +1.0600000E+005 +2.0600000E+000 +1.8044000E+004 /  
 PLOG / +2.0000000E+002 +2.3000000E-  
 004 +4.7300000E+000 +1.6037000E+004 /  
 IC4H8OH-IT+O2<=>TQC4H7OHI  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.7600000E+053 -1.9870000E+001 +9.0190000E+003 /  
 PLOG / +1.0000000E-002  
 +4.6800000E+067 -2.3920000E+001 +1.1892000E+004 /  
 PLOG / +1.0000000E-001  
 +2.0700000E+091 -3.0580000E+001 +1.7347000E+004 /  
 PLOG / +1.0000000E+000  
 +2.8400000E+100 -3.2400000E+001 +2.0041000E+004 /  
 PLOG / +1.0000000E+001  
 +1.1600000E+115 -3.5810000E+001 +2.7656000E+004 /  
 PLOG / +4.0000000E+001  
 +4.8700000E+123 -3.7830000E+001 +3.3314000E+004 /  
 PLOG / +1.0000000E+002  
 +7.9500000E+124 -3.7820000E+001 +3.5683000E+004 /  
 PLOG / +2.0000000E+002  
 +4.5800000E+122 -3.6860000E+001 +3.6374000E+004 /  
 IC4H8OH-IT+O2<=>C2CY(COC)OH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.4200000E+032 -6.9500000E+000 +6.2100000E+003 /  
 PLOG / +1.0000000E-002  
 +5.1900000E+036 -8.2400000E+000 +9.2330000E+003 /  
 PLOG / +1.0000000E-001  
 +5.7700000E+038 -8.7600000E+000 +1.1715000E+004 /  
 PLOG / +1.0000000E+000  
 +2.8600000E+036 -7.9500000E+000 +1.2823000E+004 /  
 PLOG / +1.0000000E+001  
 +1.3700000E+032 -6.5100000E+000 +1.3646000E+004 /  
 PLOG / +4.0000000E+001  
 +2.1500000E+029 -5.5600000E+000 +1.4541000E+004 /  
 PLOG / +1.0000000E+002  
 +1.2000000E+026 -4.5100000E+000 +1.4778000E+004 /



PLOG / +2.0000000E+002  
+3.3100000E+022 -3.3700000E+000 +1.4606000E+004 /  
TQJC4H8OH<=>IC4H7OH+HO2  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+9.7300000E+065 -1.8500000E+001 +4.2975000E+004 /  
PLOG / +1.0000000E-002  
+1.0400000E+064 -1.7250000E+001 +4.4419000E+004 /  
PLOG / +1.0000000E-001  
+7.9000000E+059 -1.5590000E+001 +4.4504000E+004 /  
PLOG / +1.0000000E+000  
+9.3500000E+053 -1.3490000E+001 +4.3566000E+004 /  
PLOG / +1.0000000E+001  
+4.1300000E+044 -1.0390000E+001 +4.1279000E+004 /  
PLOG / +4.0000000E+001  
+6.5700000E+038 -8.4900000E+000 +3.9745000E+004 /  
PLOG / +1.0000000E+002  
+8.3200000E+034 -7.2300000E+000 +3.8675000E+004 /  
PLOG / +2.0000000E+002  
+9.4600000E+031 -6.2800000E+000 +3.7849000E+004 /  
DUP  
TQJC4H8OH<=>IC4H7OH+HO2  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+5.2700000E+064 -1.8000000E+001 +4.2872000E+004 /  
PLOG / +1.0000000E-002  
+4.8200000E+062 -1.6740000E+001 +4.4284000E+004 /  
PLOG / +1.0000000E-001  
+3.4200000E+058 -1.5070000E+001 +4.4348000E+004 /  
PLOG / +1.0000000E+000  
+4.0500000E+052 -1.2970000E+001 +4.3402000E+004 /  
PLOG / +1.0000000E+001  
+1.9300000E+043 -9.8800000E+000 +4.1120000E+004 /  
PLOG / +4.0000000E+001  
+3.2800000E+037 -7.9900000E+000 +3.9593000E+004 /  
PLOG / +1.0000000E+002  
+4.3500000E+033 -6.7400000E+000 +3.8527000E+004 /  
PLOG / +2.0000000E+002  
+5.1300000E+030 -5.7900000E+000 +3.7706000E+004 /  
DUP  
TQJC4H8OH<=>TQC4H8OI  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+3.7800000E+050 -1.2910000E+001 +3.1539000E+004 /  
PLOG / +1.0000000E-002  
+1.4200000E+045 -1.0940000E+001 +3.0864000E+004 /  
PLOG / +1.0000000E-001  
+1.5000000E+040 -9.2100000E+000 +2.9932000E+004 /  
PLOG / +1.0000000E+000  
+3.1200000E+035 -7.6400000E+000 +2.8864000E+004 /  
PLOG / +1.0000000E+001  
+2.7300000E+029 -5.6700000E+000 +2.7243000E+004 /  
PLOG / +4.0000000E+001  
+8.8800000E+025 -4.5400000E+000 +2.6272000E+004 /

PLOG / +1.0000000E+002  
 +4.6000000E+023 -3.8000000E+000 +2.5622000E+004 /  
 PLOG / +2.0000000E+002  
 +9.0800000E+021 -3.2500000E+000 +2.5131000E+004 /  
 TQJC4H8OH<=>QC4H7OHP  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +9.1600000E+062 -1.8020000E+001 +4.5297000E+004 /  
 PLOG / +1.0000000E-002  
 +2.5600000E+062 -1.7100000E+001 +4.7393000E+004 /  
 PLOG / +1.0000000E-001  
 +1.2500000E+059 -1.5610000E+001 +4.7984000E+004 /  
 PLOG / +1.0000000E+000  
 +1.9700000E+053 -1.3490000E+001 +4.7281000E+004 /  
 PLOG / +1.0000000E+001  
 +1.9100000E+043 -1.0150000E+001 +4.4926000E+004 /  
 PLOG / +4.0000000E+001  
 +7.6800000E+036 -8.0500000E+000 +4.3267000E+004 /  
 PLOG / +1.0000000E+002  
 +3.4900000E+032 -6.6400000E+000 +4.2089000E+004 /  
 PLOG / +2.0000000E+002  
 +1.7700000E+029 -5.5700000E+000 +4.1173000E+004 /  
 TQJC4H8OH<=>TQC4H7OHI  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +9.5700000E+058 -1.5990000E+001 +3.8293000E+004 /  
 PLOG / +1.0000000E-002  
 +7.2700000E+054 -1.4250000E+001 +3.8593000E+004 /  
 PLOG / +1.0000000E-001  
 +8.3000000E+049 -1.2440000E+001 +3.8031000E+004 /  
 PLOG / +1.0000000E+000  
 +1.9000000E+044 -1.0510000E+001 +3.6905000E+004 /  
 PLOG / +1.0000000E+001  
 +2.1800000E+036 -7.9000000E+000 +3.4865000E+004 /  
 PLOG / +4.0000000E+001  
 +4.1000000E+031 -6.3600000E+000 +3.3581000E+004 /  
 PLOG / +1.0000000E+002  
 +3.0000000E+028 -5.3500000E+000 +3.2704000E+004 /  
 PLOG / +2.0000000E+002  
 +1.3400000E+026 -4.5900000E+000 +3.2035000E+004 /  
 TQC4H8OI=>CH3COCH3+CH2O+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +8.0900000E+038 -9.9100000E+000 +1.9096000E+004 /  
 PLOG / +1.0000000E-002  
 +9.0900000E+039 -9.9300000E+000 +1.9135000E+004 /  
 PLOG / +1.0000000E-001  
 +1.8900000E+041 -1.0020000E+001 +1.9407000E+004 /  
 PLOG / +1.0000000E+000  
 +7.4700000E+023 -4.1000000E+000 +1.4658000E+004 /  
 PLOG / +1.0000000E+001  
 +2.9500000E+033 -6.7500000E+000 +1.8685000E+004 /  
 PLOG / +4.0000000E+001  
 +4.2400000E+036 -7.5600000E+000 +2.0307000E+004 /

PLOG / +1.0000000E+002  
 +7.8300000E+036 -7.5400000E+000 +2.0747000E+004 /  
 PLOG / +2.0000000E+002  
 +7.6300000E+035 -7.1700000E+000 +2.0641000E+004 /  
 QC4H7OHP<=>IC4H7OH+HO2  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +3.2900000E+057 -1.5640000E+001 +2.8576000E+004 /  
 PLOG / +1.0000000E-002  
 +9.6500000E+058 -1.5750000E+001 +2.9927000E+004 /  
 PLOG / +1.0000000E-001  
 +2.1900000E+050 -1.2660000E+001 +2.8547000E+004 /  
 PLOG / +1.0000000E+000  
 +1.6700000E+049 -1.2050000E+001 +2.9204000E+004 /  
 PLOG / +1.0000000E+001  
 +7.0800000E+040 -9.2600000E+000 +2.7188000E+004 /  
 PLOG / +4.0000000E+001  
 +1.3200000E+030 -5.8200000E+000 +2.4071000E+004 /  
 PLOG / +1.0000000E+002  
 +1.1500000E+030 -5.8000000E+000 +2.4053000E+004 /  
 PLOG / +2.0000000E+002  
 +1.1200000E+030 -5.8000000E+000 +2.4050000E+004 /  
 QC4H7OHP<=>CCY(CCO)COH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.1100000E+051 -1.2970000E+001 +2.8497000E+004 /  
 PLOG / +1.0000000E-002  
 +5.5800000E+051 -1.2870000E+001 +2.9529000E+004 /  
 PLOG / +1.0000000E-001  
 +3.0300000E+044 -1.0280000E+001 +2.8326000E+004 /  
 PLOG / +1.0000000E+000  
 +1.4200000E+044 -9.9800000E+000 +2.8986000E+004 /  
 PLOG / +1.0000000E+001  
 +9.6900000E+037 -7.9300000E+000 +2.7491000E+004 /  
 PLOG / +4.0000000E+001  
 +5.9000000E+029 -5.3000000E+000 +2.5095000E+004 /  
 PLOG / +1.0000000E+002  
 +5.2700000E+029 -5.2900000E+000 +2.5081000E+004 /  
 PLOG / +2.0000000E+002  
 +5.1500000E+029 -5.2800000E+000 +2.5078000E+004 /  
 TQC4H7OHI<=>C2CY(COC)OH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.1000000E+031 -7.2100000E+000 +1.4640000E+004 /  
 PLOG / +1.0000000E-002  
 +1.3700000E+032 -7.2400000E+000 +1.4716000E+004 /  
 PLOG / +1.0000000E-001  
 +3.3400000E+033 -7.3500000E+000 +1.5127000E+004 /  
 PLOG / +1.0000000E+000  
 +1.8600000E+023 -3.6800000E+000 +1.2864000E+004 /  
 PLOG / +1.0000000E+001  
 +9.8800000E+031 -6.2300000E+000 +1.6040000E+004 /  
 PLOG / +4.0000000E+001  
 +1.2500000E+034 -6.7800000E+000 +1.7056000E+004 /

PLOG / +1.0000000E+002  
 +7.7300000E+033 -6.6700000E+000 +1.7176000E+004 /  
 PLOG / +2.0000000E+002  
 +2.1300000E+033 -6.4500000E+000 +1.7170000E+004 /  
 TQC4H7OHI<=>SC4H7OH-I+HO2  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +6.0100000E+027 -7.2700000E+000 +1.4658000E+004 /  
 PLOG / +1.0000000E-002  
 +7.7800000E+028 -7.3000000E+000 +1.4733000E+004 /  
 PLOG / +1.0000000E-001  
 +3.2700000E+030 -7.4800000E+000 +1.5191000E+004 /  
 PLOG / +1.0000000E+000  
 +2.8100000E+017 -2.8200000E+000 +1.2336000E+004 /  
 PLOG / +1.0000000E+001  
 +1.9200000E+026 -5.2200000E+000 +1.6146000E+004 /  
 PLOG / +4.0000000E+001  
 +7.6100000E+027 -5.4900000E+000 +1.7483000E+004 /  
 PLOG / +1.0000000E+002  
 +1.9100000E+026 -4.8600000E+000 +1.7429000E+004 /  
 PLOG / +2.0000000E+002  
 +2.9400000E+024 -4.1800000E+000 +1.7285000E+004 /  
 IC4H8OH-TI+O2<=>IQJC4H8OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +3.3400000E+111 -3.2670000E+001 +2.5143000E+004 /  
 PLOG / +1.0000000E-002  
 +4.8400000E+107 -3.1050000E+001 +2.5460000E+004 /  
 PLOG / +1.0000000E-001  
 +2.4100000E+100 -2.8420000E+001 +2.4474000E+004 /  
 PLOG / +1.0000000E+000  
 +4.5500000E+089 -2.4780000E+001 +2.2176000E+004 /  
 PLOG / +1.0000000E+001  
 +1.1400000E+076 -2.0310000E+001 +1.8721000E+004 /  
 PLOG / +4.0000000E+001  
 +9.2500000E+066 -1.7350000E+001 +1.6238000E+004 /  
 PLOG / +1.0000000E+002  
 +6.2000000E+060 -1.5360000E+001 +1.4499000E+004 /  
 PLOG / +2.0000000E+002  
 +1.3000000E+056 -1.3860000E+001 +1.3159000E+004 /  
 IC4H8OH-TI+O2<=>IC3H6OHCHO+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.5900000E+015 -1.6300000E+000 +8.9470000E+003 /  
 PLOG / +1.0000000E-002  
 +5.0700000E+020 -3.2400000E+000 +1.1938000E+004 /  
 PLOG / +1.0000000E-001  
 +5.0000000E+025 -4.6600000E+000 +1.5251000E+004 /  
 PLOG / +1.0000000E+000  
 +3.1800000E+026 -4.7900000E+000 +1.7388000E+004 /  
 PLOG / +1.0000000E+001  
 +6.0000000E+020 -2.9500000E+000 +1.7297000E+004 /  
 PLOG / +4.0000000E+001  
 +1.7000000E+014 -9.1000000E-001 +1.6099000E+004 /

PLOG / +1.0000000E+002  
 +7.9100000E+008 +7.3000000E-001 +1.4913000E+004 /  
 PLOG / +2.0000000E+002  
 +3.0300000E+004 +2.0800000E+000 +1.3854000E+004 /  
 IC4H8OH-TI+O2<=>IQC4H8OT  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.1200000E+102 -3.2400000E+001 +2.3496000E+004 /  
 PLOG / +1.0000000E-002  
 +4.2300000E+095 -3.0040000E+001 +2.2067000E+004 /  
 PLOG / +1.0000000E-001  
 +3.4500000E+083 -2.6080000E+001 +1.7114000E+004 /  
 PLOG / +1.0000000E+000  
 +8.1600000E+082 -2.5610000E+001 +1.6198000E+004 /  
 PLOG / +1.0000000E+001  
 +1.0400000E+097 -2.9540000E+001 +2.2648000E+004 /  
 PLOG / +4.0000000E+001  
 +7.2500000E+103 -3.1420000E+001 +2.6487000E+004 /  
 PLOG / +1.0000000E+002  
 +2.4800000E+106 -3.2060000E+001 +2.8397000E+004 /  
 PLOG / +2.0000000E+002  
 +1.3900000E+107 -3.2200000E+001 +2.9446000E+004 /  
 IC4H8OH-TI+O2=>CH3COCH3+CH2O+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +4.3900000E+048 -1.1880000E+001 +1.1603000E+004 /  
 PLOG / +1.0000000E-002  
 +9.8200000E+050 -1.2490000E+001 +1.4143000E+004 /  
 PLOG / +1.0000000E-001  
 +3.4300000E+049 -1.1940000E+001 +1.5561000E+004 /  
 PLOG / +1.0000000E+000  
 +2.4300000E+045 -1.0560000E+001 +1.6415000E+004 /  
 PLOG / +1.0000000E+001  
 +4.9800000E+039 -8.6800000E+000 +1.7473000E+004 /  
 PLOG / +4.0000000E+001  
 +7.9900000E+033 -6.8300000E+000 +1.7502000E+004 /  
 PLOG / +1.0000000E+002  
 +1.0200000E+029 -5.2800000E+000 +1.7165000E+004 /  
 PLOG / +2.0000000E+002  
 +7.1800000E+024 -3.9900000E+000 +1.6747000E+004 /  
 IC4H8OH-TI+O2<=>CH3+C3KET21  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +2.9100000E+040 -9.2300000E+000 +1.0830000E+004 /  
 PLOG / +1.0000000E-002  
 +9.6600000E+043 -1.0200000E+001 +1.3698000E+004 /  
 PLOG / +1.0000000E-001  
 +1.3400000E+044 -1.0130000E+001 +1.5661000E+004 /  
 PLOG / +1.0000000E+000  
 +2.5700000E+041 -9.1800000E+000 +1.7047000E+004 /  
 PLOG / +1.0000000E+001  
 +1.8200000E+036 -7.4600000E+000 +1.8330000E+004 /  
 PLOG / +4.0000000E+001  
 +8.8200000E+029 -5.4400000E+000 +1.8205000E+004 /

PLOG / +1.0000000E+002  
 +1.7400000E+024 -3.6500000E+000 +1.7600000E+004 /  
 PLOG / +2.0000000E+002  
 +2.1600000E+019 -2.1200000E+000 +1.6925000E+004 /  
 IC4H8OH-TI+O2<=>IQC4H7OHT  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.0300000E+115 -3.5130000E+001 +2.5407000E+004 /  
 PLOG / +1.0000000E-002  
 +1.1000000E+129 -3.8890000E+001 +3.2891000E+004 /  
 PLOG / +1.0000000E-001  
 +5.1500000E+135 -4.0380000E+001 +3.8573000E+004 /  
 PLOG / +1.0000000E+000  
 +7.2700000E+129 -3.8130000E+001 +3.9933000E+004 /  
 PLOG / +1.0000000E+001  
 +4.5000000E+112 -3.2490000E+001 +3.7045000E+004 /  
 PLOG / +4.0000000E+001  
 +7.7200000E+097 -2.7790000E+001 +3.3612000E+004 /  
 PLOG / +1.0000000E+002  
 +5.1700000E+086 -2.4260000E+001 +3.0799000E+004 /  
 PLOG / +2.0000000E+002  
 +4.7000000E+077 -2.1410000E+001 +2.8440000E+004 /  
 IC4H8OH-TI+O2=>IC3H5OH+CH2O+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +5.1000000E+024 -4.3100000E+000 +1.3009000E+004 /  
 PLOG / +1.0000000E-002  
 +6.9100000E+033 -6.9700000E+000 +1.7935000E+004 /  
 PLOG / +1.0000000E-001  
 +1.7400000E+041 -9.0300000E+000 +2.3613000E+004 /  
 PLOG / +1.0000000E+000  
 +2.2600000E+036 -7.3200000E+000 +2.5633000E+004 /  
 PLOG / +1.0000000E+001  
 +3.1500000E+017 -1.4000000E+000 +2.2782000E+004 /  
 PLOG / +4.0000000E+001  
 +9.3500000E+000 +3.7100000E+000 +1.9114000E+004 /  
 PLOG / +1.0000000E+002 +5.5900000E-  
 012 +7.4600000E+000 +1.6156000E+004 /  
 PLOG / +2.0000000E+002 +1.2700000E-  
 021 +1.0410000E+001 +1.3733000E+004 /  
 IC4H8OH-TI+O2<=>CCY(CCOC)OH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +3.0600000E+033 -7.2400000E+000 +1.1476000E+004 /  
 PLOG / +1.0000000E-002  
 +6.5600000E+042 -9.9200000E+000 +1.7197000E+004 /  
 PLOG / +1.0000000E-001  
 +8.2400000E+046 -1.0950000E+001 +2.2090000E+004 /  
 PLOG / +1.0000000E+000  
 +4.4800000E+038 -8.2200000E+000 +2.3019000E+004 /  
 PLOG / +1.0000000E+001  
 +1.0100000E+018 -1.7700000E+000 +1.9496000E+004 /  
 PLOG / +4.0000000E+001  
 +1.1600000E+001 +3.4400000E+000 +1.5637000E+004 /

PLOG / +1.0000000E+002 +4.8500000E-  
012 +7.2300000E+000 +1.2599000E+004 /  
PLOG / +2.0000000E+002 +8.6400000E-  
022 +1.0210000E+001 +1.0126000E+004 /  
!  
IQJC4H8OH<=>IC3H6OHCHO+OH  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+3.5800000E+071 -2.0620000E+001 +5.2656000E+004 /  
PLOG / +1.0000000E-002  
+9.6700000E+071 -2.0080000E+001 +5.4935000E+004 /  
PLOG / +1.0000000E-001  
+3.3900000E+067 -1.8180000E+001 +5.5330000E+004 /  
PLOG / +1.0000000E+000  
+7.2600000E+058 -1.5090000E+001 +5.4016000E+004 /  
PLOG / +1.0000000E+001  
+4.5700000E+046 -1.1010000E+001 +5.1172000E+004 /  
PLOG / +4.0000000E+001  
+4.3100000E+038 -8.3800000E+000 +4.9054000E+004 /  
PLOG / +1.0000000E+002  
+2.1200000E+033 -6.6600000E+000 +4.7587000E+004 /  
PLOG / +2.0000000E+002  
+2.7200000E+029 -5.4100000E+000 +4.6486000E+004 /  
!  
IQJC4H8OH<=>IQC4H8OT  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+1.0400000E+045 -1.1200000E+001 +3.1755000E+004 /  
PLOG / +1.0000000E-002  
+2.9000000E+040 -9.6200000E+000 +3.0945000E+004 /  
PLOG / +1.0000000E-001  
+4.8500000E+035 -8.0100000E+000 +2.9850000E+004 /  
PLOG / +1.0000000E+000  
+2.6200000E+030 -6.2800000E+000 +2.8498000E+004 /  
PLOG / +1.0000000E+001  
+3.3700000E+024 -4.3700000E+000 +2.6873000E+004 /  
PLOG / +4.0000000E+001  
+9.7500000E+020 -3.2300000E+000 +2.5861000E+004 /  
PLOG / +1.0000000E+002  
+5.6100000E+018 -2.5200000E+000 +2.5208000E+004 /  
PLOG / +2.0000000E+002  
+1.4400000E+017 -2.0100000E+000 +2.4740000E+004 /  
IQJC4H8OH<=>IQC4H7OHT  
+1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PLOG / +1.0000000E-003  
+1.3600000E+050 -1.2930000E+001 +3.6743000E+004 /  
PLOG / +1.0000000E-002  
+3.3600000E+045 -1.1270000E+001 +3.6143000E+004 /  
PLOG / +1.0000000E-001  
+1.1300000E+040 -9.4100000E+000 +3.4990000E+004 /  
PLOG / +1.0000000E+000  
+5.9300000E+033 -7.3300000E+000 +3.3438000E+004 /  
PLOG / +1.0000000E+001  
+4.2400000E+026 -5.0000000E+000 +3.1502000E+004 /

PLOG / +4.0000000E+001  
 +1.9700000E+022 -3.6100000E+000 +3.0275000E+004 /  
 PLOG / +1.0000000E+002  
 +3.4300000E+019 -2.7200000E+000 +2.9477000E+004 /  
 PLOG / +2.0000000E+002  
 +3.6900000E+017 -2.0900000E+000 +2.8900000E+004 /  
 IQC4H7OHT=>IC3H5OH+CH2O+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +4.2500000E+016 -3.6600000E+000 +1.9364000E+004 /  
 PLOG / +1.0000000E-002  
 +2.9800000E+033 -8.0100000E+000 +2.7106000E+004 /  
 PLOG / +1.0000000E-001  
 +3.4600000E+038 -8.8300000E+000 +3.1412000E+004 /  
 PLOG / +1.0000000E+000  
 +7.0700000E+028 -5.4600000E+000 +2.9633000E+004 /  
 PLOG / +1.0000000E+001  
 +2.0100000E+013 -4.3000000E-001 +2.5278000E+004 /  
 PLOG / +4.0000000E+001  
 +1.4300000E+013 -3.8000000E-001 +2.5238000E+004 /  
 PLOG / +1.0000000E+002  
 +1.3800000E+013 -3.8000000E-001 +2.5234000E+004 /  
 PLOG / +2.0000000E+002  
 +1.3700000E+013 -3.7000000E-001 +2.5233000E+004 /  
 IQC4H7OHT<=>CCY(CCOC)OH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +1.1200000E+025 -5.5900000E+000 +1.9349000E+004 /  
 PLOG / +1.0000000E-002  
 +7.2000000E+032 -7.6000000E+000 +2.3093000E+004 /  
 PLOG / +1.0000000E-001  
 +2.2200000E+034 -7.6500000E+000 +2.5130000E+004 /  
 PLOG / +1.0000000E+000  
 +2.4000000E+027 -5.2800000E+000 +2.3663000E+004 /  
 PLOG / +1.0000000E+001  
 +2.2400000E+017 -2.0400000E+000 +2.0810000E+004 /  
 PLOG / +4.0000000E+001  
 +1.8200000E+017 -2.0100000E+000 +2.0786000E+004 /  
 PLOG / +1.0000000E+002  
 +1.7800000E+017 -2.0100000E+000 +2.0783000E+004 /  
 PLOG / +2.0000000E+002  
 +1.7700000E+017 -2.0100000E+000 +2.0782000E+004 /  
 IQC4H7OHT<=>IC4H7OOH+OH  
 +1.4200000E+036 -1.5840000E+001 +1.1594000E+004 !AUTHOR: ! REF: H. SUN,  
 ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PLOG / +1.0000000E-003  
 +6.0700000E+013 -4.2100000E+000 +2.2478000E+004 /  
 PLOG / +1.0000000E-002  
 +9.7400000E+039 -1.0890000E+001 +3.3616000E+004 /  
 PLOG / +1.0000000E-001  
 +2.1800000E+049 -1.2650000E+001 +4.0359000E+004 /  
 PLOG / +1.0000000E+000  
 +3.3200000E+037 -8.4200000E+000 +3.8539000E+004 /  
 PLOG / +1.0000000E+001  
 +2.3400000E+016 -1.5600000E+000 +3.2712000E+004 /



PLOG / +4.0000000E+001  
+1.4400000E+016 -1.4900000E+000 +3.2656000E+004 /  
PLOG / +1.0000000E+002  
+1.3800000E+016 -1.4800000E+000 +3.2651000E+004 /  
PLOG / +2.0000000E+002  
+1.3700000E+016 -1.4800000E+000 +3.2649000E+004 /  
IQC4H8OT=>CH3COCH3+CH2O+OH  
+3.6400000E+009 +1.3000000E+000 +2.3700000E+004 !\AUTHOR: !\REF:  
VILLANO, L. HUYNH, H-H CARTENSEN, A M. DEAN., J. PHYS. CHEM A, 2012, 116,  
5068. !\COMMENT:  
IQC4H8OT<=>CH3+C3KET21  
+4.9500000E+010 +8.3000000E-001 +2.7900000E+004 !\AUTHOR: !\REF:  
VILLANO, L. HUYNH, H-H CARTENSEN, A M. DEAN., J. PHYS. CHEM A, 2012, 116,  
5068. !\COMMENT:  
IQC4H7OHT<=>CH2COHCH2OOH+CH3  
+4.9500000E+010 +8.3000000E-001 +2.7900000E+004 !\AUTHOR: !\REF:  
VILLANO, L. HUYNH, H-H CARTENSEN, A M. DEAN., J. PHYS. CHEM A, 2012, 116,  
5068. !\COMMENT:

!

---

!\REACTIONCLASS: \O2ROH\_O2\_PRODUCTS \A  
\N \EA

!

---

TQC4H7OHIO2<=>TQC4H7OHIQ-I  
+2.5600000E+012 -1.3000000E-001 +3.4360000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-I=>HO2CHO+CH3COCH3+OH  
+5.8190000E+005 +2.4000000E+000 +2.2790000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-I<=>IC4KETIT+HO2  
+1.8290000E+010 +7.9000000E-001 +1.5100000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
IC4KETIT=>CH3COCH3+HCO+OH  
+9.5000000E+015 +0.0000000E+000 +4.2540000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
IC4KETIT+OH<=>TC3H6O2HCO+H2O  
+6.1329948E+004 +2.6541900E+000 -4.5864000E+003 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
IC4KETIT+HO2<=>TC3H6O2HCO+H2O +1.1773000E-  
004 +4.9196600E+000 +3.6842744E+003 !\AUTHOR: !\REF: C ZHOU ESTIMATED  
SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: ! ANALOGY TO  
O2+QOOH\_2  
TC3H6O2HCO=>CH3COCH3+CO+OH  
+1.2780000E+020 -1.8900000E+000 +3.4460000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIO2<=>TQC4H7OHIQ-P  
+5.6900000E+008 +7.8000000E-001 +2.1850000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-P<=>IC3H5COHQ+HO2  
+1.8300000E+010 +7.9000000E-001 +1.5100000E+004 !\AUTHOR: !\REF: C ZHOU

ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-P<=>CH2CQCOHQ+CH3  
+5.3800000E+011 +7.0000000E-002 +2.4800000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-P=>IC3H5Q+HOCHO+OH  
+5.3800000E+011 +7.0000000E-002 +2.4800000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-P<=>COHQCYC(COC)+OH  
+2.2800000E+008 +1.2900000E+000 +9.8900000E+003 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIQ-P<=>QCYC(CCOC)OH+OH  
+4.5800000E+015 -1.0800000E+000 +1.8440000E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
IC3H5COHQ=>HOCHO+C3H5-T+OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
CH2CQCOHQ=>HOCHO+CH2CO+2OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
CH2CQCOHQ=>HCO+CH2CO+3OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
IC3H5Q=>CH2CO+CH3+OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
COHQCYC(COC)=>HOCHO+CH2O+C2H3+OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
QCYC(CCOC)OH=>HOCHO+CH2CO+CH3+OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !\REF: C ZHOU  
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION. !\COMMENT: !  
ANALOGY TO O2+QOOH\_2  
TQC4H7OHIO2<=>TQC4H7OHTO2  
+2.9560000E+009 +4.0000000E-002 +1.6350000E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
TQC4H7OHTO2<=>HOCOCQ(CH3)2+OH  
+1.7500000E+008 +1.7000000E+000 +2.6000000E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
HOCOCQ(CH3)2=>CO+CH3COCH3+2OH  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H7OHTO2<=>IQC4H7OHTQ-P  
+2.0630000E+007 +1.0000000E+000 +2.1070000E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H7OHTQ-P=>OH+CH2O+CH2COHCH2OOH  
+1.2000000E+010 +3.5000000E-001 +1.5700000E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701

CH2COHCH2OOH=>OH+CH2O+CH2CO+H  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H7OHTQ-P<=>OH+IC4H6Q2-II  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
PLOG / +1.0000000E-002  
+2.5300000E+040 -9.9100000E+000 +3.2631400E+004 /  
PLOG / +1.0000000E-001  
+2.5400000E+037 -8.7200000E+000 +3.2909500E+004 /  
PLOG / +1.0000000E+000  
+1.1200000E+031 -6.5300000E+000 +3.1806600E+004 /  
PLOG / +1.0000000E+001  
+1.9800000E+021 -3.3400000E+000 +2.9137800E+004 /  
PLOG / +1.0000000E+002  
+1.9500000E+010 +1.5400000E-001 +2.5612000E+004 /  
IC4H6Q2-II=>OH+CH2O+HO2+C3H4-A  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H7OHTO2<=>IQC4H8OTQ-I  
+4.1300000E+007 +1.0000000E+000 +2.1070000E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H8OTQ-I=>OH+CH2O+C3KET21  
+1.2000000E+010 +3.5000000E-001 +1.5700000E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H8OTQ-I<=>CH3+CO(CH2OOH)2  
+2.7400000E+013 +2.4000000E-001 +2.9830000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
CO(CH2OOH)2=>2OH+2CH2O+CO  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
IQC4H7OHTO2<=>CHOC(CH3)OHCH2Q+OH  
+1.2000000E+010 +3.5000000E-001 +1.5700000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
CHOC(CH3)OHCH2Q=>OH+CH2O+H+CH3COCHO  
+1.5900000E+020 -1.5000000E+000 +4.2879460E+004 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
CH3COCHO+OH=>2CO+CH3+H2O  
+6.1329948E+004 +2.6541900E+000 -4.5864000E+003 !\AUTHOR: !REF:S.  
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701  
TQC4H7OHI+O2<=>TQC4H7OHIO2  
+3.4900000E+014 -8.1600000E-001 -5.3649000E+002 !\AUTHOR: ! REF:  
MIYOSHI A., IJCK, 2012, 44, 59-74  
IQC4H7OHT+O2<=>IQC4H7OHTO2  
+6.8700000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: ! REF:  
MIYOSHI A., IJCK, 2012, 44, 59-74  
!=====  
!=====  
!\SUBSPECIES: \C2CY(COC)OH\CCY(CCO)COH\CCY(CCO)COH\CCY(CCOC)OH  
!=====  
!=====  
C2CY(COC)OH+OH=>IC3H6CO+OH+H2O  
+2.2600000E+003 +2.7300000E+000 -4.6880000E+003 !\AUTHOR: !\ C-W ZHOU,  
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:  
C2CY(COC)OH+HO2=>IC3H6CO+OH+H2O2  
+8.6000000E+000 +3.4600000E+000 +9.7323260E+003 !\AUTHOR: !\ J. MENDES,  
C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:

CCY(CCO)COH+OH=>IC3H5CHO+OH+H2O  
+5.6600000E+002 +2.9300000E+000 -4.0394000E+003 !\AUTHOR: !\ C-W ZHOU,  
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:  
CCY(CCO)COH+HO2=>IC3H5CHO+OH+H2O +1.8100000E-  
001 +3.9800000E+000 +9.0567000E+003 !\AUTHOR: !\ J. MENDES, C-W ZHOU,  
AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:  
CCY(CCO)COH+OH=>PC3H4OH-2+CH2O+H2O  
+1.2600000E+003 +2.9700000E+000 -2.6606000E+003 !\AUTHOR: !\ C-W ZHOU,  
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:  
CCY(CCO)COH+HO2=>PC3H4OH-2+CH2O+H2O +1.4000000E-  
005 +5.2600000E+000 +8.2679000E+003 !\AUTHOR: !\ J. MENDES, C-W ZHOU,  
AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:  
CCY(CCOC)OH+OH=>CH2O+SC3H4OH+H2O  
+5.6600000E+002 +2.9300000E+000 -4.0394000E+003 !\AUTHOR: !\ C-W ZHOU,  
J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12, 7221-7233 !\COMMENT:  
CCY(CCOC)OH+HO2=>CH2O+SC3H4OH+H2O +1.8100000E-  
001 +3.9800000E+000 +9.0567000E+003 !\AUTHOR: !\ J. MENDES, C-W ZHOU,  
AND H. J. CURRAN, JPCA, 2014, 118, 1300-1308 !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \C2CY(COC)OH\CCY(CCO)COH\CCY(CCO)COH\CCY(CCOC)OH

!=====  
=====

!=====  
=====

!\SUBSPECIES: \IC4H7OH

!=====  
=====

!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

IC4H7+OH<=>IC4H7OH  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
IC4H7O+H<=>IC4H7OH  
+4.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES !\COMMENT:  
IC4H6OH+H<=>IC4H7OH  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
CH2CCH2OH+CH3<=>IC4H7OH  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

!\IC4H6OH

IC4H7OH+O2<=>IC4H6OH+HO2  
+6.0000000E+013 +0.0000000E+000 +3.9900000E+004 !\AUTHOR: !\REF:  
Ingham,T.; Walker,R.W.; Woolford,R.E., Symp. Int. Combust. Proc. 25, 767-  
774 (1994) !\COMMENT:

IC4H7OH+OH<=>IC4H6OH+H2O  
+1.2600000E+003 +2.9700000E+000 -2.6605930E+003 !\AUTHOR: !\ REF: C  
ZHOU, ET AL. COMBUST & FLAME, 2011, 158, 726. !\COMMENT: ANALOGY TO  
ALPHA-POSITION ABSTRACTION BY OH AND HO2 FROM N-BUTANOL  
IC4H7OH+HO2<=>IC4H6OH+H2O2 +1.4500000E-  
005 +5.2600000E+000 +8.2679070E+003 !\AUTHOR: !\ REF: C ZHOU, ET AL.  
IJCK, 2012, 44, 155. !\COMMENT:  
IC4H6OH+H2<=>IC4H7OH+H  
+2.1600000E+004 +2.3800000E+000 +1.8990000E+004 !\AUTHOR: !\REF:ANALOGY  
C3H5-A+X -->PRODUCTS !\COMMENT:  
IC4H6OH+CH2O<=>IC4H7OH+HCO  
+6.3000000E+008 +1.9000000E+000 +1.8190000E+004 !\AUTHOR: !\REF:RATE  
CONSTANT ANALOGY TO C3H5-A+CH2O (X 5) !\COMMENT:  
IC4H6OH+IC4H8<=>IC4H7OH+IC4H7  
+4.7000000E+002 +3.3000000E+000 +1.9840000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
!\IC4H7O  
IC4H7O+H2<=>IC4H7OH+H  
+9.0500000E+006 +2.0000000E+000 +1.7830000E+004 !\AUTHOR: !\REF:(TSANG/  
HAMPSON 86) X 5 !\COMMENT:  
IC4H7OH+HCO<=>IC4H7O+CH2O  
+3.0200000E+011 +0.0000000E+000 +1.8160000E+004 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

C3H4-A+CH2OH<=>IC4H6OH  
+1.0000000E+011 +0.0000000E+000 +9.2000000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
IC4H7O<=>IC4H6OH  
+1.3910000E+011 +0.0000000E+000 +1.5600000E+004 !\AUTHOR:  
!\REF:EA<=>8.6+7 (RING STRAIN+EABS OF PRIMARY H BY RO) !\COMMENT:  
!\WARNING: OTHER IC4H7O DECOMPOSITIONS ARE IN THE IC4H8 MECAHNISM  
!

---

!\REACTIONCLASS: \R\_HO2 \A  
\N \EA  
!

---

IC4H6OH+HO2=>CH2CCH2OH+CH2O+OH  
+1.4460000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA  
!

---

IC4H7OH+H<=>IC4H8OH  
+1.0000000E+013 +0.0000000E+000 +1.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH IC4H9 -->IC4H8+H !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_ABSCRACTION \A  
\N \EA

!

---

IC4H7O+O2<=>IC3H5CHO+HO2  
+3.0000000E+010 +0.0000000E+000 +1.6490000E+003 !\AUTHOR: !\REF:FROM  
BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 21, 411--429, 1992 !\COMMENT:  
IC4H7O+HO2<=>IC3H5CHO+H2O2  
+3.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX !\COMMENT:  
IC4H7O+CH3<=>IC3H5CHO+CH4  
+2.4000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX !\COMMENT:  
IC4H7O+O<=>IC3H5CHO+OH  
+6.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX !\COMMENT:  
IC4H7O+OH<=>IC3H5CHO+H2O  
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX !\COMMENT:  
IC4H7O+H<=>IC3H5CHO+H2  
+1.9900000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
CH3O+X -->CH2O+HX !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \IC4H7OH

!=====  
=====

!=====  
=====

!\SUBSPECIES: \IC3H6OHCHO

!=====  
=====

IC3H6OHCHO+OH=>TC3H6OH+CO+H2O  
+6.1329900E+004 +2.6500000E+000 -4.5864000E+003 !\AUTHOR: !\REF:J.  
MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.  
!\COMMENT:  
IC3H6OHCHO+H=>TC3H6OH+CO+H2  
+8.6600000E+005 +2.3000000E+000 +1.4260000E+003 !\AUTHOR: !\REF:J.  
MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.  
!\COMMENT: UNCLEAR FROM BASEMECH2907\_C7.INP

IC3H6OHCHO+HO2=>TC3H6OH+CO+H2O2 +1.0100000E-  
004 +5.0000000E+000 +3.4290000E+003 !\AUTHOR: !\REF:J. MENDES, C-W  
ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104. !\COMMENT: UNCLEAR  
FROM BASEMECH2907\_C7.INP  
IC3H6OHCHO+CH3=>TC3H6OH+CO+CH4  
+3.9400000E+000 +3.6000000E+000 +4.2230000E+003 !\AUTHOR: !\REF:J.  
MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.  
!\COMMENT: UNCLEAR FROM BASEMECH2907\_C7.INP

!=====  
=====

!\ENDSUBSPECIES: \IC3H6OHCHO

!=====  
=====

!=====  
=====

!\SUBSPECIES: \TC3H6OH

!=====  
=====

TC3H6OH<=>CH3COCH3+H  
+8.9810000E+011 +2.7100000E-001 +3.2990000E+004 !\AUTHOR: !\REF:J.

```

MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.
!\COMMENT: UNCLEAR FROM BASEMECH2907_C7.INP
TC3H6OH<=>IC3H5OH+H
+4.2110000E+010 +1.0050000E+000 +4.0900000E+004 !\AUTHOR: !\REF:J.
MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.
!\COMMENT: UNCLEAR FROM BASEMECH2907_C7.INP
TC3H6OH+O2<=>CH3COCH3+HO2
+2.2300000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:J.
MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.
!\COMMENT: UNCLEAR FROM BASEMECH2907_C7.INP
!=====
!=====
!\ENDSUBSPECIES: \TC3H6OH
!=====
!=====
!-----
!-----
!\ENDSUBMECH: \IC4H8
!-----
!-----
!-----
!\SUBMECH: \C4H8-1\C4H8-2
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!-----
!-----
!\REACTIONCLASS: \UNIMOL \A
\N \EA
!-----
C3H5-A+CH3 (+M) <=> C4H8-1 (+M)
+1.0000000E+014 -3.2000000E-001 -2.6230000E+002 !\AUTHOR: !\REF: Yijun
Zhang et al. Combustion and Flame 159 (2012) 905`C917
LOW /
+3.9100000E+060 -1.2810000E+001 +6.2500000E+003 / !LOW-PRESSURE-LIMIT
TROE / +1.0400000E-001
+1.6060000E+003 +6.0000000E+004 +6.1184000E+003 / !TROE PARAMETERS
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES
C2H5+C2H3 (+M) <=> C4H8-1 (+M)
+1.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: Yijun
Zhang et al. Combustion and Flame 159 (2012) 905`C917
LOW /
+1.5500000E+056 -1.1790000E+001 +8.9845000E+003 / !LOW-PRESSURE-LIMIT
TROE / +1.9800000E-001
+2.2779000E+003 +6.0000000E+004 +5.7232000E+003 / !TROE PARAMETERS
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES
C4H71-4+H (+M) <=> C4H8-1 (+M)
+3.6000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: Yijun
Zhang et al. Combustion and Flame 159 (2012) 905`C917
LOW /
+3.0100000E+048 -9.3200000E+000 +5.8336000E+003 / !LOW-PRESSURE-LIMIT
TROE / +4.9800000E-001
+1.3140000E+003 +1.3140000E+003 +5.0000000E+004 / !TROE PARAMETERS

```

H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6 / 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
C4H71-3+H<=>C4H8-1  
+5.0000000E+013 +0.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF: EST  
C3H5-S+CH3(+M)<=>C4H8-2(+M)  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF  
C2H3+CH3(+M)=C3H6(+M)  
LOW /  
+8.5400000E+058 -1.1940000E+001 +9.7698000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +1.7500000E-001  
+1.3406000E+003 +6.0000000E+004 +1.0139800E+004 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6 / 3.000 / AR / 0.700 / C2H2 / 3.000 / C2H4 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
C4H8-2<=>C3H5-A+CH3  
+7.5000000E+065 -1.5600000E+001 +9.7300000E+004 !\AUTHOR: !\REF: ASSUME BY THIS WORK  
C4H8-2<=>H+C4H71-3  
+4.6000000E+084 -2.0030000E+001 +1.3278700E+005 !\AUTHOR: !\REF  
C3H6=AC3H5+H IN 2009 KIEFER ET AL. X2 25TORR/5 TO 5TORR  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

!\*\*\*\*\*ABSTRACTION BY  
OH\*\*\*\*\*!  
C4H8-1+OH<=>C4H71-3+H2O  
+7.7690000E+005 +2.2000000E+000 -4.3718000E+002 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A 2011, 115, 2549`C2556 !\COMMENT: /2.6  
C4H8-1+OH<=>C4H71-4+H2O  
+8.6000000E+006 +2.0300000E+000 +2.6231000E+003 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A 2011, 115, 2549`C2556 !\COMMENT: \*2  
C4H8-1+OH<=>C4H71-2+H2O  
+3.0000000E+006 +1.9700000E+000 +2.8476600E+003 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A 2011, 115, 2549`C2556 !\COMMENT:  
C4H8-1+OH<=>C4H71-1+H2O  
+6.9300000E+006 +1.9200000E+000 +4.9620400E+003 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A 2011, 115, 2549`C2556 !\COMMENT:  
C4H8-2+OH<=>C4H71-3+H2O  
+4.4600000E+006 +2.0720000E+000 +1.0508000E+003 !\AUTHOR: !\REF:ANALOGY WITH C3H6+OH<=>C3H5-A+H2O \*2/2  
C4H8-2+OH<=>C4H72-2+H2O  
+6.0000000E+006 +1.9700000E+000 +2.8459000E+003 !\AUTHOR: !\REF:  
ANALOGY WITH C4H8-1 \*2  
!\*\*\*\*\* ABSTRACTION BY  
HO2\*\*\*\*\*!  
C4H8-1+HO2<=>C4H71-3+H2O2 +7.8200000E-001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF:Judith Zador,Stephen J. Klippenstein,and James A. Miller J. Phys. Chem. A 2011, 115, 10218`C10225 !\COMMENT: \*2  
C4H8-2+HO2<=>C4H71-3+H2O2 +6.9000000E-001 +4.0000000E+000 +1.2103000E+004 !\AUTHOR: !\REF:Judith Zador,Stephen J. Klippenstein,and James A. Miller J. Phys. Chem. A 2011, 115, 10218`C10225 !\COMMENT: \*2



C4H8-1+HO2<=>C4H71-4+H2O2  
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C4H10+HO2<=>PC4H9+H2O2  
C4H8-1+HO2<=>C4H71-1+H2O2  
+9.5700000E+002 +3.0590000E+000 +2.0798600E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+HO2  
C4H8-1+HO2<=>C4H71-2+H2O2  
+1.5600000E+004 +2.8200000E+000 +2.4427900E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+HO2  
C4H8-2+HO2<=>C4H72-2+H2O2  
+3.1200000E+004 +2.8200000E+000 +2.4427900E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+HO2 \*2  
C4H8-1+H<=>C4H71-4+H2  
+3.8400000E+004 +2.8700000E+000 +6.6110000E+003 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS  
C4H8-1+H<=>C4H71-3+H2  
+2.4200000E+003 +3.0500000E+000 +1.9950000E+003 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS  
C4H8-1+H<=>C4H71-2+H2  
+2.3700000E+004 +2.8500000E+000 +8.9170000E+003 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS  
C4H8-1+H<=>C4H71-1+H2  
+2.6300000E+004 +2.8300000E+000 +1.2050000E+004 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS  
DUP  
C4H8-1+H<=>C4H71-1+H2  
+2.2300000E+004 +2.8500000E+000 +1.1710000E+004 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS  
DUP  
C4H8-2+H<=>C4H71-3+H2  
+5.6200000E+002 +3.5000000E+000 +1.6270000E+003 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS !\*2 Ea-1  
C4H8-2+H<=>C4H72-2+H2  
+8.4700000E+004 +2.7600000E+000 +9.3040000E+003 !\AUTHOR: !\REF:KPS,  
TST/RRHO+HRS  
C4H8-1+O<=>C4H71-3+OH  
+1.7500000E+011 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:IN  
ARAMCO  
C4H8-2+O<=>C4H71-3+OH  
+2.1900000E+011 +8.1000000E-001 +7.5500000E+003 !\AUTHOR: !\REF:IN  
ARAMCO  
C4H8-1+O<=>C4H71-1+OH  
+1.2000000E+011 +7.0000000E-001 +8.9591000E+003 !\AUTHOR: !\REF:  
ANALOGY WITH C2H4+O  
C4H8-1+O<=>C4H71-2+OH  
+6.0300000E+010 +7.0000000E-001 +7.6320000E+003 !\AUTHOR: !\REF:  
ANALOGY WITH C2H4+O  
C4H8-2+O<=>C4H72-2+OH  
+1.2060000E+011 +7.0000000E-001 +7.6320000E+003 !\AUTHOR: !\REF:  
ANALOGY WITH C2H4+O !\*2  
C4H8-1+O<=>C4H71-4+OH  
+1.1300000E+014 +0.0000000E+000 +7.8500000E+003 !\AUTHOR: !\REF:  
ANALOGY WITH C4H10+O<=>PC4H9+OH  
C4H8-1+O2<=>C4H71-3+HO2  
+1.0000000E+014 +0.0000000E+000 +3.7190000E+004 !\AUTHOR: !\REF:IN  
ARAMCO !\*5

$C_4H_8-2+O_2 \rightleftharpoons C_4H_7-3+HO_2$   
+2.0000000E+014 +0.0000000E+000 +3.9390000E+004 !\AUTHOR: !\REF:IN  
ARAMCO !\*5  
 $C_4H_8-1+O_2 \rightleftharpoons C_4H_7-1+HO_2$   
+2.0000000E+013 +0.0000000E+000 +6.2270000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH  $C_3H_6+O_2$   
 $C_4H_8-1+O_2 \rightleftharpoons C_4H_7-2+HO_2$   
+1.0000000E+013 +0.0000000E+000 +5.8770000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH  $C_3H_6+O_2$   
 $C_4H_8-2+O_2 \rightleftharpoons C_4H_7-2+HO_2$   
+2.0000000E+013 +0.0000000E+000 +5.8770000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH  $C_3H_6+O_2$  !\*2  
 $C_4H_8-1+O_2 \rightleftharpoons C_4H_7-4+HO_2$   
+6.0000000E+013 +0.0000000E+000 +5.2340000E+004 !\AUTHOR: !\REF:  
ANALOGY WITH  $C_4H_{10}+O_2 \rightleftharpoons PC_4H_9+HO_2$   
 $C_4H_8-1+CH_3 \rightleftharpoons C_4H_7-3+CH_4$   
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:IN  
ARAMCO (TSANG '91)  
 $C_4H_8-1+CH_3 \rightleftharpoons C_4H_7-4+CH_4$  +4.5200000E-  
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:IN ARAMCO (TSANG  
'91)  
 $C_4H_8-2+CH_3 \rightleftharpoons C_4H_7-3+CH_4$   
+7.1400000E+000 +3.5700000E+000 +7.6420000E+003 !\AUTHOR: !\REF:IN  
ARAMCO (TSANG '91)  
 $C_4H_8-1+CH_3 \rightleftharpoons C_4H_7-1+CH_4$   
+1.3480000E+000 +3.5000000E+000 +1.2850000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH  $C_3H_6+CH_3$   
 $C_4H_8-1+CH_3 \rightleftharpoons C_4H_7-2+CH_4$  +8.4000000E-  
001 +3.5000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:ANALOGY WITH  
 $C_3H_6+CH_3$   
 $C_4H_8-2+CH_3 \rightleftharpoons C_4H_7-2+CH_4$   
+1.6800000E+000 +3.5000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH  $C_3H_6+CH_3$  !\*2  
 $C_4H_8-1+CH_3O_2 \rightleftharpoons C_4H_7-3+CH_3O_2H$   
+2.7000000E+004 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:IN  
ARAMCO (TSANG '91)  
 $C_4H_8-1+CH_3O_2 \rightleftharpoons C_4H_7-4+CH_3O_2H$   
+2.3800000E+003 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:IN  
ARAMCO (TSANG '91)  
 $C_4H_8-1+CH_3O \rightleftharpoons C_4H_7-3+CH_3OH$   
+4.0000000E+001 +2.9000000E+000 +8.6090000E+003 !\AUTHOR: !\REF:IN  
ARAMCO (TSANG '91)  
 $C_4H_8-1+CH_3O \rightleftharpoons C_4H_7-4+CH_3OH$   
+2.1700000E+011 +0.0000000E+000 +6.4580000E+003 !\AUTHOR: !\REF:IN  
ARAMCO (TSANG '91)  
 $C_4H_8-2+CH_3O \rightleftharpoons C_4H_7-3+CH_3OH$   
+1.8000000E+001 +2.9500000E+000 +1.1990000E+004 !\AUTHOR: !\REF:IN  
ARAMCO (ESTIMATE)  
 $C_4H_8-1+CH_3CO_3 \rightleftharpoons C_4H_7-3+CH_3CO_3H$   
+1.0000000E+011 +0.0000000E+000 +8.0000000E+003 !\AUTHOR: !\REF:IN  
ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))  
 $C_4H_8-1+C_3H_5-A \rightleftharpoons C_4H_7-3+C_3H_6$   
+7.9000000E+010 +0.0000000E+000 +1.2400000E+004 !\AUTHOR: !\REF:IN  
ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))  
 $C_4H_8-1+C_2H_5O_2 \rightleftharpoons C_4H_7-3+C_2H_5O_2H$   
+1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479  
(1975).)

C4H8-1+NC3H7O2<=>C4H71-3+NC3H7O2H  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479  
 (1975).)  
 C4H8-1+IC3H7O2<=>C4H71-3+IC3H7O2H  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479  
 (1975).)  
 C4H8-1+PC4H9O2<=>C4H71-3+PC4H9O2H  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479  
 (1975).)  
 C4H8-1+SC4H9O2<=>C4H71-3+SC4H9O2H  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479  
 (1975).)  
 C4H8-2+NC3H7O2<=>C4H71-3+NC3H7O2H  
 +3.2000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (!TWICE RATE OF C3H6+HO2)  
 C4H8-2+IC3H7O2<=>C4H71-3+IC3H7O2H  
 +3.2000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (!TWICE RATE OF C3H6+HO2)  
 C4H8-2+PC4H9O2<=>C4H71-3+PC4H9O2H  
 +3.2000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (!TWICE RATE OF C3H6+HO2)  
 C4H8-2+SC4H9O2<=>C4H71-3+SC4H9O2H  
 +3.2000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (!TWICE RATE OF C3H6+HO2)  
 C4H71-3+C2H5<=>C4H8-1+C2H4  
 +2.5900000E+012 +0.0000000E+000 -1.3100000E+002 !\AUTHOR: !\REF:IN  
 ARAMCO (ESTIMATE)  
 C4H71-3+CH3O<=>C4H8-1+CH2O  
 +2.4100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:IN  
 ARAMCO (ESTIMATE)  
 IC4H9O2+C4H8-1<=>IC4H9O2H+C4H71-3  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (WESTBROOK ESTIMATE)  
 TC4H9O2+C4H8-1<=>TC4H9O2H+C4H71-3  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (WESTBROOK ESTIMATE)  
 IC4H9O2+C4H8-2<=>IC4H9O2H+C4H71-3  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (WESTBROOK ESTIMATE)  
 TC4H9O2+C4H8-2<=>TC4H9O2H+C4H71-3  
 +1.4000000E+012 +0.0000000E+000 +1.4900000E+004 !\AUTHOR: !\REF:IN  
 ARAMCO (WESTBROOK ESTIMATE)

---

!\REACTIONCLASS: \R\_DECOMPOSITION

\A

\N

\EA

!

---

C4H71-1<=>C4H6-1+H  
 +8.9500000E+008 +1.1400000E+000 +3.5636458E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-1<=>C2H5+C2H2  
 +2.8500000E+012 +6.8000000E-001 +3.3178291E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS

C4H71-2<=>C4H6-1+H  
 +9.7900000E+008 +1.2000000E+000 +3.8080714E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-2<=>C4H612+H  
 +1.9900000E+008 +1.5600000E+000 +3.7683274E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-2<=>C3H4-A+CH3  
 +1.2300000E+010 +1.1900000E+000 +3.2915981E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-3<=>C4H612+H  
 +3.9500000E+011 +9.3000000E-001 +6.1611149E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-3<=>C4H6+H  
 +8.5300000E+007 +1.9500000E+000 +4.7490106E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-4<=>C2H4+C2H3  
 +2.8400000E+010 +9.9000000E-001 +3.8998800E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-4<=>C4H6+H  
 +1.3200000E+005 +2.2800000E+000 +3.3245856E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H72-2<=>C4H6-2+H  
 +7.8700000E+009 +1.1600000E+000 +3.6173002E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H72-2<=>C4H612+H  
 +9.5400000E+007 +1.8100000E+000 +3.8992838E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H72-2<=>C3H4-P+CH3  
 +6.3000000E+011 +9.3000000E-001 +3.4754141E+004 !\AUTHOR: !\REF:YANG  
 CALCULATIONS  
 C4H71-3<=>C4H71-4  
 012 +7.1900000E+000 +3.6200822E+004 !\AUTHOR: !\REF:YANG CALCULATIONS +5.6200000E-  
 C4H71-3<=>C4H72-2  
 023 +1.0210000E+001 +4.1574211E+004 !\AUTHOR: !\REF:YANG CALCULATIONS +6.7600000E-  
 !

---

!\REACTIONCLASS: \RA\_HO2\_PRODUCTS \A  
 \N \EA  
 !

---

C4H71-3+HO2<=>C4H71-3OOH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS  
 PLOG / +1.0000000E-002  
 +2.0500000E+001 +1.2400000E+000 -2.2589000E+004 /  
 PLOG / +1.0000000E-001  
 +3.6900000E+006 +8.0000000E-002 -1.8331000E+004 /  
 PLOG / +1.0000000E+000  
 +2.0200000E+013 -1.4500000E+000 -1.1709000E+004 /  
 PLOG / +2.0000000E+000  
 +1.4900000E+015 -1.8700000E+000 -9.6040000E+003 /  
 PLOG / +5.0000000E+000  
 +1.8500000E+017 -2.3100000E+000 -6.9910000E+003 /  
 PLOG / +1.0000000E+001  
 +2.8800000E+018 -2.5500000E+000 -5.2600000E+003 /  
 PLOG / +3.0000000E+001  
 +3.4500000E+019 -2.7100000E+000 -3.1400000E+003 /

PLOG / +5.0000000E+001  
 +5.3300000E+019 -2.7000000E+000 -2.4380000E+003 /  
 C4H71-3+HO2<=>C4H71-O+OH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS \*3  
 PLOG / +1.0000000E-002  
 +6.9000000E+020 -2.6800000E+000 +2.2900000E+002 /  
 PLOG / +1.0000000E-001  
 +4.5000000E+022 -3.1800000E+000 +1.7600000E+003 /  
 PLOG / +1.0000000E+000  
 +8.6100000E+027 -4.6300000E+000 +6.4150000E+003 /  
 PLOG / +2.0000000E+000  
 +1.9200000E+030 -5.2800000E+000 +8.5780000E+003 /  
 PLOG / +5.0000000E+000  
 +5.4600000E+033 -6.2200000E+000 +1.1879000E+004 /  
 PLOG / +1.0000000E+001  
 +2.9800000E+036 -6.9700000E+000 +1.4600000E+004 /  
 PLOG / +3.0000000E+001  
 +5.5800000E+040 -8.1400000E+000 +1.9040000E+004 /  
 PLOG / +5.0000000E+001  
 +4.4400000E+042 -8.6700000E+000 +2.1071000E+004 /  
 C4H71-3+HO2<=>C2H3COCH3+H2O  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS  
 PLOG / +1.0000000E-002  
 +5.1600000E+014 -1.7400000E+000 +1.9100000E+003 /  
 PLOG / +1.0000000E-001  
 +1.6200000E+016 -2.1600000E+000 +3.1670000E+003 /  
 PLOG / +1.0000000E+000  
 +9.7300000E+020 -3.4700000E+000 +7.3390000E+003 /  
 PLOG / +2.0000000E+000  
 +1.7000000E+023 -4.0900000E+000 +9.3780000E+003 /  
 PLOG / +5.0000000E+000  
 +4.3300000E+026 -5.0200000E+000 +1.2574000E+004 /  
 PLOG / +1.0000000E+001  
 +2.5900000E+029 -5.7800000E+000 +1.5275000E+004 /  
 PLOG / +3.0000000E+001  
 +7.8500000E+033 -7.0100000E+000 +1.9801000E+004 /  
 PLOG / +5.0000000E+001  
 +8.8400000E+035 -7.5800000E+000 +2.1918000E+004 /  
 C4H71-3OOH<=>C4H71-O+OH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS  
 PLOG / +1.0000000E-002  
 +4.4100000E+035 -7.3700000E+000 +3.9745000E+004 /  
 PLOG / +1.0000000E-001  
 +6.6400000E+037 -7.6000000E+000 +4.4224000E+004 /  
 PLOG / +1.0000000E+000  
 +7.0900000E+037 -7.2400000E+000 +4.7692000E+004 /  
 PLOG / +2.0000000E+000  
 +1.9200000E+037 -6.9700000E+000 +4.8350000E+004 /  
 PLOG / +5.0000000E+000  
 +1.2000000E+036 -6.5100000E+000 +4.8849000E+004 /  
 PLOG / +1.0000000E+001  
 +7.1700000E+034 -6.0800000E+000 +4.8933000E+004 /

PLOG / +3.0000000E+001  
+3.6900000E+032 -5.3200000E+000 +4.8614000E+004 /  
PLOG / +5.0000000E+001  
+3.0400000E+031 -4.9700000E+000 +4.8341000E+004 /  
C4H71-3OOH<=>C2H3COCH3+H2O  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS  
PLOG / +1.0000000E-002  
+3.5800000E+023 -4.6400000E+000 +3.8121000E+004 /  
PLOG / +1.0000000E-001  
+2.8500000E+027 -5.3600000E+000 +4.3407000E+004 /  
PLOG / +1.0000000E+000  
+2.6300000E+029 -5.5300000E+000 +4.8042000E+004 /  
PLOG / +2.0000000E+000  
+2.8300000E+029 -5.4300000E+000 +4.9101000E+004 /  
PLOG / +5.0000000E+000  
+1.0400000E+029 -5.1800000E+000 +5.0137000E+004 /  
PLOG / +1.0000000E+001  
+2.1200000E+028 -4.8900000E+000 +5.0610000E+004 /  
PLOG / +3.0000000E+001  
+5.3900000E+026 -4.3300000E+000 +5.0818000E+004 /  
PLOG / +5.0000000E+001  
+7.7600000E+025 -4.0400000E+000 +5.0737000E+004 /  
C4H71-O<=>C2H3+CH3CHO  
+8.5200000E+025 -3.6100000E+000 +2.7863400E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
C4H71-O<=>AC3H5OCH2  
+1.3500000E+018 -1.7300000E+000 +1.7386500E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
C4H71-O<=>CH2CH2COCH3  
+1.6700000E+021 -2.7400000E+000 +2.0337700E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
C4H71-O<=>C2H3COCH3+H  
+2.5700000E+020 -2.0600000E+000 +2.2040100E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
C4H71-O<=>C2H4+CH3CO  
+4.7500000E+008 +1.1400000E+000 +2.0922500E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
AC3H5OCH2<=>C3H5-A+CH2O  
+8.8100000E+014 -3.2600000E-001 +3.1553100E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
AC3H5OCH2<=>CH2CH2COCH3  
+2.5100000E+020 -2.6300000E+000 +2.9288400E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
AC3H5OCH2<=>C2H3COCH3+H  
+3.9800000E+018 -1.6200000E+000 +3.0129800E+004 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT:  
AC3H5OCH2<=>C3H6+HCO  
+3.7300000E+014 -7.2600000E-001 +3.2008300E+004 !\AUTHOR: !\REF:

KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 CH2CH2COCH3<=>C2H3+CH3CHO  
 +1.9300000E+019 -1.9400000E+000 +4.8440000E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 CH2CH2COCH3<=>C2H3COCH3+H  
 +4.5200000E+012 +2.1400000E-001 +3.4570500E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 CH2CH2COCH3<=>C2H4+CH3CO  
 +1.5900000E+013 +6.3000000E-002 +2.4086300E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C2H3+CH3CHO<=>C2H4+CH3CO  
 +1.6500000E+001 +3.1700000E+000 +9.3998000E+003 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C4H71-3+HO2<=>C4H72-1OOH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS  
 PLOG / +1.0000000E-002  
 +1.0000000E+007 -3.3000000E-001 -1.7896000E+004 /  
 PLOG / +1.0000000E-001  
 +1.1500000E+011 -1.1600000E+000 -1.4831000E+004 /  
 PLOG / +1.0000000E+000  
 +2.9500000E+016 -2.3300000E+000 -9.4510000E+003 /  
 PLOG / +2.0000000E+000  
 +7.6800000E+017 -2.6200000E+000 -7.7050000E+003 /  
 PLOG / +5.0000000E+000  
 +2.2100000E+019 -2.8900000E+000 -5.5560000E+003 /  
 PLOG / +1.0000000E+001  
 +1.1400000E+020 -2.9900000E+000 -4.1590000E+003 /  
 PLOG / +3.0000000E+001  
 +2.8000000E+020 -2.9600000E+000 -2.5030000E+003 /  
 PLOG / +5.0000000E+001  
 +2.4000000E+020 -2.8800000E+000 -1.9710000E+003 /  
 C4H71-3+HO2<=>C4H7O2-1+OH  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS \*3  
 PLOG / +1.0000000E-002  
 +6.8100000E+020 -2.6800000E+000 +2.1700000E+002 /  
 PLOG / +1.0000000E-001  
 +2.2500000E+022 -3.1000000E+000 +1.5160000E+003 /  
 PLOG / +1.0000000E+000  
 +2.7500000E+027 -4.4900000E+000 +6.0670000E+003 /  
 PLOG / +2.0000000E+000  
 +6.2700000E+029 -5.1400000E+000 +8.2730000E+003 /  
 PLOG / +5.0000000E+000  
 +1.9600000E+033 -6.0900000E+000 +1.1661000E+004 /  
 PLOG / +1.0000000E+001  
 +1.1600000E+036 -6.8500000E+000 +1.4456000E+004 /  
 PLOG / +3.0000000E+001  
 +2.5100000E+040 -8.0400000E+000 +1.9009000E+004 /  
 PLOG / +5.0000000E+001  
 +2.1800000E+042 -8.5800000E+000 +2.1090000E+004 /

C4H71-3+HO2<=>SC3H5CHO+H2O

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS

PLOG / +1.0000000E-002  
+1.6200000E+014 -1.6000000E+000 +1.5190000E+003 /  
PLOG / +1.0000000E-001  
+3.1900000E+015 -1.9600000E+000 +2.6200000E+003 /  
PLOG / +1.0000000E+000  
+1.6900000E+020 -3.2600000E+000 +6.8000000E+003 /  
PLOG / +2.0000000E+000  
+3.3900000E+022 -3.8900000E+000 +8.9180000E+003 /  
PLOG / +5.0000000E+000  
+1.0900000E+026 -4.8500000E+000 +1.2249000E+004 /  
PLOG / +1.0000000E+001  
+7.8100000E+028 -5.6300000E+000 +1.5058000E+004 /  
PLOG / +3.0000000E+001  
+3.1400000E+033 -6.8900000E+000 +1.9743000E+004 /  
PLOG / +5.0000000E+001  
+4.0700000E+035 -7.4800000E+000 +2.1927000E+004 /

C4H72-1OOH<=>C4H7O2-1+OH

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS

PLOG / +1.0000000E-002  
+5.0700000E+035 -7.3900000E+000 +3.9733000E+004 /  
PLOG / +1.0000000E-001  
+7.6900000E+037 -7.6300000E+000 +4.3994000E+004 /  
PLOG / +1.0000000E+000  
+2.7600000E+037 -7.1400000E+000 +4.7024000E+004 /  
PLOG / +2.0000000E+000  
+4.3200000E+036 -6.8100000E+000 +4.7507000E+004 /  
PLOG / +5.0000000E+000  
+1.2100000E+035 -6.2400000E+000 +4.7760000E+004 /  
PLOG / +1.0000000E+001  
+3.9200000E+033 -5.7400000E+000 +4.7658000E+004 /  
PLOG / +3.0000000E+001  
+8.6200000E+030 -4.8800000E+000 +4.7084000E+004 /  
PLOG / +5.0000000E+001  
+5.2900000E+029 -4.5000000E+000 +4.6721000E+004 /

C4H72-1OOH<=>SC3H5CHO+H2O

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
3325? 3346 !\COMMENT: !QRRK ANALYSIS BY CHEMDIS

PLOG / +1.0000000E-002  
+1.1500000E+024 -4.7800000E+000 +3.8584000E+004 /  
PLOG / +1.0000000E-001  
+9.6500000E+027 -5.5100000E+000 +4.3561000E+004 /  
PLOG / +1.0000000E+000  
+2.3300000E+029 -5.5300000E+000 +4.7626000E+004 /  
PLOG / +2.0000000E+000  
+1.2900000E+029 -5.3500000E+000 +4.8469000E+004 /  
PLOG / +5.0000000E+000  
+1.8100000E+028 -4.9800000E+000 +4.9208000E+004 /  
PLOG / +1.0000000E+001  
+1.7600000E+027 -4.6100000E+000 +4.9458000E+004 /  
PLOG / +3.0000000E+001  
+1.5900000E+025 -3.9100000E+000 +4.9357000E+004 /



PLOG / +5.0000000E+001  
 +1.5800000E+024 -3.5800000E+000 +4.9164000E+004 /  
 C4H7O2-1<=>C3H5-S+CH2O  
 +8.5200000E+025 -3.6100000E+000 +2.7863400E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C4H7O2-1<=>SC3H5OCH2-1  
 +1.3500000E+018 -1.7300000E+000 +1.7386500E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C4H7O2-1<=>C3H6CHO-2  
 +1.6700000E+021 -2.7400000E+000 +2.0337700E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C4H7O2-1<=>SC3H5CHO+H  
 +2.5700000E+020 -2.0600000E+000 +2.2040100E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C4H7O2-1<=>C3H6+HCO  
 +4.7500000E+008 +1.1400000E+000 +2.0922500E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 SC3H5OCH2-1<=>C3H5-S+CH2O  
 +8.8100000E+014 -3.2600000E-001 +3.1553100E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 SC3H5OCH2-1<=>C3H6CHO-2  
 +2.5100000E+020 -2.6300000E+000 +2.9288400E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 SC3H5OCH2-1<=>SC3H5CHO+H  
 +3.9800000E+018 -1.6200000E+000 +3.0129800E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 SC3H5OCH2-1<=>C3H6+HCO  
 +3.7300000E+014 -7.2600000E-001 +3.2008300E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C3H6CHO-2<=>C3H5-S+CH2O  
 +1.9300000E+019 -1.9400000E+000 +4.8440000E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C3H6CHO-2<=>SC3H5CHO+H  
 +4.5200000E+012 +2.1400000E-001 +3.4570500E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C3H6CHO-2<=>C3H6+HCO  
 +1.5900000E+013 +6.3000000E-002 +2.4086300E+004 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 C3H5-S+CH2O<=>C3H6+HCO  
 +1.6500000E+001 +3.1700000E+000 +9.3998000E+003 !\AUTHOR: !\REF:  
 KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP  
 3325? 3346 !\COMMENT:  
 !

---

!\REACTIONCLASS: \RA\_RO2\_PRODUCTS

\A

\N

\EA

!

---

C4H71-3+CH3O2<=>C4H71-3OOCH3

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

ANALOGY WITH C4H71-3+HO2 /2

PLOG / +1.0000000E-002

+1.0300000E+001 +1.2400000E+000 -2.2589000E+004 /

PLOG / +1.0000000E-001

+1.8500000E+006 +8.0000000E-002 -1.8331000E+004 /

PLOG / +1.0000000E+000

+1.0100000E+013 -1.4500000E+000 -1.1709000E+004 /

PLOG / +2.0000000E+000

+7.4500000E+014 -1.8700000E+000 -9.6040000E+003 /

PLOG / +5.0000000E+000

+9.2500000E+016 -2.3100000E+000 -6.9910000E+003 /

PLOG / +1.0000000E+001

+1.4400000E+018 -2.5500000E+000 -5.2600000E+003 /

PLOG / +3.0000000E+001

+1.7300000E+019 -2.7100000E+000 -3.1400000E+003 /

PLOG / +5.0000000E+001

+2.6700000E+019 -2.7000000E+000 -2.4380000E+003 /

C4H71-3+CH3O2<=>C4H71-O+CH3O

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

ANALOGY WITH C4H71-3+HO2 /2

PLOG / +1.0000000E-002

+3.4500000E+020 -2.6800000E+000 +2.2900000E+002 /

PLOG / +1.0000000E-001

+2.2500000E+022 -3.1800000E+000 +1.7600000E+003 /

PLOG / +1.0000000E+000

+4.3100000E+027 -4.6300000E+000 +6.4150000E+003 /

PLOG / +2.0000000E+000

+9.6000000E+029 -5.2800000E+000 +8.5780000E+003 /

PLOG / +5.0000000E+000

+2.7300000E+033 -6.2200000E+000 +1.1879000E+004 /

PLOG / +1.0000000E+001

+1.4900000E+036 -6.9700000E+000 +1.4600000E+004 /

PLOG / +3.0000000E+001

+2.7900000E+040 -8.1400000E+000 +1.9040000E+004 /

PLOG / +5.0000000E+001

+2.2200000E+042 -8.6700000E+000 +2.1071000E+004 /

C4H71-3OOCH3<=>C4H71-O+CH3O

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

ANALOGY WITH C4H71-3+HO2 /2

PLOG / +1.0000000E-002

+2.2100000E+035 -7.3700000E+000 +3.9745000E+004 /

PLOG / +1.0000000E-001

+3.3200000E+037 -7.6000000E+000 +4.4224000E+004 /

PLOG / +1.0000000E+000

+3.5500000E+037 -7.2400000E+000 +4.7692000E+004 /

PLOG / +2.0000000E+000

+9.6000000E+036 -6.9700000E+000 +4.8350000E+004 /

PLOG / +5.0000000E+000

+6.0000000E+035 -6.5100000E+000 +4.8849000E+004 /

PLOG / +1.0000000E+001

+3.5900000E+034 -6.0800000E+000 +4.8933000E+004 /

PLOG / +3.0000000E+001

+1.8500000E+032 -5.3200000E+000 +4.8614000E+004 /

PLOG / +5.0000000E+001  
 +1.5200000E+031 -4.9700000E+000 +4.8341000E+004 /  
 C4H71-3+CH3O2<=>C4H72-1OCH3  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 ANALOGY WITH C4H71-3+HO2 /2  
 PLOG / +1.0000000E-002  
 +5.0000000E+006 -3.3000000E-001 -1.7896000E+004 /  
 PLOG / +1.0000000E-001  
 +5.7500000E+010 -1.1600000E+000 -1.4831000E+004 /  
 PLOG / +1.0000000E+000  
 +1.4800000E+016 -2.3300000E+000 -9.4510000E+003 /  
 PLOG / +2.0000000E+000  
 +3.8400000E+017 -2.6200000E+000 -7.7050000E+003 /  
 PLOG / +5.0000000E+000  
 +1.1100000E+019 -2.8900000E+000 -5.5560000E+003 /  
 PLOG / +1.0000000E+001  
 +5.7000000E+019 -2.9900000E+000 -4.1590000E+003 /  
 PLOG / +3.0000000E+001  
 +1.4000000E+020 -2.9600000E+000 -2.5030000E+003 /  
 PLOG / +5.0000000E+001  
 +1.2000000E+020 -2.8800000E+000 -1.9710000E+003 /  
 C4H71-3+CH3O2<=>C4H7O2-1+CH3O  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 ANALOGY WITH C4H71-3+HO2 /2  
 PLOG / +1.0000000E-002  
 +3.4100000E+020 -2.6800000E+000 +2.1700000E+002 /  
 PLOG / +1.0000000E-001  
 +1.1300000E+022 -3.1000000E+000 +1.5160000E+003 /  
 PLOG / +1.0000000E+000  
 +1.3800000E+027 -4.4900000E+000 +6.0670000E+003 /  
 PLOG / +2.0000000E+000  
 +3.1400000E+029 -5.1400000E+000 +8.2730000E+003 /  
 PLOG / +5.0000000E+000  
 +9.8000000E+032 -6.0900000E+000 +1.1661000E+004 /  
 PLOG / +1.0000000E+001  
 +5.8000000E+035 -6.8500000E+000 +1.4456000E+004 /  
 PLOG / +3.0000000E+001  
 +1.2600000E+040 -8.0400000E+000 +1.9009000E+004 /  
 PLOG / +5.0000000E+001  
 +1.0900000E+042 -8.5800000E+000 +2.1090000E+004 /  
 C4H72-1OCH3<=>C4H7O2-1+CH3O  
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
 ANALOGY WITH C4H71-3+HO2 /2  
 PLOG / +1.0000000E-002  
 +2.5400000E+035 -7.3900000E+000 +3.9733000E+004 /  
 PLOG / +1.0000000E-001  
 +3.8500000E+037 -7.6300000E+000 +4.3994000E+004 /  
 PLOG / +1.0000000E+000  
 +1.3800000E+037 -7.1400000E+000 +4.7024000E+004 /  
 PLOG / +2.0000000E+000  
 +2.1600000E+036 -6.8100000E+000 +4.7507000E+004 /  
 PLOG / +5.0000000E+000  
 +6.0500000E+034 -6.2400000E+000 +4.7760000E+004 /  
 PLOG / +1.0000000E+001  
 +1.9600000E+033 -5.7400000E+000 +4.7658000E+004 /  
 PLOG / +3.0000000E+001  
 +4.3100000E+030 -4.8800000E+000 +4.7084000E+004 /

PLOG / +5.0000000E+001  
+2.6500000E+029 -4.5000000E+000 +4.6721000E+004 /  
C4H71-3+C2H5O2<=>C4H71-O+C2H5O  
+3.8000000E+012 +0.0000000E+000 -1.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3O2+CH3  
IC3H7O2+C4H71-3<=>IC3H7O+C4H71-O  
+3.8000000E+012 +0.0000000E+000 -1.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3O2+CH3  
NC3H7O2+C4H71-3<=>NC3H7O+C4H71-O  
+3.8000000E+012 +0.0000000E+000 -1.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3O2+CH3  
C4H71-O<=>C2H3CHO+CH3  
+7.9400000E+014 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:ANALOGY  
TO BATT'S RATE FOR S-BUTOXY DECOMPOSITION  
C4H71-3+O<=>C2H3CHO+CH3  
+6.0300000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:IN  
ARAMCO (ESTIMATE)  
!

---

!\REACTIONCLASS: \RA\_R\_ABSTRACTION \A  
\N \EA  
!

---

C4H71-3+O2<=>C4H6+HO2  
+1.0700000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF: J. D.  
DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM.  
A, 107, 2003, 4415-4427 !\COMMENT:!\*2  
H+C4H71-3<=>C4H6+H2  
+3.1600000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALLARA,  
D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)  
C2H5+C4H71-3<=>C4H6+C2H6  
+3.9800000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:EDELSON  
AND ALLARA, 1980  
C2H3+C4H71-3<=>C2H4+C4H6  
+3.9800000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:EDELSON  
AND ALLARA, 1980  
C3H5-A+C4H71-3<=>C3H6+C4H6  
+6.3100000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:EDELSON  
AND ALLARA, 1980  
!

---

!\REACTIONCLASS: \RA\_RA\_RECOMBINATION \A  
\N \EA  
!

---

C4H71-3+C4H71-3<=>C8H141-5,3-4  
+4.1100000E+016 -1.2600000E+000 +1.5606200E+003 !\AUTHOR: !\REF:  
FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776  
C4H71-3+C4H71-3<=>C8H141-5,3  
+4.1100000E+016 -1.2600000E+000 +1.5606200E+003 !\AUTHOR: !\REF:  
FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776  
C4H71-3+C4H71-3<=>C8H142-6  
+4.1100000E+016 -1.2600000E+000 +1.5606200E+003 !\AUTHOR: !\REF:  
FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776  
C8H141-5,3-4+OH<=>C8H131-5,3-4,TA+H2O  
+2.5000000E+006 +2.0000000E+000 -2.6290600E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES

C8H141-5,3+OH<=>C8H131-5,3,TA+H2O  
+1.3000000E+006 +2.0000000E+000 -2.6290600E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+OH<=>C8H131-5,3,SA+H2O  
+3.2000000E+006 +2.0000000E+000 -1.4340300E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+OH<=>C8H131-5,3,PA+H2O  
+3.0000000E+006 +2.0000000E+000 -2.3901000E+002 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+OH<=>C8H132-6,SA+H2O  
+6.3000000E+006 +2.0000000E+000 -1.4340300E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+OH<=>C8H132-6,PA+H2O  
+6.0000000E+006 +2.0000000E+000 -2.3901000E+002 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3-4+HO2<=>C8H131-5,3-4,TA+H2O2  
+3.2000000E+004 +2.6000000E+000 +1.0755260E+004 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+HO2<=>C8H131-5,3,TA+H2O2  
+1.6000000E+004 +2.6000000E+000 +1.0755260E+004 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+HO2<=>C8H131-5,3,SA+H2O2  
+6.3000000E+003 +2.6000000E+000 +1.2428300E+004 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+HO2<=>C8H131-5,3,PA+H2O2  
+9.5000000E+003 +2.6000000E+000 +1.3862330E+004 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+HO2<=>C8H132-6,SA+H2O2  
+1.3000000E+004 +2.6000000E+000 +1.2428300E+004 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+HO2<=>C8H132-6,PA+H2O2  
+1.9000000E+004 +2.6000000E+000 +1.3862330E+004 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3-4+H<=>C8H131-5,3-4,TA+H2  
+5.0000000E+004 +2.5000000E+000 -2.8680700E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+H<=>C8H131-5,3,TA+H2  
+2.5000000E+004 +2.5000000E+000 -2.8680700E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+H<=>C8H131-5,3,SA+H2  
+5.0000000E+004 +2.5000000E+000 -1.6730400E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+H<=>C8H131-5,3,PA+H2  
+1.9000000E+005 +2.5000000E+000 +2.3900600E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+H<=>C8H132-6,SA+H2  
+1.0000000E+005 +2.5000000E+000 -1.6730400E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+H<=>C8H132-6,PA+H2  
+3.8000000E+005 +2.5000000E+000 +2.3900600E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3-4+O<=>C8H131-5,3-4,TA+OH  
+6.3000000E+010 +7.0000000E-001 +1.1950300E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+O<=>C8H131-5,3,TA+OH  
+3.2000000E+010 +7.0000000E-001 +1.1950300E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES

C8H141-5,3+O<=>C8H131-5,3,SA+OH  
+8.0000000E+010 +7.0000000E-001 +3.1070700E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+O<=>C8H131-5,3,PA+OH  
+6.3000000E+010 +7.0000000E-001 +5.9751400E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+O<=>C8H132-6,SA+OH  
+1.6000000E+011 +7.0000000E-001 +3.1070700E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+O<=>C8H132-6,PA+OH  
+1.3000000E+011 +7.0000000E-001 +5.9751400E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3-4+CH3<=>C8H131-5,3-4,TA+CH4  
+1.6000000E+012 +0.0000000E+000 +5.2581300E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+CH3<=>C8H131-5,3,TA+CH4  
+7.9000000E+011 +0.0000000E+000 +5.2581300E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+CH3<=>C8H131-5,3,SA+CH4  
+1.6000000E+012 +0.0000000E+000 +6.9311700E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H141-5,3+CH3<=>C8H131-5,3,PA+CH4 +1.5000000E-  
001 +3.5000000E+000 +5.7361400E+003 !\AUTHOR: !\REF: HENRY'S SLIDES  
C8H142-6+CH3<=>C8H132-6,SA+CH4  
+3.2000000E+012 +0.0000000E+000 +6.9311700E+003 !\AUTHOR: !\REF:  
HENRY'S SLIDES  
C8H142-6+CH3<=>C8H132-6,PA+CH4 +3.0000000E-  
001 +3.5000000E+000 +5.7361400E+003 !\AUTHOR: !\REF: HENRY'S SLIDES  
C8H141-5,3-4+O2<=>C8H131-5,3-4,TA+HO2  
+1.6000000E+013 +0.0000000E+000 +3.5420000E+004 !\AUTHOR: !\REF: C4H8-  
1, C4H8-2 AND LLNL ANALOGY !\COMMENT: !ESTIMATED BY THE AVERAGE  
DIFFERENCE BETWEEN PRIMARY&SECONDARY ALKANE ABSTRACTION  
C8H141-5,3+O2<=>C8H131-5,3,TA+HO2  
+8.0000000E+012 +0.0000000E+000 +3.5420000E+004 !\AUTHOR: !\REF: C4H8-  
1, C4H8-2 AND LLNL ANALOGY !\COMMENT: !ESTIMATED BY THE AVERAGE  
DIFFERENCE BETWEEN PRIMARY&SECONDARY ALKANE ABSTRACTION  
C8H141-5,3+O2<=>C8H131-5,3,SA+HO2  
+2.0000000E+013 +0.0000000E+000 +3.7190000E+004 !\AUTHOR: !\REF: C4H8-  
1, C4H8-2 AND LLNL ANALOGY  
C8H141-5,3+O2<=>C8H131-5,3,PA+HO2  
+2.0000000E+013 +0.0000000E+000 +3.9390000E+004 !\AUTHOR: !\REF: C4H8-  
1, C4H8-2 AND LLNL ANALOGY  
C8H142-6+O2<=>C8H132-6,SA+HO2  
+4.0000000E+013 +0.0000000E+000 +3.7190000E+004 !\AUTHOR: !\REF: C4H8-  
1, C4H8-2 AND LLNL ANALOGY  
C8H142-6+O2<=>C8H132-6,PA+HO2  
+4.0000000E+013 +0.0000000E+000 +3.9390000E+004 !\AUTHOR: !\REF: C4H8-  
1, C4H8-2 AND LLNL ANALOGY  
C6H101-3,3+C2H3<=>C8H131-5,3-4,TA  
+4.4000000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN INC. INT J CHEM KINET 38: 250°C275, 2006  
B13DE2M+C3H5-S<=>C8H131-5,3,TA  
+4.4000000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN INC. INT J CHEM KINET 38: 250°C275, 2006  
C6H10D24+C2H3<=>C8H131-5,3,SA  
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN INC. INT J CHEM KINET 38: 250°C275, 2006

C4H6+C4H71-3<=>C8H131-5,3,PA  
+1.3000000E+003 +2.4800000E+000 +8.5200000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN INC. INT J CHEM KINET 38: 250`C275, 2006  
C5H81-3+C3H5-S<=>C8H132-6,SA  
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN INC. INT J CHEM KINET 38: 250`C275, 2006  
C4H6+C4H71-3<=>C8H132-6,PA  
+1.3000000E+003 +2.4800000E+000 +8.5200000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN INC. INT J CHEM KINET 38: 250`C275, 2006  
C6H101-3,3<=>C2H3+C4H72-2  
+2.5000000E+015 +0.0000000E+000 +9.9500000E+004 !\AUTHOR: !\REF:  
ANALOGY TO KUIWEN'S MECH  
C6H10D24<=>C3H5-S+C3H5-S  
+2.5000000E+015 +0.0000000E+000 +9.9500000E+004 !\AUTHOR: !\REF:  
ANALOGY TO KUIWEN'S MECH  
C8H131-5,3-4,TA+HO2<=>C8H131-5,3-4,TAO+OH  
+1.6400000E+004 +2.7400000E+000 +1.1443800E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH J. PHYS. CHEM. A 2012, 116, 3325.3346  
#ALLYL+HO2=ALLYLOXY+OH#  
C8H131-5,3,TA+HO2<=>C8H131-5,3,TAO+OH  
+1.6400000E+004 +2.7400000E+000 +1.1443800E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH J. PHYS. CHEM. A 2012, 116, 3325.3346  
#ALLYL+HO2=ALLYLOXY+OH#  
C8H131-5,3,SA+HO2<=>C8H131-5,3,SAO+OH  
+1.6400000E+004 +2.7400000E+000 +1.1443800E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH J. PHYS. CHEM. A 2012, 116, 3325.3346  
#ALLYL+HO2=ALLYLOXY+OH#  
C8H131-5,3,PA+HO2<=>C8H131-5,3,PAO+OH  
+1.6400000E+004 +2.7400000E+000 +1.1443800E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH J. PHYS. CHEM. A 2012, 116, 3325.3346  
#ALLYL+HO2=ALLYLOXY+OH#  
C8H132-6,SA+HO2<=>C8H132-6,SAO+OH  
+1.6400000E+004 +2.7400000E+000 +1.1443800E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH J. PHYS. CHEM. A 2012, 116, 3325.3346  
#ALLYL+HO2=ALLYLOXY+OH#  
C8H132-6,PA+HO2<=>C8H132-6,PAO+OH  
+1.6400000E+004 +2.7400000E+000 +1.1443800E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH J. PHYS. CHEM. A 2012, 116, 3325.3346  
#ALLYL+HO2=ALLYLOXY+OH#  
C4H71-3+C2H3COCH3<=>C8H131-5,3-4,TAO  
+2.5000000E+010 +0.0000000E+000 +1.0090000E+004 !\AUTHOR: !\REF: H. J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
C4H71-3+C2H3COCH3<=>C8H131-5,3,TAO  
+2.5000000E+010 +0.0000000E+000 +1.0090000E+004 !\AUTHOR: !\REF: H. J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
C4H71-3+SC3H5CHO<=>C8H131-5,3,SAO  
+3.3300000E+010 +0.0000000E+000 +6.3970000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
C7H111-5,3,6P+CH2O<=>C8H131-5,3,PAO  
+1.0000000E+011 +0.0000000E+000 +3.4960000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
C4H71-3+SC3H5CHO<=>C8H132-6,SAO  
+3.3300000E+010 +0.0000000E+000 +6.3970000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
C7H111-5,1P+CH2O<=>C8H132-6,PAO  
+1.0000000E+011 +0.0000000E+000 +3.4960000E+003 !\AUTHOR: !\REF: H. J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.

CC5H9-A+C2H2<=>C7H111-5,3,6P  
+1.3200000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF: H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
C5H92-5+C2H2<=>C7H111-5,1P  
+1.3200000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF: H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275.  
!

---

!\REACTIONCLASS: \RP\_O2 \A  
\N \EA  
!

---

---

C4H71-4+O2<=>C4H6+HO2  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: !JET  
SURF 2.0, ADD 2505 KWZ  
C4H71-4+O2<=>C4H71-4O2  
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4+HO2<=>C4H7O1-4+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
CH3O2+C4H71-4<=>CH3O+C4H7O1-4  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+H2<=>C4H71-4OOH+H  
+3.0100000E+013 +0.0000000E+000 +2.6030000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+HO2<=>C4H71-4OOH+O2  
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+H2O2<=>C4H71-4OOH+HO2  
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+CH4<=>C4H71-4OOH+CH3  
+1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+CH3OH<=>C4H71-4OOH+CH2OH  
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+CH2O<=>C4H71-4OOH+HCO  
+5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+C2H6<=>C4H71-4OOH+C2H5  
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+CH3CHO<=>C4H71-4OOH+CH3CO  
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+C2H4<=>C4H71-4OOH+C2H3  
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
C4H71-4O2+C3H6<=>C4H71-4OOH+C3H5-A +5.3500000E-  
002 +4.2070000E+000 +1.3288100E+004 !\AUTHOR: !\REF: !\COMMENT:  
C4H71-4O2+C2H5CHO<=>C4H71-4OOH+C2H5CO  
+2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:



$C_4H_7-4O_2+C_2H_3CHO \rightleftharpoons C_4H_7-4OOH+C_2H_3CO$   
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_3H_8 \rightleftharpoons C_4H_7-4OOH+NC_3H_7$   
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_3H_8 \rightleftharpoons C_4H_7-4OOH+IC_3H_7$   
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+CH_3 \rightleftharpoons C_4H_7O_1-4+CH_3O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_2H_5 \rightleftharpoons C_4H_7O_1-4+C_2H_5O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+IC_3H_7 \rightleftharpoons C_4H_7O_1-4+IC_3H_7O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+NC_3H_7 \rightleftharpoons C_4H_7O_1-4+NC_3H_7O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_3H_5-A \rightleftharpoons C_4H_7O_1-4+C_3H_5O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+PC_4H_9 \rightleftharpoons C_4H_7O_1-4+PC_4H_9O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+SC_4H_9 \rightleftharpoons C_4H_7O_1-4+SC_4H_9O$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_4H_7-3 \rightleftharpoons C_4H_7O_1-4+C_4H_7-0$   
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4OOH \rightleftharpoons C_4H_7O_1-4+OH$   
+1.5000000E+016 +0.0000000E+000 +4.2500000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+CH_3O_2 \rightleftharpoons C_4H_7O_1-4+CH_3O+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+CH_3CO_3 \rightleftharpoons C_4H_7O_1-4+CH_3CO_2+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_2H_5O_2 \rightleftharpoons C_4H_7O_1-4+C_2H_5O+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+NC_3H_7O_2 \rightleftharpoons C_4H_7O_1-4+NC_3H_7O+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+IC_3H_7O_2 \rightleftharpoons C_4H_7O_1-4+IC_3H_7O+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+C_4H_7-4O_2 \rightleftharpoons C_4H_7O_1-4+C_4H_7O_1-4+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2+SC_4H_9O_2 \rightleftharpoons C_4H_7O_1-4+SC_4H_9O+O_2$   
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_7-4O_2 \rightleftharpoons C_4H_6-3OH_4$   
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6-3OH_4 \rightleftharpoons C_2H_3CHOCH_2+OH$   
+1.7100000E+009 +1.0600000E+000 +1.0900000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6-3OH_4 \rightleftharpoons C_4H_6O_2_5+OH$   
+1.7200000E+008 +7.6000000E-001 +1.1100000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_2H_3CHOCH_2+H \Rightarrow C_2H_3+CH_2CO+H_2$   
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:

$C_2H_3CHOCH_2+O \Rightarrow C_2H_3+CH_2CO+OH$   
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:

$C_2H_3CHOCH_2+OH \Rightarrow C_2H_3+CH_2CO+H_2O$   
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:

$C_2H_3CHOCH_2+HO_2 \Rightarrow C_2H_3+CH_2CO+H_2O_2$   
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_2H_3CHOCH_2+CH_3 \Rightarrow C_2H_3+CH_2CO+CH_4$   
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_2H_3CHOCH_2+CH_3O_2 \Rightarrow C_2H_3+CH_2CO+CH_3O_2H$   
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6O_2_5+H \rightleftharpoons CH_2CHCHCHO+H_2$   
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6O_2_5+O \rightleftharpoons CH_2CHCHCHO+OH$   
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6O_2_5+OH \rightleftharpoons CH_2CHCHCHO+H_2O$   
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6O_2_5+HO_2 \rightleftharpoons CH_2CHCHCHO+H_2O_2$   
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6O_2_5+CH_3 \rightleftharpoons CH_2CHCHCHO+CH_4$   
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6O_2_5+CH_3O_2 \rightleftharpoons CH_2CHCHCHO+CH_3O_2H$   
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:  
!\COMMENT:

$C_4H_6-3OH_4+HO_2 \rightleftharpoons C_4H_6O_1-3OH_4+OH$   
+4.1000000E+003 +2.7400000E+000 +1.1444000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C4H7-3+HO2 ADDITION, FOLLOWED BY WDM

$C_4H_6-3OH_4+HO_2 \rightleftharpoons C_4H_6O_2-1OH_4+OH$   
+4.1000000E+003 +2.7400000E+000 +1.1444000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C4H7-3+HO2 ADDITION, FOLLOWED BY WDM

$C_4H_6O_1-3OH_4 \rightleftharpoons C_2H_3CHO+CH_2O+OH$   
+6.7000000E+039 -8.3800000E+000 +2.2782000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C4H7-3+HO2 ADDITION, FOLLOWED BY WDM

$C_4H_6O_1-3OH_4 \rightleftharpoons C_2H_3+HO_2CH_2CHO$   
+2.6700000E+034 -6.6300000E+000 +2.2672000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C4H7-3+HO2 ADDITION, FOLLOWED BY WDM

!  
-----  
!\REACTIONCLASS: \RSP\_O2 \A  
\N \EA  
!

-----  
C4H71-1+O2<=>C4H71-1O2  
+4.0700000E+027 -4.6700000E+000 +5.2220000E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
C4H71-1O2<=>C3H6CHO-3+O  
+1.2200000E+029 -4.7100000E+000 +4.2340000E+004 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
C4H71-1O2<=>C2H5CHCO+OH  
+1.5500000E+024 -3.8700000E+000 +4.9850000E+004 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
!16\_03 !C2H3CHO+CH3<=>C4H7O1-1 7.26E+03 2.43 8960 !FROM PRAJAKTA PARAB'S  
CALCULATION FOR CH2CO+CH3<=>CH3COCH2  
!

-----  
!\REACTIONCLASS: \RSV\_O2 \A  
\N \EA  
!

-----  
C4H71-2+O2<=>C4H71-2O2  
+4.0700000E+027 -4.6700000E+000 +5.2220000E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
C4H71-2O2<=>C2H5COCH2+O  
+1.2200000E+029 -4.7100000E+000 +4.2340000E+004 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
!16\_03 !CH2CO+C2H5<=>C4H7O1-2 7.26E+03 2.43 8960 !FROM PRAJAKTA PARAB'S  
CALCULATION FOR CH2CO+CH3<=>CH3COCH2  
C4H72-2+O2<=>C4H72-2O2  
+4.0700000E+027 -4.6700000E+000 +5.2220000E+003 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
C4H72-2O2<=>CH3CHCOCH3+O  
+1.2200000E+029 -4.7100000E+000 +4.2340000E+004 !\AUTHOR: !\REF:C.  
FRANKLIN GOLDSMITH C2H3+O2 J. PHYS. CHEM. A  
!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  
!

-----  
!\*\*\*\*\*H  
ADDITION\*\*\*\*\*!  
C4H8-1+H<=>C2H4+C2H5  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+2.5500000E+006 +1.9300000E+000 +5.5640000E+003 /  
PLOG / +1.0000000E-002  
+5.5600000E+006 +1.8300000E+000 +5.8020000E+003 /  
PLOG / +1.0000000E-001  
+1.2100000E+009 +1.1800000E+000 +7.4720000E+003 /  
PLOG / +1.0000000E+000  
+9.4700000E+016 -1.0300000E+000 +1.3413000E+004 /

```

PLOG / +1.0000000E+001
+4.5000000E+028 -4.2400000E+000 +2.3618000E+004 /
PLOG / +1.0000000E+002
+7.0200000E+032 -5.2200000E+000 +3.1754000E+004 /
DUP
C4H8-1+H<=>C2H4+C2H5
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+3.4500000E+007 +1.8100000E+000 +2.2630000E+003 /
PLOG / +1.0000000E-002
+8.0600000E+007 +1.7100000E+000 +2.5220000E+003 /
PLOG / +1.0000000E-001
+1.1800000E+010 +1.1000000E+000 +4.0770000E+003 /
PLOG / +1.0000000E+000
+6.0200000E+015 -4.9000000E-001 +8.4520000E+003 /
PLOG / +1.0000000E+001
+7.5800000E+021 -2.1400000E+000 +1.4245000E+004 /
PLOG / +1.0000000E+002
+2.2900000E+021 -1.8700000E+000 +1.7243000E+004 /
DUP
C4H8-1+H<=>C3H6+CH3
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+7.8300000E+009 +1.1700000E+000 +1.4420000E+003 /
PLOG / +1.0000000E-002
+3.3900000E+010 +1.0000000E+000 +1.8950000E+003 /
PLOG / +1.0000000E-001
+3.7000000E+013 +1.4000000E-001 +4.1270000E+003 /
PLOG / +1.0000000E+000
+4.5700000E+019 -1.5400000E+000 +9.0610000E+003 /
PLOG / +1.0000000E+001
+8.5700000E+023 -2.6600000E+000 +1.4140000E+004 /
PLOG / +1.0000000E+002
+1.3200000E+020 -1.4600000E+000 +1.5383000E+004 /
DUP
C4H8-1+H<=>C3H6+CH3
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+1.8000000E+006 +1.7600000E+000 +5.9000000E+003 /
PLOG / +1.0000000E-002
+3.4600000E+006 +1.6800000E+000 +6.1000000E+003 /
PLOG / +1.0000000E-001
+4.0200000E+008 +1.1000000E+000 +7.5740000E+003 /
PLOG / +1.0000000E+000
+1.2100000E+016 -9.9000000E-001 +1.3175000E+004 /
PLOG / +1.0000000E+001
+7.1400000E+027 -4.2300000E+000 +2.3319000E+004 /
PLOG / +1.0000000E+002
+1.0000000E+033 -5.4900000E+000 +3.1922000E+004 /
DUP
C4H8-1+H<=>PC4H9
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+1.3500000E+015 -2.8100000E+000 +1.5700000E+003 /

```

PLOG / +1.0000000E-002  
+5.2000000E+016 -2.9700000E+000 +1.9920000E+003 /  
PLOG / +1.0000000E-001  
+1.9100000E+021 -3.9700000E+000 +4.6360000E+003 /  
PLOG / +1.0000000E+000  
+1.9000000E+031 -6.4600000E+000 +1.1968000E+004 /  
PLOG / +1.0000000E+001  
+2.1000000E+040 -8.6000000E+000 +2.1058000E+004 /  
PLOG / +1.0000000E+002  
+1.4400000E+037 -7.2100000E+000 +2.4896000E+004 /  
DUP  
C4H8-1+H<=>PC4H9  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+4.3300000E+020 -4.1600000E+000 -2.6300000E+002 /  
PLOG / +1.0000000E-002  
+1.7800000E+022 -4.3300000E+000 +1.8600000E+002 /  
PLOG / +1.0000000E-001  
+1.9800000E+026 -5.1800000E+000 +2.5180000E+003 /  
PLOG / +1.0000000E+000  
+3.7800000E+032 -6.6300000E+000 +7.2650000E+003 /  
PLOG / +1.0000000E+001  
+8.7900000E+034 -6.9100000E+000 +1.0952000E+004 /  
PLOG / +1.0000000E+002  
+7.8000000E+028 -4.7900000E+000 +1.0355000E+004 /  
DUP  
C4H8-1+H<=>SC4H9  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+4.0700000E+022 -4.5100000E+000 -7.7100000E+002 /  
PLOG / +1.0000000E-002  
+3.9000000E+024 -4.7800000E+000 -3.4000000E+001 /  
PLOG / +1.0000000E-001  
+2.0300000E+029 -5.8100000E+000 +2.9700000E+003 /  
PLOG / +1.0000000E+000  
+3.5300000E+034 -6.9500000E+000 +7.5250000E+003 /  
PLOG / +1.0000000E+001  
+1.1900000E+034 -6.4200000E+000 +9.8100000E+003 /  
PLOG / +1.0000000E+002  
+1.3700000E+026 -3.7900000E+000 +8.0120000E+003 /  
DUP  
C4H8-1+H<=>SC4H9  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+3.5200000E+012 -2.1500000E+000 +1.4660000E+003 /  
PLOG / +1.0000000E-002  
+1.0200000E+014 -2.2800000E+000 +1.7990000E+003 /  
PLOG / +1.0000000E-001  
+1.1600000E+018 -3.1300000E+000 +4.0490000E+003 /  
PLOG / +1.0000000E+000  
+5.2200000E+027 -5.5300000E+000 +1.0963000E+004 /  
PLOG / +1.0000000E+001  
+4.3300000E+037 -7.9200000E+000 +2.0354000E+004 /  
PLOG / +1.0000000E+002  
+2.2200000E+036 -7.0600000E+000 +2.5203000E+004 /

DUP

C4H8-2+H<=>C2H4+C2H5

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS

PLOG / +1.0000000E-003

+8.9600000E+006 +1.8600000E+000 +6.2090000E+003 /

PLOG / +1.0000000E-002

+1.9200000E+007 +1.7700000E+000 +6.4430000E+003 /

PLOG / +1.0000000E-001

+3.9700000E+009 +1.1100000E+000 +8.0970000E+003 /

PLOG / +1.0000000E+000

+3.0100000E+017 -1.0900000E+000 +1.4023000E+004 /

PLOG / +1.0000000E+001

+1.8800000E+029 -4.3300000E+000 +2.4297000E+004 /

PLOG / +1.0000000E+002

+5.1500000E+033 -5.3900000E+000 +3.2601000E+004 /

C4H8-2+H<=>C3H6+CH3

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS

PLOG / +1.0000000E-003

+6.3900000E+009 +1.2900000E+000 +1.8340000E+003 /

PLOG / +1.0000000E-002

+2.6000000E+010 +1.1200000E+000 +2.2670000E+003 /

PLOG / +1.0000000E-001

+2.4800000E+013 +2.9000000E-001 +4.4560000E+003 /

PLOG / +1.0000000E+000

+2.9100000E+019 -1.3900000E+000 +9.3650000E+003 /

PLOG / +1.0000000E+001

+6.1300000E+023 -2.5300000E+000 +1.4463000E+004 /

PLOG / +1.0000000E+002

+1.2300000E+020 -1.3500000E+000 +1.5762000E+004 /

C4H8-2+H<=>PC4H9

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS

PLOG / +1.0000000E-003

+3.9000000E+014 -2.5500000E+000 +1.7290000E+003 /

PLOG / +1.0000000E-002

+1.4100000E+016 -2.7100000E+000 +2.1330000E+003 /

PLOG / +1.0000000E-001

+4.3100000E+020 -3.6900000E+000 +4.7190000E+003 /

PLOG / +1.0000000E+000

+4.0300000E+030 -6.1700000E+000 +1.2020000E+004 /

PLOG / +1.0000000E+001

+5.1900000E+039 -8.3300000E+000 +2.1137000E+004 /

PLOG / +1.0000000E+002

+5.1700000E+036 -6.9800000E+000 +2.5063000E+004 /

C4H8-2+H<=>SC4H9

+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:

!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS

PLOG / +1.0000000E-003

+8.3400000E+021 -4.2100000E+000 -6.0200000E+002 /

PLOG / +1.0000000E-002

+6.7900000E+023 -4.4600000E+000 +8.2000000E+001 /

PLOG / +1.0000000E-001

+2.8500000E+028 -5.4700000E+000 +3.0030000E+003 /

PLOG / +1.0000000E+000

+5.4500000E+033 -6.6100000E+000 +7.5590000E+003 /

PLOG / +1.0000000E+001  
+2.3300000E+033 -6.1100000E+000 +9.8930000E+003 /  
PLOG / +1.0000000E+002  
+3.2700000E+025 -3.5100000E+000 +8.1450000E+003 /  
C4H8-1+H<=>C4H8-2+H  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+2.9800000E+007 +1.8600000E+000 +3.5750000E+003 /  
PLOG / +1.0000000E-002  
+6.1100000E+007 +1.7700000E+000 +3.7940000E+003 /  
PLOG / +1.0000000E-001  
+4.7800000E+009 +1.2400000E+000 +5.1520000E+003 /  
PLOG / +1.0000000E+000  
+1.0200000E+015 -2.5000000E-001 +9.2330000E+003 /  
PLOG / +1.0000000E+001  
+6.5100000E+020 -1.8200000E+000 +1.4806000E+004 /  
PLOG / +1.0000000E+002  
+4.4400000E+019 -1.3700000E+000 +1.7409000E+004 /  
DUP  
C4H8-1+H<=>C4H8-2+H  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+1.5500000E+004 +2.3200000E+000 +7.0490000E+003 /  
PLOG / +1.0000000E-002  
+2.3600000E+004 +2.2700000E+000 +7.1770000E+003 /  
PLOG / +1.0000000E-001  
+6.6000000E+005 +1.8600000E+000 +8.2010000E+003 /  
PLOG / +1.0000000E+000  
+1.1500000E+012 +1.1000000E-001 +1.2789000E+004 /  
PLOG / +1.0000000E+001  
+8.8000000E+023 -3.1700000E+000 +2.2546000E+004 /  
PLOG / +1.0000000E+002  
+3.7200000E+031 -5.1600000E+000 +3.2234000E+004 /  
DUP  
SC4H9<=>PC4H9  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+9.6000000E+037 -1.1040000E+001 +3.8840000E+004 /  
PLOG / +1.0000000E-002  
+6.0500000E+040 -1.1260000E+001 +3.9461000E+004 /  
PLOG / +1.0000000E-001  
+1.6400000E+047 -1.2490000E+001 +4.3112000E+004 /  
PLOG / +1.0000000E+000  
+6.5300000E+055 -1.4270000E+001 +5.0351000E+004 /  
PLOG / +1.0000000E+001  
+2.1300000E+056 -1.3710000E+001 +5.4866000E+004 /  
PLOG / +1.0000000E+002  
+6.0200000E+045 -1.0070000E+001 +5.3399000E+004 /  
PC4H9<=>C2H4+C2H5  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS  
PLOG / +1.0000000E-003  
+3.4400000E+034 -8.1000000E+000 +2.8397000E+004 /  
PLOG / +1.0000000E-002  
+1.1100000E+039 -9.0500000E+000 +3.1891000E+004 /

```

PLOG / +1.0000000E-001
+7.7400000E+042 -9.7800000E+000 +3.5771000E+004 /
PLOG / +1.0000000E+000
+7.4700000E+043 -9.6700000E+000 +3.8722000E+004 /
PLOG / +1.0000000E+001
+2.0600000E+039 -7.9700000E+000 +3.8955000E+004 /
PLOG / +1.0000000E+002
+1.4800000E+029 -4.7100000E+000 +3.5950000E+004 /
PC4H9<=>C3H6+CH3
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+3.7100000E+025 -5.8100000E+000 +3.4965000E+004 /
PLOG / +1.0000000E-002
+1.8500000E+027 -6.0100000E+000 +3.5481000E+004 /
PLOG / +1.0000000E-001
+2.4600000E+032 -7.1600000E+000 +3.8637000E+004 /
PLOG / +1.0000000E+000
+2.0500000E+042 -9.6100000E+000 +4.6415000E+004 /
PLOG / +1.0000000E+001
+4.9800000E+048 -1.0970000E+001 +5.4456000E+004 /
PLOG / +1.0000000E+002
+2.2300000E+042 -8.6800000E+000 +5.6601000E+004 /
SC4H9<=>C2H4+C2H5
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+8.3000000E+025 -5.7500000E+000 +3.9343000E+004 /
PLOG / +1.0000000E-002
+4.1200000E+027 -5.9400000E+000 +3.9859000E+004 /
PLOG / +1.0000000E-001
+5.5700000E+032 -7.1000000E+000 +4.3029000E+004 /
PLOG / +1.0000000E+000
+4.5400000E+042 -9.5400000E+000 +5.0839000E+004 /
PLOG / +1.0000000E+001
+1.0600000E+049 -1.0900000E+001 +5.8899000E+004 /
PLOG / +1.0000000E+002
+9.9400000E+042 -8.7000000E+000 +6.1203000E+004 /
SC4H9<=>C3H6+CH3
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:
!\COMMENT: QRRK/MSC ANALYSIS WITH CHEMDIS
PLOG / +1.0000000E-003
+2.8900000E+040 -9.7600000E+000 +3.3601000E+004 /
PLOG / +1.0000000E-002
+1.8000000E+044 -1.0500000E+001 +3.7007000E+004 /
PLOG / +1.0000000E-001
+2.5100000E+046 -1.0730000E+001 +4.0237000E+004 /
PLOG / +1.0000000E+000
+4.7400000E+044 -9.8500000E+000 +4.1841000E+004 /
PLOG / +1.0000000E+001
+3.7900000E+037 -7.4400000E+000 +4.0604000E+004 /
PLOG / +1.0000000E+002
+4.7900000E+026 -4.0100000E+000 +3.6898000E+004 /
!
```

---

```

!\REACTIONCLASS: \R_ADDITION\OH
\N \EA
```

```
\A
```



!

---

C4H71-1OH+H<=>PC4H8OH-1  
+4.2679497E+012 +4.9275069E-001 +4.4445766E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

NC3H7CHO+H<=>PC4H8OH-1  
+9.8000000E+010 +1.1920556E+000 +8.7855658E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C2H3OH+C2H5<=>PC4H8OH-1  
+3.0000000E+006 +1.8344228E+000 +7.3379231E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C4H8-1+OH<=>PC4H8OH-2  
+2.1000000E+006 +1.8058436E+000 -3.2923340E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526 !\COMMENT !\*2\*0.75

C4H71-1OH+H<=>PC4H8OH-2  
+1.6000000E+010 +1.1140330E+000 +4.3892377E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C4H72-1OH+H<=>PC4H8OH-2  
+2.7000000E+011 -1.3433162E-001 +1.5846588E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C3H6+CH2OH<=>PC4H8OH-3  
+7.0000000E+003 +2.4268073E+000 +7.0635143E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C4H71-4OH+H<=>PC4H8OH-3  
+1.5000000E+011 +8.8281162E-001 +2.7506294E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

SC4H8OH-1<=>PC4H8OH-3  
+2.9000000E+008 +1.3771432E+000 +3.7865971E+004 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C3H6+CH2OH<=>PC4H8OH-4  
+7.0000000E+003 +2.4268073E+000 +7.0635143E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

C4H71-4OH+H<=>PC4H8OH-4  
+1.5000000E+011 +8.8281162E-001 +2.7506294E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

SC4H8OH-1<=>PC4H8OH-4  
+2.9000000E+008 +1.3771432E+000 +3.7865971E+004 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

NC3H7CHO+H<=>PC4H9O  
+4.7000000E+009 +1.4346938E+000 +4.3578901E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

NC3H7+CH2O<=>PC4H9O  
+5.0000000E+003 +2.4251635E+000 +3.2388952E+003 !\AUTHOR: !\REF:J. ZA;ä  
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
519`C526

$C_4H_7-2OH+H \rightleftharpoons SC_4H_8OH-2$   
 +1.4000000E+008 +1.5155021E+000 +2.1884142E+002 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526  
 $C_2H_5COCH_3+H \rightleftharpoons SC_4H_8OH-2$   
 +7.0000000E+007 +1.8013421E+000 +1.3223122E+004 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526  
 $C_4H_8-1+OH \rightleftharpoons SC_4H_8OH-1$   
 +7.0000000E+005 +1.8018819E+000 -3.2902438E+003 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526 !\COMMENT !\*2\*0.25  
 $C_2H_3OH+C_2H_5 \rightleftharpoons SC_4H_8OH-1$   
 +6.4000000E+006 +1.6708958E+000 +1.0270243E+004 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526  
 $C_4H_8-2+OH \rightleftharpoons SC_4H_8OH-3$   
 +1.4000000E+006 +1.8018819E+000 -3.2902438E+003 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526 !\COMMENT !\*2\*0.25\*2  
 $SC_3H_5OH+CH_3 \rightleftharpoons SC_4H_8OH-3$   
 +6.4000000E+006 +1.6708958E+000 +1.0270243E+004 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526  
 $C_2H_5COCH_3+H \rightleftharpoons SC_4H_9O$   
 +2.7000000E+007 +1.7563257E+000 +6.2061519E+003 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526  
 $C_2H_5CHO+CH_3 \rightleftharpoons SC_4H_9O$   
 +1.2000000E+004 +2.2838256E+000 +7.9781023E+003 !\AUTHOR: !\REF:J. ZA;ä  
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)  
 519`C526  
 $C_4H_7-4OH+OH \rightleftharpoons C_4H_6,2-1OH+H_2O$   
 +2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: !\REF:ANALOGY  
 WITH C4H8-1+OH  
 $C_4H_7-4OH+HO_2 \rightleftharpoons C_4H_6,2-1OH+H_2O$  +3.9100000E-  
 001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF:ANALOGY WITH C4H8-  
 1+OH  
 !

---

!\REACTIONCLASS: \PC4H8OH-2\_O2\_PRODUCTS \A  
 \N \EA  
 !

---

$PC_4H_8OH-2+O_2 \rightleftharpoons PC_4H_8OH-2O_2$   
 +3.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $PC_4H_8OH-2O_2 \rightleftharpoons SQC_4H_8OP$   
 +2.9100000E+012 -2.2600000E-001 +2.2300000E+004 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $PC_4H_8OH-2O_2 \rightleftharpoons C_4H_7-1OH+HO_2$   
 +3.6400000E+014 -7.1100000E-001 +3.2710000E+004 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $PC_4H_8OH-2O_2 \rightleftharpoons C_4H_7-1OH+HO_2$   
 +2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

SQC4H8OP=>C2H5CHO+CH2O+OH  
+5.3600000E+012 -8.0000000E-002 +1.0790000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
PC4H8OH-2O2<=>NC4KET21OH+OH  
+1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF:  
!DIFFERENT FROM IC4H8 SYSTEM (ANALOGY WITH SC4H8OH-1 SYSTEM)  
C4H72-1OH+OH<=>C4H64,2-1OH+H2O  
+2.0200000E+006 +2.2000000E+000 -4.3692000E+002 !\AUTHOR: !\REF:  
!ANALOGY WITH C4H8-2+OH (CONSIDER THE NUMBER OF H ATOM AND OH GROUP  
AFFECT \*2)  
C4H72-1OH+OH<=>C4H63,1-1OH+H2O  
+2.6900000E+006 +2.2000000E+000 -4.3692000E+002 !\AUTHOR: !\REF:  
!ANALOGY WITH C4H8-2+OH (CONSIDER THE NUMBER OF H ATOM AND OH GROUP  
AFFECT \*2)  
C4H72-1OH+HO2<=>C4H64,2-1OH+H2O2 +1.7250000E-  
001 +4.0000000E+000 +1.2103000E+004 !\AUTHOR: !\REF: !ANALOGY WITH  
C4H8-2+OH (CONSIDER THE NUMBER OF H ATOM AND OH GROUP AFFECT \*2)  
C4H72-1OH+HO2<=>C4H63,1-1OH+H2O2 +2.3000000E-  
001 +4.0000000E+000 +1.2103000E+004 !\AUTHOR: !\REF: !ANALOGY WITH  
C4H8-2+OH (CONSIDER THE NUMBER OF H ATOM AND OH GROUP AFFECT \*2)  
C4H71-1OH+OH<=>C4H63,1-1OH+H2O  
+2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: !\REF:  
!ANALOGY WITH C4H8-1+OH  
C4H71-1OH+HO2<=>C4H63,1-1OH+H2O2 +3.9100000E-  
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF: !ANALOGY WITH  
C4H8-1+OH  
C4H64,2-1OH<=>C4H6+OH  
+7.0350000E+016 -1.0120000E+000 +3.6070000E+004 !\AUTHOR: !\REF:S.M.  
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028`C2055  
C4H63,1-1OH<=>C4H5OH-13+H  
+7.7220000E+012 +4.8800000E-001 +4.3940000E+004 !\AUTHOR: !\REF:S.M.  
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028`C2055  
C4H5OH-13<=>C4H5-N+OH  
+5.6100000E+021 -1.6120000E+000 +1.0600000E+005 !\AUTHOR: !\REF:S.M.  
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028`C2055  
C4H5OH-13<=>C2H3+CH2CHO  
+2.8160000E+024 -2.3810000E+000 +9.0130000E+004 !\AUTHOR: !\REF:S.M.  
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028`C2055  
NC4KET21OH+OH<=>C2H4COCH2OH+H2O  
+8.4500000E+011 +0.0000000E+000 -2.2800000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
NC4KET21OH+HO2<=>C2H4COCH2OH+H2O2  
+2.0000000E+011 +0.0000000E+000 +8.6980000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
NC4KET21OH+O<=>C2H4COCH2OH+OH  
+3.0700000E+013 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
NC4KET21OH+H<=>C2H4COCH2OH+H2  
+4.4600000E+006 +2.0000000E+000 +3.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
NC4KET21OH+O2<=>C2H4COCH2OH+HO2  
+1.5500000E+013 +0.0000000E+000 +4.1970000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
NC4KET21OH+CH3<=>C2H4COCH2OH+CH4  
+1.7400000E+000 +3.4600000E+000 +3.6800000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS

NC4KET21OH+CH3O<=>C2H4COCH2OH+CH3OH  
 +1.4500000E+011 +0.0000000E+000 +2.7710000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H5COCH3 REACTIONS  
 NC4KET21OH+CH3O2<=>C2H4COCH2OH+CH3O2H  
 +2.0000000E+012 +0.0000000E+000 +1.5250000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H5COCH3 REACTIONS  
 NC4KET21OH+C2H3<=>C2H4COCH2OH+C2H4  
 +3.0000000E+011 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H5COCH3 REACTIONS  
 NC4KET21OH+C2H5<=>C2H4COCH2OH+C2H6  
 +3.0000000E+010 +0.0000000E+000 +8.6000000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H5COCH3 REACTIONS  
 C2H4COCH2OH<=>CH3CHCO+CH2OH  
 +9.4400000E+029 -4.9300000E+000 +3.8330000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH SC4H9<=>C3H6+CH3  
 PC4H8OH-2O2<=>SQC4H7OHP-4  
 +1.4390000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:SHARMA  
 SQC4H7OHP-4<=>CY(CCCO)COH+OH  
 +2.4400000E+009 +7.8000000E-001 +1.8000000E+004 !\AUTHOR: !\REF:VILLANO  
 (FROM KUIWEN'S MECH)  
 SQC4H7OHP-4=>OH+HOCH2CHO+C2H4  
 +3.0800000E+008 +1.5000000E+000 +2.3500000E+004 !\AUTHOR: !\REF:VILLANO  
 (FROM KUIWEN'S MECH)  
 CY(CCCO)COH+H=>C2H4+HOCH2CO+H2  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+O=>C2H4+HOCH2CO+OH  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+OH=>C2H4+HOCH2CO+H2O  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+HO2=>C2H4+HOCH2CO+H2O2  
 +1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+CH3=>C2H4+HOCH2CO+CH4  
 +2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+CH3O2=>C2H4+HOCH2CO+CH3O2H  
 +1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+H=>CH2O+CH2CCH2OH+H2  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+O=>CH2O+CH2CCH2OH+OH  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+OH=>CH2O+CH2CCH2OH+H2O  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+HO2=>CH2O+CH2CCH2OH+H2O2  
 +1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CY(CCCO)COH+CH3=>CH2O+CH2CCH2OH+CH4  
 +2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

CY (CCCO) COH+CH3O2=>CH2O+CH2CCH2OH+CH3O2H  
 +1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 HOCH2CO<=>CH2OH+CO  
 +1.0700000E+012 +6.3000000E-001 +1.6900000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CO<=>CH3+CO  
 SQC4H7OHP-4+O2<=>SQC4H7OHP-4O2  
 +3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 SQC4H7OHP-4O2<=>C4H6OHOH1-4-3+HO2  
 +1.4400000E+007 +1.3800000E+000 +2.8900000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 SQC4H7OHP-4O2<=>NC4KET24OH-1+OH  
 +5.7900000E+001 +2.9000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 C4H6OHOH1-4-3=>C2H3CHO+CH2OH+OH  
 +1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 C4H6OHOH1-4-3=>HOCH2CHO+C2H3+OH  
 +1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 NC4KET24OH-1=>CH2O+HOCH2COCH2+OH  
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 HOCH2CHO+O2<=>HOCH2CO+HO2  
 +3.0100000E+013 +0.0000000E+000 +3.9150000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 HOCH2CHO+O<=>HOCH2CO+OH  
 +5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 HOCH2CHO+H<=>HOCH2CO+H2  
 +1.3100000E+005 +2.5800000E+000 +1.2200000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 HOCH2CHO+OH<=>HOCH2CO+H2O  
 +3.3700000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 HOCH2CHO+HO2<=>HOCH2CO+H2O2  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 HOCH2CHO+CH3<=>HOCH2CO+CH4 +7.0800000E-  
 004 +4.5800000E+000 +1.9660000E+003 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO  
 ABSTRACTION REACTIONS  
 HOCH2CHO+CH3O2<=>HOCH2CO+CH3O2H  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 HOCH2CHO+CH3CO3<=>HOCH2CO+CH3CO3H  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH CH3CHO ABSTRACTION REACTIONS  
 !

---

!\REACTIONCLASS: \SC4H8OH-1\_O2\_PRODUCTS \A  
 \N \EA  
 !

---

SC4H8OH-1+O2<=>SC4H8OH-1O2  
 +3.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

$\text{SC4H8OH-1O2} \rightleftharpoons \text{PQC4H8OS}$   
+9.3000000E+010 -3.6000000E-002 +2.2890000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{SC4H8OH-1O2} \rightleftharpoons \text{NC4KET12OH+OH}$   
+1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{PQC4H8OS} \Rightarrow \text{C2H5CHO+CH2O+OH}$   
+6.7000000E+039 -8.3800000E+000 +2.2782000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{PQC4H8OS} \Rightarrow \text{C2H5+HO2CH2CHO}$   
+2.6700000E+034 -6.6300000E+000 +2.2672000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{SC4H8OH-1O2} \rightleftharpoons \text{C4H71-2OH+HO2}$   
+2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR:  
!\REF:DIFFERENT FROM IC4H8 SYSTEM (ANALOGY WITH PC4H8OH-2 SYSTEM)  
 $\text{SC4H8OH-1O2} \rightleftharpoons \text{PQC4H7OHS-3}$   
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:SHARMA  
 $\text{PQC4H7OHS-3} \rightleftharpoons \text{CCY(COCC)OH+OH}$   
+2.5900000E+009 +6.9000000E-001 +1.6000000E+004 !\AUTHOR: !\REF:VILLANO  
(FROM KUIWEN'S MECH)  
 $\text{PQC4H7OHS-3} \Rightarrow \text{OH+CH2O+SC3H5OH}$   
+1.2300000E+009 +1.3000000E+000 +2.4900000E+004 !\AUTHOR: !\REF:VILLANO  
(FROM KUIWEN'S MECH)  
 $\text{C4H71-2OH+OH} \rightleftharpoons \text{C4H63,1-2OH+H2O}$   
+2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C4H8-1+OH  
 $\text{C4H71-2OH+HO2} \rightleftharpoons \text{C4H63,1-2OH+H2O2}$  +3.9100000E-  
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF:ANALOGY WITH C4H8-  
1+OH  
 $\text{C4H63,1-2OH} \rightleftharpoons \text{C4H612+OH}$   
+7.0350000E+016 -1.0120000E+000 +3.6070000E+004 !\AUTHOR: !\REF:S.M.  
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028`C2055  
 $\text{NC4KET12OH+H} \rightleftharpoons \text{C2H5CHOHCO+H2}$   
+1.0000000E+005 +2.5800000E+000 +1.2200000E+003 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+OH} \rightleftharpoons \text{C2H5CHOHCO+H2O}$   
+1.7000000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+O} \rightleftharpoons \text{C2H5CHOHCO+OH}$   
+5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+HO2} \rightleftharpoons \text{C2H5CHOHCO+H2O2}$   
+9.5000000E+003 +2.7000000E+000 +1.1520000E+004 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+CH3} \rightleftharpoons \text{C2H5CHOHCO+CH4}$  +1.4200000E-  
003 +4.5800000E+000 +1.9660000E+003 !\AUTHOR: !\REF:M. PELUCCHI ET AL.  
COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+C2H5} \rightleftharpoons \text{C2H5CHOHCO+C2H6}$   
+7.3600000E+004 +2.0000000E+000 +5.9170900E+003 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+CH3O} \rightleftharpoons \text{C2H5CHOHCO+CH3OH}$   
+1.0000000E+012 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.  
 $\text{NC4KET12OH+CH3O2} \rightleftharpoons \text{C2H5CHOHCO+CH3O2H}$   
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:M.  
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.

$\text{NC4KET12OH} + \text{O2} \rightleftharpoons \text{C2H5CHOHCO} + \text{HO2}$   
 +9.0300000E+013 +0.0000000E+000 +4.3320000E+004 !\AUTHOR: !\REF:M.  
 PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.

$\text{NC4KET12OH} + \text{C2H3} \rightleftharpoons \text{C2H5CHOHCO} + \text{C2H4}$   
 +3.2560000E+005 +2.0000000E+000 +3.9656900E+003 !\AUTHOR: !\REF:M.  
 PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.

$\text{NC4KET12OH} + \text{C2H5O} \rightleftharpoons \text{C2H5CHOHCO} + \text{C2H5OH}$   
 +6.0300000E+011 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:M.  
 PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.

$\text{C2H5CHOHCO} \rightleftharpoons \text{C3H6OH1-1} + \text{CO}$   
 +5.7800000E+014 +0.0000000E+000 +1.6843510E+004 !\AUTHOR: !\REF:M.  
 PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265`C286.

$\text{C3H6OH1-1} \rightleftharpoons \text{C2H5CHO} + \text{H}$   
 +8.9810000E+011 +2.7100000E-001 +3.2990000E+004 !\AUTHOR: !\REF:J.  
 MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.

$\text{C2H3OH} + \text{CH3} \rightleftharpoons \text{C3H6OH1-1}$   
 +2.0400000E+040 -8.2500000E+000 +2.4214000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH  $\text{C2H4} + \text{CH3} \rightleftharpoons \text{NC3H7}$   
 DUP

$\text{C2H3OH} + \text{CH3} \rightleftharpoons \text{C3H6OH1-1}$   
 +1.6600000E+021 -3.1700000E+000 +1.0241000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH  $\text{C2H4} + \text{CH3} \rightleftharpoons \text{NC3H7}$   
 DUP

$\text{CCY(COCC)OH} + \text{H} \Rightarrow \text{OH} + \text{C2H3COCH3} + \text{H2}$   
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{O} \Rightarrow \text{OH} + \text{C2H3COCH3} + \text{OH}$   
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{OH} \Rightarrow \text{OH} + \text{C2H3COCH3} + \text{H2O}$   
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{HO2} \Rightarrow \text{OH} + \text{C2H3COCH3} + \text{H2O2}$   
 +1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{CH3} \Rightarrow \text{OH} + \text{C2H3COCH3} + \text{CH4}$   
 +2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{CH3O2} \Rightarrow \text{OH} + \text{C2H3COCH3} + \text{CH3O2H}$   
 +1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{H} \Rightarrow \text{OH} + \text{SC3H5CHO} + \text{H2}$   
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{O} \Rightarrow \text{OH} + \text{SC3H5CHO} + \text{OH}$   
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{OH} \Rightarrow \text{OH} + \text{SC3H5CHO} + \text{H2O}$   
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{HO2} \Rightarrow \text{OH} + \text{SC3H5CHO} + \text{H2O2}$   
 +1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH} + \text{CH3} \Rightarrow \text{OH} + \text{SC3H5CHO} + \text{CH4}$   
 +2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE

CCY (COCC) OH+CH3O2=>OH+SC3H5CHO+CH3O2H  
 +1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+H=>C2H3OH+CH3CO+H2  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+O=>C2H3OH+CH3CO+OH  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+OH=>C2H3OH+CH3CO+H2O  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+HO2=>C2H3OH+CH3CO+H2O2  
 +1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+CH3=>C2H3OH+CH3CO+CH4  
 +2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+CH3O2=>C2H3OH+CH3CO+CH3O2H  
 +1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+H=>HCO+SC3H5OH+H2  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+O=>HCO+SC3H5OH+OH  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+OH=>HCO+SC3H5OH+H2O  
 +5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+HO2=>HCO+SC3H5OH+H2O2  
 +1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+CH3=>HCO+SC3H5OH+CH4  
 +2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 CCY (COCC) OH+CH3O2=>HCO+SC3H5OH+CH3O2H  
 +1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:  
 !\REF:WESTBROOK ESTIMATE  
 PQC4H7OHS-3+O2<=>PQC4H7OHS-3O2  
 +1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 PQC4H7OHS-3O2<=>NC4KET13OH-2+OH  
 +1.0900000E+004 +2.4000000E+000 +1.9900000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 NC4KET13OH-2=>CH3CHO+HOCHCHO+OH  
 +1.0500000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 PQC4H7OHS-3O2<=>C4H7O2-1,3OOH  
 +2.9100000E+012 -2.2600000E-001 +2.2300000E+004 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PQC4H7OHS-3O2<=>C4H6OHOOH1-3-4+HO2  
 +3.6400000E+014 -7.1100000E-001 +3.2710000E+004 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 PQC4H7OHS-3O2<=>C4H6OHOOH2-2-1+HO2  
 +2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR: !\REF: H.  
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.



$C_4H_7O_2-1, 3OOH \Rightarrow C_3KET12 + CH_2O + OH$   
+5.3600000E+012 -8.0000000E-002 +1.0790000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $C_4H_7O_2-1, 3OOH \Rightarrow HO_2CH_2CHO + CH_3CHO + OH$   
+6.7000000E+039 -8.3800000E+000 +2.2782000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $PQC_4H_7OHS-3O_2 \Leftrightarrow NC_4KET24OH-3 + OH$   
+1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $HOCHCHO + O \Leftrightarrow CHOCHO + OH$  +1.4600000E-  
003 +4.7300000E+000 +1.7270000E+003 !\AUTHOR: !\REF: ANALOGY WITH  
 $C_2H_5OH + OH \Leftrightarrow C_2H_5O + H_2O$   
 $HOCHCHO + OH \Leftrightarrow CHOCHO + H_2O$  +5.8100000E-  
003 +4.2800000E+000 -3.5600000E+003 !\AUTHOR: !\REF: ANALOGY WITH  
 $C_2H_5OH + OH \Leftrightarrow C_2H_5O + H_2O$   
 $HOCHCHO + H \Leftrightarrow CHOCHO + H_2$   
+9.4500000E+002 +3.1400000E+000 +8.7011000E+003 !\AUTHOR: !\REF: ANALOGY  
WITH  $C_2H_5OH + OH \Leftrightarrow C_2H_5O + H_2O$   
 $HOCHCHO + HO_2 \Leftrightarrow CHOCHO + H_2O_2$  +6.4700000E-  
007 +5.3000000E+000 +1.0533100E+004 !\AUTHOR: !\REF: ANALOGY WITH  
 $C_2H_5OH + OH \Leftrightarrow C_2H_5O + H_2O$   
 $HOCHCHO + CH_3 \Leftrightarrow CHOCHO + CH_4$   
+2.0350000E+000 +3.5700000E+000 +7.7210000E+003 !\AUTHOR: !\REF: ANALOGY  
WITH  $C_2H_5OH + OH \Leftrightarrow C_2H_5O + H_2O$   
 $HOCHCHO + CH_3O_2 \Leftrightarrow CHOCHO + CH_3O_2H$  +3.2360000E-  
007 +5.3000000E+000 +1.0533100E+004 !\AUTHOR: !\REF: ANALOGY WITH  
 $C_2H_5OH + OH \Leftrightarrow C_2H_5O + H_2O$   
 $C_4H_6OHO_2H1-3-4 \Rightarrow CH_2O + PC_3H_4OH-3 + OH$   
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF: Miyoshi  
A/2 compared to R+O2  
 $C_4H_6OHO_2H2-2-1 \Rightarrow CH_2O + PC_3H_4OH-1 + OH$   
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF: Miyoshi  
A/2 compared to R+O2  
 $NC_4KET24OH-3 \Rightarrow CH_2O + CH_3COCHOH + OH$   
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF: Miyoshi  
A/2 compared to R+O2  
 $PC_3H_4OH-3 \Leftrightarrow C_2H_3CHO + H$   
+5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS  
 $PC_3H_4OH-3 \Leftrightarrow C_3H_5O$   
+5.4800000E+045 -1.1630000E+001 +4.4328000E+004 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS  
 $PC_3H_4OH-3 \Leftrightarrow CH_2CCH_2OH$   
+2.6500000E+036 -8.8600000E+000 +5.1019000E+004 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS  
 $PC_3H_4OH-3 + O_2 \Leftrightarrow C_2H_3CHO + HO_2$   
+5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS  
 $PC_3H_4OH-1 \Leftrightarrow CH_3CHCO + H$   
+5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS  
 $PC_3H_4OH-1 \Leftrightarrow PC_3H_4OH-2$   
+2.6500000E+036 -8.8600000E+000 +5.1019000E+004 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS  
 $PC_3H_4OH-1 + O_2 \Leftrightarrow CH_3CHCO + HO_2$   
+5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF: ANALOGY  
WITH SC2H4OH REACTIONS

CH3COCHOH<=>CH3COCHO+H  
+5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH SC2H4OH REACTIONS  
CH3COCHOH<=>CH3COCH2O  
+5.4800000E+045 -1.1630000E+001 +4.4328000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH SC2H4OH REACTIONS  
CH3COCHOH+O2<=>CH3COCHO+HO2  
+5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH SC2H4OH REACTIONS  
!

---

!\REACTIONCLASS: \SC4H8OH-3\_O2\_PRODUCTS \A  
\N \EA  
!

---

SC4H8OH-3+O2<=>SC4H8OH-3O2  
+3.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
SC4H8OH-3O2<=>SQC4H8OS  
+2.9100000E+012 -2.2600000E-001 +2.2300000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
SC4H8OH-3O2<=>C4H71-3OH+HO2  
+3.6400000E+014 -7.1100000E-001 +3.2710000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
SC4H8OH-3O2<=>C4H72-2OH+HO2  
+2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
SQC4H8OS=>CH3CHO+CH3CHO+OH  
+2.6800000E+013 -8.0000000E-002 +1.0790000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT: !\*5  
SC4H8OH-3O2<=>NC4KET23OH+OH  
+1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
SC4H8OH-3O2<=>SQC4H7OHS-4  
+1.4390000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:SHARMA  
SQC4H7OHS-4<=>CCY(COCC)OH+OH  
+2.4400000E+009 +7.8000000E-001 +1.8000000E+004 !\AUTHOR: !\REF:VILLANO  
(FROM KUIWEN'S MECH)  
SQC4H7OHS-4=>OH+CH3CHO+C2H3OH  
+3.0800000E+008 +1.5000000E+000 +2.3500000E+004 !\AUTHOR: !\REF:VILLANO  
(FROM KUIWEN'S MECH)  
C4H71-3OH+OH<=>C4H63,1-3OH+H2O  
+2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: \REF:ANALOGY  
WITH C4H8-1+OH  
C4H71-3OH+HO2<=>C4H63,1-3OH+H2O +3.9100000E-  
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: \REF:ANALOGY WITH C4H8-  
1+OH  
C4H72-2OH+OH<=>C4H63,1-3OH+H2O  
+2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: \REF:ANALOGY  
WITH C4H8-1+OH  
C4H72-2OH+HO2<=>C4H63,1-3OH+H2O +3.9100000E-  
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: \REF:ANALOGY WITH C4H8-  
1+OH  
C4H63,1-3OH<=>C4H6+OH  
+7.0350000E+016 -1.0120000E+000 +3.6070000E+004 !\AUTHOR: !\REF:S.M.  
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028~C2055

$\text{NC4KET23OH+OH} \rightleftharpoons \text{CH3COCOCH3+H2O}$   
+8.4500000E+011 +0.0000000E+000 -2.2800000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+HO2} \rightleftharpoons \text{CH3COCOCH3+H2O2}$   
+2.0000000E+011 +0.0000000E+000 +8.6980000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+O} \rightleftharpoons \text{CH3COCOCH3+OH}$   
+3.0700000E+013 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+H} \rightleftharpoons \text{CH3COCOCH3+H2}$   
+4.4600000E+006 +2.0000000E+000 +3.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+O2} \rightleftharpoons \text{CH3COCOCH3+HO2}$   
+1.5500000E+013 +0.0000000E+000 +4.1970000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+CH3} \rightleftharpoons \text{CH3COCOCH3+CH4}$   
+1.7400000E+000 +3.4600000E+000 +3.6800000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+CH3O} \rightleftharpoons \text{CH3COCOCH3+CH3OH}$   
+1.4500000E+011 +0.0000000E+000 +2.7710000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+CH3O2} \rightleftharpoons \text{CH3COCOCH3+CH3O2H}$   
+2.0000000E+012 +0.0000000E+000 +1.5250000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+C2H3} \rightleftharpoons \text{CH3COCOCH3+C2H4}$   
+3.0000000E+011 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{NC4KET23OH+C2H5} \rightleftharpoons \text{CH3COCOCH3+C2H6}$   
+3.0000000E+010 +0.0000000E+000 +8.6000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{CH3COHCO+CH3} \rightleftharpoons \text{CH3COCOCH3}$   
+1.2300000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{CH3COHCO+OH} \rightleftharpoons \text{SC2H4OH+CO2}$   
+1.7300000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{CH3COHCO+H} \rightleftharpoons \text{SC2H4OH+CO}$   
+4.4000000E+012 +0.0000000E+000 +1.4590000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH C2H5COCH3 REACTIONS  
 $\text{SQC4H7OHS-4+O2} \rightleftharpoons \text{SQC4H7OHS-4O2}$   
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:MIYOSHI  
A/2 COMPARED TO R+O2  
 $\text{SQC4H7OHS-4O2} \rightleftharpoons \text{NC4KET24OH-3+OH}$   
+5.7900000E+001 +2.9000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:MIYOSHI  
A/2 COMPARED TO R+O2  
 $\text{SQC4H7OHS-4O2} \rightleftharpoons \text{C4H7O2-1,3OOH}$   
+9.3000000E+010 -3.6000000E-002 +2.2890000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{SQC4H7OHS-4O2} \rightleftharpoons \text{C4H6OHOH1-2-3+HO2}$   
+2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{SQC4H7OHS-4O2} \rightleftharpoons \text{NC4KET13OH-2+OH}$   
+1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.  
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.  
 $\text{C4H6OHOH1-2-3} \rightleftharpoons \text{CH2COHCHO+CH3+OH}$   
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:MIYOSHI  
A/2 COMPARED TO R+O2

C4H6OHOH1-2-3=>CH3CHO+SC2H2OH+OH  
 +1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:MIYOSHI  
 A/2 COMPARED TO R+O2  
 SC2H2OH+HCO<=>CH2COHCHO  
 +1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+H<=>CH2COHCO+H2  
 +1.3400000E+013 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+O<=>CH2COHCO+OH  
 +5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+OH<=>CH2COHCO+H2O  
 +9.2400000E+006 +1.5000000E+000 -9.6200000E+002 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+O2<=>CH2COHCO+HO2  
 +1.0050000E+013 +0.0000000E+000 +4.0700000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+HO2<=>CH2COHCO+H2O2  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+CH3<=>CH2COHCO+CH4  
 +2.6080000E+006 +1.7800000E+000 +5.9110000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+C2H3<=>CH2COHCO+C2H4  
 +1.7400000E+012 +0.0000000E+000 +8.4400000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+CH3O<=>CH2COHCO+CH3OH  
 +1.0000000E+012 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 CH2COHCHO+CH3O2<=>CH2COHCO+CH3O2H  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 SC2H2OH+CO<=>CH2COHCO  
 +1.5100000E+011 +0.0000000E+000 +4.8100000E+003 !\AUTHOR: !\REF:ANALOGY  
 WITH C2H3CHO REACTIONS  
 SC2H2OH<=>CH2CO+H  
 +5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH SC2H4OH REACTIONS  
 SC2H2OH<=>HCCOH+H  
 +5.4000000E+046 -1.1630000E+001 +4.4323000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH SC2H4OH REACTIONS  
 SC2H2OH<=>C2H2OH  
 +2.6500000E+036 -8.8600000E+000 +5.1019000E+004 !\AUTHOR: !\REF:ANALOGY  
 WITH SC2H4OH REACTIONS  
 SC2H2OH+O2<=>CH2CO+HO2  
 +5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF:ANALOGY  
 WITH SC2H4OH REACTIONS  
 SC2H2OH+O2<=>HCCOH+HO2  
 +5.5120000E+003 +2.4950000E+000 -4.1400000E+002 !\AUTHOR: !\REF:ANALOGY  
 WITH SC2H4OH REACTIONS

!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\O

\A

\N

\EA

!

---

C4H8-1+O<=>NC3H7+HCO  
+7.4500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+O  
C4H8-1+O=>CH2CO+C2H5+H  
+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+O  
C4H8-1+O=>C2H5CHCO+H+H  
+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+O  
C4H8-2+O<=>CH3+C2H5CO  
+7.4500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+O  
C4H8-2+O=>CH2CO+C2H5+H  
+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+O  
C4H8-2+O=>C2H5CHCO+H+H  
+3.0500000E+006 +1.8800000E+000 +1.8300000E+002 !\AUTHOR: !\REF:ANALOGY  
WITH C3H6+O

!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\HO2 \A  
\N \EA

!

---

SC4H9O2<=>C4H8-2+HO2  
+7.2500000E+009 +8.0000000E-001 +2.9900000E+004 !\AUTHOR: !\REF:VILLANO  
(FROM KUIWEN'S MECH)  
DUP  
SC4H9O2<=>C4H8-2+HO2  
+1.7000000E+010 +6.7000000E-001 +3.0700000E+004 !\AUTHOR: !\REF:VILLANO  
(FROM KUIWEN'S MECH)  
DUP  
C4H8OOH1-2<=>C4H8-1+HO2  
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF:VILLANO  
!\COMMENT: QRRK  
PLOG / +1.0000000E-002  
+1.0900000E+013 -1.3800000E+000 +9.1130000E+003 /  
PLOG / +1.0000000E-001  
+2.9300000E+018 -2.6000000E+000 +1.3142000E+004 /  
PLOG / +1.0000000E+000  
+7.8000000E+024 -4.0500000E+000 +1.8999000E+004 /  
PLOG / +2.0000000E+000  
+1.7600000E+026 -4.3200000E+000 +2.0657000E+004 /  
PLOG / +5.0000000E+000  
+7.8600000E+026 -4.3500000E+000 +2.2246000E+004 /  
PLOG / +1.0000000E+001  
+1.7300000E+026 -4.0600000E+000 +2.2736000E+004 /  
PLOG / +3.0000000E+001  
+1.3900000E+023 -3.0400000E+000 +2.2032000E+004 /  
PLOG / +5.0000000E+001  
+1.4500000E+021 -2.4300000E+000 +2.1227000E+004 /  
C4H8-1+HO2<=>C4H8OOH2-1 +1.4600000E-  
001 +3.4500000E+000 +5.7980000E+003 !\AUTHOR: !\REF:JUDIT ZADOR,STEPHEN  
J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011, 115,  
10218`C10225  
PLOG / +1.3300000E-002  
+9.7400000E+005 +4.1000000E-001 +7.5700000E+003 /

PLOG / +1.0000000E+000  
 +8.4300000E+014 -1.7600000E+000 +1.2124000E+004 /  
 PLOG / +1.0000000E+001  
 +1.8200000E+020 -3.0300000E+000 +1.6135000E+004 /  
 PLOG / +1.0000000E+002  
 +8.7900000E+017 -2.0400000E+000 +1.7111000E+004 /  
 C4H8-1+HO2<=>C4H8O1-2+OH  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:JUDIT  
 ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011,  
 115, 10218\C10225  
 PLOG / +1.3300000E-002  
 +2.9600000E+003 +2.4500000E+000 +1.2199000E+004 /  
 PLOG / +1.0000000E+000  
 +1.6900000E+010 +5.1000000E-001 +1.6606000E+004 /  
 PLOG / +1.0000000E+001  
 +2.1900000E+017 -1.4800000E+000 +2.2209000E+004 /  
 PLOG / +1.0000000E+002  
 +2.7300000E+021 -2.5100000E+000 +2.7857000E+004 /  
 C4H8OOH2-1<=>C4H8O1-2+OH  
 +3.9200000E+006 +1.6500000E+000 +1.2124000E+004 !\AUTHOR: !\REF:JUDIT  
 ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011,  
 115, 10218\C10225  
 PLOG / +1.3300000E-002  
 +2.7500000E+022 -4.3900000E+000 +1.2349000E+004 /  
 PLOG / +1.0000000E+000  
 +2.4400000E+029 -5.9000000E+000 +1.7573000E+004 /  
 PLOG / +1.0000000E+001  
 +1.5200000E+030 -5.8400000E+000 +1.9702000E+004 /  
 PLOG / +1.0000000E+002  
 +1.9300000E+020 -2.6600000E+000 +1.6454000E+004 /  
 C4H8-2+HO2<=>C4H8OOH2-3  
 +9.5500000E+003 +2.5800000E+000 +1.0347000E+004 !\AUTHOR: !\REF:JUDIT  
 ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011,  
 115, 10218\C10225  
 PLOG / +1.3300000E-002  
 +2.5300000E+012 -1.2700000E+000 +1.0098000E+004 /  
 PLOG / +1.0000000E+000  
 +1.3400000E+011 -4.8000000E-001 +8.4800000E+003 /  
 PLOG / +1.0000000E+001  
 +1.9300000E+017 -2.0400000E+000 +1.2122000E+004 /  
 PLOG / +1.0000000E+002  
 +4.4500000E+019 -2.4500000E+000 +1.4812000E+004 /  
 C4H8-2+HO2<=>C4H8O2-3+OH  
 +1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:JUDIT  
 ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011,  
 115, 10218\C10225  
 PLOG / +1.3300000E-002  
 +7.6500000E+005 +1.9262200E+000 +1.0745000E+004 /  
 PLOG / +1.0000000E+000  
 +1.7900000E+008 +1.2508900E+000 +1.2370000E+004 /  
 PLOG / +1.0000000E+001  
 +1.7500000E+015 -7.4000000E-001 +1.7220000E+004 /  
 PLOG / +1.0000000E+002  
 +8.3700000E+020 -2.2831400E+000 +2.2838000E+004 /  
 C4H8OOH2-3<=>C4H8O2-3+OH  
 +1.0500000E+010 +6.8000000E-001 +1.1964000E+004 !\AUTHOR: !\REF:JUDIT  
 ZADOR,STEPHEN J. KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011,  
 115, 10218\C10225

PLOG / +1.3300000E-002  
+3.0200000E+019 -3.5100000E+000 +9.7460000E+003 /  
PLOG / +1.0000000E+000  
+6.3700000E+024 -4.5500000E+000 +1.3480000E+004 /  
PLOG / +1.0000000E+001  
+1.3900000E+028 -5.2500000E+000 +1.6470000E+004 /  
PLOG / +1.0000000E+002  
+1.5400000E+027 -4.6900000E+000 +1.7832000E+004 /  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\RO2 \A  
\N \EA  
!

---

C4H8-1+CH3O2<=>C4H8O1-2+CH3O  
+1.0000000E+012 +0.0000000E+000 +1.4340000E+004 !\AUTHOR: !\REF:IN  
ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479  
(1975).

C4H8-2+CH3O2<=>C4H8O2-3+CH3O  
+5.6200000E+011 +0.0000000E+000 +1.2310000E+004 !\AUTHOR: !\REF:IN  
ARAMCO (SEATTLE, AUGUST, 1988)

!\ENDSUBMECH: \C4H8-1\C4H8-2

!\SUBMECH: \C4H6

!\MECHCOMMENTS: KPS, 22/07/2015 TWO ABSTRACTION REACTIONS FROM C4H6 ARE  
DEFINED IN THE WRONG DIRECTION. THERE APPEARS TO BE MANY MANY  
INCONSITENCIES FOR THE DECOMPOSITION OF C4H7 AND C4H5 RADICALS: TREAT ALL  
OR NONE AS PRESSURE-DEPENDENT??

!\MECHWARNINGS: C4H4O IS STILL BEING USED FOR FURAN/VINYL KETENE

!\MECHWARNINGS: KPS, 03/08/2015 CH3CHCHCHO HAS BEEN RENAMED SC3H5CHO BY  
SOMEONE IN BASEMECH\_2907\_C7.INP THIS CHANGE MUST BE DISCUSSED.

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

C4H6<=>C4H5-I+H  
+5.7000000E+036 -6.2700000E+000 +1.1235300E+005 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C4H6<=>C4H5-N+H  
+5.3000000E+044 -8.6200000E+000 +1.2360800E+005 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C4H6<=>C4H4+H2  
+2.5000000E+015 +0.0000000E+000 +9.4700000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

H2CC+C2H4<=>C4H6  
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WARNING  
NO REFERENCE !\COMMENT:

!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

C4H6+H<=>C4H5-N+H2  
+1.3300000E+006 +2.5300000E+000 +1.2240000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H5-N+HO2<=>C4H6+O2  
+6.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING SOURCE UNCLEAR DEFINED IN WRONG  
DIRECTION  
C4H6+O<=>C4H5-N+OH  
+7.5000000E+006 +1.9000000E+000 +3.7400000E+003 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+OH<=>C4H5-N+H2O  
+6.2000000E+006 +2.0000000E+000 +3.4300000E+003 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H5-N+H2O2<=>C4H6+HO2  
+1.2100000E+010 +0.0000000E+000 -5.9600000E+002 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING SOURCE UNCLEAR DEFINED IN WRONG  
DIRECTION  
C4H6+CH3<=>C4H5-N+CH4  
+2.0000000E+014 +0.0000000E+000 +2.2800000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+C2H3<=>C4H5-N+C2H4  
+5.0000000E+013 +0.0000000E+000 +2.2800000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+C3H3<=>C4H5-N+C3H4-A  
+1.0000000E+013 +0.0000000E+000 +2.2500000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+C3H5-A<=>C4H5-N+C3H6  
+1.0000000E+013 +0.0000000E+000 +2.2500000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+H<=>C4H5-I+H2  
+6.6500000E+005 +2.5300000E+000 +9.2400000E+003 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H5-I+HO2<=>C4H6+O2  
+6.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING SOURCE UNCLEAR DEFINED IN WRONG  
DIRECTION  
C4H6+O<=>C4H5-I+OH  
+7.5000000E+006 +1.9000000E+000 +3.7400000E+003 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+OH<=>C4H5-I+H2O  
+3.1000000E+006 +2.0000000E+000 +4.3000000E+002 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H5-I+H2O2<=>C4H6+HO2  
+1.2100000E+010 +0.0000000E+000 -5.9600000E+002 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING SOURCE UNCLEAR DEFINED IN WRONG  
DIRECTION  
C4H6+CH3<=>C4H5-I+CH4  
+1.0000000E+014 +0.0000000E+000 +1.9800000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+C2H3<=>C4H5-I+C2H4  
+2.5000000E+013 +0.0000000E+000 +1.9800000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.



C4H6+C3H3<=>C4H5-I+C3H4-A  
+5.0000000E+012 +0.0000000E+000 +1.9500000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+C3H5-A<=>C4H5-I+C3H6  
+5.0000000E+012 +0.0000000E+000 +1.9500000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
!

---

!\REACTIONCLASS: \R\_ADDITION\H \A  
\N \EA  
!

---

C4H6+H<=>C2H4+C2H3  
+1.4600000E+030 -4.3400000E+000 +2.1647000E+004 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
PLOG / +1.0000000E+000  
+1.4600000E+030 -4.3400000E+000 +2.1647000E+004 /  
PLOG / +1.0000000E+001  
+5.4500000E+030 -4.5100000E+000 +2.1877000E+004 /  
C4H6+H<=>C3H4-P+CH3  
+2.0000000E+012 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
C4H6+H<=>C3H4-A+CH3  
+2.0000000E+012 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:  
WARNING SOURCE UNCLEAR!\COMMENT: WARNING PROBABLY LASKIN ET AL.  
!

---

!\REACTIONCLASS: \R\_ADDITION\O \A  
\N \EA  
!

---

C4H6+O<=>C2H2+C2H4O1-2  
+1.0000000E+008 +1.4500000E+000 -8.6000000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H6+O<=>SC3H5CO+H  
+5.0000000E+007 +1.4500000E+000 -8.6000000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: WARNING  
THIS PATHWAY IS NOT IN BASEMECH\_2907\_C7  
C4H6+O<=>CH2CHCHCHO+H  
+4.5000000E+008 +1.4500000E+000 -8.6000000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_ADDITION\OH \A  
\N \EA  
!

---

C4H6+OH<=>C2H3CHO+CH3  
+1.3700000E+012 +0.0000000E+000 -1.0400000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: TEST,  
0525 KWZ  
C4H6+OH<=>C3H5-A+CH2O  
+1.3700000E+012 +0.0000000E+000 -1.0400000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: TEST,  
0525 KWZ  
!

---

!\REACTIONCLASS: \R\_ADDITION\HO2 \A  
\N \EA  
!

---

C4H6+HO2<=>C4H6O25+OH  
+1.2000000E+012 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H6+HO2<=>C2H3CHOCH2+OH  
+4.8000000E+012 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!=====  
=====  
!\SUBSPECIES: \C2H3CHOCH2\C4H6O25\C4H6O23  
!=====  
=====  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

C4H6O25<=>C4H4O+H2  
+5.3000000E+012 +0.0000000E+000 +4.8500000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C2H3CHOCH2<=>C4H6O23  
+2.0000000E+014 +0.0000000E+000 +5.0600000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H6O23<=>SC3H5CHO  
+1.9500000E+013 +0.0000000E+000 +4.9400000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H6O23<=>C2H4+CH2CO  
+5.7500000E+015 +0.0000000E+000 +6.9300000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H6O23<=>C2H2+C2H4O1-2  
+1.0000000E+016 +0.0000000E+000 +7.5800000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!=====  
=====  
!\ENDSUBSPECIES: \C2H3CHOCH2\C4H6O25\C4H6O23  
!=====  
=====  
!=====  
=====  
!\SUBSPECIES: \FURAN  
!=====  
=====  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

C4H4O<=>CO+C3H4-P  
+1.7800000E+015 +0.0000000E+000 +7.7500000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: WARNING:  
SHOULD BE UPDATED BASED ON KPS FURANS WORK  
C4H4O<=>C2H2+CH2CO  
+5.0100000E+014 +0.0000000E+000 +7.7500000E+004 !\AUTHOR: !\REF:

WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: WARNING:  
SHOULD BE UPDATED BASED ON KPS FURANS WORK

!=====  
=====

!\ENDSUBSPECIES: FURAN

!=====  
=====

!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A

\N \EA

!

---

C2H3+C2H2<=>C4H4+H

+7.2000000E+013 -4.8000000E-001 +6.1000000E+003 !\AUTHOR: !\REF:

WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

PLOG / +1.3200000E-002

+7.2000000E+013 -4.8000000E-001 +6.1000000E+003 /

PLOG / +2.6300000E-002

+5.0000000E+014 -7.1000000E-001 +6.7000000E+003 /

PLOG / +1.2000000E-001

+4.6000000E+016 -1.2500000E+000 +8.4000000E+003 /

PLOG / +1.0000000E+000

+2.0000000E+018 -1.6800000E+000 +1.0600000E+004 /

PLOG / +1.0000000E+001

+4.9000000E+016 -1.1300000E+000 +1.1800000E+004 /

C2H3+C2H2<=>C4H5-N

+1.1000000E+031 -7.1400000E+000 +5.6000000E+003 !\AUTHOR: !\REF:

WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

PLOG / +1.3200000E-002

+1.1000000E+031 -7.1400000E+000 +5.6000000E+003 /

PLOG / +2.6300000E-002

+1.1000000E+032 -7.3300000E+000 +6.2000000E+003 /

PLOG / +1.2000000E-001

+2.4000000E+031 -6.9500000E+000 +5.6000000E+003 /

PLOG / +1.0000000E+000

+9.3000000E+038 -8.7600000E+000 +1.2000000E+004 /

PLOG / +1.0000000E+001

+8.1000000E+037 -8.0900000E+000 +1.3400000E+004 /

C2H3+C2H2<=>C4H5-I

+5.0000000E+034 -8.4200000E+000 +7.9000000E+003 !\AUTHOR: !\REF:

WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

PLOG / +1.3200000E-002

+5.0000000E+034 -8.4200000E+000 +7.9000000E+003 /

PLOG / +2.6300000E-002

+2.1000000E+036 -8.7800000E+000 +9.1000000E+003 /

PLOG / +1.2000000E-001

+1.0000000E+037 -8.7700000E+000 +9.8000000E+003 /

PLOG / +1.0000000E+000

+1.6000000E+046 -1.0980000E+001 +1.8600000E+004 /

PLOG / +1.0000000E+001

+5.1000000E+053 -1.2640000E+001 +2.8800000E+004 /

C2H3+C2H3<=>C4H6

+7.0000000E+057 -1.3820000E+001 +1.7629000E+004 !\AUTHOR: !\REF:

WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT: WARNING:  
THIS REACTION IS IN THE WRONG PLACE!!

PLOG / +2.6300000E-002

+7.0000000E+057 -1.3820000E+001 +1.7629000E+004 /

PLOG / +1.2000000E-001  
+1.5000000E+052 -1.1970000E+001 +1.6056000E+004 /  
PLOG / +1.0000000E+000  
+1.5000000E+042 -8.8400000E+000 +1.2483000E+004 /  
C2H3+C2H3<=>C4H5-I+H  
+1.5000000E+030 -4.9500000E+000 +1.2958000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
PLOG / +2.6300000E-002  
+1.5000000E+030 -4.9500000E+000 +1.2958000E+004 /  
PLOG / +1.2000000E-001  
+7.2000000E+028 -4.4900000E+000 +1.4273000E+004 /  
PLOG / +1.0000000E+000  
+1.2000000E+022 -2.4400000E+000 +1.3654000E+004 /  
C2H3+C2H3<=>C4H5-N+H  
+1.1000000E+024 -3.2800000E+000 +1.2395000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
PLOG / +2.6300000E-002  
+1.1000000E+024 -3.2800000E+000 +1.2395000E+004 /  
PLOG / +1.2000000E-001  
+4.6000000E+024 -3.3800000E+000 +1.4650000E+004 /  
PLOG / +1.0000000E+000  
+2.4000000E+020 -2.0400000E+000 +1.5361000E+004 /  
C4H5-N<=>C4H5-I  
+2.4000000E+060 -1.6080000E+001 +4.7500000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
PLOG / +1.3200000E-002  
+2.4000000E+060 -1.6080000E+001 +4.7500000E+004 /  
PLOG / +2.6300000E-002  
+1.3000000E+062 -1.6380000E+001 +4.9600000E+004 /  
PLOG / +1.2000000E-001  
+4.9000000E+066 -1.7260000E+001 +5.5400000E+004 /  
PLOG / +1.0000000E+000  
+1.5000000E+067 -1.6890000E+001 +5.9100000E+004 /  
PLOG / +1.0000000E+001  
+2.0000000E+060 -1.4460000E+001 +5.8600000E+004 /  
C4H4+H<=>C4H5-N  
+1.2000000E+051 -1.2570000E+001 +1.2300000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
PLOG / +1.3200000E-002  
+1.2000000E+051 -1.2570000E+001 +1.2300000E+004 /  
PLOG / +2.6300000E-002  
+4.2000000E+050 -1.2340000E+001 +1.2500000E+004 /  
PLOG / +1.2000000E-001  
+1.1000000E+050 -1.1940000E+001 +1.3400000E+004 /  
PLOG / +1.0000000E+000  
+1.3000000E+051 -1.1920000E+001 +1.6500000E+004 /  
PLOG / +1.0000000E+001  
+6.2000000E+045 -1.0080000E+001 +1.5800000E+004 /  
C4H4+H<=>C4H5-I  
+6.1000000E+053 -1.3190000E+001 +1.4200000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
PLOG / +1.3200000E-002  
+6.1000000E+053 -1.3190000E+001 +1.4200000E+004 /  
PLOG / +2.6300000E-002  
+9.6000000E+052 -1.2850000E+001 +1.4300000E+004 /  
PLOG / +1.2000000E-001  
+2.1000000E+052 -1.2440000E+001 +1.5500000E+004 /

PLOG / +1.0000000E+000  
+4.9000000E+051 -1.1920000E+001 +1.7700000E+004 /  
PLOG / +1.0000000E+001  
+1.5000000E+048 -1.0580000E+001 +1.8800000E+004 /  
!

---

!\REACTIONCLASS: \R\_R\_PRODUCTS \A  
\N \EA  
!

---

---

C4H5-N+H<=>C4H5-I+H  
+3.1000000E+026 -3.3500000E+000 +1.7423000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+H<=>C4H4+H2  
+1.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+OH<=>C4H4+H2O  
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+HCO<=>C4H6+CO  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+HO2=>C2H3+CH2CO+OH  
+6.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+O2<=>CH2CHCHCHO+O  
+3.0000000E+011 +2.9000000E-001 +1.1000000E+001 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+O2<=>HCO+C2H3CHO  
+9.2000000E+016 -1.3900000E+000 +1.0100000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-N+O2=>H+CO+C2H3CHO  
+5.1900000E+015 -1.2600000E+000 +3.3126200E+003 !<BASED ON C2H3+O2 FROM  
KLIPPENSTEIN>  
!\C2  
C4H5-I+H<=>C4H4+H2  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-I+H<=>C3H3+CH3  
+2.0000000E+013 +0.0000000E+000 +2.0000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-I+OH<=>C4H4+H2O  
+4.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-I+HCO<=>C4H6+CO  
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-I+HO2=>C2H3+CH2CO+OH  
+6.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-I+O2<=>CH2CO+CH2CHO  
+2.1600000E+010 +0.0000000E+000 +2.5000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-2<=>C4H5-I  
+1.5000000E+067 -1.6890000E+001 +5.9100000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H5-2+H<=>C4H5-I+H  
+3.1000000E+026 -3.3500000E+000 +1.7423000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-2+HO2=>OH+C2H2+CH3CO  
+8.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-2+O2<=>CH3CO+CH2CO  
+2.1600000E+010 +0.0000000E+000 +2.5000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-2+OH<=>CH2OH+C3H3  
+3.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H5-2+O<=>CH2O+C3H3  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

---

!\REACTIONCLASS: \AROMATIC\_GROWTH \A  
\N \EA  
!

---

---

C4H6+C2H3=>C6H6+H2+H  
+5.6200000E+011 +0.0000000E+000 +3.2400000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H5-I+C2H2<=>FULVENE+H  
+9.7380000E+026 -3.7600000E+000 +2.1329000E+004 !\AUTHOR: !\  
10ATM/SENOSIAIN&MILLER, J.PHYS.CHEM.A, 2007, PP. 3740-3747 !\COMMENT:  
C4H5-N+C2H2<=>FULVENE+H  
+1.7400000E+019 -1.8600000E+000 +1.2384000E+004 !\AUTHOR: !\  
10ATM/SENOSIAIN&MILLER, J.PHYS.CHEM.A, 2007, PP. 3740-3747 !\COMMENT:  
C4H5-N+C2H2<=>C6H6+H  
+1.6000000E+016 -1.3300000E+000 +5.4000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H5-N+C2H3<=>C6H6+H2 +1.8400000E-  
013 +7.0700000E+000 -3.6110000E+003 !\AUTHOR: !\REF:LASKIN ET AL. IJCK  
32 589-614 2000 !\COMMENT:  
C4H5-2+C2H<=>C3H3+C3H3  
+4.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\ JAM6  
!\COMMENT:  
C4H5-2+C2H2<=>C6H6+H  
+5.0000000E+014 +0.0000000E+000 +2.5000000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H5-2+C2H4<=>C5H6+CH3  
+5.0000000E+014 +0.0000000E+000 +2.5000000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
!

---

!\ENDSUBMECH: \C4H6

!

---

!\SUBMECH: \C4H612

!\MECHCOMMENTS:

!\MECHWARNINGS:

!

---

!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA

---

---

C4H612<=>C4H5-I+H  
+4.2000000E+015 +0.0000000E+000 +9.2600000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H612<=>C4H6  
+3.0000000E+013 +0.0000000E+000 +6.5000000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C3H3+CH3(+M)<=>C4H612(+M)  
+1.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
LOW /  
+2.6000000E+057 -1.1940000E+001 +9.7700000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +1.7500000E-001  
+1.3410000E+003 +6.0000000E+004 +9.7700000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA

---

---

C4H612+H<=>C4H5-I+H2  
+1.7000000E+005 +2.5000000E+000 +2.4900000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H612+CH3<=>C4H5-I+CH4  
+7.0000000E+013 +0.0000000E+000 +1.8500000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H612+O<=>C4H5-I+OH  
+1.8000000E+011 +7.0000000E-001 +5.8800000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H612+OH<=>C4H5-I+H2O  
+3.1000000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

---

---

!\REACTIONCLASS: \H\_CAT\_ISO \A  
\N \EA

---

---

C4H612+H<=>C4H6+H  
+2.0000000E+013 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

---

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA

---

---

C4H612+H<=>C3H4-A+CH3  
+2.0000000E+013 +0.0000000E+000 +2.0000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H612+H<=>C3H4-P+CH3  
+2.0000000E+013 +0.0000000E+000 +2.0000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\O \A  
\N \EA  
!

---

C4H612+O<=>CH2CO+C2H4  
+1.2000000E+008 +1.6500000E+000 +3.2700000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

!\ENDSUBMECH: \C4H612  
!

!\SUBMECH: \C4H6-2

!\MECHCOMMENTS: 2-BUTYNE SUBMECHANISM HAS LITTLE TO NO CHEMISTRY. 1-BUTYNE IS COMPLETELY ABSENT. KPS UPDATED MANY REACTIONS IN C4 MECHANISM AS PART OF FURANS WORK. THIS SHOULD BE INCORPORATED INTO MECHANISM WITH CWZ/YL WORK

!\MECHWARNINGS:  
!

---

C4H6-2<=>C4H6  
+3.0000000E+013 +0.0000000E+000 +6.5000000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H6-2<=>C4H612

+3.0000000E+013 +0.0000000E+000 +6.7000000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H6-2+H<=>C4H612+H

+2.0000000E+013 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H6-2+H<=>C4H5-2+H2

+3.4000000E+005 +2.5000000E+000 +2.4900000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H6-2+H<=>CH3+C3H4-P

+2.6000000E+005 +2.5000000E+000 +1.0000000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H6-2<=>H+C4H5-2

+5.0000000E+015 +0.0000000E+000 +8.7300000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

C4H6-2+CH3<=>C4H5-2+CH4

+1.4000000E+014 +0.0000000E+000 +1.8500000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

!\ENDSUBMECH: \C4H6-2  
!

!\SUBMECH: \C4H4



!\MECHCOMMENTS: THE C3H3+HCCO REACTION IS HARD TO FIND A LOCATION FOR.  
DOES THIS REACTION PROCEED THROUGH 1,3,4-PENTATRIENE-1-ONE? KPS HAS  
CHEMISTRY IN FURANS MECHANISM.

!\MECHWARNINGS:

!-----  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

C4H3-I+H<=>C4H4  
+3.4000000E+043 -9.0100000E+000 +1.2120000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

C4H4+H<=>C4H3-N+H2  
+6.6500000E+005 +2.5300000E+000 +1.2240000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H4+OH<=>C4H3-N+H2O  
+3.1000000E+007 +2.0000000E+000 +3.4300000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H4+H<=>C4H3-I+H2  
+3.3300000E+005 +2.5300000E+000 +9.2400000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H4+OH<=>C4H3-I+H2O  
+1.5500000E+007 +2.0000000E+000 +4.3000000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H4+CH3<=>C4H3-I+CH4  
+5.0000000E+013 +0.0000000E+000 +1.9800000E+004 !<KPS: HALF THE RATES  
OF ABSTRACTION FROM 1,3-BUTADIENE>  
C4H4+CH3<=>C4H3-N+CH4  
+1.0000000E+014 +0.0000000E+000 +2.2800000E+004 !<KPS: HALF THE RATES  
OF ABSTRACTION FROM 1,3-BUTADIENE>  
!

---

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA  
!

---

---

C3H3+CH2<=>C4H4+H  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!

---

---

!\REACTIONCLASS: \RADICAL\_ADDITION\O \A  
\N \EA  
!

---

---

C4H4+O<=>C3H3+HCO  
+6.0000000E+008 +1.4500000E+000 -8.6000000E+002 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

```

!
!
! \REACTIONCLASS: \RADICAL_ADDITION\OH \A
! \N \EA
!


---


C4H4+OH<=>CH2O+C3H3
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\ JAM
!\COMMENT:
!


---


! \REACTIONCLASS: \RADICAL_DECOMPOSITION \A
! \N \EA
!


---


C2H2+C2H(+M)<=>C4H3-N(+M)
+8.3000000E+010 +8.9900000E-001 -3.6300000E+002 !\AUTHOR: !\REF:
!\COMMENTS:
LOW /
+1.2400000E+031 -4.7180000E+000 +1.8710000E+003 / !LOW-PRESSURE-LIMIT
TROE / +1.0000000E+000
+1.0000000E+002 +5.6130000E+003 +1.3390000E+004 / !TROE PARAMETERS
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6
/ 3.000 / C2H2 / 2.500 / C2H4 / 2.500 / !3RD BODY COLLIDER EFFICIENCIES
C2H2+C2H(+M)<=>C4H3-I(+M)
+8.3000000E+010 +8.9900000E-001 -3.6300000E+002 !\AUTHOR: !\REF:
!\COMMENTS:
LOW /
+1.2400000E+031 -4.7180000E+000 +1.8710000E+003 / !LOW-PRESSURE-LIMIT
TROE / +1.0000000E+000
+1.0000000E+002 +5.6130000E+003 +1.3390000E+004 / !TROE PARAMETERS
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6
/ 3.000 / C2H2 / 2.500 / C2H4 / 2.500 / !3RD BODY COLLIDER EFFICIENCIES
C4H2+H<=>C4H3-N
+1.1000000E+042 -8.7200000E+000 +1.5300000E+004 !\AUTHOR: !\REF:LASKIN
ET AL. IJCK 32 589-614 2000 !\COMMENT:
C4H2+H<=>C4H3-I
+1.1000000E+030 -4.9200000E+000 +1.0800000E+004 !\AUTHOR: !\REF:
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
C4H3-N<=>C4H3-I
+4.1000000E+043 -9.4900000E+000 +5.3000000E+004 !\AUTHOR: !\REF:
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
!


---


! \REACTIONCLASS: \R_R_PRODUCTS \A
! \N \EA
!


---


C4H3-N+H<=>C4H3-I+H
+2.5000000E+020 -1.6700000E+000 +1.0800000E+004 !\AUTHOR: !\REF:
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
C4H3-N+H<=>C2H2+H2CC
+6.3000000E+025 -3.3400000E+000 +1.0014000E+004 !\AUTHOR: !\REF:
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:
C4H3-N+H<=>C4H4
+2.0000000E+047 -1.0260000E+001 +1.3070000E+004 !\AUTHOR: !\REF:
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

```

C4H3-N+H<=>C4H2+H2  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-N+OH<=>C4H2+H2O  
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-N+C2H3<=>C3H3+C3H3  
+4.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\ JAM6  
!\COMMENT:  
C3H3+CH<=>C4H3-I+H  
+5.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-I+H<=>C2H2+H2CC  
+2.8000000E+023 -2.5500000E+000 +1.0780000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-I+H<=>C4H2+H2  
+6.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-I+OH<=>C4H2+H2O  
+4.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-I+O2<=>HCCO+CH2CO  
+7.8600000E+016 -1.8000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
C4H3-I+CH2<=>C3H4-A+C2H  
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ZIEGLER  
ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005) !\COMMENT:  
!

---

!\REACTIONCLASS: \AROMATIC\_GROWTH \A  
\N \EA  
!

---

C4H4+C2H<=>L-C6H4+H  
+1.2000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT: WARNING: NOT SURE ON REFERENCE  
C4H3-N+C2H2<=>L-C6H4+H  
+2.5000000E+014 -5.6000000E-001 +1.0600000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H3-N+C2H2<=>C-C6H4+H  
+6.9000000E+046 -1.0010000E+001 +3.0100000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H3-N+C2H2<=>C6H5  
+9.6000000E+070 -1.7770000E+001 +3.1300000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H3-I+CH3<=>C5H6  
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ZIEGLER  
ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005) !\COMMENT:  
!

---

!\REACTIONCLASS: \MISCELLANEOUS \A  
\N \EA  
!

---

C3H3+HCCO<=>C4H4+CO  
+2.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:

!-----  
!-----  
!\ENDSUBMECH: \C4H4  
!-----  
!-----  
!\SUBMECH: \C4H2  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

---

H2CC+C2H2 (+M) <=> C4H4 (+M)  
+3.5000000E+005 +2.0550000E+000 -2.4000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
LOW /  
+1.4000000E+060 -1.2599000E+001 +7.4170000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +9.8000000E-001  
+5.6000000E+001 +5.8000000E+002 +4.1640000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / C2H2 / 3.000 / C2H4 / 3.000 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

---

!\REACTIONCLASS: \RADICAL\_ADDITION\OH \A  
\N \EA  
!

---

---

C2H2+C2H<=>C4H2+H  
+9.6000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H2+OH<=>H2C4O+H  
+6.6000000E+012 +0.0000000E+000 -4.1000000E+002 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C4H2+OH<=>CO+C3H3  
+2.5800000E+019 -2.4400000E+000 +3.0340000E+003 !\AUTHOR: !\ PROC COMB  
INST 31 185-193 (2007) !\COMMENT:  
H2C4O+H<=>C2H2+HCCO  
+5.0000000E+013 +0.0000000E+000 +3.0000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
H2C4O+OH<=>CH2CO+HCCO  
+1.0000000E+007 +2.0000000E+000 +2.0000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
!

---

---

!\REACTIONCLASS: \AROMATIC\_GROWTH \A  
\N \EA  
!

---

---

C4H2+C2H<=>C6H2+H  
+9.6000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

C4H2+C2H<=>C6H3  
+4.5000000E+037 -7.6800000E+000 +7.1000000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

!-----

!\ENDSUBMECH: \C4H2

!-----

!-----

!\SUBMECH: \NC3H7CHO

!\MECHCOMMENTS: THIS SUBMECH IS COMPLETELY STAND-ALONE WITHIN THE C4  
MODULE, THIS SPECIES IS NOT FORMED FROM ANY C4/C5 INTERMEDIATES. MATTEO  
PELUCCHI ALDEHYDES MECHANISMS NEED TO BE INCORPORATED.

!\MECHCOMMENTS: NAMING SCHEMES FOR PELUCCHI ALDEHYDE CHEMISTRY MAY BE  
DIFFERENT IN HIS MECHANISM

!\MECHWARNINGS:

!-----

!-----

!\REACTIONCLASS: \UNIMOL \A

\N \EA

!-----

!\WARNING: MATTEO PELUCCHI CHEMISTRY SHOULD BE INCORPORATED HERE?

!-----

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A

\N \EA

!-----

!\NC3H7CHO+O2<=>NC3H7CO+HO2 1.200E+005 2.500 37560.0 !\AUTHOR:

!\REF:ANALOGY WITH ACETALDEHYDE !\COMMENT:

!\NC3H7CHO+OH<=>NC3H7CO+H2O 2.000E+006 1.800 -1300.0 !\AUTHOR:

!\REF:ANALOGY WITH ACETALDEHYDE !\COMMENT:

!\NC3H7CHO+H<=>NC3H7CO+H2 4.140E+009 1.120 2320.0 !\AUTHOR: !\REF:ANALOGY  
WITH ACETALDEHYDE !\COMMENT:

!\NC3H7CHO+O<=>NC3H7CO+OH 5.940E+012 0.000 1868.0 !\AUTHOR: !\REF:ANALOGY  
WITH ACETALDEHYDE !\COMMENT:

!\NC3H7CHO+HO2<=>NC3H7CO+H2O2 4.090E+004 2.500 10200.0 !\AUTHOR:

!\REF:HALF OF CH2O+HO2 !\COMMENT:

!\NC3H7CHO+CH3<=>NC3H7CO+CH4 2.890E-003 4.620 3210.0 !\AUTHOR:

!\REF:ANALOGY WITH ACETALDEHYDE !\COMMENT:

!\NC3H7CHO+CH3O<=>NC3H7CO+CH3OH 1.000E+012 0.000 3300.0 !\AUTHOR:

!\REF:ANALOGY WITH ACETALDEHYDE !\COMMENT:

!\NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H 4.090E+004 2.500 10200.0 !\AUTHOR:

!\REF:PITZ ESTIMATE !\COMMENT:

NC3H7CHO+O2<=>NC3H7CO+HO2

+3.0100000E+013 +0.0000000E+000 +3.9150000E+004 !\AUTHOR:

!\REF:ANALOGY TO CH3CHO

NC3H7CHO+O<=>NC3H7CO+OH

+5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR:

!\REF:ANALOGY TO CH3CHO

NC3H7CHO+H<=>NC3H7CO+H2

+1.3100000E+005 +2.5800000E+000 +1.2200000E+003 !\AUTHOR:

!\REF:ANALOGY TO CH3CHO

NC3H7CHO+OH<=>NC3H7CO+H2O  
 +3.3700000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR:  
 !\REF:!ANALOGY TO CH3CHO  
 NC3H7CHO+HO2<=>NC3H7CO+H2O2  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR:  
 !\REF:!ANALOGY TO CH3CHO  
 NC3H7CHO+CH3<=>NC3H7CO+CH4 +7.0800000E-  
 004 +4.5800000E+000 +1.9660000E+003 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO  
 NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H  
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR:  
 !\REF:!ANALOGY TO CH3CHO  
 NC3H7CHO+OH<=>C3H6CHO-3+H2O  
 +5.5200000E+002 +3.1200000E+000 -1.1760000E+003 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+HO2<=>C3H6CHO-3+H2O2  
 +3.4400000E+012 +5.0000000E-002 +1.7880000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+CH3O2<=>C3H6CHO-3+CH3O2H  
 +3.4400000E+012 +5.0000000E-002 +1.7880000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+OH<=>C3H6CHO-2+H2O  
 +4.6800000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+HO2<=>C3H6CHO-2+H2O2  
 +9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+CH3O2<=>C3H6CHO-2+CH3O2H  
 +9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+OH<=>C3H6CHO-1+H2O  
 +5.2800000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+HO2<=>C3H6CHO-1+H2O2  
 +2.3790000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 NC3H7CHO+CH3O2<=>C3H6CHO-1+CH3O2H  
 +2.3790000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 !

---

!\REACTIONCLASS: \RADICAL\_DECOMP \A  
 \N \EA  
 !

---

NC3H7CO<=>NC3H7+CO  
 +1.0000000E+011 +0.0000000E+000 +9.6000000E+003 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 C2H5CHCO+H<=>C3H6CHO-3  
 +5.0000000E+012 +0.0000000E+000 +1.2000000E+003 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 C2H3CHO+CH3<=>C3H6CHO-3  
 +1.2300000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:CURRAN  
 ESTIMATE !\COMMENT:  
 C3H6CHO-1<=>C2H4+CH2CHO  
 +7.4000000E+011 +0.0000000E+000 +2.1970000E+004 !\AUTHOR: !\REF:REVERSE  
 ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95. !\COMMENT:  
 !=====

!\SUBSPECIES: \C2H5CHCO  
!  
=====

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

C2H5CHCO+OH<=>NC3H7+CO2  
+3.7300000E+012 +0.0000000E+000 -1.0100000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
C2H5CHCO+H<=>NC3H7+CO  
+4.4000000E+012 +0.0000000E+000 +1.4590000E+003 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:  
C2H5CHCO+O<=>C3H6+CO2  
+3.2000000E+012 +0.0000000E+000 -4.3700000E+002 !\AUTHOR: !\REF:CURRAN  
ESTIMATE !\COMMENT:

!  
=====

!\ENDSUBSPECIES: \C2H5CHCO  
!  
=====

!\SUBSPECIES: \SC3H5CHO  
!  
=====

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

SC3H5CHO<=>C3H6+CO  
+3.9000000E+014 +0.0000000E+000 +6.9000000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CO+H<=>SC3H5CHO  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
CH2CHCHCHO+H<=>SC3H5CHO  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: PITZ  
ESTIMATE !\COMMENT:  
!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

SC3H5CHO+OH<=>SC3H5CO+H2O  
+3.3700000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: !\REF:BILL  
ADDED !\COMMENT:  
SC3H5CHO+HO2<=>SC3H5CO+H2O2  
+1.0000000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H5CHO+X -->IC3H5CO+HX !\COMMENT:  
SC3H5CHO+CH3<=>SC3H5CO+CH4  
+3.9800000E+012 +0.0000000E+000 +8.7000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H5CHO+X -->IC3H5CO+HX !\COMMENT:

SC3H5CHO+O<=>SC3H5CO+OH  
+7.1800000E+012 +0.0000000E+000 +1.3890000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H5CHO+X -->IC3H5CO+HX !\COMMENT:  
SC3H5CHO+O2<=>SC3H5CO+HO2  
+4.0000000E+013 +0.0000000E+000 +3.7600000E+004 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H5CHO+X -->IC3H5CO+HX !\COMMENT:  
SC3H5CHO+H<=>SC3H5CO+H2  
+2.6000000E+012 +0.0000000E+000 +2.6000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H5CHO+X -->IC3H5CO+HX !\COMMENT:  
SC3H5CHO+C2H3<=>SC3H5CO+C2H4  
+1.1100000E+000 +3.5000000E+000 +4.6820000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CHO+H<=>CH2CHCHCHO+H2  
+1.7000000E+005 +2.5000000E+000 +2.4900000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CHO+O<=>CH2CHCHCHO+OH  
+5.2400000E+011 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CHO+OH<=>CH2CHCHCHO+H2O  
+4.4600000E+006 +2.0720000E+000 +1.0510000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CHO+CH3<=>CH2CHCHCHO+CH4  
+2.1000000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CHO+C2H3<=>CH2CHCHCHO+C2H4  
+2.2100000E+000 +3.5000000E+000 +4.6820000E+003 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!  
\_\_\_\_\_

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA  
!  
\_\_\_\_\_

SC3H5CHO+H<=>CH3+C2H3CHO  
+4.0000000E+021 -2.3900000E+000 +1.1180000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
SC3H5CHO+H<=>C3H6+HCO  
+4.0000000E+021 -2.3900000E+000 +1.1180000E+004 !\AUTHOR: !\REF:  
WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL. !\COMMENT:  
!  
\_\_\_\_\_

!\REACTIONCLASS: \R\_DECOMPOSITION \A  
\N \EA  
!  
\_\_\_\_\_

C3H5-S+CO<=>SC3H5CO  
+5.0000000E+012 +0.0000000E+000 +8.0000000E+003 !\AUTHOR: !\REF:PITZ  
ESTIMATE !\COMMENT:  
CH2CHCHCHO<=>C3H5-A+CO  
+6.1000000E+005 +9.2000000E-001 -1.1200000E+003 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 32: 498-522, 2000. !\COMMENT: SPECIES HAS BEEN RENAMED  
CH2CHCHCHO+O2<=>C2H3CHO+HOCO  
+1.2000000E+036 -7.2500000E+000 +3.3600000E+004 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 32: 498-522, 2000. !\COMMENT: SPECIES HAS BEEN RENAMED  
!  
=====  
=====  
!\ENDSUBSPECIES: \SC3H5CHO



!=====  
=====  
!=====  
=====  
!\\SUBSPECIES: \\C2H3COCH3  
!=====  
=====  
!

---

!\\REACTIONCLASS: \\RADICAL\_ADDITION \\A  
\\N \\EA  
!

---

C2H3COCH3+OH<=>CH3CHO+CH3CO  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\\AUTHOR: !\\REF:CURRAN  
ESTIMATE !\\COMMENT:  
C2H3COCH3+OH=>CH2CO+C2H3+H2O  
+5.1000000E+011 +0.0000000E+000 +1.1920000E+003 !\\AUTHOR: !\\REF:CURRAN  
ESTIMATE !\\COMMENT:  
C2H3COCH3+HO2=>CH2CHO+CH3CO+OH  
+6.0300000E+009 +0.0000000E+000 +7.9490000E+003 !\\AUTHOR: !\\REF:CURRAN  
ESTIMATE !\\COMMENT:  
C2H3COCH3+HO2=>CH2CO+C2H3+H2O2  
+8.5000000E+012 +0.0000000E+000 +2.0460000E+004 !\\AUTHOR: !\\REF:CURRAN  
ESTIMATE !\\COMMENT:  
C2H3COCH3+CH3O2=>CH2CHO+CH3CO+CH3O  
+3.9700000E+011 +0.0000000E+000 +1.7050000E+004 !\\AUTHOR: !\\REF:CURRAN  
ESTIMATE !\\COMMENT:  
C2H3COCH3+CH3O2=>CH2CO+C2H3+CH3O2H  
+3.0100000E+012 +0.0000000E+000 +1.7580000E+004 !\\AUTHOR: !\\REF:CURRAN  
ESTIMATE !\\COMMENT:

!=====  
=====  
!\\ENDSUBSPECIES: \\C2H3COCH3  
!=====  
=====  
!

!-----  
-----  
!\\ENDSUBMECH: \\NC3H7CHO  
!-----  
-----  
!-----  
-----  
!

!\\SUBMECH: \\C2H5COCH3  
!\\MECHCOMMENTS: KPS, 22/07/2015 THIS SUBMECH IS COMPLETELY STAND-ALONE  
WITHIN THE C4 MODULE, THIS SPECIES IS NOT FORMED FROM ANY C4  
INTERMEDIATES. IS THERE ANY REQUIREMENT TO HAVE IT IN?  
!\\MECHCOMMENTS: KPS HAS MORE DETAILED CHEMISTRY FOR C2H3COCH3 (METHYL  
VINYL KETONE) IN HIS FURANS MECHANISMS.  
!\\MECHWARNINGS:  
!-----  
-----  
!

---

!\\REACTIONCLASS: \\UNIMOL \\A  
\\N \\EA  
!

---

!\WARNING: REACTION CLASS MISSING?

!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA

---

C2H5COCH3+OH<=>CH2CH2COCH3+H2O  
+7.5500000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+HO2<=>CH2CH2COCH3+H2O2  
+2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995 !\COMMENT:  
C2H5COCH3+O<=>CH2CH2COCH3+OH  
+2.2500000E+013 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+H<=>CH2CH2COCH3+H2  
+9.1600000E+006 +2.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+O2<=>CH2CH2COCH3+HO2  
+2.0500000E+013 +0.0000000E+000 +5.1310000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+CH3<=>CH2CH2COCH3+CH4  
+3.1900000E+001 +3.1700000E+000 +7.1720000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3OH  
+2.1700000E+011 +0.0000000E+000 +6.4600000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995 !\COMMENT:  
C2H5COCH3+CH3O2<=>CH2CH2COCH3+CH3O2H  
+3.0100000E+012 +0.0000000E+000 +1.9380000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995 !\COMMENT:  
C2H5COCH3+C2H3<=>CH2CH2COCH3+C2H4  
+5.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+C2H5<=>CH2CH2COCH3+C2H6  
+5.0000000E+010 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 !\COMMENT:  
C2H5COCH3+OH<=>CH3CHCOCH3+H2O  
+8.4500000E+011 +0.0000000E+000 -2.2800000E+002 !\AUTHOR: !\REF:ANALOGY  
TO C2H5COC2H5+OH<=>PRODUCTS; CURRAN 1995 !\COMMENT:  
C2H5COCH3+HO2<=>CH3CHCOCH3+H2O2  
+2.0000000E+011 +0.0000000E+000 +8.6980000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+O<=>CH3CHCOCH3+OH  
+3.0700000E+013 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
C2H5COCH3+H<=>CH3CHCOCH3+H2  
+4.4600000E+006 +2.0000000E+000 +3.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+O2<=>CH3CHCOCH3+HO2  
+1.5500000E+013 +0.0000000E+000 +4.1970000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
C2H5COCH3+CH3<=>CH3CHCOCH3+CH4  
+1.7400000E+000 +3.4600000E+000 +3.6800000E+003 !\AUTHOR: !\REF:ANALOGY

TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3OH  
+1.4500000E+011 +0.0000000E+000 +2.7710000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+CH3O2<=>CH3CHCOCH3+CH3O2H  
+2.0000000E+012 +0.0000000E+000 +1.5250000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+C2H3<=>CH3CHCOCH3+C2H4  
+3.0000000E+011 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
C2H5COCH3+C2H5<=>CH3CHCOCH3+C2H6  
+3.0000000E+010 +0.0000000E+000 +8.6000000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
C2H5COCH3+OH<=>C2H5COCH2+H2O  
+5.1000000E+011 +0.0000000E+000 +1.1920000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995 !\COMMENT:  
C2H5COCH3+HO2<=>C2H5COCH2+H2O2  
+2.3800000E+004 +2.5500000E+000 +1.4690000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+O<=>C2H5COCH2+OH  
+5.0000000E+012 +0.0000000E+000 +5.9620000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995 !\COMMENT:  
C2H5COCH3+H<=>C2H5COCH2+H2  
+9.3000000E+012 +0.0000000E+000 +6.3570000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995 !\COMMENT:  
C2H5COCH3+O2<=>C2H5COCH2+HO2  
+2.0500000E+013 +0.0000000E+000 +4.9150000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
C2H5COCH3+CH3<=>C2H5COCH2+CH4  
+1.6200000E+011 +0.0000000E+000 +9.6300000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995 !\COMMENT:  
C2H5COCH3+CH3O<=>C2H5COCH2+CH3OH  
+2.1700000E+011 +0.0000000E+000 +4.6600000E+003 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+CH3O2<=>C2H5COCH2+CH3O2H  
+3.0100000E+012 +0.0000000E+000 +1.7580000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN  
1995 !\COMMENT:  
C2H5COCH3+C2H3<=>C2H5COCH2+C2H4  
+6.1500000E+010 +0.0000000E+000 +4.2780000E+003 !\AUTHOR: !\REF:ANALOGY  
TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995 !\COMMENT:  
C2H5COCH3+C2H5<=>C2H5COCH2+C2H6  
+5.0000000E+010 +0.0000000E+000 +1.1600000E+004 !\AUTHOR: !\REF:ANALOGY  
TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995  
!\COMMENT:  
!

---

!\REACTIONCLASS: \R\_DECOMP  
\N \EA

\A

!  
-----  
C2H3COCH3+H<=>CH3CHCOCH3  
+5.0000000E+012 +0.0000000E+000 +1.2000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H6CHO+X -->PRODUCTS !\COMMENT:  
CH3CHCO+CH3<=>CH3CHCOCH3  
+1.2300000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:ANALOGY  
WITH IC3H6CHO+X -->PRODUCTS !\COMMENT:  
C2H5COCH2<=>CH2CO+C2H5  
+1.0000000E+014 +0.0000000E+000 +3.5000000E+004 !\AUTHOR: !\REF: WKM  
19/ 04/ 2010 !\COMMENT:  
!

-----  
!\REACTIONCLASS: \R\_02 \A  
\N \EA  
!

-----  
CH3CHCOCH3+O2<=>CH3CHOOCH3  
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: CURRAN  
AND GAFFURI, 1995 !\COMMENT:  
CH3CHOOCH3<=>CH2CHOOHCOCH3  
+8.9000000E+012 +0.0000000E+000 +2.9700000E+004 !\AUTHOR: !\REF: CURRAN  
AND GAFFURI, 1995 !\COMMENT:  
C2H3COCH3+HO2<=>CH2CHOOHCOCH3  
+7.0000000E+010 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF: CURRAN  
AND GAFFURI, 1995 !\COMMENT:  
!

-----  
!\ENDSUBMECH: \C2H5COCH3  
!

-----  
!+++++  
!+++++  
!+++++  
!\END\_KINETICS\_MODULE: \C4  
!+++++  
!+++++  
!+++++  
!+++++  
!+++++  
!+++++  
!\KINETICS\_MODULE: \C5  
!\MODCOMMENTS:  
!\MODWARNINGS: KPS, 22/07/2015. WHEN COMBINING JBs PENTANE MECAHNISMS  
WITH CWs IC4H8 MECHANISMS I NOTICED THAT BOTH AUTHORS APPEAR TO HAVE  
UNIQUE AND DUPLICATE  
!\MODWARNINGS: CHEMICAL KINETICS FOR THE SPECIES "\AC5H10". THEREFORE, I  
HAVE SEPERATED THE C5 ALKENES/DIENES  
!\MODWARNINGS: AC5H10\BC5H10\CC5H10\B13DE2M INTO SEPERATE SUBMECHANISMS.  
I HAVE ALSO MOVED JBs AC5H10 KINETICS INTO CWs AC5H10 MECHANISM  
!\MODWARNINGS: PLEASE SEARCH FOR "!\WARNING: DUPLICATED KINETICS" TO  
FIND THIS.  
!\MODWARNINGS: THERE ARE ALSO OTHER REASONS WHY I HAVE DONE THIS RELATED  
TO THE FACT  
!\MODWARNINGS: RELATING TO THE FACT THAT THESE ISOMERS COULD BE IMPORTANT  
FOR GASOLINE SURROGATES AS THEY ARE REQUIRED TO ACCURATELY PREDICT  
!\MODWARNINGS: THE DISTILLATION CURVE (HOW MUCH FUEL HAS EVAPORATED AT A  
GIVEN TEMPERATURE) OF REAL FUELS.

```

!\MODWARNINGS: FOR THIS REASON, IT IS LIKELY THAT A REAL GASOLINE
SURROGATE NEEDS AT LEAST:
!\MODWARNINGS: HEPTANE/OCTANE/TOLUENE/IC4H8/C5H10/C2H5OH AND DI-
ISOBUTYLENE MECHANISMS TO PREDICT BOTH THE EVAPORATION AND CHEMICAL
KINETICS
!\MODWARNINGS: OF REAL FUELS.
!\MODWARNINGS: KPS, 22/07/2015. SOME REACTIONS HAVE BEEN INCORPORATED
INTO THIS MECHANISM FROM KWS C6/C7 MECHANISM. THERE ARE SOME "FLOATING"
SPECIES AND REACTIONS IN C5/C6/C7 ALKANES.
!\MODWARNINGS: MODELLERS NEED TO DISCUSS.
!\MODWARNINGS: SPECIES "C5H81-3" IS 1,3-PENTADIENE. THIS SPECIES IS
ALREADY IN AROMATIC MECAHNISM. MODELLERS NEED TO DISCUSS.
!\MODWARNINGS: JB, 06/10/2015. 2- AND 3-PENTANONE SUBMECHANISMS INCLUDED.
!\MODSUBMECHS:
!+++++
!+++++
!+++++
!-----
!\SUBMECH: \NC5H12
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!
!\REACTIONCLASS: \OTHER_DECOMPOSITIONS,ETC. \A
\N \EA
!
!\WARNING: KPS, NEED TO DISCUSS THESE SPECIES AND REACTIONS WITH JB
C5H81-3+OH<=>CH2O+C4H71-3
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H81-3+OH<=>C2H3CHO+C2H5
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H81-3+OH<=>CH3CHO+C3H5-S
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C4H7O1-4<=>CH2O+C3H5-A
+1.3260000E+021 -2.3490000E+000 +2.5084000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!16_03 !C4H8-1+OH<=>SC4H8OH-1 6.534E+015 -1.240 -71.0 !\AUTHOR: JB !\REF:
J. ZADOR, A. W. JASPER, J. A. MILLER, PHYS. CHEM. CHEM. PHYS., 2009, 11,
11040-11053 !\COMMENT: FIRST HPL TERM IN HIGH T FIT FOR HYDROXYL ADDITION
TO PROP
!-----
!\ENDSUBMECH: \NC5H12
!-----
!
!\SUBMECH: \C5H10-1\C5H10-2
!\MECHCOMMENTS: KPS, 22/07/2015 THERE SEVERAL REASONS WHY I HAVE ADDED
THE C5-ENES AS SUBMECHANISMS

```

!\MECHCOMMENTS: 1) SO THEY CAN BE EASILY RECOGNISED/SEPERATED FROM  
 OXIDATION PATHWAYS  
 !\MECHCOMMENTS: 2. THEY ARE COMPONENTS OF GASOLINES AND GOOD MODEL  
 COMPONENTS FOR GASOLINE SURROGATES, AND SO UPDATING THEIR CHEMISTRY WITH  
 MORE DETAIL BASED ON  
 !\MECHCOMMENTS: CWS IC4H8 MECHANISM COULD BE WORTHWILE, AS THEY ARE  
 REQUIRED TO ACCURATELY MODEL THE DISTILLATION CURVE OF A REAL FUEL AND  
 CAN BE USED AS  
 !\MECHCOMMENTS: SENSITIVITY INDUCING COMPONENT AS THEIR RON IS NOT EQUAL  
 MON. 1-PENTENE IS ALSO A GOOD CANDIDATE FOR SURROGATE FUELS.  
 !\MECHWARNINGS: KPS, 22/07/215 JB HAD PATHWAYS FORMING AC5H10 AND ITS  
 DERIVATIVES IN HIS PENTANE MECHANISM  
 !\MECHWARNINGS: THE SPECIES AC5H9-A2 APPEARS TO HAVE 4 REACTIONS IN JB's  
 PENTANES BUT NO FORMATION PATHWAYS.  
 !\MECHWARNINGS: CWZ APPEARS TO HAVE MUCH MORE DETAILED CHEMISTRY FOR  
 AC5H10 SO WE NEED TO DISCUSS C5H10 ISOMERS AS SEPERATE SUBMECHANISMS

!-----  
 !-----  
 !

---

!\REACTIONCLASS: \E\_UNIMOL \A  
 \N \EA  
 !

---

C5H10-1<=>C2H5+C3H5-A  
 +9.8640000E+021 -2.0860000E+000 +7.5060000E+004 !\AUTHOR: !\REF:  
 WARNING NO REFERENCE !\COMMENT: WARNING!  
 !ANALOGY WITH C3H5-A+CH3  
 C4H71-3+CH3(+M)<=>C5H10-2(+M)  
 +1.0000000E+014 -3.2000000E-001 -2.6230000E+002 !\AUTHOR: !\REF:  
 !\COMMENTS:  
 LOW /  
 +3.9100000E+060 -1.2810000E+001 +6.2500000E+003 / !LOW-PRESSURE-LIMIT  
 TROE / +1.0400000E-001  
 +1.6060000E+003 +6.0000000E+004 +6.1180000E+003 / !TROE PARAMETERS  
 H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
 / 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
 !

---

!\REACTIONCLASS: \E\_R\_ABSTRACTION \A  
 \N \EA  
 !

---

!\SITE: \PRIMARY  
 C5H10-1+O2<=>C5H91-5+HO2  
 +3.0000000E+013 +0.0000000E+000 +5.2290000E+004 !\AUTHOR: !\REF:  
 WARNING NO REFERENCE !\COMMENT: WARNING!  
 C5H10-1+O<=>C5H91-5+OH  
 +9.8000000E+005 +2.4300000E+000 +4.7500000E+003 !\AUTHOR: !\REF:  
 WARNING NO REFERENCE !\COMMENT: WARNING!  
 C5H10-1+H<=>C5H91-5+H2  
 +6.6500000E+005 +2.5400000E+000 +6.7560000E+003 !\AUTHOR: !\REF:  
 WARNING NO REFERENCE !\COMMENT: WARNING!  
 C5H10-1+OH<=>C5H91-5+H2O  
 +5.2700000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:  
 WARNING NO REFERENCE !\COMMENT: WARNING!

C5H10-1+HO2<=>C5H91-5+H2O2  
+2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3<=>C5H91-5+CH4 +4.5210000E-  
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF: WARNING NO  
REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3O<=>C5H91-5+CH3OH  
+2.1700000E+011 +0.0000000E+000 +6.4580000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3O2<=>C5H91-5+CH3O2H  
+2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+O2<=>C5H92-5+HO2  
+3.0000000E+013 +0.0000000E+000 +5.2290000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+O<=>C5H92-5+OH  
+9.8000000E+005 +2.4300000E+000 +4.7500000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+H<=>C5H92-5+H2  
+6.6510000E+005 +2.5400000E+000 +6.7560000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+OH<=>C5H92-5+H2O  
+5.2700000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+HO2<=>C5H92-5+H2O2  
+2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3<=>C5H92-5+CH4 +4.5210000E-  
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF: WARNING NO  
REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3O<=>C5H92-5+CH3OH  
+2.1700000E+011 +0.0000000E+000 +6.4580000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3O2<=>C5H92-5+CH3O2H  
+2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!\SITE: \SECONDARY  
C5H10-1+O2<=>C5H91-4+HO2  
+2.0000000E+013 +0.0000000E+000 +4.9640000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+O<=>C5H91-4+OH  
+5.5100000E+005 +2.4500000E+000 +2.8300000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+H<=>C5H91-4+H2  
+1.3000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+OH<=>C5H91-4+H2O  
+4.6700000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+HO2<=>C5H91-4+H2O2  
+9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3<=>C5H91-4+CH4  
+1.5100000E+000 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3O<=>C5H91-4+CH3OH  
+1.4500000E+011 +0.0000000E+000 +4.5710000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!

C5H10-1+CH3O2<=>C5H91-4+CH3O2H  
+9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!\SITE: \ALLYLIC\_PRIMARY  
C5H10-2+O2<=>C5H91-3+HO2  
+3.3000000E+012 +0.0000000E+000 +3.9900000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+O<=>C5H91-3+OH  
+4.4100000E+005 +2.4200000E+000 +3.1500000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+H<=>C5H91-3+H2  
+1.7300000E+005 +2.5000000E+000 +2.4920000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+OH<=>C5H91-3+H2O  
+3.1200000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+HO2<=>C5H91-3+H2O2  
+9.6390000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3<=>C5H91-3+CH4  
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3O<=>C5H91-3+CH3OH  
+9.0000000E+001 +2.9500000E+000 +1.1990000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3O2<=>C5H91-3+CH3O2H  
+9.6390000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!\SITE: \ALLYLIC\_SECONDARY  
C5H10-1+O2<=>C5H91-3+HO2  
+2.2000000E+012 +0.0000000E+000 +3.7220000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+O<=>C5H91-3+OH  
+6.6000000E+005 +2.4300000E+000 +1.2100000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+H<=>C5H91-3+H2  
+3.3760000E+005 +2.3600000E+000 +2.0700000E+002 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+OH<=>C5H91-3+H2O  
+2.7640000E+004 +2.6400000E+000 -1.9190000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+HO2<=>C5H91-3+H2O2  
+4.8200000E+003 +2.5500000E+000 +1.0530000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3<=>C5H91-3+CH4  
+3.6900000E+000 +3.3100000E+000 +4.0020000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3O<=>C5H91-3+CH3OH  
+4.0000000E+001 +2.9000000E+000 +8.6090000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-1+CH3O2<=>C5H91-3+CH3O2H  
+4.8200000E+003 +2.5500000E+000 +1.0530000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+O2<=>C5H92-4+HO2  
+2.2000000E+012 +0.0000000E+000 +3.7220000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!



C5H10-2+O<=>C5H92-4+OH  
+9.9000000E+005 +2.4300000E+000 +1.2100000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+H<=>C5H92-4+H2  
+3.3760000E+005 +2.3600000E+000 +2.0700000E+002 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+OH<=>C5H92-4+H2O  
+2.7640000E+004 +2.6400000E+000 -1.9190000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+HO2<=>C5H92-4+H2O2  
+4.8200000E+003 +2.5500000E+000 +1.0530000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3<=>C5H92-4+CH4  
+3.6900000E+000 +3.3100000E+000 +4.0020000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3O<=>C5H92-4+CH3OH  
+4.0000000E+001 +2.9000000E+000 +8.6090000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H10-2+CH3O2<=>C5H92-4+CH3O2H  
+4.8200000E+003 +2.5500000E+000 +1.0530000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

---

!\REACTIONCLASS: \E\_RADICAL\_BETA\_SCISSION \A  
\N \EA  
!

---

C4H6+CH3<=>C5H91-3  
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H81-3+H<=>C5H91-3  
+2.5000000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C3H6+C2H3<=>C5H91-4  
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C2H4+C3H5-A<=>C5H91-5  
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H81-3+H<=>C5H92-4  
+4.2400000E+011 +5.1000000E-001 +1.2300000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C2H4+C3H5-S<=>C5H92-5  
+2.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

---

!\REACTIONCLASS: \PEROXYL\_ADDITION \A  
\N \EA  
!

---

C5H9O1-3+OH<=>C5H91-3+HO2  
+6.0880000E+015 -1.0700000E+000 +1.5720000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O1-3+CH3O<=>C5H91-3+CH3O2  
+5.9460000E+017 -1.6500000E+000 +2.0480000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!

C5H9O1-3+C2H5O<=>C5H91-3+C2H5O2  
+3.8930000E+014 -7.2000000E-001 +1.8330000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O2-4+OH<=>C5H92-4+HO2  
+7.0270000E+015 -1.2400000E+000 +1.5890000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O2-4+CH3O<=>C5H92-4+CH3O2  
+6.8630000E+017 -1.8200000E+000 +2.0650000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O2-4+C2H5O<=>C5H92-4+C2H5O2  
+4.4930000E+014 -8.9000000E-001 +1.8490000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

---

!\REACTIONCLASS: \ALLYLOXY\_RADICAL\_BETA\_SCISSION \A  
\N \EA  
!

---

C5H9O1-3<=>C2H3CHO+C2H5  
+3.1310000E+019 -1.8500000E+000 +1.0670000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O1-3<=>C2H5CHO+C2H3  
+1.4170000E+018 -1.5600000E+000 +2.3340000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O2-4<=>SC3H5CHO+CH3  
+5.9830000E+015 -1.1300000E+000 +9.9410000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
C5H9O2-4<=>CH3CHO+C3H5-S  
+1.0730000E+022 -2.6600000E+000 +2.9650000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

!\ENDSUBMECH: \C5H10-1\C5H10-2  
!

!\SUBMECH: \CC5H10\BC5H10

!\MECHCOMMENTS:

!\MECHWARNINGS: KPS, 22/07/2015 REACTION CLASS \E\_RADICAL\_BETA\_SCISSION IS EMPTY

!\MECHWARNINGS: KPS, 22/07/2015 WHEN COMBINING JBS PENTANE WITH CWS ISO-BUTENE KPS NOTICED THAT BOTH MECAHNISMS HAVE COMMON REACTIONS

!\MECHWARNINGS: FOR AC5H10 AND BOTH AUTHORS ARE USING DIFFERENT KINETIC PARAMETERS. THIS WILL HAVE TO BE DISCUSSED

!\MECHWARNINGS: I HAVE COMBINED JOHNS AC5H10 REACTIONS WITH CWS AND SEPERATED THEM INTO THEIR REACTION CLASSES MEANING THAT SOME REACTIONS

!\MECHWARNINGS: HAVE BEEN REMOVED FROM THIS SUBMECHANISM. EACH RATE CONSTANT IS COMMENTED

!\MECHWARNINGS: SEARCH FOR "!\WARNING: DUPLICATED KINETICS" AT THE TOP OF THE AC5H10 SUBMECH. IT LOOKS LIKE CWS KINETICS ARE MUCH MORE DETAILED.

!

---

!\REACTIONCLASS: \E\_UNIMOL \A  
\N \EA

!  
-----  
BC5H10<=>C4H72-2+CH3  
+1.2170000E+023 -1.9260000E+000 +1.0140000E+005 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10<=>IC4H7+CH3  
+2.6100000E+019 -1.0170000E+000 +7.9020000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!ANALOGY WITH C3H5-A+CH3  
C4H71-3+CH3 (+M) <=> CC5H10 (+M)  
+1.0000000E+014 -3.2000000E-001 -2.6230000E+002 !\AUTHOR: !\REF:  
!\COMMENTS:  
LOW /  
+3.9100000E+060 -1.2810000E+001 +6.2500000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +1.0400000E-001  
+1.6060000E+003 +6.0000000E+004 +6.1180000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

-----  
!\REACTIONCLASS: \E\_R\_ABSTRACTION \A  
\N \EA  
!

-----  
!\SITE: \PRIMARY  
CC5H10+H<=>CC5H9-A+H2  
+3.9000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+OH<=>CC5H9-A+H2O  
+1.4000000E+008 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+HO2<=>CC5H9-A+H2O2  
+2.8920000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+CH3<=>CC5H9-A+CH4  
+4.5300000E+000 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+CH3O<=>CC5H9-A+CH3OH  
+4.3500000E+011 +0.0000000E+000 +4.5710000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+CH3O2<=>CC5H9-A+CH3O2H  
+2.8920000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!\SITE: \ALLYLIC\_PRIMARY  
BC5H10+H<=>AC5H9-C+H2  
+3.4600000E+005 +2.5000000E+000 +2.4920000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+H<=>CC5H9-B+H2  
+1.7300000E+005 +2.5000000E+000 +2.4920000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+OH<=>AC5H9-C+H2O  
+6.2400000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+OH<=>CC5H9-B+H2O  
+3.1200000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!

BC5H10+HO2<=>AC5H9-C+H2O2  
+1.9280000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+HO2<=>CC5H9-B+H2O2  
+9.6390000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+CH3<=>AC5H9-C+CH4  
+4.4200000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+CH3<=>CC5H9-B+CH4  
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+CH3O<=>AC5H9-C+CH3OH  
+1.8000000E+002 +2.9500000E+000 +1.1990000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+CH3O<=>CC5H9-B+CH3OH  
+9.0000000E+001 +2.9500000E+000 +1.1990000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+CH3O2<=>AC5H9-C+CH3O2H  
+1.9280000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
BC5H10+CH3O2<=>CC5H9-B+CH3O2H  
+9.6390000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!\SITE: \ALLYLIC\_TERTIARY  
CC5H10+H<=>CC5H9-B+H2  
+2.6500000E+006 +2.2000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+OH<=>CC5H9-B+H2O  
+6.1400000E+002 +3.2000000E+000 -3.5000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+HO2<=>CC5H9-B+H2O2  
+1.8100000E+003 +2.5000000E+000 +7.1540000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+CH3<=>CC5H9-B+CH4  
+4.6130000E+000 +3.1000000E+000 +2.3300000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+CH3O<=>CC5H9-B+CH3OH  
+1.0000000E+001 +2.8500000E+000 +5.2310000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+CH3O2<=>CC5H9-B+CH3O2H  
+1.8100000E+003 +2.5000000E+000 +7.1540000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

---

!\REACTIONCLASS: \WADDINGTON \A  
\N \EA  
!

---

BC5H10+OH<=>IC3H7+CH3CHO  
+2.0000000E+010 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
CC5H10+OH<=>IC4H9+CH2O  
+2.0000000E+010 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

---

!\REACTIONCLASS: \PEROXYL\_ADDITION \A  
\N \EA  
!

---

CC5H9-B+HO2<=>CC5H9O-B+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
CC5H9-B+CH3O2<=>CC5H9O-B+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
CC5H9-B+C2H5O2<=>CC5H9O-B+C2H5O  
+9.6400000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!

---

!\REACTIONCLASS: \ALLYLOXY\_RADICAL\_BETA\_SCISSION \A  
\N \EA  
!

---

AC5H9-D<=>AC5H9-A2  
+1.1130000E+012 +0.0000000E+000 +3.1700000E+004 !\AUTHOR: !\REF:  
WARNING NO REFERENCE !\COMMENT: WARNING!  
!-----  
!\ENDSUBMECH: \BC5H10\CC5H10  
!-----  
!\SUBMECH: \AC5H10  
!\MECHCOMMENTS: AC5H10 SUBMECH CONTAINS B13DE2M (BUTA-1,3-DIENE-2-METHYL  
OR 2-METHYL-1,3-BUTADIENE AS A SUBMECH BELOW  
!\MECHCOMMENTS: IF SIMULATING IC4H10, AC5H10 SUBMECHANISM IN C5-MODULE IS  
NECESSARY ALONG WITH B13DE2M SUBMECH.  
!\MECHWARNINGS: KPS, 22/07/2015 WHEN COMBINING JB'S PENTANE WITH CWS ISO-  
BUTENE KPS NOTICED THAT BOTH MECHANISMS HAVE COMMON REACTIONS  
!\MECHWARNINGS: FOR AC5H10 AND BOTH AUTHORS ARE USING DIFFERENT KINETIC  
PARAMETERS. THIS WILL HAVE TO BE DISCUSSED  
!\MECHWARNINGS: I HAVE COMBINED JOHN'S AC5H10 REACTIONS WITH CWS AND  
SEPERATED THEM INTO THEIR REACTION CLASSES. EACH RATE CONSTANT IS  
COMMENTED  
!\MECHWARNINGS: SEARCH FOR "!\WARNING: DUPLICATED KINETICS" AT THE TOP  
OF THE AC5H10 SUBMECH. IT LOOKS LIKE CWS KINETICS ARE MUCH MORE DETAILED.  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

AC5H10<=>C3H5-T+C2H5  
+8.9220000E+024 -2.4090000E+000 +1.0050000E+005 !\AUTHOR: KPS, THIS  
REACTION IS FROM CWS IC4H8  
IC4H7+CH3(+M)<=>AC5H10(+M)  
+1.5000000E+014 -3.2000000E-001 -2.6230000E+002 !\AUTHOR: KPS, THIS  
REACTION IS FROM CWS IC4H8

LOW /  
+5.8650000E+060 -1.2810000E+001 +6.2500000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +1.0400000E-001  
+1.6060000E+003 +6.0000000E+004 +6.1180000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

AC5H10+H<=>AC5H9-A2+H2  
+1.7300000E+005 +2.5000000E+000 +2.4920000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+O<=>AC5H9-A2+OH  
+3.7000000E+005 +2.5600000E+000 -1.1300000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+OH<=>AC5H9-A2+H2O  
+3.1200000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+HO2<=>AC5H9-A2+H2O2  
+9.6390000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3<=>AC5H9-A2+CH4  
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3O2<=>AC5H9-A2+CH3O2H  
+9.6390000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3O<=>AC5H9-A2+CH3OH  
+9.0000000E+001 +2.9500000E+000 +1.1990000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+H<=>AC5H9-C+H2  
+3.3760000E+005 +2.3600000E+000 +2.0700000E+002 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+OH<=>AC5H9-C+H2O  
+2.7640000E+004 +2.6400000E+000 -1.9190000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+HO2<=>AC5H9-C+H2O2  
+4.8200000E+003 +2.5500000E+000 +1.0530000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3<=>AC5H9-C+CH4  
+3.6900000E+000 +3.3100000E+000 +4.0020000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3O2<=>AC5H9-C+CH3O2H  
+4.8200000E+003 +2.5500000E+000 +1.0530000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3O<=>AC5H9-C+CH3OH  
+4.0000000E+001 +2.9000000E+000 +8.6090000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+H<=>AC5H9-D+H2  
+1.9500000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+OH<=>AC5H9-D+H2O  
+7.0100000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:

AC5H10+CH3<=>AC5H9-D+CH4  
+2.2700000E+000 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+HO2<=>AC5H9-D+H2O2  
+1.4500000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3O<=>AC5H9-D+CH3OH  
+2.1800000E+011 +0.0000000E+000 +4.5710000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+CH3O2<=>AC5H9-D+CH3O2H  
+1.4500000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

AC5H9-A2<=>C3H4-A+C2H5  
+1.9830000E+020 -1.6300000E+000 +5.9240000E+004 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
B13DE2M+H<=>AC5H9-C  
+4.0000000E+013 +0.0000000E+000 +1.3000000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
C4H612+CH3<=>AC5H9-C  
+1.7600000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275. EXTERNAL CH3 ATOM  
ADDITION TO PROPENE  
B13DE2M+H<=>AC5H9-D  
+2.5000000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275. INTERNAL H ATOM  
ADDITION TO PROPENE  
AC5H9-D<=>C3H5-T+C2H4  
+1.2200000E+012 +6.4000000E-001 +2.9370000E+004 !\AUTHOR: !\REF:CURRAN  
IJCK, 2006, 38, 250-275.  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

!\WARNING: DUPLICATED KINETICS

AC5H10+OH<=>SC4H9+CH2O  
+2.0000000E+010 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: KPS, THIS  
REACTION IS FROM CWS IC4H8  
AC5H10+O<=>SC4H9+HCO  
+7.2300000E+005 +2.3400000E+000 -1.0500000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+O<=>IC3H7+CH3CO  
+7.2300000E+005 +2.3400000E+000 -1.0500000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
AC5H10+O<=>IC4H9+HCO  
+7.2300000E+005 +2.3400000E+000 -1.0500000E+003 !\AUTHOR: !\REF:FROM  
LLNL C8-C16 N-ALKANES MECH !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_RO2 \A  
\N \EA

!

---

!\WARNING: DUPLICATED REACTIONS THESE ARE NO DUPLICATES, BUT WE ALL NEED TO DISCUSS COMBINING THESE REACTIONS

AC5H9-C+HO2<=>AC5H9O-C+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: KPS, THIS REACTION IS FROM CWS IC4H8

AC5H9-C+CH3O2<=>AC5H9O-C+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: KPS, THIS REACTION IS FROM CWS IC4H8

AC5H9-C+C2H5O2<=>AC5H9O-C+C2H5O  
+9.6400000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: KPS, THIS REACTION IS FROM JBS PENTANE

CH3CHO+C3H5-T<=>AC5H9O-C  
+9.4500000E+002 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: J. P. ORME, H. J. CURRAN,\* AND J. M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131.  
INTERNAL ADDITION TWO LARGE SPECIES

AC5H9-C+HO2<=>B2E2M1OJ+OH  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH !\COMMENT:

AC5H9-C+CH3O2<=>B2E2M1OJ+CH3O  
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH !\COMMENT:

CH2O+C4H72-2<=>B2E2M1OJ  
+8.8000000E+003 +2.4800000E+000 +6.1000000E+003 !\AUTHOR: !\REF: J. P. ORME, H. J. CURRAN,\* AND J. M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-131. INTERNAL ADDITION TWO LARGE SPECIES !\COMMENT:

!-----  
!-----  
!\ENDSUBMECH: \AC5H10  
!-----  
!-----  
!\SUBMECH: \B13DE2M  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----  
!-----

---

!\REACTIONCLASS: \UNIMOL \A  
\n \EA  
!

---

C2H3+C3H5-T<=>B13DE2M  
+8.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:  
H+B13DE2MJ<=>B13DE2M  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:  
!\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\n \EA  
!

---



B13DE2M+H<=>B13DE2MJ+H2  
+3.6440000E+005 +2.4550000E+000 +4.3612000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
B13DE2M+O2<=>B13DE2MJ+HO2  
+5.9600000E+019 -1.6700000E+000 +4.6192100E+004 !\AUTHOR: !\REF:  
!\COMMENT:  
B13DE2M+OH<=>B13DE2MJ+H2O  
+4.4600000E+006 +2.0720000E+000 +1.0508000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
B13DE2M+HO2<=>B13DE2MJ+H2O2 +3.0700000E-  
002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: !\COMMENT:  
B13DE2M+CH3<=>B13DE2MJ+CH4  
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:  
!\COMMENT:  
B13DE2M+CH3O2<=>B13DE2MJ+CH3O2H +7.6800000E-  
002 +4.4030000E+000 +1.3547200E+004 !\AUTHOR: !\REF: !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

C2H3+C3H4-A<=>B13DE2MJ  
+9.4500000E+002 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: !\REF: J. P.  
ORME, H. J. CURRAN,\* AND J. M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-  
131. INTERNAL ADDITION TWO LARGE SPECIES  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION\H \A  
\N \EA  
!

---

B13DE2M+H<=>CC5H9-B  
+4.2400000E+011 +5.1000000E-001 +1.2300000E+003 !\AUTHOR: !\REF:H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275. EXTERNAL H ATOM  
ADDITION TO PROPENE  
B13DE2M+H<=>CC5H9-A  
+2.5000000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275. INTERNAL H ATOM  
ADDITION TO PROPENE  
B12DE3M+H<=>CC5H9-B  
+4.2400000E+011 +5.1000000E-001 +1.2300000E+003 !\AUTHOR: !\REF:H.J.  
CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275. EXTERNAL H ATOM  
ADDITION TO PROPENE  
C2H3+C3H6<=>CC5H9-A  
+9.4500000E+002 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: !\REF: J. P.  
ORME, H. J. CURRAN,\* AND J. M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-  
131. INTERNAL ADDITION TWO LARGE SPECIES  
!

---

!\REACTIONCLASS: \R\_RO2 \A  
\N \EA  
!

---

C2H3+CH3COCH3<=>CC5H9O-B  
+9.4500000E+002 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: !\REF: !J. P.  
ORME, H. J. CURRAN,\* AND J. M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-  
131. INTERNAL ADDITION TWO LARGE SPECIES\COMMENT:

```

CC5H9-B+HO2<=>B2E3M1OJ+OH
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003   !\AUTHOR: !\REF:
!\COMMENT:
CC5H9-B+CH3O2<=>B2E3M1OJ+CH3O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003   !\AUTHOR: !\REF:
!\COMMENT:
CH2O+IC4H7-I1<=>B2E3M1OJ
+8.8000000E+003 +2.4800000E+000 +6.1000000E+003   !\AUTHOR: !\REF:J. P.
ORME, H. J. CURRAN,* AND J. M. SIMMIE J. PHYS. CHEM. A 2006, 110, 114-
131. INTERNAL ADDITION TWO LARGE SPECIES
!-----
!\ENDSUBMECH: \B13DE2M
!-----
!-----
!\SUBMECH: \TC4H8CHO
!\MECHCOMMENTS: KPS, 22/07/2015 NOT SURE WHY THIS IS INCLUDED IN
MECHANISM AS THERE ARE NO OBVIOUS FORMATION PATHWAYS
!\MECHWARNINGS:
!-----
!-----
!\REACTIONCLASS: \RADICAL_DECOMPOSITION           \A
\N           \EA
!-----

TC4H8CHO<=>IC3H5CHO+CH3
+1.0000000E+013 +0.0000000E+000 +2.6290000E+004   !\AUTHOR: !\REF:REVERSE
ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95 !\COMMENT:
TC4H8CHO<=>IC4H8+HCO
+8.5200000E+012 +0.0000000E+000 +2.0090000E+004   !\AUTHOR: !\REF:REVERSE
ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95 !\COMMENT:
!-----

!\REACTIONCLASS: \R_O2_PRODUCTS                   \A
\N           \EA
!-----

TC4H8CHO+O2<=>O2C4H8CHO
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:CURRAN
ESTIMATE !\COMMENT:
O2C4H8CHO<=>O2HC4H8CO
+2.1600000E+011 +0.0000000E+000 +1.5360000E+004   !\AUTHOR: !\REF:CURRAN
ESTIMATE !\COMMENT:
IC4H8O2H-T+CO<=>O2HC4H8CO
+1.5000000E+011 +0.0000000E+000 +4.8090000E+003   !\AUTHOR: !\REF:CURRAN
ESTIMATE !\COMMENT:
!-----
!\ENDSUBMECH: \TC4H8CHO
!-----
!+++++
+++++
+++++

```

```
!\END_KINETICS_MODULE: \C5
!+++++
!+++++
!+++++
!+++++
!+++++
!\KINETICS_MODULE: \C6
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS: \NC6H14 \C6H12-1 \C6H12-2 \C6H12-3 \NC5H11CHO \C6H10-15
!+++++
!+++++
!-----
!\SUBMECH: \C6H101-5
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!
```

---

```
!\REACTIONCLASS: \UNIMOL \A
\N \EA
!
```

---

---

```
C6H101-5<=>C3H5-A+C3H5-A
+4.9000000E+022 -2.0600000E+000 +6.3355500E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
PLOG / +1.0000000E+000
+5.0700000E+047 -9.7000000E+000 +7.2680000E+004 /
PLOG / +4.0000000E+000
+4.2200000E+039 -7.3000000E+000 +6.9390000E+004 /
PLOG / +1.0000000E+001
+2.1200000E+035 -6.0000000E+000 +6.7620000E+004 /
!
```

---

---

```
!\REACTIONCLASS: \RH_R_ABSTRACTION \A
\N \EA
!
```

---

---

```
C6H101-5+H<=>C6H9-A+H2
+6.7520000E+005 +2.3600000E+000 +2.0700000E+002 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+O2<=>C6H9-A+HO2
+4.0000000E+014 +0.0000000E+000 +3.8890000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+O<=>C6H9-A+OH
+1.3200000E+006 +2.4300000E+000 +1.2100000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+OH<=>C6H9-A+H2O
+5.5280000E+004 +2.6400000E+000 -1.9190000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+CH3<=>C6H9-A+CH4
+7.3800000E+000 +3.3100000E+000 +4.0020000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
```

```

!
-----
!\REACTIONCLASS:  \RADICAL_DECOMPOSITION          \A
\N                \EA
!
-----

C4H6+C2H3<=>C6H9-A
+8.8000000E+005 +2.5000000E+000 +6.1300000E+003    !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
!
-----

!\REACTIONCLASS:  \RADICAL_ADDITION\H          \A
\N                \EA
!
-----

C6H101-5+H=>C3H4-A+C3H5-A+H2
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000    !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C6H101-5+H<=>C3H5-A+C3H6
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000    !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
!-----
!-----
!\ENDSUBMECH:  \C6H101-5
!-----
!-----
!+++++
!+++++
!+++++
!\COMMENTS:
!\WARNINGS:
!\END_KINETICS_MODULE:  \C6
!+++++
!+++++
!+++++
!+++++
!+++++
!\KINETICS_MODULE:  \AROMATIC
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
!+++++
!+++++
!+++++
!-----
!-----
!\SUBMECH:  \CORE_TO_AROMATIC_LINKERS
!\MECHCOMMENTS:  THESE REACTIONS MAY FORM A LINK BETWEEN THE C2/C3/C4
MECHANISM AND THE AROMATIC MECHANISM. THEY ARE STANDALONE WITHIN AROMATIC
MODULE, BUT ARE REQUIRED IF ADDING AROMATIC CHEMISTRY TO THE CORE
MECHANISM.
!\MECHCOMMENTS:  PROBABLY NEED A BETTER NAME FOR THIS SUBMECH.
!\MECHWARNINGS:
!-----
!-----
!
-----

```

!\REACTIONCLASS: \MISC \A  
\N \EA  
!

---

L-C6H4+H<=>C-C6H4+H  
+1.4000000E+054 -1.1700000E+001 +3.4500000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C-C6H4+H<=>C6H5  
+2.4000000E+060 -1.3660000E+001 +2.9500000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
L-C6H4+H<=>C6H5  
+1.7000000E+078 -1.9720000E+001 +3.1400000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C6H3+H<=>L-C6H4  
+3.4000000E+043 -9.0100000E+000 +1.2120000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
L-C6H4+H<=>C6H3+H2  
+1.3300000E+006 +2.5300000E+000 +9.2400000E+003 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
L-C6H4+OH<=>C6H3+H2O  
+3.1000000E+006 +2.0000000E+000 +4.3000000E+002 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C6H2+H<=>C6H3  
+1.1000000E+030 -4.9200000E+000 +1.0800000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C6H3+H<=>C6H2+H2  
+3.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C6H3+OH<=>C6H2+H2O  
+4.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:  
C6H3+H<=>C4H2+C2H2  
+2.8000000E+023 -2.5500000E+000 +1.0780000E+004 !\AUTHOR: !\REF:LASKIN  
ET AL. IJCK 32 589-614 2000 !\COMMENT:

!-----  
!-----  
!\ENDSUBMECH: \CORE\_TO\_AROMATIC\_LINKERS  
!-----  
!-----  
!-----  
!-----  
!\SUBMECH: \C6H6  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

C6H5+H (+M) <=>C6H6 (+M)  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:WANG ET  
AL. C&F, 110: 173. 1994 !\COMMENT:  
LOW /  
+6.6000000E+075 -1.6300000E+001 +7.0000000E+003 / !LOW-PRESSURE-LIMIT

TROE / +1.0000000E+000 +1.0000000E-001 +5.8490000E+002 +6.1130000E+003 / !TROE PARAMETERS  
H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / !3RD  
BODY COLLIDER EFFICIENCIES  
FULVENE<=>C6H6  
+2.9500000E+031 -4.9700000E+000 +8.8470000E+004 !\AUTHOR:  
!\REF:PITZ2001 !\COMMENT:  
FULVENE<=>C6H5+H  
+8.5110000E+024 -2.5050000E+000 +1.1333000E+005 !\AUTHOR:  
!\REF:10ATM/MILLER&KLIPPENSTEIN, J.PHYS.CHEM.A, 2003, PP. 7783-7799  
!\COMMENT:  
!

---

!\REACTIONCLASS: \R\_CAT\_ISO \A  
\N \EA  
!

---

C6H6+H<=>FULVENE+H  
+8.4300000E+032 -4.9500000E+000 +5.1244000E+004 !\AUTHOR: !\REF:  
1997BUR/DVI505-514 !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

C6H6+H<=>C6H5+H2  
+2.5000000E+014 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:EMDEE  
ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 !\COMMENT:  
C6H6+O2<=>C6H5+HO2  
+6.3000000E+013 +0.0000000E+000 +6.0000000E+004 !\AUTHOR: !\REF:EMDEE  
ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 !\COMMENT:  
C6H6+O<=>C6H5+OH  
+2.0000000E+013 +0.0000000E+000 +1.4700000E+004 !\AUTHOR: !\REF:EMDEE  
ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 !\COMMENT:  
C6H6+OH<=>C6H5+H2O  
+1.2000000E+000 +4.1000000E+000 -3.0100000E+002 !\AUTHOR:  
!\REF:CHEN&BOZ J. PHYS. CHEM. A 108: 4632 - 4652 2004 !\COMMENT:  
C6H6+HO2<=>C6H5+H2O2  
+5.5000000E+012 +0.0000000E+000 +2.8900000E+004 !\AUTHOR:  
!\REF:ESTIMATED !\COMMENT:  
C6H6+CH3<=>C6H5+CH4  
+7.3200000E+012 +0.0000000E+000 +1.8920000E+004 !\AUTHOR:  
!\REF:ESTIMATED !\COMMENT:  
C6H5+CH2O<=>C6H6+HCO  
+8.5500000E+004 +2.1900000E+000 +3.8000000E+001 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA  
!

---

C6H5+HCO<=>C6H6+CO  
+8.5500000E+004 +2.1900000E+000 +3.8000000E+001 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:

```

!
-----
!\REACTIONCLASS:  \RADICAL_DECOMPOSITION          \A
\N                \EA
!
-----
C6H5=>H+C4H2+C2H2
+4.3000000E+012 +6.2000000E-001 +7.7294000E+004   !\AUTHOR: !\REF:CHAOS
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007
!\COMMENT:
!
-----
!\REACTIONCLASS:  \R_ADDITION                      \A
\N                \EA
!
-----
C6H6+O<=>C6H5O+H
+2.2000000E+013 +0.0000000E+000 +4.5300000E+003   !\AUTHOR: !\REF:ALZUETA
ET AL. IJCK 32: 498-522 (2000) !\COMMENT:
C6H6+OH<=>C6H5OH+H
+1.3200000E+002 +3.2500000E+000 +5.5900000E+003   !\AUTHOR:
!\REF:TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA MIYOSHI J. PHYS. CHEM.
A, 2006, 110 (15), 5081-5090 !\COMMENT:
!
-----
!\REACTIONCLASS:  \R_HO2                          \A
\N                \EA
!
-----
C6H5+HO2<=>C6H5O+OH
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:DA
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:
!
-----
!\REACTIONCLASS:  \R_O2                          \A
\N                \EA
!
-----
C6H5+O2<=>C6H5O+O
+2.6000000E+013 +0.0000000E+000 +6.1200000E+003   !\AUTHOR: !\REF:FRANK
ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833. !\COMMENT:
C6H5+O2<=>O-C6H4O2+H
+3.0000000E+013 +0.0000000E+000 +8.9800000E+003   !\AUTHOR: !\REF:FRANK
ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833. !\COMMENT:
C6H5+O2<=>C6H5OO
+1.8600000E+013 -2.2000000E-001 -7.1100000E+002   !\AUTHOR: !\REF:DA
SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575 !\COMMENT:
C6H5OO<=>C6H5O+O
+1.2700000E+015 -2.4600000E-001 +3.8536000E+004   !\AUTHOR: !\REF:DA
SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575 !\COMMENT:
C6H5O+OH<=>C6H5OOH
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000   !\AUTHOR: !\REF:WKM
ESTIMATED !\COMMENT:
!-----
!
!-----
!\ENDSUBMECH:  \C6H6
!-----
!-----

```

!-----  
!-----  
!\SUBMECH: \C6H5OH  
!\MECHCOMMENTS:  
!\MECHWARNINGS:  
!-----  
!-----  
!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

---

C6H5O+H(+M)<=>C6H5OH(+M)  
+2.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:EMDEE  
ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 !\COMMENT: WKM ESTIMATED  
LOW /  
+1.0000000E+094 -2.1840000E+001 +1.3880000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +4.3000000E-002  
+3.0420000E+002 +6.0000000E+004 +5.8960000E+003 / !TROE PARAMETERS  
C6H4OH+H<=>C6H5OH  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH<=>C5H6+CO  
+4.3100000E+015 -6.1000000E-001 +7.4115000E+004 !\AUTHOR: !\REF:WKM A  
FACTOR \*0.5 TO FIT PYROLYSIS DATA !\COMMENT:  
!

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

C6H5OH+H<=>C6H5O+H2  
+1.2000000E+014 +0.0000000E+000 +1.2400000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+O2<=>C6H5O+HO2  
+1.0000000E+013 +0.0000000E+000 +3.8800000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+O<=>C6H5O+OH  
+1.3000000E+013 +0.0000000E+000 +2.9000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+OH<=>C6H5O+H2O  
+1.4000000E+008 +1.4000000E+000 -9.6000000E+002 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+HO2<=>C6H5O+H2O2  
+1.0000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+CH3<=>C6H5O+CH4  
+1.8000000E+011 +0.0000000E+000 +7.7000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+C3H5-A<=>C6H5O+C3H6  
+4.9000000E+011 +0.0000000E+000 +9.4000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+C4H5-I<=>C6H5O+C4H6  
+4.9000000E+011 +0.0000000E+000 +9.4000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:



C6H5OH+C6H5<=>C6H5O+C6H6  
+4.9000000E+012 +0.0000000E+000 +4.4000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+C6H5OO<=>C6H5O+C6H5OOH  
+1.3300000E+011 +0.0000000E+000 +1.4000000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+H<=>C6H4OH+H2  
+1.7000000E+014 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+O<=>C6H4OH+OH  
+2.0000000E+013 +0.0000000E+000 +1.4700000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+OH<=>C6H4OH+H2O  
+1.4000000E+013 +0.0000000E+000 +4.6000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+HO2<=>C6H4OH+H2O2  
+4.0000000E+011 +0.0000000E+000 +2.8900000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
C6H5OH+CH3<=>C6H4OH+CH4  
+2.0000000E+012 +0.0000000E+000 +1.5000000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_ADDITION\O \A  
\N \EA  
!

---

C6H5OH+O<=>OC6H4OH+H  
+1.6000000E+013 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_DECOMPOSITION \A  
\N \EA  
!

---

C6H5O<=>CO+C5H5  
+2.0000000E+011 +0.0000000E+000 +4.3900000E+004 !\AUTHOR: !\REF:WKM A  
FACTOR REDUCED FROM 2.5E+11 TO 2.0E+11 TO FIT DATA BENZENE FLOW REACTOR  
DATA (LOVELL) !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_PRODUCTS \A  
\N \EA  
!

---

C6H5O+H<=>CO+C5H6  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:  
C6H5O+O<=>C5H5+CO2  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:  
C6H5O+O<=>OC6H4OH  
+2.6000000E+010 +4.7000000E-001 +8.0000000E+002 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:

!

---

!\REACTIONCLASS: \R\_O2\_PRODUCTS \A  
\N \EA  
!

---

C6H4OH+O2<=>OC6H4OH+O  
+2.1000000E+013 +0.0000000E+000 +6.1000000E+003 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
OC6H4OH<=>C5H4OH+CO  
+7.4000000E+011 +0.0000000E+000 +4.3800000E+004 !\AUTHOR: !\REF:DA  
COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003 !\COMMENT:  
!

---

---

!\REACTIONCLASS: \R\_O\_PRODUCTS \A  
\N \EA  
!

---

C6H5O+O<=>P-C6H4O2+H  
+4.2500000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
C6H5O+O<=>O-C6H4O2+H  
+8.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
!

---

---

!\REACTIONCLASS: \R\_HO2\_PRODUCTS \A  
\N \EA  
!

---

C6H5O+HO2<=>O-OC6H5OJ+OH  
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:UP AND  
IT IS NOT SEEN IN THE EXPERIMENT !\COMMENT:  
P-C6H4O2+H<=>P-OC6H5OJ  
+4.0000000E+012 +0.0000000E+000 +9.7400000E+003 !\AUTHOR: !\REF:WKM  
ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38: 250-275,  
2006 !\COMMENT:  
O-C6H4O2+H<=>O-OC6H5OJ  
+4.0000000E+012 +0.0000000E+000 +6.9600000E+003 !\AUTHOR: !\REF:WKM  
ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38: 250-275,  
2006 !\COMMENT:

!=====  
=====  
!\SUBSPECIES: O-C6H4O2\P-C6H4O2  
!=====  
=====  
!

---

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

O-C6H4O2<=>C5H4O+CO  
+1.0000000E+012 +0.0000000E+000 +4.0000000E+004 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
P-C6H4O2<=>C5H4O+CO  
+3.7000000E+011 +0.0000000E+000 +5.9000000E+004 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:

P-C6H3O2+H<=>P-C6H4O2  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

P-C6H4O2+H<=>P-C6H3O2+H2  
+2.0000000E+012 +0.0000000E+000 +8.1000000E+003 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
P-C6H4O2+O<=>P-C6H3O2+OH  
+1.4000000E+013 +0.0000000E+000 +1.4700000E+004 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
P-C6H4O2+OH<=>P-C6H3O2+H2O  
+1.0000000E+006 +2.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

P-C6H4O2+H<=>C5H5O+CO  
+2.5000000E+013 +0.0000000E+000 +4.7000000E+003 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
P-C6H4O2+O=>2CO+C2H2+CH2CO  
+3.0000000E+013 +0.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_PRODUCTS \A  
\N \EA  
!

---

P-C6H3O2+H<=>2C2H2+2CO  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:  
P-C6H3O2+O=>C2H2+HCCO+2CO  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 30: 683-697, 1998 !\COMMENT:

!\ENDSUBSPECIES: \O-C6H4O2\P-C6H4O2

!\ENDSUBMECH: \C6H5OH

!\SUBMECH: \C5H6

!\MECHCOMMENTS: C4H4O IS STILL BEING USED AS NAME FOR BOTH VINYL KETENE  
AND FURAN, WHICH ARE ISOMERS. KPS UPDATED MUCH OF THIS CHEMISTRY DURING

FURANS MECHANISM DEVELOPMENT. INCORPORATE INTO LATES BUTENES BEFORE ALL ARE FINALISED.

!\MECHWARNINGS:

!-----  
!-----  
!

---

!\REACTIONCLASS: \AROMATIC\_GROWTH \A  
\N \EA  
!

---

---

C5H6+C2H3<=>C6H6+CH3  
+2.1000000E+067 -1.6080000E+001 +4.2460000E+004 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
!

---

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA  
!

---

---

C5H5+H(+M)<=>C5H6(+M)  
+2.6000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:  
LOW /  
+4.4000000E+080 -1.8280000E+001 +1.2994000E+004 / !LOW-PRESSURE-LIMIT  
TROE / +6.8000000E-002  
+4.0070000E+002 +4.1360000E+003 +5.5020000E+003 / !TROE PARAMETERS  
CO / 1.500 / CO2 / 2.000 / H2O / 6.000 / H2 / 2.000 / CH4 / 2.000 / !3RD  
BODY COLLIDER EFFICIENCIES  
C5H6(+M)<=>C3H4-A+C2H2(+M)  
+3.8000000E+017 +0.0000000E+000 +1.0400000E+005 !\AUTHOR: !\REF:MACKIE  
ET AL. PHYS CHEM CHEM PHYS 3 2467 2001 !\COMMENT:  
LOW /  
+1.0000000E+098 -2.2250000E+001 +1.2632150E+005 / !LOW-PRESSURE-LIMIT  
TROE / +1.4410000E-001  
+5.3580000E+000 +3.2840000E+003 +6.7100000E+009 / !TROE PARAMETERS  
CO / 1.500 / CO2 / 2.000 / H2O / 6.000 / H2 / 2.000 / CH4 / 2.000 / !3RD  
BODY COLLIDER EFFICIENCIES  
C#CCVCCJ+H<=>C5H6  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:LIN J  
COMPUT CHEM 21 415-425 2000 !\COMMENT:  
!

---

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

---

C5H6+H<=>C5H5+H2  
+7.2000000E+013 +0.0000000E+000 +3.5000000E+003 !\AUTHOR: !\REF:ROY AND  
FRANK, 21ST INTERNATIONAL SYMPOSIUM ON SHOCKWAVES, 1997 PPER 1560  
!\COMMENT:  
C5H6+O2<=>C5H5+HO2  
+4.0000000E+013 +0.0000000E+000 +3.7150000E+004 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
C5H6+O<=>C5H5+OH  
+4.8000000E+004 +2.7100000E+000 +1.1000000E+003 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:

C5H6+OH<=>C5H5+H2O  
 +3.0800000E+006 +2.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+HO2<=>C5H5+H2O2  
 +1.1000000E+004 +2.6000000E+000 +1.2900000E+004 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+CH3<=>C5H5+CH4 +1.8000000E-  
 001 +4.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ZHONG & BOZZELI J  
 PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+HCO<=>C5H5+CH2O  
 +1.0800000E+008 +1.9000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+C2H3<=>C5H5+C2H4 +1.2000000E-  
 001 +4.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ZHONG & BOZZELI J  
 PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+C3H5-A<=>C5H5+C3H6  
 +5.5000000E+010 +0.0000000E+000 +5.5050000E+003 !\AUTHOR:  
 !\1997BUR/DVI505-514 !\COMMENT: WARNING NOTED IN MEHL MECHANISM SAYS THIS  
 WAS DIVIDED BY 2  
 C5H6+C4H5-I<=>C5H5+C4H6  
 +6.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:EMDEE  
 ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 !\COMMENT:  
 C5H6+C4H5-N<=>C5H5+C4H6  
 +6.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: KPS !\REF:  
 ADOPTED FROM MEHL AROMATIC!\COMMENT: WARNING: ADDED ON 06/08/2015 WAS  
 MISSING FROM PREVIOUS VERSIONS OF MECHANISM  
 C5H6+C6H5<=>C5H5+C6H6 +1.0000000E-  
 001 +4.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ZHONG & BOZZELI J  
 PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+C6H5O<=>C5H5+C6H5OH  
 +3.1600000E+011 +0.0000000E+000 +8.0000000E+003 !\AUTHOR: !\REF:EMDEE  
 ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 !\COMMENT:  
 C5H6+C5H5<=>C6H6+C4H5-N  
 +5.0000000E+009 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ON  
 OTHER CONDITIONS. !\COMMENT: WARNING  
 !

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
 \N \EA  
 !

---

C5H6+H<=>C2H2+C3H5-A  
 +1.5480000E+037 -6.1800000E+000 +3.2890000E+004 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+H<=>C5H7  
 +2.4000000E+073 -1.7850000E+001 +3.1500000E+004 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 C5H6+O<=>C5H5O+H  
 +8.9000000E+012 -1.5000000E-001 +5.9000000E+002 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 DUP  
 C5H6+O<=>C5H5O+H  
 +5.6000000E+012 -6.0000000E-002 +2.0000000E+002 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
 DUP  
 C5H6+H<=>CVCCJCVC  
 +1.1000000E+014 -1.6000000E-001 +3.1000000E+003 !\AUTHOR: !\REF:ZHONG &  
 BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:

C5H6+OH<=>CVCCJCVCOH  
+1.1000000E+013 -7.0000000E-002 +8.7000000E+002 !\AUTHOR: !\REF:ZHONG &  
BOZZELLI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
CVCCJCVCOH+O2<=>HOCVCCVO+CH2CHO  
+1.2000000E+036 -7.2500000E+000 +3.3600000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

!=====  
=====

!\SUBSPECIES: \C5H7

!=====  
=====

!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA

!

---

C5H7<=>CVCCJCVC  
+3.2000000E+015 +0.0000000E+000 +3.9500000E+004 !\AUTHOR: !\REF:ARENDS  
ET AL. J PHYS CHEM 97: 7914 1993 !\COMMENT:  
CVCCJCVC<=>CVCCVCCJ  
+5.4000000E+011 -7.0000000E-001 +6.0000000E+001 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

!\WARNING: CVCCVCCJ+H<=>CVCCVCC 2.300E+020 -1.600 3020.0 !\AUTHOR:  
!\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

!\COMMENT:WARNING 1,3-PENTADIENE HAS BEEN RENAMED IN KZ VERSION. THIS  
REACTION HAS BEEN GIVEN PRESSURE-DE

CVCCVCCJ+H(+M)<=>C5H81-3(+M)

+2.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: KPS !\REF:  
THIS IS RATE CONSTANT IN MOST RECENT MEHL MECHANISM !\COMMENT: REACTION  
WAS MISSING FROM PREVIOUS VERSIONS OF ARAMCO

LOW /

+1.3300000E+060 -1.2000000E+001 +5.9678000E+003 / !LOW-PRESSURE-LIMIT  
TROE / +2.0000000E-002

+1.0966000E+003 +1.0966000E+003 +6.8595000E+003 / !TROE PARAMETERS

H2 / 2.000 / H2O / 6.000 / CH4 / 2.000 / CO / 1.500 / CO2 / 2.000 / C2H6  
/ 3.000 / AR / 0.700 / !3RD BODY COLLIDER EFFICIENCIES

CVCCJCVC+O2<=>C2H3CHO+CH2CHO

+1.2000000E+036 -7.2500000E+000 +3.3600000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

CVCCJCVC+O<=>C2H3CHO+C2H3

+2.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
ET AL. COMBUST SCI TECH 116:211 1996 !\COMMENT:

!=====  
=====

!\ENDSUBSPECIES: \C5H7

!=====  
=====

!

!\SUBSPECIES: \CVCCVC

!=====  
=====

!

---

!\REACTIONCLASS: \UNIMOL\_CHEMACT \A  
\N \EA

!  
-----  
CVCCVCCJ+H<=>C4H5-N+CH3  
+2.9000000E+026 -2.1800000E+000 +3.6770000E+004 !\AUTHOR: !\REF:MARINOV  
ET AL. COMBUST SCI TECH 116:211 1996 !\COMMENT: WARNING RATE CONSTANT HAS  
STRANGE REVERSE RATE CONSTANT  
!

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

-----  
C5H81-3+H<=>CVCCVCCJ+H2  
+7.0000000E+006 +2.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF:MARINOV  
ET AL. COMBUST SCI TECH 116:211 1996 !\COMMENT:  
C5H81-3+OH<=>CVCCVCCJ+H2O  
+7.0000000E+006 +2.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:MARINOV  
ET AL. COMBUST SCI TECH 116:211 1996 !\COMMENT:  
!

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

-----  
C5H81-3+H<=>C4H6+CH3  
+5.2000000E+071 -1.6380000E+001 +5.1000000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
!

!\REACTIONCLASS: \R\_R\_PRODUCTS \A  
\N \EA  
!

-----  
CVCCVCCJ+OH<=>CVCCVCCOH  
+1.5000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
CVCCVCCJ+O2<=>CH2CHCHCHO+CH2O  
+8.2000000E+010 +1.8000000E-001 +9.1400000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
CVCCVCCOH+H<=>C4H6+CH2OH  
+2.5000000E+034 -6.1200000E+000 +1.6250000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
!=====

!\ENDSUBSPECIES: \CVCCVC  
!=====

!\REACTIONCLASS: \RADICAL\_OXIDATION \A  
\N \EA  
!

-----  
C5H7+O2<=>OC5H7O  
+8.9000000E+024 -3.8000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

OC5H7O+O2<=>OC4H6O+HOCO  
+6.3000000E+005 -7.2500000E+000 +3.3600000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
OC4H6O+H<=>OC4H5O+H2  
+2.3000000E+010 +1.0500000E+000 +3.2790000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
OC4H6O+OH<=>OC4H5O+H2O  
+3.5000000E+009 +1.1800000E+000 -4.4700000E+002 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
OC4H5O+O2<=>O2CCHOOJ+C2H4  
+1.6000000E+045 -9.9200000E+000 +2.0670000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
O2CCHOOJ<=>HOCO+CO2  
+3.0000000E+013 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
\N \EA  
!

---

C5H7+H<=>C5H6+H2  
+3.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 32: 498-522, 2000. !\COMMENT:  
C5H7+O<=>C5H6+OH  
+1.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 32: 498-522, 2000. !\COMMENT:  
C5H7+OH<=>C5H6+H2O  
+2.4000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H6+HO2<=>C5H7+O2  
+1.3000000E+015 -1.0700000E+000 +9.5300000E+003 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
!

!\ENDSUBSPECIES: \C5H7  
!  
!  
!  
!

!\SUBSPECIES: \HOCVCCVO  
!  
!  
!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA  
!

---

HOCVCCVO+OH<=>HOCVCCJVO+H2O  
+2.6900000E+010 +7.6000000E-001 -3.4000000E+002 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
HOCVCCVO+HO2<=>HOCVCCJVO+H2O2  
+1.0000000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
HOCVCCVO+CH3<=>HOCVCCJVO+CH4  
+3.9800000E+012 +0.0000000E+000 +8.7000000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:



HOCVCCVO+O<=>HOCVCCJVO+OH  
+7.1800000E+012 +0.0000000E+000 +1.3890000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
HOCVCCVO+O2<=>HOCVCCJVO+HO2  
+2.0000000E+013 +0.0000000E+000 +4.0700000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
HOCVCCVO+H<=>HOCVCCJVO+H2  
+2.6000000E+012 +0.0000000E+000 +2.6000000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

C2H2OH+CO<=>HOCVCCJVO  
+1.5100000E+011 +0.0000000E+000 +4.8100000E+003 !\AUTHOR: !\REF:WKM  
ANALOGY TO C2H5+CO<=>C2H5CO !\COMMENT:  
!=====  
=====  
!\ENDSUBSPECIES: \HOCVCCVO  
!=====  
=====  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

C5H5<=>C3H3+C2H2  
+1.9800000E+068 -1.5000000E+001 +1.2490000E+005 !\AUTHOR: !\REF:LIN J  
COMPUT CHEM 21 415-425 2000 !\COMMENT:  
C#CCVCCJ<=>C5H5  
+8.0000000E+013 +0.0000000E+000 +3.4058300E+004 !\AUTHOR: !\REF:LIN J  
COMPUT CHEM 21 415-425 2000 !\COMMENT:  
C3H3+C2H2<=>C#CCVCCJ  
+4.1100000E+072 -1.8200000E+001 +4.5400000E+004 !\AUTHOR: !\REF:LIN J  
COMPUT CHEM 21 415-425 2000 !\COMMENT:  
C#CCVCCJ+H<=>C5H6-L  
+1.0000000E+010 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:LINDSTEDT C&F 99:551-561 (1994) !\COMMENT:  
C5H6-L+O<=>C#CCVCCJ+OH  
+1.0000000E+010 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:LINDSTEDT C&F 99:551-561 (1994) !\COMMENT:  
C5H6-L+OH<=>C#CCVCCJ+H2O  
+1.0000000E+010 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:  
!\REF:LINDSTEDT C&F 99:551-561 (1994) !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_OXIDATION \A  
\N \EA  
!

---

C5H5+HO2<=>C5H5O+OH  
+6.3000000E+029 -4.6900000E+000 +1.1650000E+004 !\AUTHOR: !\REF:RISTORI  
ET AL. COMBUST. SCI. AND TECH 2001. VOL. 167. PP. 223-256 !\COMMENT:

C5H5+O2<=>C4H4O+HCO  
+6.0000000E+018 -2.4800000E+000 +1.0970000E+004 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
C5H5+O<=>C4H5-N+CO  
+3.2000000E+013 -1.7000000E-001 +4.4000000E+002 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
C5H5+O<=>C5H4O+H  
+5.8000000E+013 -2.0000000E-002 +2.0000000E+001 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
C5H5+OH<=>C5H5OH  
+6.5000000E+014 -8.5000000E-001 -2.7300000E+003 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
DUP  
C5H5+OH<=>C5H5OH  
+1.1000000E+043 -8.7600000E+000 +1.8730000E+004 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
DUP  
C5H5+OH<=>C5H5OH  
+1.1000000E+059 -1.3080000E+001 +3.3450000E+004 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
DUP  
C5H5+OH<=>C5H4OH+H  
+3.5000000E+057 -1.2180000E+001 +4.8350000E+004 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:  
C5H5+OH<=>C4H6+CO  
+4.0000000E+014 +0.0000000E+000 +4.5000000E+003 !\AUTHOR: !\REF:ZHONG &  
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:

!=====  
=====

!\SUBSPECIES: C5H5OH

!=====  
=====

!

---

!\REACTIONCLASS: \UNIMOL \A  
\N \EA

!

---

C5H4OH+H<=>C5H5OH  
+1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 32: 498-522, 2000. !\COMMENT:

!

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
\N \EA

!

---

C5H5OH+H<=>C5H5O+H2  
+4.0000000E+013 +0.0000000E+000 +6.0940000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELI (ZHONG'S THESIS) !\COMMENT:  
C5H5OH+O<=>C5H5O+OH  
+1.0000000E+013 +0.0000000E+000 +4.6830000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELI (ZHONG'S THESIS) !\COMMENT:  
C5H5OH+OH<=>C5H5O+H2O  
+1.0000000E+013 +0.0000000E+000 +1.6970000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELI (ZHONG'S THESIS) !\COMMENT:

C5H5OH+HO2<=>C5H5O+H2O2  
+1.0000000E+013 +0.0000000E+000 +1.5800000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H5OH+H<=>C5H4OH+H2  
+3.2000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H5OH+O<=>C5H4OH+OH  
+4.7000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H5OH+OH<=>C5H4OH+H2O  
+5.5000000E+012 +0.0000000E+000 +1.7310000E+003 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H5OH+HO2<=>C5H4OH+H2O2  
+3.6000000E+003 +2.5500000E+000 +1.0531000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA

!

---

C5H5O<=>C5H4O+H  
+2.9000000E+032 -6.5000000E+000 +2.1220000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H5O<=>C4H5-N+CO  
+1.1000000E+079 -1.9620000E+001 +6.6250000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H5O<=>CJVCCVCCVO  
+2.0000000E+013 +0.0000000E+000 +1.4338000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA

!

---

C5H5O+O2<=>C5H4O+HO2  
+6.0000000E+010 +0.0000000E+000 +1.6000000E+003 !\AUTHOR: KPS: !\REF:  
ADDED FROM MEHL AROMATIC !\COMMENT: WARNING WAS NOT PRESENT IN PREVIOUS  
VERSIONS OF GALWAY AROMATIC

!=====  
=====

!\SUBSPECIES: CJVCCVCCVO

!=====  
=====

CJVCCVCCVO<=>CVCCVCCJVO  
+4.3000000E+011 -1.0500000E+000 +4.1180000E+003 !\AUTHOR:  
!\REF:ESTIMATED FROM METHODS DESCRIBED IN CURRAN'S N-HEPTANE C&F 114:  
149-177 (1998) !\COMMENT:  
C4H5-N+CO<=>CVCCVCCJVO  
+1.5100000E+011 +0.0000000E+000 +4.8100000E+003 !\AUTHOR: !\REF:WKM  
ANALOGY TO C2H5+CO<=>C2H5CO !\COMMENT:

CJVCCVCCVO<=>C2H2+CJVCCVO  
+3.0000000E+013 +0.0000000E+000 +4.3710000E+004 !\AUTHOR: !\REF:SAKAI  
ET AL PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418  
!\COMMENT:

CJVCCVO<=>C2H3CO  
+1.4000000E+009 +9.8000000E-001 +3.2100000E+004 !\AUTHOR: !\REF:SAKAI

ET AL PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418  
 !\COMMENT:  
 C2H2+HCO<=>CJVCCVO  
 +7.7700000E+006 +1.4100000E+000 +7.7550000E+003 !\AUTHOR: !\REF:SAKAI  
 ET AL PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418  
 !\COMMENT:  
 !=====

---

!\ENDSUBSPECIES: CJVCCVCCVO  
 !=====

---

!\REACTIONCLASS: \R\_R\_ABSTRACTION \A  
 \N \EA  
 !

---

C5H4OH+H<=>C5H4O+H2  
 +2.1000000E+013 +0.0000000E+000 +5.4000000E+004 !\AUTHOR: !\REF:ALZUETA  
 & GLARBORG IJCK 32: 498-522, 2000. !\COMMENT:  
 C5H4OH+O2<=>C5H4O+HO2  
 +3.0000000E+013 +0.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF:ALZUETA  
 & GLARBORG IJCK 32: 498-522, 2000. !\COMMENT:  
 !=====

---

!\SUBSPECIES: \C5H4O  
 !=====

---

!\REACTIONCLASS: \UNIMOL \A  
 \N \EA  
 !

---

C5H4O=>CO+C2H2+C2H2  
 +5.7000000E+032 -6.7600000E+000 +6.8500000E+004 !\AUTHOR: !\REF:WANG  
 AND BREZINSKY J PHYS CHEM A 102: 1530 1998 !\COMMENT:  
 DUP  
 C5H4O=>CO+C2H2+C2H2  
 +6.2000000E+041 -7.8700000E+000 +9.8700000E+004 !\AUTHOR: !\REF:WANG  
 AND BREZINSKY J PHYS CHEM A 102: 1530 1998 !\COMMENT:  
 DUP  
 C5H3O+H<=>C5H4O  
 +1.0000000E+014 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
 & GLARBORG IJCK 30: 683, 1998. !\COMMENT:  
 !

---

!\REACTIONCLASS: \RH\_R\_ABSTRACTION \A  
 \N \EA  
 !

---

C5H4O+H<=>C5H3O+H2  
 +2.0000000E+012 +0.0000000E+000 +8.1000000E+003 !\AUTHOR: !\REF:ALZUETA  
 & GLARBORG IJCK 30: 683, 1998. !\COMMENT:  
 C5H4O+O<=>C5H3O+OH  
 +1.4000000E+013 +0.0000000E+000 +1.4700000E+003 !\AUTHOR: !\REF:ALZUETA  
 & GLARBORG IJCK 30: 683, 1998. !\COMMENT:

C5H4O+OH<=>C5H3O+H2O  
+1.1000000E+008 +1.4200000E+000 +1.4500000E+003 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 30: 683, 1998. !\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_DECOMPOSITION \A  
\N \EA  
!

---

C5H3O=>C2H2+CO+C2H  
+2.0000000E+013 +0.0000000E+000 +5.1000000E+004 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 30: 683, 1998. !\COMMENT:  
!

---

!\REACTIONCLASS: \R\_O2\_PRODUCTS \A  
\N \EA  
!

---

C5H3O+O2=>CO2+C2H2+HCCO  
+9.7000000E+058 -1.3470000E+001 +3.8180000E+004 !\AUTHOR: !\REF:CHAOS  
ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES) 2007  
!\COMMENT:  
!

---

!\REACTIONCLASS: \RADICAL\_ADDITION \A  
\N \EA  
!

---

C5H4O+H<=>C4H5-N+CO  
+2.1000000E+061 -1.3270000E+001 +4.0810000E+004 !\AUTHOR: !\REF:PRIVATE  
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:  
C5H4O+O<=>C4H4+CO2  
+1.0000000E+013 +0.0000000E+000 +2.0000000E+003 !\AUTHOR: !\REF:ALZUETA  
& GLARBORG IJCK 30: 683, 1998. !\COMMENT:  
!=====

!\ENDSUBSPECIES: \C5H4O  
!=====

!\ENDSUBSPECIES: \C5H5OH  
!=====

!\SUBSPECIES: \C4H4O  
!=====

---

C4H4O+H<=>C3H5-A+CO  
+6.6000000E+013 -2.0000000E-002 +2.7400000E+003 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 32: 498-522, 2000 !\COMMENT: WARNING C4H4O IS  
DUPLICATE SPECIES  
DUP

C4H4O+H<=>C3H5-A+CO  
+5.9000000E+006 +2.0000000E+000 +1.3000000E+003 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 32: 498-522, 2000 !\COMMENT: WARNING C4H4O IS  
DUPLICATE SPECIES

DUP  
C4H4O+O<=>CH2CHO+HCCO  
+3.0000000E+008 +1.4500000E+000 -8.6000000E+002 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 32: 498-522, 2000 !\COMMENT: WARNING C4H4O IS  
DUPLICATE SPECIES  
C4H4O+OH<=>C3H5-A+CO2  
+3.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ALZUETA  
ET AL. INT J CHEM KINET: 32: 498-522, 2000 !\COMMENT: WARNING C4H4O IS  
DUPLICATE SPECIES  
C4H4O+OH=>C2H2+HCCO+H2O  
+2.0200000E+013 +0.0000000E+000 +5.9330000E+003 !\AUTHOR: KPS !\REF:  
!PITZ2001 !\COMMENT: WARNING ADDED BY KPS ON 06/08/2015 WAS MISSING FROM  
GALWAY VERSIONS OF AROMATICS  
!=====  
=====  
!\ENDSUBSPECIES: \C4H4O  
!=====  
=====  
!-----  
-----  
!\ENDSUBMECH: \C5H6  
!-----  
-----  
!+++++  
+++++  
+++++  
!\END\_KINETICS\_MODULE: \AROMATIC  
!+++++  
+++++  
+++++  
!\END\_KINETICS\_INPUT  
!Supplementary Material II  
!Pyrolysis and oxidation of methyl acetate in a shock tube: a multi-  
species time-history study  
!Wei Rena\*, King-Yiu Lamb, David F. Davidsonb, Ronald K. Hansonb,  
Xueliang Yangc  
!a Department of Mechanical and Automation Engineering, The Chinese  
University of Hong Kong, New Territories, Hong Kong  
!b Department of Mechanical Engineering, Stanford University, Stanford,  
CA 94305, USA  
!c Department of Mechanical and Aerospace Engineering, Princeton  
University, Princeton, NJ 08544, USA  
!\*\*\*\*\*  
\*\*\*\*\*  
! CH3OCOCH3 sub-mechanism  
!\*\*\*\*\*  
\*\*\*\*\*  
CH3COOCH3<=>CH3+CH3+CO2 8.05E+087 -21.00 125195.4  
PLOG /0.05 1.10E+88 -21.00 125195.4/  
PLOG /0.50 1.94E+84 -19.60 126405.6/  
PLOG /1.00 8.07E+78 -18.00 123551.9/  
PLOG /10 4.30E+65 -14.00 117470.9/  
PLOG /100 4.17E+45 -8.20 105384.4/  
PLOG /1000 6.97E+28 -3.40 94422.7/  
CH3COOCH3<=>CH3+CH3OCO 7.78E+086 -21.00 127983.5  
PLOG /0.05 1.06E+87 -21.00 127983.5/  
PLOG /0.50 2.59E+82 -19.30 128623.4/  
PLOG /1.00 1.91E+77 -17.75 126063.8/

```

PLOG /10.0 1.76E+69 -15.15 124545.6/
PLOG /100 6.14E+49 -9.45 113561.9/
PLOG /1000 6.50E+30 -4.00 101447.6/
CH3COOCH3<=>CH3OH+CH2CO 2.25E+075 -17.90 110934.8
PLOG /0.05 6.75E+75 -17.90 109434.8/
PLOG /0.50 2.03E+70 -16.10 108755.2/
PLOG /1.00 1.95E+64 -14.35 105178.1/
PLOG /10.0 4.11E+51 -10.60 98661.90/
PLOG /100 3.12E+25 -5.95 88699.70/
PLOG /1000 2.52E+11 0.85 71533.80/
dup
CH3COOCH3<=>CH3OH+CH2CO 2.25E+075 -17.90 110934.8
PLOG /0.05 8.28E+68 -16.10 102718.1/
PLOG /0.5 2.25E+59 -13.20 98650.80/
PLOG /1.0 1.34E+53 -11.40 94821.80/
PLOG /10. 4.38E+39 -7.45 87336.80/
PLOG /100. 2.34E+22 -2.50 76183.80/
PLOG /1000. 1.94E+12 0.38 69594.90/
dup
CH3COOCH3+O2<=>CH2COOCH3+HO2 6.00E+13 0.00 47640.0
CH3COOCH3+O2<=>CH3COOCH2+HO2 6.00E+13 0.00 47910.0
CH3COOCH3+O<=>CH2COOCH3+OH 2.30E+04 2.93 7040.3
CH3COOCH3+O<=>CH3COOCH2+OH 2.35E+04 2.965 5404.
CH3COOCH3+H<=>CH2COOCH3+H2 1.11E+05 2.68 7087.4
CH3COOCH3+H<=>CH3COOCH2+H2 4.24E+04 2.84 6927.0
CH3COOCH3+OH<=>CH2COOCH3+H2O 3.07E+01 3.505 0.
CH3COOCH3+OH<=>CH3COOCH2+H2O 5.71E+00 3.79 -1211.5
CH3COOCH3+CH3<=>CH2COOCH3+CH4 6.72E-01 3.80 8254.3
CH3COOCH3+CH3<=>CH3COOCH2+CH4 12.00E-01 3.99 9115.3
CH3COOCH3+HO2<=>CH2COOCH3+H2O2 4.36E-05 5.04 15275.7
CH3COOCH3+HO2<=>CH3COOCH2+H2O2 2.46E-06 5.53 13717.5
!CH3+CH2CO=C2H5+CO 1.05E+06 2.0396 10672.0 DUPLICATE 2492
CH2COOCH3<=>CH2CO+CH3O 6.01E+09 -0.95 43298
PLOG /0.010 6.01E+09 -0.95 43298
PLOG /0.025 3.02E+18 -3.21 46073/
PLOG /0.079 2.08E+23 -4.45 48250/
PLOG /0.158 4.89E+27 -5.55 50536.87/
PLOG /1.000 2.01E+35 -7.28 55568/
PLOG /1.600 1.03E+36 -7.37 56263/
PLOG /2.500 2.49E+36 -7.37 56776/
PLOG /5.000 2.58E+36 -7.22 57306.79/
PLOG /10.00 6.66E+36 -7.19 58167/
PLOG /20.00 5.12E+36 -7.01 58831/
PLOG /100.0 1.51E+34 -5.99 59249/
CH2COOCH3<=>CH3CO+CH2O 5.45E+36 -7.93 38118
PLOG /0.010 5.45E+36 -7.93 38118/
PLOG /0.025 4.95E+37 -8.00 39967/
PLOG /0.079 3.57E+38 -8.14 41197/
PLOG /0.158 3.22E+39 -8.31 42566/
PLOG /1.000 3.78E+41 -8.62 46492/
PLOG /1.600 1.38E+42 -8.71 47676/
PLOG /2.500 1.17E+42 -8.63 48439/
PLOG /5.000 9.40E+41 -8.50 49767/
PLOG /10.00 8.37E+41 -8.38 51239/
PLOG /20.00 1.97E+42 -8.39 53197/
PLOG /100.0 1.62E+38 -7.04 54529/
CH2COOCH3<=>CH3COOCH2 1.25E+23 -4.23 23321
PLOG /0.010 1.25E+23 -4.23 23321/

```

PLOG /0.025 5.15E+24 -4.51 25081/  
 PLOG /0.079 6.80E+25 -4.74 26157/  
 PLOG /0.158 4.29E+26 -4.88 27085/  
 PLOG /1.000 8.39E+28 -5.31 29764/  
 PLOG /1.600 1.32E+29 -5.30 30257/  
 PLOG /2.500 1.43E+29 -5.26 30650/  
 PLOG /5.000 6.66E+28 -5.08 31051/  
 PLOG /10.00 2.29E+28 -4.87 31385/  
 PLOG /20.00 2.57E+27 -4.52 31432/  
 PLOG /100.0 4.79E+23 -3.30 30538/  
 CH3COOCH2=CH2CO+CH3O 2.43E+11 -1.44 43150  
 PLOG /0.010 2.43E+11 -1.44 43150/  
 PLOG /0.025 4.51E+19 -3.58 45661/  
 PLOG /0.079 1.14E+24 -4.70 47586/  
 PLOG /0.158 2.05E+28 -5.77 49788/  
 PLOG /1.000 1.06E+37 -7.82 55678/  
 PLOG /1.600 2.23E+38 -8.09 56974/  
 PLOG /2.500 2.88E+39 -8.30 58220/  
 PLOG /5.000 4.14E+40 -8.47 60013/  
 PLOG /10.00 1.40E+41 -8.47 61646/  
 PLOG /20.00 7.82E+40 -8.25 62992/  
 PLOG /100.0 1.79E+40 -7.75 66910/  
 CH3COOCH2=CH3CO+CH2O 1.79E+32 -6.62 35044  
 PLOG /0.010 1.79E+32 -6.62 35044/  
 PLOG /0.025 6.59E+33 -6.89 36838/  
 PLOG /0.079 1.57E+34 -6.90 37549/  
 PLOG /0.158 3.23E+34 -6.90 38242/  
 PLOG /1.000 6.17E+33 -6.47 39294/  
 PLOG /1.600 6.54E+33 -6.42 39707/  
 PLOG /2.500 1.60E+33 -6.19 39724/  
 PLOG /5.000 1.67E+32 -5.84 39728/  
 PLOG /10.00 5.08E+30 -5.33 39398/  
 PLOG /20.00 1.79E+29 -4.85 39083/  
 PLOG /100.0 4.81E+24 -3.43 37465/  
 O2+CH2COOCH3=>HO2+CH2O+CH2CO 1.00E+12 0.00 2000.  
 O2+CH2COOCH3=>OH+2CH2O+CO 4.50E+10 0.00 0.  
 O+CH2COOCH3=CH2O+CH3OCO 3.00E+13 0.00 0.  
 O2+CH3COOCH2=>OH+2CH2O+CO 4.50E+10 0.00 0.  
 O2+CH3COOCH2=>HO2+CH2O+CH2CO 1.00E+12 0.00 2000.  
 O+CH3COOCH2=CH2O+CH3+CO2 3.00E+13 0.00 0.  
 O+CH3COOCH2=HCO+CH3COOH 3.00E+13 0.00 0.  
 H+CH2COOCH3=CH3+CH3+CO2 1.94E+14 -0.07 920.3  
 H+CH2COOCH3=CH3+CH3OCO 1.25E+14 -0.59 963.5  
 H+CH2COOCH3=CH3OH+CH2CO 1.22E+18 -1.36 1347.7  
 H+CH2COOCH3=CH3O+CH3CO 2.41E+12 0.477 2004.6  
 OH+CH2COOCH3=CH2OH+CH3OCO 1.00E+13 0.00 0.  
 HO2+CH2COOCH3=>OH+CH2O+CH3OCO 1.00E+13 0.00 0.  
 CH3+CH2COOCH3=C2H5+CH3OCO 1.00E+13 0.00 0.  
 H+CH3COOCH2=CH3+CH3+CO2 1.94E+14 -0.07 920.3  
 H+CH3COOCH2=CH3+CH3OCO 1.25E+14 -0.59 963.5  
 H+CH3COOCH2=CH3OH+CH2CO 1.22E+18 -1.36 1347.7  
 H+CH3COOCH2=CH3O+CH3CO 2.41E+12 0.477 2004.6  
 OH+CH3COOCH2=CH2OH+CH3+CO2 1.00E+13 0.00 0.00  
 HO2+CH3COOCH2=>OH+CH2O+CH3+CO2 1.00E+13 0.00 0.00  
 CH3+CH3COOCH2=CH3COOH+C2H4 1.00E+13 0.00 0.00  
 !CH3COOCH2+O2(+M)=CH3COOCH2O2(+M) 5.82E+12 0.00 0.00  
 !LOW /1.04E+16 0.00 -6436/  
 !Troel /0.312 246. 5.9E-4/



```

!AR/1.0/ H2/3.0/ H2O/9.0/ CH4/3.0/ CO/3.0/ CO2/4.5/ C2H6/4.5/ CH3OH/3.0/
HE/1.2/ CH3COOCH3/6.0/
!CH3COOCH2O2(+M)=CH2COOCH2OOH(+M) 6.54E+10 0.00 18220.
!LOW /2.33E+15 0.00 11430./
!Troee /0.25 2088. 1.04E-4/
!AR/1.0/ H2/3.0/ H2O/9.0/ CH4/3.0/ CO/3.0/ CO2/4.5/ C2H6/4.5/ CH3OH/3.0/
HE/1.2/ CH3COOCH3/6.0/
!CH2COOCH2OOH(+M)<=>OH+CH2O+CO+CH2O(+M) 1.16E+14 0.00 20560.
!LOW /3.2E+19 0.00 19400./
!Troee /-2.69 163. 1.09E-5/
!AR/1.0/ H2/3.0/ H2O/9.0/ CH4/3.0/ CO/3.0/ CO2/4.5/ C2H6/4.5/ CH3OH/3.0/
HE/1.2/ CH3COOCH3/6.0/
!CH3COOCH2O2<=>HO2+CH2O+CH2CO 6.90e+33 -7.03 36543.5
!CH3COOCH2O2+CH3COOCH2O2=O2+2HCO+2CH3COOH 1.00E+13 0.00 0.
!CH2COOCH2OOH+O2 = OH+HOCH2COOCHO 3.70E+27 -5.03 8654.43
!HOCH2COOCHO=OH+CH2O+CO2+HCO 1.00E+16 0.00 30000.
!CH2COOCH2OOH+O2=2OH+CH2O+CO2+HCO 1.00E+16 0.00 30000.
!HO2+CH3OCOCH2O2=O2+OH+CH3OCO+CH2O 2.28E+11 0.00 -1788.
!CH2COOCH3+O2(+M)=CH3OCOCH2O2(+M) 5.82E+12 0.00 0.00
!LOW /1.04E+16 0.00 -6436/
!Troee /0.312 246. 5.9E-4/
!AR/1.0/ H2/3.0/ H2O/9.0/ CH4/3.0/ CO/3.0/ CO2/4.5/ C2H6/4.5/ CH3OH/3.0/
HE/1.2/ CH3COOCH3/6.0/
!CH3OCOCH2O2(+M)=CH2OCOCH2OOH(+M) 6.54E+10 0.00 18220.
!LOW /2.33E+15 0.00 11430./
!Troee /0.25 2088. 1.04E-4/
!AR/1.0/ H2/3.0/ H2O/9.0/ CH4/3.0/ CO/3.0/ CO2/4.5/ C2H6/4.5/ CH3OH/3.0/
HE/1.2/ CH3COOCH3/6.0/
!CH2OCOCH2OOH(+M)<=>OH+CH2O+CO+CH2O(+M) 1.16E14 0.00 20560.
!LOW /3.2E+19 0.00 19400./
!Troee /-2.69 163. 1.09E-5/
!AR/1.0/ H2/3.0/ H2O/9.0/ CH4/3.0/ CO/3.0/ CO2/4.5/ C2H6/4.5/ CH3OH/3.0/
HE/1.2/ CH3COOCH3/6.0/
!CH3OCOCH2O2<=>HO2+CH2O+CH2CO 6.90e+33 -7.03 36543.5
!CH3OCOCH2O2+CH3OCOCH2O2=O2+2CH3OCO+2CH2O 1.00E+13 0.00 0.
!CH2OCOCH2OOH+O2=OH+HOCH2OCOCHO 3.70E+27 -5.03 8654.43
!HOCH2OCOCHO=OH+CH2O+CO2+HCO 1.00E+16 0.00 30000.0
!CH2OCOCH2OOH+O2=2OH+CH2O+CO2+HCO 1.00E+16 0.00 30000.0

```

!Reactions of methyl chloroacetate pyrolysis

```

CH3OCOCH2CL=CH3+OCOCH2CL 4.55E+35 -19.60 1.26E+05
!Estimated as CH3COOCH3=CH3+CH3OCO, Peukert et al., 2012
CH3OCOCH2CL=CL+CH3COOCH2 1.0E+15 0.0 8.0E+04
!Estimated as CH3Cl=CH3+Cl, Shilov 1959 CH3Cl with corrected Ea.
CH3OCOCH2CL=CH2CL+CH3OCO 7.78E+086 -21.00 127983.5
!Estimated as methyl acetate CH3COOCH3=CH3OCO+CH3, Ren et al. 2017
PLOG /0.05 1.06E+87 -21.00 127983.5/
PLOG /0.50 2.59E+82 -19.30 128623.4/
PLOG /1.00 1.91E+77 -17.75 126063.8/
PLOG /10.0 1.76E+69 -15.15 124545.6/
PLOG /100 6.14E+49 -9.45 113561.9/
PLOG /1000 6.50E+30 -4.00 101447.6/
CH3OCOCH2CL=COCH2CL+CH3O 0.7E+0016 0.000 193645
!Estimated methyl undecanoate (calcul par kingas)

```

CH3OCOCH2CL=CH3+CH2CL+CO2 8.05E+087 -21.00 125195  
!Estimated as methyl acetate CH3COOCH3=CH3+CH3+CO2, Ren et al. 2017  
PLOG /0.05 1.10E+88 -21.00 125195.4/  
PLOG /0.50 1.94E+84 -19.60 126405.6/  
PLOG /1.00 20.0E+78 -18.00 123551.9/ ! 8.07  
PLOG /10 4.30E+65 -14.00 117470.9/  
PLOG /100 4.17E+45 -8.20 105384.4/  
PLOG /1000 6.97E+28 -3.40 94422.7/

!H-atom abstraction with H

CH3OCOCH2CL+H=>CH3COOCH2+HCL 5.18E+07 2.027 8061  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3COOCH2+HCL=>CH3OCOCH2CL+H 4.76E+05 2.184 33748  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCH2CL+H=>CH3OCOCHCL+H2 2.04E+06 2.36 5838  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCHCL+H2=>CH3OCOCH2CL+H 6.16E+06 1.933 19184  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCH2CL+H=>CH2OCOCH2CL+H2 7.32E+05 2.598 8563  
!Kinetic parameters determined by Quantum calculations, see paper  
CH2OCOCH2CL+H2=>CH3OCOCH2CL+H 7.04E+06 1.602 13352  
!Kinetic parameters determined by Quantum calculations, see paper

!H-atom abstraction with CH3

CH3OCOCH2CL+CH3=>CH3COOCH2+CH3CL 4.46E+03 2.883 12523  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3COOCH2+CH3CL=>CH3OCOCH2CL+CH3 2.02E+05 2.421 19971  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCH2CL+CH3=>CH3OCOCHCL+CH4 7.48E+01 3.237 5935  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCHCL+CH4=>CH3OCOCH2CL+CH3 1.784E+03 3.116 19477  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCH2CL+CH3=>CH2OCOCH2CL+CH4 8.04E+01 3.42 10091  
!Kinetic parameters determined by Quantum calculations, see paper  
CH2OCOCH2CL+CH4=>CH3OCOCH2CL+CH3 6.08E+03 2.73 15077  
!Kinetic parameters determined by Quantum calculations, see paper

!H-atom abstraction with Cl

CH3OCOCH2CL+CL=CH3COOCH2+CL2 1.15E+09 1.63 2.54E+04  
!estimated as CH3Cl+Cl=CH3+Cl2 Brudnik et al., 2013  
CH3OCOCH2CL+CL=>CH3OCOCHCL+HCL 9E+03 3.039 -3929  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCHCL+HCL=>CH3OCOCH2CL+CL 6.49E+03 2.514 8474  
!Kinetic parameters determined by Quantum calculations, see paper  
CH3OCOCH2CL+CL=>CH2OCOCH2CL+HCL 1.05E+02 3.723 -3958  
!Kinetic parameters determined by Quantum calculations, see paper  
CH2OCOCH2CL+HCL=>CH3OCOCH2CL+CL 2.41E+02 2.629 -113  
!Kinetic parameters determined by Quantum calculations, see paper

!H-atom abstraction with CH2Cl

CH3OCOCH2CL+CH2CL=>CH3COOCH2+CH2CL2 0.372E+03 2.883 12523  
!estimated with H-atom abstraction with CH3 radicals A/4  
CH3COOCH2+CH2CL2=>CH3OCOCH2CL+CH2CL 0.505E+05 2.421 19971  
!estimated with H-atom abstraction with CH3 radicals A/4  
CH3OCOCH2CL+CH2CL=>CH3OCOCHCL+CH3CL 1.8675E+01 3.237 5935  
!estimated with H-atom abstraction with CH3 radicals A/4

CH3OCOCHCL+CH3CL=>CH3OCOCH2CL+CH2CL 0.3345E+03 3.116 19477  
!estimated with H-atom abstraction with CH3 radicals A/4  
CH3OCOCH2CL+CH2CL=>CH2OCOCH2CL+CH3CL 2.01E+01 3.42 10091  
!estimated with H-atom abstraction with CH3 radicals A/4  
CH2OCOCH2CL+CH3CL=>CH3OCOCH2CL+CH2CL 1.14E+03 2.73 15077  
!estimated with H-atom abstraction with CH3 radicals A/4

!Beta-scission  
CH3OCOCHCL=COCHCL+CH3O 5.45E+13 0.66 4.93E+04  
!estimated as CH2COOCH3=CH2CO+CH3O Huynh et al., 2008  
COCHCL+CL=>CO+CHCL2 1.51E+14 0.0 0.0  
!estimated as COCH2+CL=CO+CH2CL NIST database  
OCOCH2CL=CH2CL+CO2 8.691E+17 -1.81 1.3657E+04  
!estimated as CH3OCO=CH3+CO2 Zhou et al., 2008  
CH2OCOCH2CL=>CH2O+COCH2CL 5.5E+07 1.565 28908  
!Kinetic parameters determined by Quantum calculations, see paper  
CH2O+COCH2CL=>CH2OCOCH2CL 6.37E-02 3.648 7304  
!Kinetic parameters determined by Quantum calculations, see paper

!alpha scission  
COCH2CL=>CO+CH2CL 2.32E+15 -0.334 14186  
!Kinetic parameters determined by Quantum calculations, see paper  
CO+CH2CL=>COCH2CL 1.48E+06 1.71 7410  
!Kinetic parameters determined by Quantum calculations, see paper

!Isomerization  
CH3OCOCHCL=>CH2OCOCH2CL 4.65E+06 1.841 30594  
!Kinetic parameters determined by Quantum calculations  
CH2OCOCH2CL=>CH3OCOCHCL 2.22E+07 1.272 22037  
!Kinetic parameters determined by Quantum calculations

!Terminations

CH2CL+H=CH3CL 1.0E+14 0.0 0.0  
!estimated  
CH2CL+CL=CH2CL2 1.0E+13 0.0 0.0  
!estimated  
CH2CH2CL+H=C2H5CL 1.0E+14 0.0 0.0  
!estimated  
CH2CCL+H=CH2CHCL 1.0E+14 0.0 0.0  
!estimated  
CH3CHCL+H=C2H5CL 1.0E+14 0.0 0.0  
!estimated  
CHCL2+H=CH2CL2 1.0E+14 0.0 0.0  
!estimated

!Reactions for H/Cl system (Pelucchi et al., 2016)

H+CL+M=HCL+M 2.0E+23 -2.45 0.0! Schading  
and Roth, 1994  
H2/2.0/ CL2/2.0/ N2/2.0/  
CL+H2=HCL+H 9.5E+07 1.72 3060 ! Kumaran et  
al., 1994  
CL+CL+M=CL2+M 2.3E+19 -1.50 0.0 ! See text  
H2/2.0/ CL2/6.9/ N2/2.0/  
CL2+M=CL+CL+M 5.7E+15 0.00 55596 ! Leylegian et  
al., 2005

CL2+H=HCL+CL	8.6E+13	0.00	1172.0 !
Baulch et al., 1981			
HCL+H=CL+H2	7.9E+12	0.0	3.4 ! Wu et
al., 1987			

!Reactions of alkyl chlorine

!Reactions chloromethane

CH3CL+CL=CH3+CL2	1.24E+13	1.63	2.54E+04
!Brudnik et al., 2013			
CH3CL+CL=CH2CL+HCL	2.18E+08	1.73	1580
!Brudnik et al., 2013			
CH3CL+H=CH3+HCL	36.7E+08	1.73	8575
!Louis et al., 2004 A*10			
CH3CL+H=H2+CH2CL	2.8E+05	2.59	7645
!Bryukov et al., 2001			
CH3+CL=CH3CL	3.07E+13	0.3	-109
!Parker et al., 2007			
CH3+HCL=CH3CL+H	8.33E+07	2.56	26290
!Bryukov et al., 2001			
CH3CL+O=OH+CH2CL	2.0E+13	0.0	7750
!Herron et al., 1988			
CH3CL+CH3=CH4+CH2CL	1.26E+12	0	1.16E+04
!Macken et al., 1979			
CH3CL=CH3+CL	1E+15	0	8.54E+04
!Shilov et al., 1959			

!Reactions chloroethene

CH2CH2CL+CL=CH2CHCL+HCL	9.9932E+12	0.0	3001
!Howlett et al., 1952			
C2H3+CL2=CH2CHCL+CL	2.79E+12	0	746
!Eskola et al., 2003			
CH2CH2CL=CH2CHCL+H	1.40E+13	0.0	4.21E+04
!Barat et al., 1992			
CH2CCL+HCL=CH2CHCL+CL	1.0E+12	0.0	3994
!Schneider et al., 1986			
CH3CHCL2=CH2CHCL+HCL	1.91E+13	0.0	5.35E+04
!Jonas et al., 1978			
CH3CHCL=CH2CHCL+H	2.02E+12	1.22	3.88E+04
!knyazev et al., 1994			
CH2CHCL+H=CH3CHCL	2.02E+10	0.86	149
!Knyazev et al., 1994			
CH2CHCL+H=CH2CH2CL	1.50E+13	0.0	5803
!Barat et al., 1992			
CH2CHCL+H=>C2H4+CL	2.46e+08	1.528	3454
!Kinetic parameters determined by Quantum calculations, see paper			
CH2CHCL+CH3=>C3H6+CL	6.55e+03	2.428	6803
!Kinetic parameters determined by Quantum calculations, see paper			

!Reactions dichloromethane

CH2CL+HCL=CH2CL2+H	1.16E+09	2.85	2.84E+04
!Bryukov et al., 2001			
CH2CL2+CL=CH2CL+CL2	1.28E+10	1.23	2.18E+04
!Brudnik et al., 2013			
CH2CL2+CL=CHCL2+HCL	8.91E+07	1.58	715
!Bryukov et al., 2002			

CH2CL2+H=CH2CL+HCL	8.31E+07	1.79	5884	
!Bryukov et al., 2001				
CH2CL2+H=H2+CHCL2	9.15E+04	2.66	6091	
!Bryukov et al., 2001				
CH2CL2+OH=CHCL2+H2O	2.43E+09	1.09	1532	
!Taylor et al., 1993				
CH2CL2=CH2CL+CL	1.33E+16	0	7.75E+04	!Lim
et al.,1994				
CH2CL2=CHCL+HCL	3.1E+14	0	7.57E+04	!Lim
et al., 1994				
!CH2CL+CL=CH2CL2				
!Reactions dichloroethane				
CH2CLCH2CL=CH2CH2CL+CL	1.26E+16	0	8.10E+04	
!Karra et al., 1988				
CH2CLCH2CL=CH2CL+CH2CL	8.68E+15	0	8.70E+04	
!Karra et al., 1988				
CH2CLCH2CL=CH2CHCL+HCL	4.79E+13	0	5.83E+04	
!Rajakumar et al., 2003				
CH2CLCH2CL=C2H4+CL2	4.25E+11	0.83	9.34E+04	!Zhu
et al., 2002				
!Reactions chloroethane				
C2H5+CL2=C2H5CL+CL	7.59E+12	0.0	-238	
!Timonen et al., 1988				
CH3CHCL+HCL=C2H5CL+CL	3.16E+11	0.0	8008	
!Manion et al. 1988				
CH3CHCL+H2=C2H5CL+H	1.26E+12	0.0	1.62E+04	
!Manion et al. 1988				
C2H5CL+H=CH2CH2CL+H2	1.94E+11	2.9	6898	
!Sheng et al., 2004				
C2H5CL+H=CH3CHCL+H2	5.07E+11	2.38	5411	
!Sheng et al., 2004				
C2H5CL+H=C2H5+HCL	1.62E+12	1.46	8108	
!Sheng et al., 2004				
C2H5CL+CL=HCL+CH3CHCL	5.03E+07	1.7	-1153	!He
et al., 2006				
C2H5CL+CL=HCL+CH2CH2CL	1.88E+04	2.8	-503	!He
et al., 2012				
C2H5CL+OH=CH3CHCL+H2O	1.56E+13	0.5	1195	
!Herndon et al. 2001				
C2H5CL=CH3+CH2CL	1.71E+16	0.0	88910	
!Karra et al., 1988				
C2H5CL=C2H5+CL	5E+15	0.0	82935	
!Karra et al., 1988				
C2H5CL=C2H4+HCL	9.12E+13	0.0	5.33E+04	
!Ahubelem et al., 2014				
!Autres réactions				
CH3+CL=HCL+CH2	2.20E+13	0.0	8247	
!Goldbach et a., 1990				
C2H6+CL=C2H5+HCL	4.35E+11	0.70	-233	
!Bryukov et al., 2003				
C2H3+HCL=C2H4+CL	1.26E+12	0.0	503	
!Manion et al., 1988				

CH2O+CL=HCO+HCL	4.94E+13	0.0	67.57
!Atkinson et al., 2001			
C2H6+CH2CL=C2H5+CH3CL	4.33E+09	4	8287
!Estimated as C2H6+CL=HCL+C2H5			
C3H6+CL=C3H5-A+HCL	2.95E+13	0.0	179
!Pilgrim et al., 1997			

END