

```
+++++
+++++
ELEMENTS
C
H
N
O
AR
HE
END
!+++++
+++++
+++++
SPECIES
!+++++
+++++
+++++
!\SPECIES_MODULE: DILUENTS
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS:
AR
N2
HE
H2
H
O2
O
H2O
OH
OHV
H2O2
HO2
CO
CO2
HOCO
CH4
CH3
CH2
CH2 (S)
C
CH
CHV
CH3O2H
CH3O2
CH2O2H
CH3OH
CH3O
CH2OH
CH2O
HCO
HCOH
HO2CHO
HOCH2O2H
HOCH2O2
OCH2O2H
HOCH2O
O2CHO
```

HOCHO
OCHO
C2H6
C2H5
C2H5O2H
C2H5O2
C2H4
C2H3
CHOCHO
C2H3OOH
C2H3OO
CHCHO
C2H2
C2H
H2CC
C2H5OH
C2H5O
PC2H4OH
SC2H4OH
O2C2H4OH
C2H4O2H
C2H4O1-2
C2H3O1-2
CH3CHO
CH3CO
CH2CHO
O2CH2CHO
HO2CH2CO
C2H3OH
C2H2OH
CH2CO
HCCO
HCCOH
CH3CO3H
CH3CO3
CH3CO2
CH3OCH3
CH3OCH2
CH3OCH2O2H
CH3OCH2O2
CH2OCH2O2H
O2CH2OCH2O2H
HO2CH2OCHO
OCH2OCHO
HOCH2OCO
CH3OCH2O
CH3OCHO
CH3OCO
CH2OCHO
C3H8
IC3H7
NC3H7
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
C3H6
C3H5-A
C3H5-S
C3H5-T
CC3H6
C3H5O
CH2CHOCH2
CH3CHCHO
AC4H7OOH
C3H6OH1-2
CH3CHCO
AC3H5OOH
C3H6OH2-1
HOC3H6O2
SC3H5OH
IC3H5OH
C3H5OH
CH2CCH2OH
C3H4-P
C3H4-A
C3H3
CC3H4
C3H2
H2CCC (S)
C3H2 (S)
C3H2C
PC3H4OH-2
SC3H4OH
C3H3O
C3H3O2H
C2HCHO
C2H5CHO
C2H5CO
CH2CH2CHO
C2H3CHO
C2H3CO
CH3COCH3
CH3COCH2
CH3COCH2O2
CH3COCH2O
C3KET21
C4H10
PC4H9
SC4H9

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
IC4H10
IC4H9
TC4H9
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
IC4H8
IC4H7
IC4H7-I1
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
C4H8-1
C4H8-2
C4H71-1
C4H71-2
C4H71-3
C4H71-4
C4H72-2
C4H71-0
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
C4H6OHOOH1-4-3
C4H6OHOOH2-2-1
C4H6OHOOH1-3-4
C4H6OHOOH1-2-3
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
C4H6
C4H612
C4H6-2
C4H5-I
C4H5-N
C4H5-2
C4H4
C4H3-I
C4H3-N
C4H2
!\OXIDSPEC:
C4H6O25
C2H3CHOCH2
C4H4O
C4H6O23
CH2CHCHCHO
H2C4O
NC3H7CHO
NC3H7CO
C3H6CHO-1
C3H6CHO-2
C3H6CHO-3
SC3H5CHO
SC3H5CO
C2H5COCH3
C2H5COCH2
CH2CH2COCH3
CH3CHCOCH3
C2H3COCH3
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CH2CHOOHCOCH3
C2H5CHCO
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C5H11-2
C5H11-3
!\OXIDSPEC:
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C5H11O2H-3
C5H11O2-1
C5H11O2-2
C5H11O2-3
C5H11O-1
C5H11O-2
C5H11O-3
C5H10OOH1-2
C5H10OOH1-3
C5H10OOH1-4
C5H10OOH1-5

C5H1000H2-1
C5H1000H2-3
C5H1000H2-4
C5H1000H2-5
C5H1000H3-1
C5H1000H3-2
C5H1001-2
C5H1001-3
C5H1001-4
C5H1001-5
C5H1002-3
C5H1002-4
C5H1000H1-202
C5H1000H1-302
C5H1000H1-402
C5H1000H1-502
C5H1000H2-102
C5H1000H2-302
C5H1000H2-402
C5H1000H2-502
C5H1000H3-102
C5H1000H3-202
C5H91-2,300H
C5H91-2,400H
C5H91-2,500H
C5H91-3,400H
C5H91-3,500H
C5H91-4,500H
C5H92-1,300H
C5H92-1,400H
C5H92-1,500H
C5H92-3,400H
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C5H93-1,400H
C5H93-1,500H
C5H93-2,400H
C5H91-300H
C5H91-400H
C5H91-500H
C5H92-100H
C5H92-400H
C5H92-500H
C5H901-200H-3
C5H901-200H-4
C5H901-200H-5
C5H901-300H-2
C5H901-300H-4
C5H901-300H-5
C5H901-400H-2
C5H901-400H-3
C5H901-400H-5
C5H901-500H-2
C5H901-500H-3
C5H902-300H-1
C5H902-300H-4
C5H902-300H-5

C5H9O2-4OOH-1
C5H9O2-4OOH-3
C5H9O1-2O-5
CH2CH2OCH2CH2CHO
NC5KET12
NC5KET13
NC5KET14
NC5KET15
NC5KET21
NC5KET23
NC5KET24
NC5KET25
NC5KET31
NC5KET32
NC5KET12O
NC5KET13O
NC5KET14O
NC5KET15O
NC5KET21O
NC5KET23O
NC5KET24O
NC5KET25O
NC5KET31O
NC5KET32O
NC5DIONE13
NC5DIONE24
C5H10OH23
O2C5H10OH23
OCH2CHO
CH2OCH2CHO
C2H4OCHO
C5H10OOH1-3OH
C5H10OOH2-4OH
C5H10OOH3-1OH
NC5CYCPER13
NC5CYCPER24
NC5CYCPER31
IC5H12
AC5H11
BC5H11
CC5H11
DC5H11
AC5H9O-A2
AC5H11O2H
BC5H11O2H
CC5H11O2H
DC5H11O2H
AC5H11O2
BC5H11O2
CC5H11O2
DC5H11O2
AC5H11O
BC5H11O
CC5H11O
DC5H11O
AC5H10OOH-A
AC5H10OOH-B
AC5H10OOH-C

AC5H1000H-D
BC5H1000H-A
BC5H1000H-C
BC5H1000H-D
CC5H1000H-A
CC5H1000H-B
CC5H1000H-D
DC5H1000H-A
DC5H1000H-B
DC5H1000H-C
A-AC5H100
A-BC5H100
A-CC5H100
A-DC5H100
B-CC5H100
B-DC5H100
C-DC5H100
AC5H1000H-AO2
AC5H1000H-BO2
AC5H1000H-CO2
AC5H1000H-DO2
BC5H1000H-AO2
BC5H1000H-CO2
BC5H1000H-DO2
CC5H1000H-AO2
CC5H1000H-BO2
CC5H1000H-DO2
DC5H1000H-AO2
DC5H1000H-BO2
DC5H1000H-CO2
C5H9A-A, BOOH
C5H9A-A, COOH
C5H9A-A, DOOH
C5H9A-B, COOH
C5H9A-B, DOOH
C5H9A-C, DOOH
C5H9B-A, AOOH
C5H9B-A, COOH
C5H9B-A, DOOH
C5H9B-C, DOOH
C5H9C-A, AOOH
C5H9C-A, BOOH
C5H9C-A, DOOH
C5H9C-B, DOOH
C5H9D-A, AOOH
C5H9D-A, BOOH
C5H9D-A, COOH
C5H9D-B, COOH
C5H9A-AOOH
C5H9A-COOH
C5H9A-DOOH
C5H9B-AOOH
C5H9B-DOOH
C5H9C-AOOH
C5H9C-BOOH
C5H9OA-AOOH-B
C5H9OA-AOOH-C
C5H9OA-AOOH-D

C5H9OA-BOOH-A
C5H9OA-BOOH-C
C5H9OA-BOOH-D
C5H9OA-COOH-A
C5H9OA-COOH-B
C5H9OA-COOH-D
C5H9OA-DOOH-A
C5H9OA-DOOH-B
C5H9OA-DOOH-C
C5H9OB-COOH-A
C5H9OB-COOH-D
C5H9OB-DOOH-A
C5H9OB-DOOH-C
C5H9OC-DOOH-A
C5H9OC-DOOH-B
CH3COCH2OCH2CH2
IC5KETAA
IC5KETAB
IC5KETAC
IC5KETAD
IC5KETCA
IC5KETCB
IC5KETCD
IC5KETDA
IC5KETDB
IC5KETDC
IC5KETAAO
IC5KETABO
IC5KETACO
IC5KETADO
IC5KETCAO
IC5KETCBO
IC5KETCDO
IC5KETDAO
IC5KETDBO
IC5KETDCO
AC5H10OH
BC5H10OH
CC5H10OH
AO2C5H10OH
BO2C5H10OH
CO2C5H10OH
IC3H5COCH3
IC3H5COCH2
AC3H4COCH3
NEOC5H12
NEOC5H11
NEOC5H11O2H
NEOC5H11O2
NEOC5H11O
NEOC5H10OOH
NEO-C5H10O
NEOC5H10OOH-O2
NEOC5H9Q2
NEOC5KET
NEOC5KETOX
NEOC5KEJOL
NEOC5H9O-OOH

C5H10-1
C5H81-3
C5H901-3
BC5H10
CC5H9-A
CC5H9-B
AC5H9O-C
CC5H9O-B
AC5H10
AC5H9-A2
AC5H9-C
AC5H9-D
B2E2M1OJ
B13DE2M
B13DE2MJ
B12DE3M
B2E3M1OJ
TC4H8CHO
O2C4H8CHO
O2HC4H8CO
PC4H8CHO-1O2
PC4H8CHO-2O2
PC4H8CHO-3O2
PC4H8CHO-4O2
C4H7CHO-2
C4H7CHO-3
C4H7CHO-4
NC3H7COCH3
C2H5COC2H5
NC3H7COCH2
CH3CH2CHCOCH3
CH3CHCH2COCH3
CH2CH2CH2COCH3
CH2CH2COC2H5
CH3CHCOC2H5
!\OXIDSPEC:
NC52ONEO2-3
NC52ONEO2-4
NC52ONEO2-5
NC53ONEO2-1
NC53ONEO2-2
NC52ONE-3
NC52ONE-4
NC53ONE-1
NC5H11OH
C5H10OH11
C5H10OH12
C5H10OH13
C5H10OH14
C5H10OH15
!\OXIDSPEC:
C5H10OH-1O2
C5H10OH-2O2
C5H10OH-3O2
C5H10OH-4O2
C5H10OH-5O2
C5H9OH1-1
C5H9OH1-2

C5H9OH1-3
C5H9OH1-4
C6H101-5
C6H9-A
H15DE25DM
H15DE25DM-S
H15DE25DM-A
!\OXIDSPEC:
H15DE25DM-AO
H15DE25DM-SO
H15DE2M-T
IC4H7CHO
L-C6H4
C-C6H4
C6H3
C6H2
C6H6
FULVENE
C6H5
!\OXIDSPEC:
C6H5OO
C6H5OOH
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

!-----

!++++
++++
++++
!\END_SPECIES_MODULE: \AROMATIC
!++++
++++
++++

PC4H9CHO
PC4H8CHO-1
PC4H8CHO-2
PC4H8CHO-3
PC4H8CHO-4
CH3COOH
C2H5COOH
AC3H5CHO
PC4H9CO
C5H9O12-5
C5H9O13-5
C5H9O14-5
C5H9O23-1
C5H9O23-5
C5H9O24-1

!
!
!-----

!----- AJOUT HP PRINCETON -----

!-----

C2O C4H C5H2 HCCCHCCH H2CCCCCH C4H5C2H N NH NH2 NH3 NNH N2H2 N2H3 N2H4
NO3
HNO3 O3

!-----

!
!----- AJOUT DAGAUT -----

NO NO2 HNO HONO H2NO CH3NO CH3NO2 CH3ONO CH3ONO2 H2CNO2 N2O

!-----

HNO2 C2H5NO2 NC3H7NO2 IC3H7NO2 PC4H9NO2 SC4H9NO2 C5H11-1NO2 C5H11-2NO2
C5H11-3NO2

!
END
!\END_SPECIES_LIST
!\END_SPECIES_LIST
!\START_KINETICS_INPUT
REACTIONS

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

!\KINETICS_MODULE: \H2_O2

!\MODCOMMENTS:

!\MODWARNINGS:

!\MODSUBMECHS:

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

!-----

!\SUBMECH: \H2

!-----

CH2O+TC4H9<=>NEOC5H11O

+5.0000000E+010 +0.0000000E+000 +2.3300000E+003 !\AUTHOR: !\REF:H. J.
CURRAN INT. J. CHEM. KIN. 2006, 38, 4, 250-275

!

!\REACTIONCLASS: \QOOH<=>CETH+OH

\A

\N \EA

!

NEOC5H10OOH<=>NEO-C5H10O+OH

+3.7100000E+009 +7.0000000E-001 +1.5900000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089

!

!\REACTIONCLASS: \QOOH_DECOMPOSITION

\A

\N \EA

!

NEOC5H10OOH=>OH+CH2O+IC4H8

+3.6400000E+009 +1.3000000E+000 +2.3700000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089

NEOC5H10OOH<=>IC4H7OOH+CH3

+1.6400000E+007 +2.0000000E+000 +2.8300000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089

!

!\REACTIONCLASS: \QOOH+O2<=>O2QOOH

\A

\N \EA

!

NEOC5H10OOH+O2<=>NEOC5H10OOH-O2

+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.5

!

!\REACTIONCLASS: \O2QOOH<=>P(OOH)2

\A

\N \EA

!

NEOC5H10OOH-O2<=>NEOC5H9Q2
+7.9870000E+008 +1.2000000E+000 +2.1600000E+004 !\AUTHOR: !\REF:
!\COMMENT:
!

!\REACTIONCLASS: \O2QOOH<=>KET+OH \A
\N \EA
!

NEOC5H10OOH-O2<=>NEOC5KET+OH
+5.1880000E+004 +1.9000000E+000 +1.8800000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
!O2CH2CH2CH2OOH<=>HO2CH2CH2CHO+OH ANALOGY
!

!\REACTIONCLASS: \P(OOH)2_DECOMPOSITION \A
\N \EA
!

NEOC5H9Q2<=>IC4H7OOH+CH2O2H
+3.6400000E+009 +1.3000000E+000 +2.3700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H9Q2<=>IC4H6Q2-II+CH3
+1.6400000E+007 +2.0000000E+000 +2.8300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \KET_DECOMPOSITION \A
\N \EA
!

NEOC5KET<=>NEOC5KETOX+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5KETOX<=>TC3H6CHO+CH2O
+2.4750000E+021 -2.5400000E+000 +1.5830000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \P(OOH)2<=>CETH-OOH+OH \A
\N \EA
!

NEOC5H9Q2<=>NEOC5H9O-OOH+OH
+3.7100000E+009 +7.0000000E-001 +1.5900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \CETH-OOH_DECOMPOSITION \A
\N \EA
!

NEOC5H9O-OOH=>C3H5-T+CH2O+CH2O+OH
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \CETH_DECOMPOSITION \A
\N \EA
!

NEO-C5H10O+OH<=>TC4H8CHO+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEO-C5H10O+OH=>IC4H7+CH2O+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEO-C5H10O+HO2<=>TC4H8CHO+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEO-C5H10O+HO2=>IC4H7+CH2O+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEO-C5H10O+H<=>TC4H8CHO+H2
+3.5440000E+007 +2.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEO-C5H10O+H=>IC4H7+CH2O+H2
+1.3300000E+006 +2.5400000E+000 +6.7560000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEO-C5H10O<=>IC4H8+CH2O
+3.8000000E+015 +0.0000000E+000 +6.0700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \OTHER_DECOMPOSITIONS \A
\N \EA
!

NEOC5KETOX<=>NEOC5KEJOL
+1.2030000E+009 +1.1990000E+000 +1.3600700E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5KEJOL<=>IC4H8OH+CO
+2.2730000E+021 -2.3400000E+000 +1.1020000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!\WARNING: KPS, FROM WHERE IS THIS SPECIES FORMED?? IS THIS A DUPLICATE?
!IC4H6Q2-II=>C3H4-A+CH2O+HO2+OH 1.000E+16 0.000 43000.0 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: RMVD, DUPLICATE WITH IC4 MEC
!-----

!\ENDSUBMECH: \NEOC5H12
!-----
!-----
!-----
!-----

!\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 JB'S PENTANE WITH CW'S 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 CW'S AND SEPARATED 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 CW'S 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 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 CLASSED. 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

!-----

!-----

!-----

!\SUBMECH: \PC4H8CHO-1\PC4H8CHO-2\PC4H8CHO-3

!\MECHCOMMENTS:

!\MECHWARNINGS: KPS, 22 /07 /2015 THESE SPECIES HAVE BEEN MOVED FROM KWS
C6 /C7 MECHANISM. WE SHOULD DISCUSS.

!-----

!-----

!\REACTIONCLASS: \1. \A
\N \EA
!

C2H5+C2H3CHO<=>PC4H8CHO-1
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH3+AC3H5CHO<=>PC4H8CHO-2
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C4H8-1+HCO<=>PC4H8CHO-2
+1.0000000E+011 +0.0000000E+000 +6.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C3H6+CH2CHO<=>PC4H8CHO-3
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C2H4+CH2CH2CHO<=>PC4H8CHO-4
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!\WARNING: KPS, 22 /07 /2015 REACTION MOVED FROM KUIWENS "OTHER
DECOMPOSITIONS" PART OF C6 /C7 MECHANISM
C3H5-A+HCO<=>AC3H5CHO
+1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \2. \A
\N \EA
!

PC4H9CHO+O2<=>PC4H9CO+HO2
+3.0100000E+013 +0.0000000E+000 +3.9150000E+004 !\AUTHOR:
!\REF:!ANALOGY TO CH3CHO
PC4H9CHO+O<=>PC4H9CO+OH
+5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR:
!\REF:!ANALOGY TO CH3CHO
PC4H9CHO+H<=>PC4H9CO+H2
+1.3100000E+005 +2.5800000E+000 +1.2200000E+003 !\AUTHOR:
!\REF:!ANALOGY TO CH3CHO
PC4H9CHO+OH<=>PC4H9CO+H2O
+3.3700000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR:
!\REF:!ANALOGY TO CH3CHO
PC4H9CHO+HO2<=>PC4H9CO+H2O2
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR:
!\REF:!ANALOGY TO CH3CHO
PC4H9CHO+CH3<=>PC4H9CO+CH4 +7.0800000E-
004 +4.5800000E+000 +1.9660000E+003 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+CH3O2<=>PC4H9CO+CH3O2H
+3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR:
!\REF:!ANALOGY TO CH3CHO
PC4H9CHO+OH<=>PC4H8CHO-1+H2O
+5.5200000E+002 +3.1200000E+000 -1.1760000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+OH<=>PC4H8CHO-2+H2O
+4.6800000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

PC4H9CHO+OH<=>PC4H8CHO-3+H2O
+4.6800000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+OH<=>PC4H8CHO-4+H2O
+5.2800000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+HO2<=>PC4H8CHO-1+H2O2
+3.4400000E+012 +5.0000000E-002 +1.7880000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+HO2<=>PC4H8CHO-2+H2O2
+9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+HO2<=>PC4H8CHO-3+H2O2
+9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+HO2<=>PC4H8CHO-4+H2O2
+2.3790000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+CH3O2<=>PC4H8CHO-1+CH3O2H
+3.4400000E+012 +5.0000000E-002 +1.7880000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+CH3O2<=>PC4H8CHO-2+CH3O2H
+9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+CH3O2<=>PC4H8CHO-3+CH3O2H
+9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
PC4H9CHO+CH3O2<=>PC4H8CHO-4+CH3O2H
+2.3790000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \3. \A
\N \EA
!

!\WARNING: KPS, WHERE ARE DECOMPOSITION REACTIONS FOR OTHER PC4H8CHO
RADICALS?? THERE APPEAR TO BE NONE?
PC4H9CO<=>NC3H7+CH2CO
+1.0000000E+011 +0.0000000E+000 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING DECOMPOSITION RATE COSNTANTS FOR
OTHER RADICALS MISSING?
PC4H9CO<=>PC4H9+CO
+5.7800000E+014 +0.0000000E+000 +1.6843500E+004 !\AUTHOR: JB !\REF: J.
M. SIMMIE, J. PHYS. CHEM. A, 116, 2012, 4528-4538 !\COMMENT: SAME RATE
CONSTANT USED IN PELUCCHI ET AL., COMBUST. FLAME, 162, 2015, 265-286
!

!\REACTIONCLASS: \R+O2<=>RO2 \A
\N \EA
!

!\PC4H9CO+O2<=>PC4H9CO3 1.000E+011 0.000 0.0 !\AUTHOR: JB !\REF: ESTIMATED
BY JB !\COMMENT: REMOVED FOR NOW TO TEST EFFECT OF OTHER RELATED
REACTIONS
PC4H8CHO-1+O2<=>PC4H8CHO-1O2
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED BY JB !\COMMENT:

PC4H8CHO-2+O2<=>PC4H8CHO-2O2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
PC4H8CHO-3+O2<=>PC4H8CHO-3O2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
PC4H8CHO-4+O2<=>PC4H8CHO-4O2
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
!

!\REACTIONCLASS: \RO2<=>E+HO2 \A
\N \EA
!

PC4H8CHO-1O2<=>C4H7CHO-2+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
PC4H8CHO-2O2<=>C4H7CHO-2+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
PC4H8CHO-2O2<=>C4H7CHO-3+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
PC4H8CHO-3O2<=>C4H7CHO-3+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
PC4H8CHO-3O2<=>C4H7CHO-4+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
PC4H8CHO-4O2<=>C4H7CHO-4+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
!

!\REACTIONCLASS: \OTHER_DECOMPOSITIONS, ETC. \A
\N \EA
!

C4H7CHO-2+OH=>C4H7-1+CO+H2O
+1.7000000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: JB !\REF: M.
PELUCCHI, K. P. SOMERS, K. YASUNAGA, U. BURKE, A. FRASSOLDATI, E. RANZI,
H. J. CURRAN, T. FARAVELLI, COMBUST. FLAME, 2015, 162, 265-286
!\COMMENT: ALDE
C4H7CHO-3+OH=>C4H7-2+CO+H2O
+1.7000000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: JB !\REF: M.
PELUCCHI, K. P. SOMERS, K. YASUNAGA, U. BURKE, A. FRASSOLDATI, E. RANZI,
H. J. CURRAN, T. FARAVELLI, COMBUST. FLAME, 2015, 162, 265-286
!\COMMENT: ALDE

C4H7CHO-3+OH=>C4H6+HCO+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED

C4H7CHO-4+OH=>C4H71-4+CO+H2O
+1.7000000E+012 +0.0000000E+000 -6.1900000E+002 !\AUTHOR: JB !\REF: M.
PELUCCHI, K. P. SOMERS, K. YASUNAGA, U. BURKE, A. FRASSOLDATI, E. RANZI,
H. J. CURRAN, T. FARAVELLI, COMBUST. FLAME, 2015, 162, 265-286
!\COMMENT: ALDE

C4H7CHO-4+OH=>C4H6+HCO+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED

!-----
!-----
!\ENDSUBMECH: \PC4H8CHO-1\PC4H8CHO-2\PC4H8CHO-3
!-----
!-----

!\SUBMECH: \C5H9O12-5\C5H9O13-5\C5H9O14-5\C5H9O23-1\C5H9O23-5\C5H9O24-1
!\MECHCOMMENTS:

!\MECHWARNINGS: KPS, 22 /07 /2015 THESE SPECIES HAVE BEEN MOVED FROM THE
"OTHER DECOMPOSITIONS" SECTION OF KWS C6 /C7 CHEMISTRY. WE NEED TO TALK
ABOUT HOW BEST TO INCLUDE THESE SPECIES

!-----
!-----
C3H5O+C2H4<=>C5H9O12-5
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH2CH2CHO+C2H4<=>C5H9O13-5
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH2O+C4H71-4<=>C5H9O14-5
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C2H3CHO+C2H5<=>C5H9O23-1
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH3CHCHO+C2H4<=>C5H9O23-5
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH3CHO+C3H5-A<=>C5H9O24-1
+1.0000000E+011 +0.0000000E+000 +7.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

!-----
!-----
!\ENDSUBMECH: \C5H9O12-5\C5H9O13-5\C5H9O14-5\C5H9O23-1\C5H9O23-5\C5H9O24-1
1
!-----
!-----

!\SUBMECH: \NC3H7COCH3\C2H5COC2H5
!\MECHCOMMENTS:
!\MECHWARNINGS:

!-----

!

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

CH3CO+NC3H7<=>NC3H7COCH3
+2.0000000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
NC3H7COCH3+OH<=>NC3H7COCH2+H2O
+3.9900000E+002 +3.0800000E+000 +9.4400000E+002 !\AUTHOR: JB !\REF: C.
-W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011,
11175-11192 !\COMMENT: ETHYL METHYL KETONE RATE CONSTANT
NC3H7COCH3+HO2<=>NC3H7COCH2+H2O2 +4.1400000E-
002 +4.0700000E+000 +1.6253300E+004 !\AUTHOR: JB !\REF: J. MENDES, C. -
W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525 !\COMMENT:
N-PROPYL METHYL KETONE RATE CONSTANT
NC3H7COCH3+OH<=>CH3CH2CHCOCH3+H2O
+2.3600000E+002 +3.1500000E+000 +3.0504000E+003 !\AUTHOR: JB !\REF: C.
-W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011,
11175-11192 !\COMMENT: ETHYL METHYL KETONE RATE CONSTANT
NC3H7COCH3+HO2<=>CH3CH2CHCOCH3+H2O2 +3.5600000E-
001 +3.6900000E+000 +1.3099600E+004 !\AUTHOR: JB !\REF: J. MENDES, C. -
W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525 !\COMMENT:
N-PROPYL METHYL KETONE RATE CONSTANT
NC3H7COCH3+OH<=>CH3CHCH2COCH3+H2O
+4.1400000E+002 +3.0000000E+000 +2.4400000E+003 !\AUTHOR: JB !\REF:
ESTIMATED BY JB !\COMMENT:
NC3H7COCH3+HO2<=>CH3CHCH2COCH3+H2O2 +1.1500000E-
003 +4.4300000E+000 +1.1364800E+004 !\AUTHOR: JB !\REF: J. MENDES, C. -
W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525 !\COMMENT:
N-PROPYL METHYL KETONE RATE CONSTANT
NC3H7COCH3+OH<=>CH2CH2CH2COCH3+H2O
+2.7320000E+007 +1.8130000E+000 +8.6840000E+002 !\AUTHOR: JB !\REF: R.
SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060
!\COMMENT: ASSUMED ANALOGOUS TO ALKANE. P1 RATE CONSTANT (SEE REFERENCE)
NC3H7COCH3+HO2<=>CH2CH2CH2COCH3+H2O2 +4.4400000E-
001 +3.8800000E+000 +1.5814100E+004 !\AUTHOR: JB !\REF: J. MENDES, C. -
W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525 !\COMMENT:
N-PROPYL METHYL KETONE RATE CONSTANT
C2H5COC2H5+OH<=>CH2CH2COC2H5+H2O
+2.7000000E+000 +3.8100000E+000 +2.8993000E+003 !\AUTHOR: JB !\REF: C.
-W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011,
11175-11192 !\COMMENT: ETHYL METHYL KETONE RATE CONSTANT
C2H5COC2H5+HO2<=>CH2CH2COC2H5+H2O2 +6.1800000E-
005 +4.9100000E+000 +1.4081300E+004 !\AUTHOR: JB !\REF: J. MENDES, C. -
W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525 !\COMMENT:
ETHYL METHYL KETONE RATE CONSTANT
C2H5COC2H5+OH<=>CH3CHCOC2H5+H2O
+2.3600000E+002 +3.1500000E+000 +3.0504000E+003 !\AUTHOR: JB !\REF: C.
-W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011,
11175-11192 !\COMMENT: ETHYL METHYL KETONE RATE CONSTANT
C2H5COC2H5+HO2<=>CH3CHCOC2H5+H2O2 +8.4200000E-
002 +3.9300000E+000 +1.3389800E+004 !\AUTHOR: JB !\REF: J. MENDES, C. -
W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525 !\COMMENT:
ETHYL METHYL KETONE RATE CONSTANT

!

!\REACTIONCLASS: \RADICAL_BETA_SCISSION \A
\N \EA
!

NC3H7+CH2CO<=>NC3H7COCH2
+3.6300000E+003 +2.4300000E+000 +8.9600000E+003 !\AUTHOR: JB !\REF:
FROM PRAJACTA PARAB'S CALCULATIONS FOR KETENE+METHYL<=>ACETONYL RADICAL
!\COMMENT: DIVIDED BY 2
C2H3COCH3+CH3<=>CH3CH2CHCOCH3
+1.7600000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:
PROPENE+METHYL RATE CONSTANT
C3H6+CH3CO<=>CH3CHCH2COCH3
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:
PROPENE+ETHYL RATE CONSTANT
C2H4+CH3COCH2<=>CH2CH2CH2COCH3
+1.3200000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:
ETHYLENE+ETHYL RATE CONSTANT
C2H4+C2H5CO<=>CH2CH2COC2H5
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:
PROPENE+ETHYL RATE CONSTANT
CH3CHCO+C2H5<=>CH3CHCOC2H5
+3.6300000E+003 +2.4300000E+000 +8.9600000E+003 !\AUTHOR: JB !\REF:
FROM PRAJACTA PARAB'S CALCULATIONS FOR KETENE+METHYL<=>ACETONYL RADICAL
!\COMMENT: DIVIDED BY 2
!

!\REACTIONCLASS: \R+O2<=>RO2 \A
\N \EA
!

CH3CH2CHCOCH3+O2<=>NC52ONEO2-3
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED BY JB !\COMMENT:
CH3CHCH2COCH3+O2<=>NC52ONEO2-4
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
CH2CH2CH2COCH3+O2<=>NC52ONEO2-5
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
CH2CH2COC2H5+O2<=>NC53ONEO2-1
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
CH3CHCOC2H5+O2<=>NC53ONEO2-2
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED BY JB !\COMMENT:
!

!\REACTIONCLASS: \RO2<=>E+HO2 \A
\N \EA

!

NC52ONEO2-3<=>NC52ONE-3+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
NC52ONEO2-4<=>NC52ONE-3+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
NC52ONEO2-4<=>NC52ONE-4+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
NC52ONEO2-5<=>NC52ONE-4+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
NC53ONEO2-1<=>NC53ONE-1+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
NC53ONEO2-2<=>NC53ONE-1+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
!

!\REACTIONCLASS: \OTHER_DECOMPOSITIONS,ETC. \A
\N \EA
!

NC52ONE-3+OH=>CH2CO+C3H5-S+H2O
+4.4600000E+006 +2.0720000E+000 +1.0508000E+003 !\AUTHOR: JB !\REF:
ANALOGY TO C3H6+OH<=>C3H5-A+H2O !\COMMENT: ALLYLIC H-ATOM ABSTRACTION
FOLLOWED BY BETA-SCISSION
NC52ONE-4+OH=>CH2CO+C3H5-A+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH<=>C4H7-1-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED
NC53ONE-1+OH=>CH3CHCO+C2H3+H2O
+2.3600000E+002 +3.1500000E+000 +3.0504000E+003 !\AUTHOR: JB !\REF: C.
-W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011,
11175-11192 !\COMMENT: ETHYL METHYL KETONE RATE CONSTANT. SECONDARY H-
ATOM ABS
!-----
!-----
!\ENDSUBMECH: \NC3H7COCH3\C2H5COC2H5
!-----
!-----
!-----
!\SUBMECH: \NC5H11OH
!\MECHCOMMENTS: ADOPTED LARGELY FROM ALEX HEUFER'S N-PENTANOL MECHANISM.
JB
!\MECHWARNINGS:

!-----

!

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

NC5H11OH+OH<=>C5H10OH15+H2O
+5.2800000E+009 +9.7000000E-001 +1.5900000E+003 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+HO2<=>C5H10OH15+H2O2
+2.0400000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+OH<=>C5H10OH14+H2O
+4.6700000E+007 +1.6100000E+000 -3.5000000E+001 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+HO2<=>C5H10OH14+H2O2
+6.3200000E+001 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+OH<=>C5H10OH13+H2O
+1.1410000E+003 +2.8700000E+000 -2.9260000E+003 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+HO2<=>C5H10OH13+H2O2 +2.7600000E-
004 +4.7600000E+000 +1.1850000E+004 !\AUTHOR: !\REF: !\COMMENT:
NC5H11OH+OH<=>C5H10OH12+H2O
+1.5400000E+000 +3.7000000E+000 -3.7360000E+003 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+HO2<=>C5H10OH12+H2O2 +7.5100000E-
003 +4.5200000E+000 +1.4710000E+004 !\AUTHOR: !\REF: !\COMMENT:
NC5H11OH+OH<=>C5H10OH11+H2O
+3.6100000E+003 +2.8900000E+000 -2.2910000E+003 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+HO2<=>C5H10OH11+H2O2 +3.5000000E-
005 +5.2600000E+000 +8.2680000E+003 !\AUTHOR: !\REF: !\COMMENT:
NC5H11OH+OH<=>C5H11O-1+H2O
+5.8800000E+002 +2.8200000E+000 -5.8500000E+002 !\AUTHOR: !\REF:
!\COMMENT:
NC5H11OH+HO2<=>C5H11O-1+H2O2 +6.4700000E-
007 +5.3000000E+000 +1.0530000E+004 !\AUTHOR: !\REF: !\COMMENT:
!

!\REACTIONCLASS: \RADICAL_BETA_SCISSION \A
\N \EA
!

C5H10OH15=>C2H4+C2H4+CH2OH
+5.1680000E+013 +1.0300000E-001 +2.9083800E+004 !\AUTHOR: !\REF:
!\COMMENT:
C3H6+PC2H4OH<=>C5H10OH14
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4OH+CH3<=>C5H10OH13
+1.7600000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H8-1+CH2OH<=>C5H10OH13
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:

C3H5OH+C2H5<=>C5H10OH12
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C2H3OH+NC3H7<=>C5H10OH11
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
!

!\REACTIONCLASS: \R+O2<=>RO2 \A
\N \EA
!

C5H10OH11+O2<=>C5H10OH-1O2
+5.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED BY JB !\COMMENT:
C5H10OH12+O2<=>C5H10OH-2O2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
C5H10OH13+O2<=>C5H10OH-3O2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
C5H10OH14+O2<=>C5H10OH-4O2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
C5H10OH15+O2<=>C5H10OH-5O2
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: ASSUMED TO BE THE
SAME AS REGULAR ALKYL RADICAL
!

!\REACTIONCLASS: \RO2<=>E+HO2 \A
\N \EA
!

C5H10OH-1O2<=>C5H9OH1-1+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
C5H10OH-2O2<=>C5H9OH1-1+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
C5H10OH-2O2<=>C5H9OH1-2+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
C5H10OH-3O2<=>C5H9OH1-2+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
C5H10OH-3O2<=>C5H9OH1-3+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION

C5H10OH-4O2<=>C5H9OH1-3+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
C5H10OH-4O2<=>C5H9OH1-4+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
C5H10OH-5O2<=>C5H9OH1-4+HO2
+2.8850000E+009 +9.3000000E-001 +2.9800000E+004 !\AUTHOR: JB !\REF: J.
BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119,
2015, 7510-7527 !\COMMENT: RATE RULE FOR CONCERTED ELIMINATION
!

!\REACTIONCLASS: \OTHER_DECOMPOSITIONS,ETC. \A
\N \EA
!

!16_03 !C4H7OH1-3+OH=>C4H6+OH+H2O 1.010E+006 2.200 -437.2 !\AUTHOR: JB
!\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556
!\COMMENT: ANALOGY TO C4H8-1+OH<=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-
ATOM ABSTRACTION FOLLOWED
C5H9OH1-1+OH=>C4H7CHO-2+H+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH<=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED
C5H9OH1-2+OH=>C4H7CHO-2+H+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH<=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED
C5H9OH1-2+OH=>C5H81-3+OH+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH<=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED
C5H9OH1-3+OH=>C5H81-3+OH+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH<=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED
C5H9OH1-4+OH=>C4H6+CH2OH+H2O
+1.0100000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: JB !\REF: S.
S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549-2556 !\COMMENT: ANALOGY
TO C4H8-1+OH<=>C4H71-3+H2O. DIVIDED BY 2. ALLYLIC H-ATOM ABSTRACTION
FOLLOWED
!-----
!-----
!\ENDSUBMECH: \NC5H11OH
!-----
!-----
!++++
!++++
!++++
!\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<=>CVCCJCVCC
+3.2000000E+015 +0.0000000E+000 +3.9500000E+004 !\AUTHOR: !\REF:ARENDS
ET AL. J PHYS CHEM 97: 7914 1993 !\COMMENT:
CVCCJCVCC<=>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

CVCCJCVCC+O2<=>C2H3CHO+CH2CHO

+1.2000000E+036 -7.2500000E+000 +3.3600000E+004 !\AUTHOR: !\REF:PRIVATE
COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:

CVCCJCVCC+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: \CVCCCVCC

!=====
=====

!

!\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:

$C_5H_5+O_2 \rightleftharpoons C_4H_4O+HCO$
+6.0000000E+018 -2.4800000E+000 +1.0970000E+004 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
 $C_5H_5+O \rightleftharpoons C_4H_5-N+CO$
+3.2000000E+013 -1.7000000E-001 +4.4000000E+002 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
 $C_5H_5+O \rightleftharpoons C_5H_4O+H$
+5.8000000E+013 -2.0000000E-002 +2.0000000E+001 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
 $C_5H_5+OH \rightleftharpoons C_5H_5OH$
+6.5000000E+014 -8.5000000E-001 -2.7300000E+003 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
DUP
 $C_5H_5+OH \rightleftharpoons C_5H_5OH$
+1.1000000E+043 -8.7600000E+000 +1.8730000E+004 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
DUP
 $C_5H_5+OH \rightleftharpoons C_5H_5OH$
+1.1000000E+059 -1.3080000E+001 +3.3450000E+004 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
DUP
 $C_5H_5+OH \rightleftharpoons C_5H_4OH+H$
+3.5000000E+057 -1.2180000E+001 +4.8350000E+004 !\AUTHOR: !\REF:ZHONG &
BOZZELI J PHYS CHEM A 102: 3537 1998 !\COMMENT:
 $C_5H_5+OH \rightleftharpoons C_4H_6+CO$
+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
!

 $C_5H_4OH+H \rightleftharpoons C_5H_5OH$
+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
!

 $C_5H_5OH+H \rightleftharpoons C_5H_5O+H_2$
+4.0000000E+013 +0.0000000E+000 +6.0940000E+003 !\AUTHOR: !\REF:PRIVATE
COMMUNICATION WITH BOZZELI (ZHONG'S THESIS) !\COMMENT:
 $C_5H_5OH+O \rightleftharpoons C_5H_5O+OH$
+1.0000000E+013 +0.0000000E+000 +4.6830000E+003 !\AUTHOR: !\REF:PRIVATE
COMMUNICATION WITH BOZZELI (ZHONG'S THESIS) !\COMMENT:
 $C_5H_5OH+OH \rightleftharpoons C_5H_5O+H_2O$
+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
!+++++
+++++
+++++

CH3COOH<=>CH4+CO2
+1.5000000E+013 +0.0000000E+000 +7.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
CH3COOH<=>H2O+CH2CO
+1.4000000E+012 +0.0000000E+000 +6.5000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
CH3COOH=>CO+OH+CH3
+7.5000000E+015 +0.0000000E+000 +9.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
CH3COOH=>CH3+CO2+H
+2.5000000E+014 +0.0000000E+000 +8.8000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C2H5COOH=>C2H6+CO2
+1.5000000E+013 +0.0000000E+000 +7.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C2H5COOH=>H2O+CH3CHCO
+1.4000000E+012 +0.0000000E+000 +6.5000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C2H5COOH=>CO+OH+C2H5
+7.5000000E+015 +0.0000000E+000 +9.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING
C2H5COOH=>CO2+C2H5+H
+2.5000000E+014 +0.0000000E+000 +8.8000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT: WARNING

!\END_KINETICS_INPUT
!
```

!

!-----

!----- AJOUT HP PRINCETON -----

!-----

!*****

! H2/O2 mechanism of Burke et al. IJCK (2011)

!

!

!

!*****

!=====

! H2-O2 Dissociation Reactions

!=====

! Srinivasan and Michael, International Journal of Chemical Kinetic

(2006) Vol. 38

H2O+H2O<=>H+OH+H2O 1.006E+26 -2.440 120180.0

!=====

!Formation and Consumption of H2O2

!=====

! Hippler et al., Journal of Physical Chemistry (1990) Vol. 93, pp.1755

!HO2+HO2<=>H2O2+O2 4.200E+14 0.000 11982.0

! DUPLICATE

!HO2+HO2<=>H2O2+O2 1.300E+11 0.000 -1629.3

! DUPLICATE

! Hong et al., Journal of Physical Chemistry A (2010) Vol. 114, pp.

5718-5727

!H2O2+OH<=>HO2+H2O 1.740E+12 0.000 318.0

! DUPLICATE

!H2O2+OH<=>HO2+H2O 7.590E+13 0.000 7270.0

! DUPLICATE

!*****

! CO/CO2 mechanism-HPMECH

!

!

!

!*****

! Joshi and Wang, International Journal of Chemical Kinetics (2006) Vol.

38, pp. 57-73

! The rate used is the low pressure limit value.

!CO+OH<=>CO2+H 7.046E+04 2.053 -276.2

!DUPLICATE

!CO+OH<=>CO2+H 5.757E+12 -0.664 331.9

!DUPLICATE

!*****

! HCO/CH2O mechanism-HPMECH
!

!*****

HCO+HO2<=>CO+H2O2 1.500E+13 0.000 0.0

!!
! HCOH RADICAL REACTION SET
!!

! Estimation

HCOH+O=>CO+H2O 8.00E+13 0.000 0.0
HCOH+OH=>CO+H2O+H 3.00E+13 0.000 0.0
HCOH+H<=>HCO+H2 3.00E+13 0.000 0.0
HCOH+O2=HCO+HO2 6.00E+12 0.000 0.0

!*****

! C mechanism-HPMECH
!

!*****

!*****

! CH mechanism-HPMECH
!

!*****

! Huang et al. (Journal of Physical Chemistry A (2002) Vol. 106, pp. 5490-5497) calculated the PES of the CH+O2 reactions. However, they only find the CO+OH and CO2+H channels.

! Rohrig et al. reported an overall experimental rate constant of $1.00 \times 10^{14} \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ for T btween 2200-2600K

! Berman et al. (Symposium International on Combustion (1982) Vol. 19, pp. 73-) reported a rate of $3.25 \times 10^{13} \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ for T between 300-700K

! Taatjes (Journal of Physical Chemistry (1996) Vol. 100, pp. 17840-) reported a rate of $3.37 \times 10^{14} \times T^{-0.48} \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$ for T between 20-300K

! I performed a fit on all these data point, and obtained the overall expression $3.3 \times 10^{10} \times T^{1.008} \times \text{EXP}(489.9/RT) \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$

! The branching ratio are taken for the ReCOmmendations of Baulch et al. (the CO+H+O path is included in the CO+OH channel)

CH+O2<=>CO2+H 9.900E+09 1.008 -489.9
CH+O2<=>CO+OH 6.600E+09 1.008 -489.9
CH+O2=>CO+O+H 9.900E+09 1.008 -489.9

!

!*****

! CH2 mechanism-HPMECH

!

!

!

!*****

! Triplet methylene

! Kiefer and Kumaran, Journal of Physical Chemistry (1993) Vol. 97, pp. 414-420

CH2+M=>C+H2+M 1.148E+14 0.000 55820.0
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/

CH2+O<=>CO+H2 8.190E+13 0.000 536.5

!

! Lee et al., Journal of Physical Chemistry A (2012) Vol. 116, pp. 9245-9256

! The overall rate constant is $1.650E+13 \times \text{EXP}(-874/T)$

! Complex system with few experimental measurements

! The branching ratio between all the different channels is not well established.

! Blitz et al. (Z. Phys. Chem. (2011) Vol. 225, pp. 957-967) determined the following

! branching ratios at 298 K : CO+OH+H 32%, CO2+H+H 23%, CO2+H2 21%, CH2O+O 18%, CO+H2O 6%

! whereas Lee et al. determined at T about 1935 K the following

! branching ratios: CO+OH+H and CO2+H+H 58%, O+CH2O 23%, CO2+H2 and CO+H2O 19%

! Temperature dependence was derived from those two temperatures and applied to the overall rate constant.

CH2+O2=>CO+OH+H 5.673E+12 0.000 1779.2
CH2+O2<=>CO2+H2 3.968E+12 0.000 1908.4
CH2+O2<=>CH2O+O 2.328E+12 0.000 1501.3
CH2+O2<=>CO+H2O 6.130E+11 0.000 1453.0

! Lu et al., Journal of Physical Chemistry A (2010) Vol. 114, pp. 5493-5502

CH2+H2<=>H+CH3 4.408E+05 2.300 7350.7

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

CH2+HO2<=>OH+CH2O 2.000E+13 0.000 0.0

! Wang et al., Theoretical Chemistry Accounts (2006) Vol. 115, pp. 205-211

CH2+CH2O<=>CH3+HCO 7.407E-02 4.210 1623.9

! Braun et al., Journal of Chemical Physics (1981) Vol. 56, pp. 355-

CH2+CH<=>H+C2H2 4.000E+13 0.000 0.0

! Jasper et al., Journal of Physical Chemistry A (2007) Vol. 111, pp. 8699-8707

! The overall rate constant is $8.867E+13 \times T^{0.002} \times \text{EXP}(-4.5/T)$

! The branching ratio between the two channels was calculated as

C2H2+2H/C2H2+H2 4/1

CH2+CH2<=>C2H2+2H 7.094E+13 0.002 8.9
CH2+CH2<=>C2H2+H2 1.773E+13 0.002 8.9

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087

CH2+CO2<=>CH2O+CO 2.350E+10 0.000 0.0

! Singlet methylene

! K. L. Gannon, M. A. Blitz, T. Kovacs, M. J. Pilling, and P. W. Seakins
J. Chem. Phys. 132, 024302(2010)

CH2(S)+HE<=>CH2+HE 5.37E+11 0.52 781.
CH2(S)+H2<=>CH2+H2 1.07E+12 0.52 781.
CH2(S)+O2<=>CH2+O2 1.10E+10 1.13 -280.
CH2(S)+C2H2<=>CH2+C2H2 0.80E+15 -0.57 -4.85 !! Pilling and
Harding 20%

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol.
34, pp. 757-1397

CH2(S)+C2H4<=>CH2+C2H4 1.144E+13 0.000 -556.4
CH2(S)+CH4<=>CH2+CH4 1.867E+12 0.000 -496.8

CH2(S)+M<=>CH2+M 1.200E+13 0.000 0.0
HE/0.0/ AR/0.0/ N2/0.0/ H2/0.0/ O2/0.0/ H2O/0.0/ CO2/0.0/ CH4/0.0/
C2H2/0.0/ C2H4/0.0/ CO/0.0/

!!===== above energy
transfer=====

! estimated

CH2(S)+O<=>H+CO+H 4.505E+13 0.000 0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087

CH2(S)+HO2<=>CH2O+OH 3.010E+13 0.000 0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087

CH2(S)+H2O2<=>CH3O+OH 3.010E+13 0.000 0.0

! GRI-Mech 3.0 http://www.me.berkeley.edu/gri_mech/

CH2(S)+H2O<=>CH2O+H2 6.820E+10 0.250 -935.0

!
!*****

! CH3 mechanism-HPMECH

!
!
!

!*****

! Lim and Michael, Symposium International on Combustion, 1994, Vol. 25,
pp. 713-719

! Nitrogen set as the bath gas

! Efficiencies taken from GRI-Mech 3.0

http://www.me.berkeley.edu/gri_mech/

CH3+M=>CH+H2+M 3.569E+15 0.000 81046.0

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

AR/0.7/ HE/0.70/ CH3OH/3.0/

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol. 34, pp. 757-1397

CH3+O=>CO+H2+H 1.686E+13 0.000 0.0

! Miller and Bowman, Progress in Energy and Combustion Sciences (1989) Vol. 15, pp. 287-338

CH3+CH<=>H+C2H3 3.000E+13 0.000 0.0

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol. 34, pp. 757-1397

CH4+CH2(S)<=>CH3+CH3 1.867E+13 0.000 -496.8

!
!*****

! CH3O mechanism-HPMECH

!
!
!
!
!*****

! Xu et al., Molecular Physics (2007) Vol. 105, pp. 2763-2776

CH3O+H<=>CH2(S)+H2O 3.280E+12 0.088 -152.6

! estimated

CH3O+O=OH+CH2O 8.00E+13 0.00 0.

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

CH3O+OH<=>CH2O+H2O 1.810E+13 0.000 0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

CH3O+CO<=>CH3+CO2 1.570E+13 0.000 11804.0

! Tsang, Journal of Physical Chemical Reference Data (1987) Vol. 16, pp. 471-508

! rate similar as the rate of the reaction CH3O+CH3CO<=>CH3CHO+CH2O

CH3O+HCO<=>CH2O+CH2O 6.030E+12 0.000 0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

CH3O+CH2<=>CH2O+CH3 1.810E+13 0.000 0.0

!
!*****

! CH2OH mechanism-HPMECH

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!
!
!
!*****

! The rate constant has been calculated by Stephen Klippenstein

! Troe fitting valid between 300 and 2000 K, 0.001 and 100 atm

! The rate constant below is for Nitrogen as the bath gas

CH2OH<=>CH3O 3.797E+22 -4.681 35559.6

PLOG / 0.001 1.158E+18 -4.592 36016.8 /
PLOG / 0.010 3.810E+19 -4.628 35229.3 /
PLOG / 0.100 2.870E+21 -4.771 35111.7 /
PLOG / 1.000 3.797E+22 -4.681 35559.6 /
PLOG / 5.000 9.756E+22 -4.499 36133.6 /
PLOG / 10.000 1.449E+23 -4.416 36465.8 /
PLOG / 50.000 2.935E+23 -4.199 37365.2 /
PLOG / 100.000 2.423E+23 -4.046 37725.5 /

!

! Xu et al., Molecular Physics (2007) Vol. 105, pp. 2763-2776
CH2OH+H<=>CH2(S)+H2O 9.020E+09 0.870 -785.9

! Xu et al., Molecular Physics (2007) Vol. 105, pp. 2763-2776
CH2OH+H<=>CH3O+H 2.460E+07 1.595 7194.1

!

! Tsang, Journal of Physical Chemical Reference Data (1987) Vol. 16, pp. 471-508

CH2OH+CH2<=>OH+C2H4 2.410E+13 0.000 0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

! Scaled by 10

CH2OH+CH2<=>CH2O+CH3 1.210E+13 0.000 0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

CH2OH+CH3<=>CH2O+CH4 2.410E+12 0.000 0.0

!

!

!*****

! CH3OH mechanism-HPMECH

!

!

!

!*****

!

! Jasper Paper

! The present fitting is valid for pressures between 100 and 1000000 torr
! and temperatures between 750 and 3000 K

CH3OH(+M)<=>CH2O+H2(+M) 1.660E+12 0.199
89678.5

LOW/ 6.190E+25 -2.750 84971.1 /

TROE/ 0.014 737.2 740.2 206499.5 /

AR/0.70/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3OH/3.0/

! Jasper Paper

! The present fitting is valid for pressures above 100 torr
! and temperatures between 750 and 3000 K

CH3OH(+M)<=>HCOH+H2(+M) 2.917E+07 1.950
85035.0

LOW/ 7.786E+37 -5.994 86236.9 /

TROE/ 0.686 1718.3 153.9 499615.0 /

AR/0.70/ H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH3OH/3.0/

! Jasper paper, Bath gas is Argon
! The present fitting is valid between 750 and 3000 K
CH3OH<=>CH2OH+H 4.089E+44 -9.428 107414.2 ! 1
atmosphere rate constant
PLOG / 0.000132 3.110E+34 -7.944 111085.7 /
PLOG / 0.001320 1.110E+37 -8.323 109174.3 /
PLOG / 0.013200 6.733E+38 -8.510 107101.1 /
PLOG / 0.132000 4.959E+41 -8.969 105978.8 /
PLOG / 1.320000 4.086E+44 -9.382 107251.7 /
PLOG / 13.200000 4.080E+45 -9.263 109268.3 /
PLOG / 132.000000 7.717E+43 -8.419 110568.1 /
PLOG / 13200.000000 1.638E+29 -3.838 105074.8 /

! Jasper paper, Bath gas is Argon
! The present fitting is valid between 750 and 3000 K
CH3OH<=>CH3O+H 3.068E+34 -7.332 116789.8 ! 1
atmosphere rate constant
PLOG / 0.000132 9.241E+28 -7.012 134030.3 /
PLOG / 0.001320 9.218E+28 -6.689 130040.2 /
PLOG / 0.013200 2.179E+30 -6.772 127194.7 /
PLOG / 0.132000 3.517E+31 -6.819 121849.3 /
PLOG / 1.320000 3.053E+34 -7.292 115732.5 /
PLOG / 13.200000 2.060E+39 -8.158 114301.0 /
PLOG / 132.000000 3.311E+42 -8.531 117206.4 /
PLOG / 13200.000000 5.484E+39 -6.946 123154.3 /

! Moses et al. (Klippenstein), The Astrophysical Journal (2011) Vol. 737,
Paper 15.
! QCISD(T)/CBS//QCISD(T)/cc-pVTZ calculations were performed with the
spin-restricted formalism
CH3OH+H<=>CH3+H2O 2.957E+05 2.485 20627.0

! Johnson et al., Physical Chemistry Chemical Physics (2000) Vol. 2, pp.
2549-2553
! Assuming a branching ratio k(CH2OH)/k equal to 95%
CH3OH+CH<=>CH2+CH3O 4.522E+17 -1.930 0.0
CH3OH+CH<=>CH2+CH2OH 8.592E+18 -1.930 0.0

! Tsang, Journal of Physical Chemical Reference Data (1987) Vol. 16, pp.
471-508
CH3OH+CH2<=>CH3+CH3O 1.443E+01 3.100 6935.0
CH3OH+CH2<=>CH3+CH2OH 3.192E+01 3.200 7174.0

! Estimation
CH3OH+CH2(S)<=>C2H4+H2O 1.000E+13 0.000 0.0
CH3OH+CH2(S)<=>CH3+CH2OH 1.000E+14 0.000 0.0

!!=====

!!=====

!!=====C2

SPECIES=====

!!=====

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!*****

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!           C2H mechanism-HPMECH
!
!
!*****
!*****
!
! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol.
34, pp. 757-1397
C2H+HO2<=>HCCO+OH          1.806E+13      0.000      0.0

!estimated
C2H+HCO=C2H2+CO            6.00E+13      0.00      0.0

C2H+CH3=C3H3+H             5.00E+13      0.00      0.0

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol.
34, pp. 757-1397
C2H+CH4<=>CH3+C2H2          2.168E+10      0.940      651.8

! estimated
C2H+CH3OH=C2H2+CH2OH       6.03E+13      0.00      0.
C2H+CH3OH=C2H2+CH3O        1.21E+13      0.00      0.

!*****
!*****
!           C2O mechanism-HPMECH
!
!
!*****
!*****
!
! Miller and Melius, Combustion and Flame (1992) Vol. 91, pp. 21-
C2O+H<=>CH+CO              5.000E+13      0.000      0.0
C2O+O<=>CO+CO              5.000E+13      0.000      0.0
C2O+OH=>CO+CO+H           2.000E+13      0.000      0.0
C2O+O2=>CO+CO+O           2.000E+13      0.000      0.0
!
!*****
!*****
!           HCCO mechanism-HPMECH
!
!
!*****
!*****
!
! Klippenstein et al., Proceedings of the Combustion Institute (2002)
Vol. 29, pp. 1209-
HCCO+O2=>O+CO+HCO          2.180E+02      2.690      3541.0

! Miller and Melius, Combustion and Flame (1992) Vol. 91, pp. 21-
HCCO+OH<=>C2O+H2O          3.000E+13      0.000      4.1  ! new
reaction pathway
HCCO+CH2<=>C2H3+CO         3.000E+13      0.000      0.0
HCCO+HCCO=>C2H2+CO+CO     1.000E+13      0.000      0.0

```

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol. 34, pp. 757-1397

HCCO+O<=>CH+CO2 2.951E+13 0.000 1112.8

!

!*****

! C2H2 mechanism-HPMECH

!

!

!

!*****

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986) Vol. 15, pp. 1087

C2H2+O2<=>C2H+HO2 1.204E+13 0.000 74520.0

! Thiesemann, H.; MacNamara, J.; Taatjes, C. A. J. Phys. Chem. A 1997, 101, 1881

C2H2+CH=C3H2+H 1.00E+14 0.00 0.00

!

!

!=====H2CC chemistry=====

!

! Laskin and Wang, Chemical Physics Letters (1999) Vol. 303, pp. 43-49

! The rate constant is for Argon

! Wang et al., USC-Mech II, http://ignis.usc.edu/USC_Mech_II.htm, May 2007.

H2CC+O2<=>CH2+CO2 1.000E+13 0.000 0.0

H2CC+O<=>CH2+CO 1.000E+14 0.000 0.0

!

!*****

! C2H2O mechanism-HPMECH

!

!

!

!*****

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol. 34, pp. 757-1397

CH2CO+O<=>CH2O+CO 3.613E+11 0.000 1351.3

CH2CO+O<=>HCO+HCO 3.613E+11 0.000 1351.3

! Baulch et al., Journal of Physical Chemical Reference Data (2005) Vol. 34, pp. 757-1397

! Baoshan Wang has calculated the PES

CH2CO+OH<=>CH3+CO2 6.745E+11 0.000 -1013.0

!estimated

OH+HCCOH=H2O+HCCO 2.000E+13 0.000

0.0

O+HCCOH=HCCO+OH 8.000E+13 0.000 0.0

!*****

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!           C2H3 mechanism-HPMECH
!
!
!
!*****
*****

! Harding et al., Proceedings of the Combustion Institute (2005) Vol. 30,
pp. 985
! The rate constant of the abstraction channel is estimated to be 10% of
the addition channel
C2H3+O<=>CH2CO+H           1.030E+13      0.205      -848.5
C2H3+O<=>OH+C2H2           1.030E+12      0.205      -848.5

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
C2H3+OH<=>CH2CHO+H         3.011E+13      0.000      0.0

! Wang et al., USC-Mech II, http://ignis.usc.edu/USC\_Mech\_II.htm, May
2007.
C2H3+HO2<=>CH2CHO+OH       1.000E+13      0.000      0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
!! too fat decrease by a factor of 8
C2H3+HCO<=>C2H4+CO         1.033E+13      0.000      0.0

!estimated
C2H3+CH2=CH3+C2H2         2.00E+13      0.00      0.

C2H3+C2H3=CH3+C3H3         3.00E+12      0.00      -800.
C2H+C2H3=C2H2+C2H2         2.00E+13      0.00      0.
!estimated

!*****
*****

!           C2H3O mechanism-HPMECH
!
!
!
!*****
*****

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
CH3CO+H<=>CH3+HCO          9.635E+13      0.000      0.0

! Bartels et al., Symposium International on Combustion (1991) Vol. 23,
pp. 131-138
! Scaled by a factor 2
! Original rate is 1.2E+14 mol.cm^-3.s^-1 at 298 K, but this reaction is
radical-radical reaction, the rate will decrease to two thirds at higher
temp
CH3CO+O<=>CH3+CO2          6.000E+13      0.000      0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
CH3CO+OH<=>CH2CO+H2O       1.204E+13      0.000      0.0

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! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087

CH3CO+OH<=>CH3+CO+OH 3.011E+13 0.000 0.0

! Estimation

CH3CO+CH2<=>CH2CO+CH3 1.810E+13 0.000 0.0

! Estimation

CH2CHO+H<=>CH3+HCO 8.000E+13 0.000 0.0

CH2CHO+H<=>CH2CO+H2 2.000E+13 0.000 0.0

! Estimation

CH2CHO+O<=>CH2O+HCO 5.000E+13 0.000 0.0

! GRI-Mech 3.0 http://www.me.berkeley.edu/gri_mech/

CH2CHO+OH<=>H2O+CH2CO 1.200E+13 0.000 0.0

CH2CHO+OH<=>HCO+CH2OH 3.010E+13 0.000 0.0

!

!*****

! C2H4 mechanism-HPMECH

!

!

!

!*****

!

! GRI-Mech 3.0 http://www.me.berkeley.edu/gri_mech/

C2H4 (+M) <=> C2H2 + H2 (+M) 8.000E+12 0.440 88770.0

LOW / 1.580E+51 -9.310 97800.0 /

TROE / 0.7345 180.0 1035.0 5417.0 /

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

AR/0.7/ HE/0.70/ CH3OH/3.0/

! Nguyen, et al., Journal of Physical Chemistry A (2005) Vol. 109, pp.
7489-7499

! The overall rate is $1.018E+08 \times T^{1.66} \times \text{EXP}(-657.8/RT)$.

! The temperature dependent branching ratios of the six channels are
given in Table 7 of the paper.

! The present rates are a fit on the temperature dependent rate constants
for each channel.

C2H4+O<=>CH2+CH2O 9.547E+05 2.121 1233.8

C2H4+O<=>CH3CO+H 3.134E+04 2.325 384.9

C2H4+O<=>CH2CO+H2 4.032E+04 2.282 341.4

C2H4+O<=>CH4+CO 1.275E+05 2.108 449.7

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087

C2H4+HO2<=>CH3CHO+OH 6.022E+09 0.000 7948.8

! ! Estimated for whole temp range

!! Phys. Chem. Chem. Phys., 2009, 11, 655?64

C2H4+CH=C3H4-A+H 1.70E+14 -0.31 0.

! Baulch et al., J. Phys. Chem. Ref. Data, 34:757 (2005)

C2H4+CH2=C3H5-A+H 3.20E+12 0.00 5285.

! estimated


```

! estimated
C2H5+CH=H+C3H5-A          5.00E+13      0.00      0.

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
C2H5+CH2<=>C2H4+CH3      1.810E+13      0.000      0.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
C2H5+CH2 (S) <=>C2H4+CH3  9.000E+12      0.000      0.0

! Estimation
C2H5+CH2OH<=>C2H4+CH3OH  1.000E+13      0.000      0.0
C2H5+CH2OH<=>C2H6+CH2O   1.000E+13      0.000      0.0
C2H5+CH3O<=>C2H6+CH2O   1.000E+13      0.000      0.0
C2H5+C2H=C2H2+C2H4      1.00E+13       0.00       0.
C2H5+C2H3=C3H5-A+CH3    3.00E+13       0.00       0.
!
!*****
!
!               C2H5O mechanism-HPMECH
!
!
!
!*****
!*****

!make it 10% of C2H4+OH channel. MC calculations showed it!
PC2H4OH+O=CH2O+CH2OH    8.00E+13      0.00      0.00
H+PC2H4OH=CH3+CH2OH     9.00E+13      0.00      0.00
H+PC2H4OH=C2H4+H2O      3.00E+13      0.00      0.00
PC2H4OH+OH=H2O+C2H3OH   3.00E+13      0.00      0.00
PC2H4OH+O2=C2H3OH+HO2   1.00E+12      0.00      -1100.  ! Judit Zador et
al., Proc Combust Inst 32(2009)271-277
!
!*****
!*****

!               C2H6 mechanism-HPMECH
!
!
!
!*****
!*****

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
C2H6+HCO<=>CH2O+C2H5      4.700E+04      2.720      18235.0

! Activation energy: Berman and Lin, Chemical Physics (1983), Vol. 82,
pp. 435-42
! Preexponential factor: Galland et al., Journal of Physical Chemistry A
(2003) Vol. 107, pp. 5419-5426
C2H6+CH<=>C2H4+CH3      6.185E+13      0.000      -262.3

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
C2H6+CH2OH<=>CH3OH+C2H5   1.990E+02      3.000      13976.0

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! Ceursters, et al Phys. Chem. Chem. Phys., 2001, 3, 3070-3074
C2H6+C2H<=>C2H2+C2H5 7.200E+11 0.540 -358.0

! Tsang and Hampson, Journal of Physical Chemical Reference Data (1986)
Vol. 15, pp. 1087
C2H6+C2H3<=>C2H4+C2H5 6.010E+02 3.300 10502.0

!*****

! C2H6o mechanism-HPMECH

!
!
!

!*****

! Sivaramakrishnan ET AL., J. Phys. Chem. A 2010, 114, 9425-9439
!C2H5OH=C2H4+H2O 3.41E+59 -14.22 83672.
!PLOG /0.01 2.62E+57 -13.29 85262./
!PLOG /0.10 1.65E+52 -11.52 84745./
!PLOG /1.00 5.23E+43 -8.90 81507./
!PLOG /10.0 4.59E+32 -5.60 76062./
!PLOG /10.0 3.84E+20 -2.06 69466./

!C2H5OH=CH3+CH2OH 1.20E+54 -12.94 100006.
!PLOG /0.01 5.18E+59 -13.98 99906./
!PLOG /0.10 1.62E+66 -15.30 105390./
!PLOG /1.00 5.55E+64 -14.47 107099./
!PLOG /10.0 1.55E+58 -12.29 105768./
!PLOG /10.0 1.78E+47 -8.96 101058./

!C2H5OH=C2H5+OH 8.10E+46 -11.33 111053.
!PLOG /0.01 1.82E+56 -13.49 107028./
!PLOG /0.10 4.65E+63 -14.99 109623./
!PLOG /1.00 1.46E+65 -14.89 112344./
!PLOG /10.0 2.79E+61 -13.40 113080./
!PLOG /10.0 6.17E+51 -10.34 109040./

!C2H5OH+H=CH3CHOH+H2 8.80e+04 2.68 2914.
!C2H5OH+H=PC2H4OH+H2 5.30e+04 2.81 7442.
!C2H5OH+H=CH3CH2O+H2 9.42e+02 3.14 9407.
!C2H5OH+OH=CH3CHOH+H2O 7.20E+05 2.54 -1534.
!C2H5OH+OH=PC2H4OH+H2O 5.70E+00 3.38 -2394.
!C2H5OH+OH=CH3CH2O+H2O 5.80E-03 4.28 -3561.

! Wu et al. J. Phys. Chem. A 2007, 111, 6693-6703
!C2H5OH+O=CH3CHOH+OH 1.44E+05 2.47 876.
!C2H5OH+O=PC2H4OH+OH 9.60E+02 3.23 4657.
!C2H5OH+O=CH3CH2O+OH 1.44E-03 4.73 1727.

!! could also produce H+CH2CHCH2OH

!!! Xu et al., J. Chem. Phys.120(2004) 6593

!C2H5OH+CH3=CH3CHOH+CH4 1.98E+01 3.37 7634.
!C2H5OH+CH3=PC2H4OH+CH4 2.03E+00 3.57 7721.
!C2H5OH+CH3=CH3CH2O+CH4 3.30E+02 3.30 12290.

! Raghu Sivaramakrishnan et al., Combustion and Flame 158 (2011) 618-632

!CH3OCH3(+M)=CH3O+CH3(+M) 2.33E+19 -0.66
84139.

! Low /1.72E+59 -11.40

93295.6/

```

! Troe /1.0 1.0E-30 880./
! H2/3.0/ H2O/9.0/ CH4/3.0/ CO/2.25/ CO2/3.0/ C2H6/4.5/ AR/1.0/
N2/1.50/ CH3OCH3/5.0/ HE/1.20/

!CH3OCH3+H=H2+CH3OCH2          3.94E+00          4.13          1780.
! make it 30% smaller
!CH3OCH3+H=H2+CH3OCH2          3.00E+00          4.13          1780.
! K. TAKAHASHI, O. YAMAMOTO, T. INOMATA, M. KOGOMA Int J Chem Kinet 39:
97-108, 2007
!CH3OCH3+O=CH3OCH2+OH          2.69E+07          2.00          2629.
! Cook et al., J. Phys. Chem. A 2009, 113, 9974
!CH3OCH3+OH=H2O+CH3OCH2        6.32E+06          2.00          -652.
!CH3OCH3+HO2=CH3OCH2+H2O2      1.02E+02          3.48          17424.
! estimate from J. Phys. Chem. A 2008, 112, 7047-7054
!CH3OCH3+O2=CH3OCH2+HO2        4.10E+13          0.00          4.491E+04
! Tranter Patrick and Yang
!CH3OCH3+CH3=CH4+CH3OCH2        6.22E+00          3.78          9631.
! 30% uncertainty from 10 to 6.22
!*****
!
!           C3H2 mechanism-HPMECH
!
!
!
!*****
!!HC=C=CH is in triplet state, and the most stable isomer is
cyclic(singlet), the difference is about 10 kcal/mol
!! now the question is how it is generated in combustion enviroments,
!!for CH+C2H2, the main product channel is triplet HC=C=CH, but for
C3H3+O, the main products channel is very complicated
!! thermo is also a huge problem for C3H2 in Burcat's thermo!!
C3H2+O=C2H2+CO          6.02E+13          0.00          0. !
Warnatz J. Ber. Bunsenges. Phys. Chem. 87 (1983) 1008.
!! looks alright, C3H2 is a resonant stablized radical. the association
should be very fast
!! The product is no doubt C2H2+CO. The TS to it is around 70 kcal/mol
!! the simple bond-fission barrier is just too high
C3H2+OH=C2H2+HCO        6.80E+13          0.00          0. !
Warnatz J. Ber. Bunsenges. Phys. Chem. 87 (1983) 1008.
!!The products may be alittle tricky. the first etep is HCCCHOH, then
decompose??

C3H2+H(+M)=C3H3(+M)      3.41E+14          0.00          291.95
LOW/2.47E+31 -3.92 4411.25/
Troe/0.419 3165.06 177.35 204926.14/
H2/3.0/ H2O/9.0/ CO/2.30/ CO2/4.0/ AR/1.0/ CH4/3.0/
C2H6/4.0/ N2/1.50/ HE/1.0/ CH3OH/6.0/ O2/1.5/

C3H2+O2=HCO+HCCO        1.00E+13          0.00          1000. !
Miller, J.A. et al Prog. Energy Combust. Sci., 1989, v. 15, pp. 287-338.

C3H2+CH=C4H2+H          1.00E+14          0.00          0. !
estimated!
!! THIS REACTION IS VERY FAST. I ASSUME IT IS LOWER LIMIT
C3H2+CH2=C4H3-I+H        5.00E+13          0.00          0. !
Wang H., and Frenklach M. Combust. Flame 110 (1997) 173

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C3H2+CH2(S)=C4H3-I+H           5.00E+13     0.00     0.  !
estimated
!! ADDITION-ELIMINATION C4H3-I is more stable
C3H2+CH3=C4H4+H           1.00E+13     0.00     0.  !
estimated
!! assuming no entrance barrier
C3H2+C2H=C5H2+H           1.00E+14     0.00     0.  !
estimated
C3H2+HCCO=C4H3-N+CO           1.00E+13     0.00     0.  !
Wang H., and Frenklach M. Combust. Flame 110 (1997) 173
C3H2+C2H2=HCCCHCCH+H       5.00E+12     0.00    5000.  !
estimated
!! I have no idea about this reaction. Jim Miller's est.
!! similar to Ch2 system
C3H2C+O=C2H+HCO           1.00E+13     0.00    12000.  !
estimated
!! complete C3H2 chemistry
!*****
!*****
!
!           C3H3 mechanism-HPMECH
!
!
!*****
!*****

C3H3+C2H=HCCCHCCH+H       3.00E+13     0.00     0.
!JAM&SJK
C3H3+C2H=H2CCCCCH+H       1.00E+13     0.00     0.
!JAM&SJK
!! the rates should be even higher

C3H3+C3H3=C4H5C2H           1.3177E+77   -19.00   33332.  !bpick jul03
PLOG /0.03947   1.3177E+77   -19.00   33332./
PLOG /1.         4.8957E+60   -14.02   25733./
PLOG /10.        1.4785E+55   -12.30   23622./
C4H5C2H=FULVENE           5.7544E+76   -18.67   95531.  !bpick
jul03
PLOG /0.03947   5.7544E+76   -18.67   95531./
PLOG /1.         2.3442E+56   -12.55   86405./
PLOG /10.        4.8978E+26   -4.144   65424./
C4H5C2H=C6H6             6.7608E+98   -24.58   122310.  !bpick
jul03
PLOG /0.03947   6.7608E+98   -24.58   122310./
PLOG /1.         1.6218E+53   -11.34   100210./
PLOG /10.        2.8184E+51   -10.68   106950./
C4H5C2H=C6H5+H           2.6915E+84   -20.14   121900.  !bpick
jul03
PLOG /0.03947   2.6915E+84   -20.14   121900./
PLOG /1.         4.1687E+77   -17.68   133520./
PLOG /10.        3.0903E+43   -7.928   118650./
C6H6=C6H5+H             1.3490E+108  -25.81   181750.  !bpick
jul03
PLOG /0.03947   1.3490E+108  -25.81   181750./
PLOG /1.         6.3096E+60   -12.40   148070./
PLOG /10.        5.4954E+38   -6.178   132000./
!! C3H3 self reactions are from Jim Miller's mechanism. Should be the
most reliable source for now.

```

!! the collision efficiency of different partners can't simply apply for this system.

!*****

! C3H4 mechanism-HPMECH

!

!

!

!*****

C3H4-A+OH=CH2O+C2H3	1.00E+12	0.0	-198.7	!
JAM/Liu(1988)/Butler(07)				
C3H4-A+OH=CH2CO+CH3	3.04E+12	0.0	-198.7	!
C3H4-A+CH2=C4H5-I+H	2.00E+13	0.0	4000.	!
JAM&SJK				
C3H4-A+CH2(S)=C4H5-I+H	2.00E+13	0.0	0.0	!
JAM&SJK				

C3H4-P+OH=HCCO+CH4	5.00E+12	0.00	5000.	!
JAM				

C3H4-P+CH=C4H4+H	1.20E+14	0.00	0.	!
ESTIMATED				

!!Phys. Chem. Chem. Phys., 2009, 11, 655?664 iC4H4 CH2CHCCH

C3H4-P+CH2=C4H5-I+H	2.00E+13	0.00	4000.	!
JAM&SJK				

C3H4-P+CH2(S)=C4H5-I+H	1.00E+14	0.00	0.	
------------------------	----------	------	----	--

! PRODUCTS ESTIMATED, SHOULD BE RIGHT

!

!*****

! C3H5 mechanism-HPMECH

!

!

!

!*****

! S-C3H5===CH3CHCH
! T-C3H5===CH3CCH2
! A-C3H5===CH2CHCH2

C3H5-A+H(+M)=C3H6(+M)	2.00E+14	0.00	0.	!
Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)				
LOW	/1.33E+60	-12.00	5967.8/	

TROE /0.02 1097 10967 6860/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/ AR/0.7/

C3H5-A+O=>C2H4+H+CO	6.00E+13	0.00	0.	!
---------------------	----------	------	----	---

Hoyermann et al Proc Combust Inst. 32 (2009) 157?164

C3H5-A+O2=>C2H2+CH2O+OH	9.71E+20	-2.70	24980.	!
-------------------------	----------	-------	--------	---

Lee et al., Proc Combust Inst 30:1015(2005)				
C3H5-A+O2=CH2O+CH2CHO	3.08E+09	0.37	16910.	!

Lee et al., Proc Combust Inst 30:1015(2005)				
C3H5-A+HO2=>C2H3CHO+OH+H	1.00E+13	0.00	0.	!

Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)

!! makes more sense

C3H5-A+CH2=C4H6+H	3.00E+13	0.00	0. !	Tsang
W, J. Phys. Chem. Ref. Data 20:221(1991)				
C3H5-A+CH2(S)=C4H6+H	1.00E+14	-0.00	0. !	Tsang
W, J. Phys. Chem. Ref. Data 20:221(1991)				
C3H5-A+C2H=C2H3+C3H3	4.00E+13	0.00	0. !	
Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)				
!! OTHER CHANNELS ARE NEGLIGIBLE				
C3H5-A+C2H3=C3H6+C2H2	4.80E+12	0.00	0. !	
Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)				
C3H5-A+C3H2=C6H6+H	2.00E+13	0.00	0.0 !	
JAM&SJK 2004				
!!CH bond are weak, similar to C2H3				
C3H5-S+H=C3H5-A+H	1.00E+13	0.00	0. !	
estimated				
C3H5-S+O=CH2CO+CH3	0.75E+14	0.00	0. !	
estimated				
C3H5-S+O=C2H5+CO	0.75E+14	0.00	0. !	
estimated				
C3H5-S+OH=C3H4-P+H2O	1.00E+13	0.00	0. !	
estimated				
C3H5-S+OH=C3H4-A+H2O	1.00E+13	0.00	0. !	
estimated				
C3H5-S+OH=CH2CO+CH3+H	0.50E+13	0.00	0. !	
estimated				
!! addition-elimination				
C3H5-S+O2=CH3CO+CH2O	4.34E+12	0.00	0. !	
Davis et al., J. Phys. Chem. A 103:5889(1999)				
!! for H atom reaction abstraction is usually fast than addition-elimination with shallow well				
!! remain question				
!*****				
!*****				
!	C3H3O	mechanism-HPMECH		
!		!		
!				
!*****				
!*****				
C2H3CO+H=C2H3+HCO	1.00E+13	0.000	00.00	
!Estimated				
C2H3CO+H=C2H4+CO	1.00E+14	0.00	0. !	
Estimated				
!*****				
!*****				
!	C3H4O	mechanism-HPMECH		
!		!		
!				
!*****				
!*****				
C2H3CHO=C2H4+CO	2.00E+12	0.00	56300. !	
estimated				
! same as C3H2O, may not be very good, but no other sources can be referenced				
C2H3CHO+H=C2H4+HCO	1.08E+11	0.45	5820.	
C2H3CHO+O=C2H3+OH+CO	3.00E+13	0.00	3540.	
C2H3CHO+O=CH2O+CH2CO	1.90E+07	1.80	220.	

C2H3CHO+OH=C2H3+H2O+CO 3.43E+09 1.18 -447.
C2H3CHO+C2H3=C4H6+HCO 2.80E+21 -2.44 14720.

!! from USC-Mech II, looks reasonable

!*****

! C3H6 mechanism-HPMECH

!
!
!

!*****

C3H6+O=CH3+CH2CHO 0.77E+07 1.83 -546. !

Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)

C3H6+O=C2H3CHO+H+H 1.31E+07 1.83 -546. !

Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)

C3H6+O=C2H4+CH2O 0.43E+07 1.83 -546. !

Tsang W, J. Phys. Chem. Ref. Data 20:221(1991)

! C3H6+O chemistry is not right in these rates

!! Let's take the abstrac rates and rearrange the addition-elimination rates

!! The first step on triplrt surface CH3CHCH2O is H- atom release or H2CO+CH3CH via bond fission

!! on singlet sruface, it must go through the intersystem crossing first

!! CH3CHCH2O will isomerized to CH3CH2CHO then forming C2H5+HCO and

CH3+CH2HCO, C2H4+H2CO is also a product channel in low temp

!! on Triplet surface, the branching ratio is 75:25

!! on singlet it is about 56:44:0 when temp >1000 K, at room temp

C2H4+H2CO is dominant

!! aussming isc is about 50:50(which is normal), then branching ratio of

H+H+C2H3CHO: H2CO+C2H4: C2H5+HCO: Ch3+CH2CHO is 75:25:56:44

!! k=3.48E+7*T^1.83*exp(275/T) from Wing Tsang

!! Other channel are not important at low pressure flame conditions

C3H6+CH=C4H6+H 1.20E+14 0.00 0. !

ESTIMATED

!! Phys. Chem. Chem. Phys., 2009, 11, 655?664 C4H6 CH2CHCHCH2

C3H6+CH2=C3H5-A+CH3 2.00E+13 0.00 0.

!!Berichte der Bunsengesellschaft f♦r physikalische Chemie

!!Volume 93, Issue 2, pages 165?170, Februar 1989

C3H6+C2H=C2H2+C3H5-A 0.50E+14 0.00 140. !

half of C2H+C2H6 rate

C3H6+C2H=CH3+C4H4 0.70E+14 0.00 -140. !

estimated

!*****

! C3H7 mechanism-HPMECH

!
!
!

!*****

C3H6+H=C3H5-S+H2 3.97E+02 3.252
12007.

dup

C3H6+H=C3H5-S+H2 5.10E+02 3.234

12357.

dup

!*****

! C4H mechanism-HPMECH
!

!*****

C4H+O=C2O+C2H	6.00E+13	0.00	0.0 !
estimated			
C4H+O2=HCCO+C2O	5.00E+13	0.00	1500.0 !
estimated			
C4H+H2=H+C4H2	2.10E+06	2.32	882. !
estimated			

!!all from C2H chemistry, should be reasonable

!*****

! C4H2 mechanism-HPMECH
!

!*****

C4H2+OH=H2O+C4H	9.15E+09	1.03	21746. !
Senosiain J. P., Klippenstein S. J., Miller J. A. Proc. Combust. Inst. 31 (2007) 185-192.			
C4H2+H(+M)=C4H3-I(+M)	4.31E+10	1.16	1753. !
Klippenstein S. J., Miller J. A. J. Phys. Chem. A 109 (2005) 4285-4295.			
LOW	/2.30E+45	-8.10	2507. /
TROE /0.0748 1.0E-50 -4215.9 1.0E50/ H2/2.0/ CO/2.0/ CO2/3.0/ H2O/9.0/			
C4H2+O=C3H2+CO	2.70E+13	0.00	1720. !
Warnatz J., in Combustion Chemistry, Gardiner, W. C. Jr. Springer-Verlag, New York (1984).			
C4H2+CH=C5H2+H	1.00E+14	0.00	0. !
estimate			
C4H2+CH2=H2CCCCCH+H	1.30E+13	0.00	4326. !
Bohland, T et al., Symp. Int. Combust. Proc. 21:841(1988)			
C4H2+CH2(S)=H2CCCCCH+H	1.70E+15	-0.39	0. !
Estimate from CH2sing+C2H2			

!*****

! C4H3 mechanism-HPMECH
!

!*****

C4H3-I+O=CH2CO+C2H	6.00E+13	0.00	0. !
estimated			

!*****

! C4H5 mechanism-HPMECH
!

!

!*****

!! I will assume the abstraction is fast with very little temp dependence
!! different from USC-Mech II and Jim Miller's. H-atom abstraction from
Radicals is always fast.

!! since C-H bond is weak, for example C2H3,
!! however, addition-elimination is also a possibility for unsaturated
species

C4H5-N+OH=HCO+C3H5-A 3.00E+13 0.00 0.
!estimated

!! again from Jim Miller, The OH in the intermediate is weak, H is ready
to transfer via four center or six center TS

!! products could be HCO+CH3CHCH or HCO+CH2CHCH2, using the latter

!! radical-radical reaction fast, increase a factor of 2

C4H5-N+O=CO+C3H5-A 6.00E+13 0.00 0. !
estimated

!! should be very fast CH2CHCHCH. RADICAL SITE SIMILAR AS C2H3+O

C4H5-N+O2=CH2CO+CH2CHO 1.00E+13 0.00 0. !
estimated

!! this actually is from Jim Miller's. make more sense to me via five
center TS

!! analogy to C2H3+O2 for entrance channel, no barrier

!! these three may be true, but I guess they wont be important

!! ignore them for now

C4H5-N+C2H=FULVENE 4.00E+12 0.00 0. !
JAM6

C4H5-N+C2H=C6H5+H 1.60E+13 0.00 0. ! JAM6

C4H5-N+C2H=C4H4+C2H2 3.00E+12 0.00 5000. !
JAM6

C4H5-I+O=C2H3+CH2CO 3.00E+13 0.00 0.0 !
JAM

C4H5-I+O=CH2O+C3H3 3.00E+13 0.00 0.0 ! JAM

!! resonant structure. O addition equally on two C-sites

C4H5-I+H=C2H2+C2H4 3.00E+13 0.00 0. !
JAM&SJK

!! make sense from simple structure estimation

! that's is what it is supposed to be

C4H5-I+OH=C2H4+CH2CO 2.00E+13 0.00 0. ! JAM

C4H5-I+OH=CH2O+C3H4-A 2.00E+13 0.00 0. !
JAM

C4H5-I+OH=CH2OH+C3H3 3.00E+12 0.00 0. ! JAM

!! two sites barrierless addition, products make sense

C4H5-I+O2=C2H3CO+CH2O 4.52E+19 -2.20 9990. ! Rutz
et al. J. Phys. Chem. A 2011, 115, 1018?1026

!C4H5-I+O2=CH2CHO+CH2CO 2.14E+11 0.21 12760. !
Rutz et al. J. Phys. Chem. A 2011, 115, 1018?1026

!! make sense for me

C4H5-I+C2H=FULVENE 1.00E+13 0.00 0.0
! JAM6

C4H5-I+C2H=C6H5+H 6.00E+12 0.00 0.0
! JAM6

C4H5-I+C2H=2C3H3 4.00E+12 0.00 0.0 ! JAM6

C4H5-I+C2H=C4H4+C2H2 3.00E+12 0.00 5000.0
! JAM6

!! trust Jim Miller no other choice

!! Important Note: the following rates are calculated using N2 as the collider
 !! recombination are not important for the reaction systems. So will not think about the collision efficiencies

C4H5-I+C2H2=H+C6H6 1.47E+23 -3.28 24907.
 ! Senosiain, et al., J. Phys. Chem. A 2007, 111, 3740
 PLOG /0.01 1.47E+23 -3.28 24907./
 PLOG /0.025 1.47E+23 -3.28 24907./
 PLOG /0.1 1.47E+23 -3.28 24907./
 PLOG /1. 1.67E+23 -3.30 24959./
 PLOG /10. 8.25E+24 -3.76 24562./
 PLOG /100. 5.37E+32 -5.84 35023./

C4H5-I+C2H2=H+C4H5C2H 5.70E+18 -1.43 30351. !
 Senosiain, et al., J. Phys. Chem. A 2007, 111, 3740
 PLOG /0.01 5.59E+18 -1.43 30341./
 PLOG /0.025 5.70E+18 -1.43 30351./
 PLOG /0.1 7.29E+18 -1.46 30465./
 PLOG /1. 5.59E+18 -1.43 30341./
 PLOG /10. 5.62E+19 -1.69 31434./
 PLOG /100. 4.70E+23 -2.73 36142./

!*****

! C4H6 mechanism-HPMECH

!
 !
 !

!*****

!! C4H6 ! CH2CHCHCH2 54.0924 CH2=CH-
 CH=CH2
 !! C4H612 ! CH3CHCCH2 54.0924 CH3-
 CH=C=CH2
 !! iiC4H6 ! CH3CCCH3

C4H6+O=IC3H5CO+H 1.50E+08 1.45 -860. !USC-
 Mech II

!!20 Torr data

!! these reactions should have an entrance barrier. for example
 H+C2H2=C2H3, H+C2H4=C2H5

!! But the barrier is small to form CH3CHCHCH2, the following
 isomerizations have high barrier to form final products

C4H6+OH=CH3CHO+C2H3 6.30E+12 0.00 -874. !

From Jim Miller's

!! addition equally to carbon sites, products channel energy are lower
 !! assuming rates are the same

!! iiC4H6 ! CH3CCCH3

C4H6-2+H=C4H5-I+H2 3.40E+05 2.50 2490. !=
 C3H6+H

C4H6-2=H+C4H5-I 5.00E+15 0.00 87300.

!96HID/HIG

C4H6-2+CH3=C4H5-I+CH4 1.40E+14 0.00 18500.

!Estimated

!! USC-Mech II and reference therein is the most reliable source

!! most of the reaction products and rates are reasonable

!*****

! C5H2 and C5H3 mechanism-HPMECH
!

!*****

!! C5H2----HCCCCCH radicals triplet state

C5H2+O=C4H2+CO 6.00E+13 0.00 0. !
estimated

C5H2+OH=C4H2+CO+H 2.50E+13 0.00 0. !
estimated

!! product is not too right, however, dont want to bother with new thermo
!! negelect C5H3 dissociation or C5H2+H association for now
!! reaction with O2

C5H2+CH=C6H2+H 1.00E+14 0.00 0.0 !
estimated

!!C5H2+C2H=C7H2+H 1.00E+14 0.00 0.0 !
estimated

!!Should be in the right range

H2CCCCCH+OH=C5H2+H2O 2.00E+13 0.00 0. !
estimated

HCCCHCCH+OH=C5H2+H2O 2.00E+13 0.00 0. !
estimated

H2CCCCCH+O=C4H+CH2O 8.00E+13 0.00 0. !
estimated

HCCCHCCH+O=C3H2+HCCO 8.00E+13 0.00 0. !
estimated

H2CCCCCH+H=C5H2+H2 4.00E+13 0.00 0. !
estimated

HCCCHCCH+H=C5H2+H2 4.00E+13 0.00 0. !
estimated

H2CCCCCH+CH3=C5H2+CH4 3.00E+12 0.00 5000. !
estimated

HCCCHCCH+CH3=C5H2+CH4 3.00E+12 0.00 5000. !
estimated

!! right range for all above, not too important anyway I guess
HCCCHCCH+H=H2CCCCCH+H 1.00E+13 0.00 0. !
estimated

!! depdening on thermo, if reactant is less stable, the rate could be
1.0E14 or at least 6.0E13

H2CCCCCH+CH3=FULVENE 1.00E+11 0.00 0.0
! JAM 11/2007

H2CCCCCH+CH3=C6H5+H 1.00E+11 0.00 0.0
! JAM 11/2007

H2CCCCCH+CH3=C6H6 5.00E+10 0.00 0.0
! JAM 11/2007

! These need some work
HCCCHCCH+CH3=FULVENE 1.00E+11 0.00 0. !
JAM 11/2007

HCCCHCCH+CH3=C6H5+H 1.00E+11 0.00 0.
! JAM 11/2007

!! The thermo of C5H3 has to re-evaluated before assessing the rates
!*****

```

!           C6H2  mechanism-HPMECH
!
!
!
!*****
*****
C6H2+O=C5H2+CO           2.70E+13      0.00      1720.  !
Estimated
C6H2+OH=HCCCHCCH+CO     1.68E+28      -4.59      20140. !
Estimated
!! this channel should be pretty good
!! but the other channels are too complicated to write the rate and
thermo---H+C5H2O
!*****
*****
!           C6H3  mechanism-HPMECH
!
!
!
!*****
*****
!! linear species HCC-C*=CH-CCH
C6H3+O2=>CO+C3H2+HCCO    5.00E+11      0.00      0.  !
Wang, H.; Frenklach, M. Combust.Flame 1997, 110, 173.
!! this one is slow, no doubt about it
!*****
*****
!           C6H4  mechanism-HPMECH
!
!
!
!*****
*****

!!C-C6H4 decomposition
!!L-C6H4 HCC-CH=CH-CCH
!! remember to check the thermo
C-C6H4=C2H2+C4H2          1.95E+90      -21.30     139390. !
Moskaleva et al., Phys. Chem. Chem. Phys., 1999, 1, 3967-3972
!! 100 Torr data
!C-C6H4=L-C6H4            4.77E119      -30.10     151502. !
Moskaleva et al., Phys. Chem. Chem. Phys., 1999, 1, 3967-3972
!! 100 Torr data for C-C6H4 to p-C6H4, but p-C6H4 will isomerize to L-
C6H4 very quickly
!!L-C6H4+H=n-C6H5         3.30E+44      -10.04     18800.  !
(54) Wang 97
!! it wont be stablized at all. I can hardly believe the existence of n-
C6H5 in combustion enviroments
C-C6H4+OH=C5H5+CO         1.00E+13      0.00      0.  !
Estimated
!! Hai Wang has the same number
C-C6H4+O=OH+C6H3          1.00E+13      0.00      0.  !
Estimated
!! at least at this level for high temp
!L-C6H4+H=C6H5             3.60E+77      -20.09     28100.  !
Wang, H.; Frenklach, M. Combust.Flame 1997, 110, 173.
!L-C6H4+OH=C6H3+H2O       3.10E+06      2.00      430.  !
Wang, H.; Frenklach, M. Combust.Flame 1997, 110, 173.

```

```
!!reasonable
!*****
*****
!           C6H5  mechanism-HPMECH
!
!
!
!*****
*****
```

```
!!!! I dont like the idea of linear C6H5, it can easily stablize to
phenyl
C6H5(+M)=C-C6H4+H(+M)           4.30E+12      0.62      77313.  ! Hai
Wang et al., Proc combust. Inst. 28(2000) 1545-1555
```

```
LOW/ 1.00E+84 -18.87      90064      /
TROE/ 0.902, 696., 358., 3856.      /
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/
```

```
!! will check collision efficiency
!! I am not sure about the rate either
!! C6H5+H=C-C6H4+H2           2.00E+11      1.10      24500.  !
01-MEB-LIN 1 atm wenjun cited this from USC_II
!! I am very surprised to see this rate, it is terribly wrong.
Misinterpretation of the paper.
```

```
C6H5+H=C-C6H4+H2           1.10E+06      2.36      4931.  !
Mebel, et al., J Chem Phys 114(2001) 8421
```

```
C6H5+O=C5H5+CO           1.00E+14      0.00      0.  !
FRANK et al., Symposium (International) on Combustion 25(1994) 833-840
```

```
C6H5+OH=C6H5O+H           5.00E+13      0.00      0.  !
estimate
!C6H5+OH=C6H5O+H           5.00E+13      0.00      0.  !
estimate
```

```
C6H5+OH=C-C6H4+H2O           1.00E+07      2.00      1000.  !
estimate
```

```
!! very high pressure expts with big errors of temperature. Rates are not
too good to believe.
```

```
!!O-C6H4O2=C5H4O+CO           7.40E+11      0.00      59000.  !
94-FRA-HER
```

```
!! MC has a very good calculation results
C6H5+C2H4=C6H6+C2H3           5.69E-02      4.47      4471.  !
Tokmakov et al., J. Phys. Chem. A 2004, 108, 9697-9714
```

```
!*****
*****
```

```
!           O-C6H4O2  mechanism-HPMECH
!
!
!
!*****
*****
```

```
!! experiments are at 1.3~2.3 atm. decrease the rate a factor of 10 may
be OK for the 30 Torr experiments considering the falloff
```

```
!!O-C6H4O2+OH rate is about 3.0E12 at 300K, but the products is very hard
to check
```

```
O-C6H4O2+H=CO+C5H5O           4.30E+09      1.45      3900.  !
USC Mech II
```

```
O-C6H4O2+O=2CO+C2H2+CH2CO           3.00E+13      0.00      5000.  !
USC Mech II
```

```
!*****
*****
```

```

!           C6H6  mechanism-HPMECH
!
!
!*****
*****
C6H6+O=C6H5OH          1.50E+29   -4.72   13342.  !
Taatjes et al., J. Phys. Chem. A 2010, 114, 3355?3370
  DUPLICATE
C6H6+O=C6H5OH          8.31E+04   -5.04    9356.  !
Taatjes et al., J. Phys. Chem. A 2010, 114, 3355?3370
  DUPLICATE
C6H6+O=C5H6+CO         7.20E+13    0.12   11777.  !
Taatjes et al., J. Phys. Chem. A 2010, 114, 3355?3370
!!C6H6+O=C6H5+OH
!! Abstraction is minor at low temp for sure, but might be important at
higher temp
!! however, all the results conclude it is not important except J. Phys.
Chem. A 2007, 111, 3836-3849

!*****
*****
!           C6H5OH  mechanism-HPMECH
!
!
!*****
*****
!*****
*****
!           O3  mechanism-HPMECH
!
!
!*****
*****
!!The following reactiosn are from
!!Luther, K.; Oum, K.; Troe, J. Phys. Chem. Chem. Phys. 2005,7,2764-2770.
!! and
!!Atkinson, R.; Baulch, D.L.; Cox, R.A.; Crowley, J.N.; Hampson, R.F.;
Hynes, R.G.; Jenkin, M.E.; Rossi, M.J.; Troe, J.
!!Evaluated kinetic and photochemical data for atmospheric chemistry:
Volume I - gas phase reactions of Ox, HOx, NOx and SOx species
!!Atmos. Chem. Phys. 4(2004) 1461 - 1738
!O2+O+AR=O3+AR          4.29E+17   -1.50    0.
!duplicate
!O2+O+AR=O3+AR          5.10E+21   -3.20    0.
!duplicate
!O2+O+HE=O3+HE          5.16E+17   -1.50    0.
!duplicate
!O2+O+HE=O3+HE          6.12E+21   -3.20    0.
!duplicate
!!put HE efficiency 20% higher than AR, it is usually true for most of
reactions
!O2+O+M=O3+M             6.53E+17   -1.50    0.
!  H2/2.0/ O2/0.95/ O3/2.5/ O/4.0/ AR/0.0/ HE/0.0/
!duplicate

```

```

!O2+O+M=O3+M          1.33E+22   -3.30      0.
!  H2/2.0/ O2/1.07/ O3/2.5/ O/4.0/ AR/0.0/ HE/0.0/
!duplicate

O3(+M)=O2+O(+M)        1.37E+15   -0.67 25990
LOW /2.275E+28 -4.37 27297/
TroE /0.6417   3.91E-04  8680.74   6060.75/
AR/1.0/ HE/1.2/ N2/1.5/ H2/3.0/ O2/1.50/ O3/3.75/ O/6.0/
!!O3+O is taken from
!!Atkinson, R.; Baulch, D.L.; Cox, R.A.; Crowley, J.N.; Hampson, R.F.;
Hynes, R.G.; Jenkin, M.E.; Rossi, M.J.; Troe, J.
!!Evaluated kinetic and photochemical data for atmospheric chemistry:
Volume I - gas phase reactions of Ox, HOx, NOx and SOx species
!!Atmos. Chem. Phys. 4(2004) 1461 - 1738
O3+O=O2+O2            4.82E+12   0.00 4094.
!! O3+H=O2+OH is taken from
!!DeMore, W.B.; Sander, S.P.; Golden, D.M.; Hampson, R.F.; Kurylo, M.J.;
Howard, C.J.; Ravishankara, A.R.; Kolb, C.E.; Molina, M.J.
!!Chemical kinetics and photochemical data for use in stratospheric
modeling. Evaluation number 12
!!JPL Publication 97-4 1997 1-266
O3+H=O2+OH            8.43E+13   0.00 934
!! O3+H=O+HO2 is taken from
!!C.J. Howard, B.J. Finlayson-Pitts J. Chem. Phys., 72 (6) (1980), pp.
3842-3843
O3+H=O+HO2            4.52E+11   0.00 0.
!! O3+OH=O2+HO2 is from
!!A. Mansergas, J.M. Anglada ChemPhysChem, 8 (2007), pp. 1534-1539
O3+OH=O2+HO2          1.85E+11   0.00 831
!!O3+H2O=O2+H2O2 is from
!! S. Hatakeyama, M.T. Leu J. Phys. Chem., 93 (1989), pp. 5784-5789
O3+H2O=O2+H2O2        6.62E+01   0.00 0
!! O3+HO2=OH+O2+O2 is from
!!DeMore, W.B.; Sander, S.P.; Golden, D.M.; Hampson, R.F.; Kurylo, M.J.;
Howard, C.J.; Ravishankara, A.R.; Kolb, C.E.; Molina, M.J.
!!Chemical kinetics and photochemical data for use in stratospheric
modeling. Evaluation number 12
!!JPL Publication 97-4 1997 1-266
O3+HO2=OH+O2+O2       6.62E+09   0.00 994
!! the following two are from
!!R. Atkinson, D.L. Baulch, R.A. Cox, J.N. Crowley, R.F. Hampson, R.G.
Hynes, M.E. Jenkin, M.J. Rossi, J. Troe
!! Atmos. Chem. Phys., 4 (2004), pp. 1461-1738
!O3+NO=O2+NO2         8.43E+11   0.00 2603

O3+CO<=>O2+CO2         6.02E+02   0.00      0.00
O3+HCO<=>O2+H+CO2     5.00E+11   0.00      0.00

!!O3+CH3=CH3O+O2 is from
!!J. Albaladejo, E. Jimenez, A. Notario, B. Cabanas, E. Martinez
!!J. Phys. Chem. A, 106 (2002), pp. 2512-2519
O3+CH3=CH3O+O2        5.83E+10   0.00 0

!*****
*****
!
! N mechanism-HPMECH
!

```



```

!
!
!*****
*****
! Capitelli et al., Plasma Kinetics in Atmospheric Gases (2000), Springer
2N+M<=>N2+M          6.53E+14  0.00  -218.90
  N2/0.0/ AR/0.5/ O/3.0/ N/3.0/ CO2/3.5/
2N+N2<=>2N2          3.01E+14  0.00  -
251.61

!*****
*****
!
!          NO  mechanism-HPMECH
!
!
!*****
*****
! Capitelli et al., Plasma Kinetics in Atmospheric Gases (2000), Springer
N+O+M<=>NO+M          1.96E+19 -1.00
0.00
  N2/0.0/ O2/0.0/ CO2/2.9/ AR/0.05/
N+O+N2<=>NO+N2        6.28E+16 -0.50
0.00
N+O+O2<=>NO+O2        6.28E+16 -0.50
0.00
N+HO2<=>NO+OH         1.02E+13  0.00
1987.20

! Bromly et al., Combustion Science and Technology (1996), Vol. 115, pp.
259-296
N+NO<=>N2+O           3.27E+12  0.30
0.00
N+O2<=>NO+O           6.40E+09  1.00
6280.00
N+OH<=>NO+H           3.80E+13  0.00
0.00

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-
Phase Combustion Chemistry (2000), Gardiner ed., Springer
NO+C<=>CO+N           1.70E+13  0.00
0.00

! Glassman and Yetter, Combustion (2008), 4th ed., Academic Press
N+O3<=>NO+O2          6.00E+07  0.00
0.00

!*****
*****
!
!          NO2  mechanism-HPMECH
!
!
!*****
*****

```

! Mueller et al., International Journal of Chemical Kinetics (1999), Vol. 31, pp. 705-724

NO+O(+M)<=>NO2(+M) 1.30E+15 -0.75
0.00
LOW/4.72E+24 -2.87

1550.00/
TROE/0.957 1E-90 8.332E+03/ !Exponential fit to Fc=0.95-0.0001*T
AR/0.0/ H2O/12.0/ H2/2.0/ CO/1.9/ CO2/3.8/
NO+O(+AR)<=>NO2(+AR) 1.30E+15 -0.75 0.00
LOW/7.56E+19 -1.41

0.00/
TROE/0.957 1E-90 8.332E+03/ !Exponential fit to Fc=0.95-0.0001*T

NO2+O<=>O2+NO 1.05E+14 -0.52
0.00

NO2+H<=>NO+OH 1.32E+14 0.00
362.00

HO2+NO<=>NO2+OH 2.05E+12 0.00 -497.00

!NO2+ HO2 = HONO+ O2 7.230E+10 0.0 0.0 !
(DAGAUT, DME, 75COX/DER)
NO2+ HO2 = HONO+ O2 1.900E+00 3.3 3044.0 !
(DAGAUT, DME, 75COX/DER) !*0.2 1.446E+10 0.0 0.0

CH2O+ NO2 = HCO+ HONO 8.000E+02 2.77 13730.0 !
(DAGAUT, DME, 91STA/HER)

NO2+NO2<=>2NO+O2 1.63E+12 0.00 26100.00

CO+NO2<=>CO2+NO 9.03E+13 0.00
33800.00

HCO+NO2<=>H+CO2+NO 8.39E+15 -0.75
1930.00

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-Phase Combustion Chemistry (2000), Gardiner ed., Springer

!NO2+CH3<=>NO+CH3O 1.40E+13 0.00
0.00

NO2+CH3<=>NO+CH3O 1.40E+15 0.00
0.00 !/*100

!!agree with Srinivasan, N.K.; Su, M.C.; Sutherland, J.W.; Michael, J.V.
!!Reflected shock tube studies of high-temperature rate constants for
OH+CH4 -> CH3+H2O and CH3+NO2 -> CH3O+NO
!! J. Phys. Chem. A 109(2005)1857-1863

!*****

! N2O mechanism-HPMECH

!

!

!

!*****

! ? Skreiberg, P. Kilpinen, P. Glarborg, Combust. Flame 136 (2004)
501?518.

N2O(+M)<=>N2+O(+M) 1.30E+12 0.00
62570.00

LOW/4.00E+14 0.00

56600.00/
 AR/0.63/ H2O/7.5/
 N2O+O<=>O2+N2 3.70E+12 0.00
 15936.00
 N2O+O<=>2NO 9.20E+13 0.00
 27679.00

!! S.J. Klippenstein et al. / Combustion and Flame 158 (2011) 774-789
 N2O+H<=>N2+OH 6.40E+07 1.835
 13492.00 !

! Skreiberg, P. Kilpinen, P. Glarborg, Combust. Flame 136 (2004)
 501-518.
 N2O+OH<=>HO2+N2 1.30E-02 4.72
 36560.00
 N2O+OH<=>HNO+NO 1.20E-04 4.33
 25080.00

!! this is not too important and have large uncertainties
 N2O+NO<=>NO2+N2 1.00E+14 0.00
 49700.00

! Mueller et al., International Journal of Chemical Kinetics (1999), Vol.
 31, pp. 705-724
 CO+N2O<=>CO2+N2 5.01E+13 0.00
 44000.00

! Wennberg et al., Journal of Geophysical Research: Atmospheres (1994),
 pp. 18839-18846
 N+NO2<=>N2O+O 3.49E+12 0.00 -
 437.18

!*****

 ! HNO mechanism-HPMECH
 !
 !
 !
 !*****

! Mueller et al., International Journal of Chemical Kinetics (1999), Vol.
 31, pp. 705-724
 NO+H(+M)<=>HNO(+M) 1.52E+15 -0.41
 0.00
 LOW/2.40E+14 0.206

-1550.00/
 SRI/0.82 1.0E-30 1.0E+30/
 N2/1.60/
 HNO+H<=>NO+H2 4.40E+11 0.72
 650.00
 HNO+O<=>OH+NO 2.30E+13 0.00
 0.00
 HNO+OH<=>H2O+NO 1.30E+07 0.00 -
 956.00

!! Tsang, W.; Herron, J.T.
 !! Chemical kinetic data base for propellant combustion. I. Reactions
 involving NO, NO2, HNO, HNO2, HCN and N2O
 !! J. Phys. Chem. Ref. Data 20(1991) 609-663

```

!! this is the original reference
HNO+HNO<=>H2O+N2O          8.51E+08  0.00
3080.00
!! Dammeier, J.; Colberg, M.; Friedrichs, G.
!! Wide temperature range (T=295 K and 770-1305 K) study of the kinetics
of the reactions HCO plus NO and HCO+N02 using frequency modulation
spectroscopy
!! Phys. Chem. Chem. Phys.
!! 9(2007) 4177-4188
HCO+NO<=>HNO+CO          7.23E+12  0.00
0.00

!! Bryukov, M.G.; Kachanov, A.A.; Timonnen, R.; Seetula, J.; Vandoren,
J.; Sarkisov, O.M.
!! Kinetics of HNO reactions with O2 and HNO
!! Chem. Phys. Lett. 208(1993) 392-398
!! Original reference
HNO+O2<=>HO2+NO          2.20E+10  0.00
9140.00

! Xu and Lin, International Journal of Chemical Kinetics (2004), Vol. 36,
Iss. 4, pp.205-215
HNO+HCO<=>NO+CH2O          5.83E-01  3.84
115.26

! Choi and Lin, International Journal of Chemical Kinetics (2005), Vol.
37, Iss. 5, pp. 261-274
HNO+CH3<=>NO+CH4          1.47E+11  0.76  347.76

!*****
*****
!           HONO  mechanism-HPMECH
!
!
!
!*****
*****

! Mueller et al., International Journal of Chemical Kinetics (1999), Vol.
31, pp. 705-724
NO+OH(+M)=HONO(+M)          .110E+14  -0.300  .0
!\AUTHOR: AS !\REF: Fulle D Hamann HF Hippler H Troe J JCP 108:5391 1998
!\COMMENT:
LOW / .3392E24 -2.50 .0/          ! He
.110E+15
TROE / 0.75 1E-30 1E30 1E30/
AR/0.1/
HNO+NO2<=>HONO+NO          6.02E+11  0.00
1990.00
HONO+O<=>OH+NO2          1.20E+13  0.00
5960.00
HONO+OH<=>H2O+NO2          8.50E+11  0.00  -
517.00 !1.70E+12  0.00  -520.00
HCO+NO2<=>CO+HONO          1.24E+23  -3.29
2350.00

! Mueller et al., Combustion and Flame (2000), Vol. 120, pp. 589-594

```

$\text{NO}_2 + \text{H}_2 \rightleftharpoons \text{HONO} + \text{H}$ 7.33E+11 0.00
 28800.00

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-Phase Combustion Chemistry (2000), Gardiner ed., Springer
 $\text{HONO} + \text{H} \rightleftharpoons \text{H}_2\text{O} + \text{NO}$ 8.10E+06 1.89
 3845.24
 $\text{HONO} + \text{H} \rightleftharpoons \text{OH} + \text{HNO}$ 5.60E+10 0.86
 4968.01
 $\text{HONO} + \text{CH}_3 \rightleftharpoons \text{NO}_2 + \text{CH}_4$ 8.10E+05 1.87
 5504.56 ! Might be better to give reverse rate. cf. "Kinetics of hydrogen-oxygen and methane-oxygen ignition sensitized by NO or NO₂" by Slack and Grillo

! Mebel et al., Journal of Physical Chemistry (1998), Vol. 102, pp.1803-1807
 $2\text{HONO} \rightleftharpoons \text{NO} + \text{NO}_2 + \text{H}_2\text{O}$ 3.49E-01 3.64
 12139.83

!*****

 ! NH mechanism-HPMECH
 !
 !
 !*****

!! P. Glarborg, M.U. Alzueta, K. Dam-Johansen, J.A. Miller
 !! Combust. Flame, 115 (1998), pp. 1-27
 $\text{NH} + \text{O}_2 \rightleftharpoons \text{HNO} + \text{O}$ 4.60E+05 2.00 6500.
 $\text{NH} + \text{O}_2 \rightleftharpoons \text{NO} + \text{OH}$ 1.30E+06 1.50 100.
 $\text{NH} + \text{O} \rightleftharpoons \text{NO} + \text{H}$ 9.20E+13 0.00
 0.00
 !! S.J. Klippenstein, L.B. Harding, B. Ruscic, R. Sivaramakrishnan, N.K. Srinivasan,
 !! M.-C. Su, J.V. Michael, J. Phys. Chem. A 113 (2009) 10241-10259.
 $\text{NH} + \text{OH} \rightleftharpoons \text{HNO} + \text{H}$ 3.20E+14 -0.376 -
 46.
 $\text{NH} + \text{OH} \rightleftharpoons \text{N} + \text{H}_2\text{O}$ 1.60E+07 1.733 -
 576.
 !! S.J. Klippenstein et al. / Combustion and Flame 158 (2011) 774-789
 $\text{NH} + \text{NO} \rightleftharpoons \text{N}_2\text{O} + \text{H}$ 1.80E+14 0.351
 244.
 $\text{NH} + \text{NO} \rightleftharpoons \text{N}_2 + \text{OH}$ 2.70E+12 0.0721 512.
 !! P. Glarborg, M.U. Alzueta, K. Dam-Johansen, J.A. Miller
 !! Combust. Flame, 115 (1998), pp. 1-27
 $\text{NH} + \text{NO}_2 \rightleftharpoons \text{NO} + \text{HNO}$ 5.90E+12 0.00
 0.00
 $\text{NH} + \text{NO}_2 \rightleftharpoons \text{N}_2\text{O} + \text{OH}$ 4.10E+12 0.00
 0.00
 $\text{NH} + \text{NH} \rightleftharpoons \text{N}_2 + \text{H} + \text{H}$ 2.50E+13 0.00
 0.00

! Caridade et al., Journal of Physical Chemistry A (2005), Vol. 109, pp. 2356-2363
 $\text{NH} + \text{N} \rightleftharpoons \text{N}_2 + \text{H}$ 6.41E+11 0.51
 18.48

NH+N<=>N+N+H 7.57E+14 -0.20
54159.26

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-Phase Combustion Chemistry (2000), Gardiner ed., Springer
NH+O2<=>H+NO2 2.30E+10 0.00
2484.01
NO+CH<=>N+HCO 2.90E+13 0.00
0.00
NO+CH<=>NH+CO 5.50E+12 0.00
0.00
!! accept this NO+CH for now. the branching ratio and total rate is too far off
!NH+CH3<=>CH4+N 8.20E+05 1.87
5852.32

! Deppe et al., Berichte der Bunsengesellschaft für physikalische Chemie (1998), Vol. 102, Iss. 10, pp. 1474-1485
NH+M<=>N+H+M 1.80E+14 0.00
74808.81
N/0.0/
! Davidson and Hanson, International Journal of Chemical Kinetics (1990), Vol. 22, Iss. 8, pp. 843-861
N+H2<=>H+NH 1.60E+14 0.00
25138.13
!*****

!
!
! NH2 mechanism-HPMECH
!
!
!
!*****

!!Z. Tian, Y. Li, L. Zhang, P. Glarborg, F. Qi, Combust. Flame 156 (2009) 1413-1426.
NH2+O<=>HNO+H 6.60E+13 0.00
0.00
NH2+O<=>NH+OH 7.00E+12 0.00 0.
DUPLICATE
NH2+O<=>NH+OH 8.60E-01 4.010 1673.
DUPLICATE
!! D.P. Linder, X. Duan, M. Page
!! J. Phys. Chem., 99 (1995), pp. 11458-11463
NH2+H<=>NH+H2 7.20E+05 2.32
1590.00
!!S.J. Klippenstein, L.B. Harding, B. Ruscic, R. Sivaramakrishnan, N.K. Srinivasan,
!!M.-C. Su, J.V. Michael, J. Phys. Chem. A 113 (2009) 10241-10259.
NH2+OH<=>NH+H2O 3.30E+06 1.95 -
217.
! Skreiberg, P. Kilpinen, P. Glarborg, Combust. Flame 136 (2004) 501-518.
NH2+HO2=NH3+O2 9.20E+05 1.94 -
1152.

```

!! S.J. Klippenstein et al. / Combustion and Flame 158 (2011) 774-789
NH2+O2=H2NO+O          2.60E+11    0.4872
  29050
NH2+O2<=>HNO+OH        2.90E-02    3.764
18185.
NH2+NO<=>N2+H2O        1.30E+16   -1.25
0.00
  DUPLICATE
NH2+NO<=>N2+H2O        -3.10E+13  -0.48
1180.00
  DUPLICATE
NH2+NO<=>NNH+OH        3.10E+13  -0.48
1180.00
!! Stephen J. Klippenstein et al J.Phys.Chem.A 2013, 117, 9011-9022
NH2+NO2<=>N2O+H2O      2.60E+18  -2.191
455.00
NH2+NO2<=>H2NO+NO      9.69E+11  0.0321   -
1512.00
! S. Skreiberg, P. Kilpinen, P. Glarborg, Combust. Flame 136 (2004)
501-518.
NH2+HNO=NH3+NO         3.60E+06   1.630 -
1250.
NH2+HONO=NH3+NO2       7.10E+01   3.02 -4940.
!!! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-
Phase Combustion Chemistry (2000), Gardiner ed., Springer
NH2+CH3<=>NH+CH4        2.80E+06   1.94   9210.69
NO+CH2<=>NH2+CO         2.30E+16  -1.43
1331.43
NH2+N<=>N2+2H           7.10E+13   0.00
0.00

! Deppe et al., Berichte der Bunsengesellschaft f#ur physikalische Chemie
(1998), Vol. 102, Iss. 10, pp. 1474-1485
NH2+M<=>NH+H+M         1.20E+15   0.00
76003.75

!*****
*****
!
!
!           NH3  mechanism-HPMECH
!
!
!*****
*****

!! S.J. Klippenstein et al. / Combustion and Flame 158 (2011) 774-789
NH3+M<=>NH2+H+M        2.20E+16   0.00
93500.00
NH3+H<=>NH2+H2         6.38E+05   2.39
10200.00
NH3+O<=>NH2+OH         2.80E+02   3.29
4471.0
NH3+OH<=>NH2+H2O       2.04E+06   2.04   566.00
NH3+HO2<=>NH2+H2O2     3.00E+11   0.00
22000.00

```

!*****

! NNH mechanism-HPMECH

!

!

!*****

!! S.J. Klippenstein et al. / Combustion and Flame 158 (2011) 774-789

NNH<=>N2+H	3.00E+08	0.00		
0.00				
NNH+H<=>N2+H2	1.00E+14	0.00		
0.00				
NNH+O<=>N2+OH	1.20E+13	0.145	-	
217.				
NNH+O<=>N2O+H	1.90E+14	-0.274	-	
22.				
NNH+O<=>NH+NO	5.20E+11	0.388	-	
409.				
NNH+O2<=>HO2+N2	5.60E+14	-0.385	-	
13.				
NNH+OH<=>N2+H2O	5.00E+13	0.00	0.	
NNH+NO<=>N2+HNO	5.00E+13	0.00	0.	

!*****

! H2NO mechanism-HPMECH

!

!

!*****

H2NO+M=HNO+H+M	2.80E+24	-2.830		
64915				
H2O /10/				
H2NO+H=HNO+H2	3.00E+07	2.000	2000	
H2NO+H=NH2+OH	5.00E+13	0.000	0	
H2NO+O=HNO+OH	3.00E+07	2.000	2000	
H2NO+OH=HNO+H2O	2.00E+07	2.000	1000	
H2NO+HO2=HNO+H2O2	2.90E+04	2.690	1600	
H2NO+O2=HNO+HO2	3.00E+12	0.000	25000	

!*****

! N2H2 mechanism-HPMECH

!

!

!*****

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-Phase Combustion Chemistry (2000), Gardiner ed., Springer

NH2+NH<=>N2H2+H	1.50E+15	-0.50		
0.00				


```

N2H2<=>NNH+H                                1.80e+40 -8.41
73397.38 ! 1 atm
  DUPLICATE
  PLOG / 0.1 5.60E+36 -7.75 70257.60 /
  PLOG / 1.0 1.80E+40 -8.41 73397.38 /
  PLOG / 10.0 3.10E+41 -8.42 76050.30 /
N2H2<=>NNH+H                                2.60E+40 -8.53
72930.39 ! 1 atm
  DUPLICATE
  PLOG / 0.1 1.60E+37 -7.94 70764.34 /
  PLOG / 1.0 2.60E+40 -8.53 72930.39 /
  PLOG / 10.0 1.30E+44 -9.22 77083.65 /
N2H2+H<=>NNH+H2                              4.80E+08 1.50
1579.83
N2H2+O<=>NNH+OH                              3.30E+08 1.50
496.80
N2H2+OH<=>NNH+H2O                            2.40E+06 2.00 -
1192.32
N2H2+NH2<=>NNH+NH3                           1.80E+06 1.94 -
1152.58
N2H2+CH3<=>NNH+CH4                           1.60E+06 1.87
2970.87
N2H2+NH<=>NNH+NH2                            2.40E+06 2.00 -
1192.32
N2H2+NO<=>N2O+NH2                            4.00E+12 0.00
11923.22

! Allen et al., Combustion and Flame (1997), Vol. 109, pp. 449-470
N2H2+M<=>NH+NH+M                             3.16E+16 0.00 99400.00
NH2+NH2<=>N2H2+H2                            3.98E+13 0.00
11900.00
NNH+NNH<=>N2H2+N2                            1.00E+13 0.00
9940.00
N2H2+HO2<=>NNH+H2O2                          1.00E+13 0.00
1990.00

!*****
!*****
!
!
!
!*****
!*****

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-
Phase Combustion Chemistry (2000), Gardiner ed., Springer
NH2+NH2<=>N2H3+H                             1.20E+12 -0.03 10085.06 ! 1
atm
  PLOG / 0.1 9.20E+11 -0.01 10015.51 /
  PLOG / 1.0 1.20E+12 -0.03 10085.06 /
  PLOG / 10.0 4.70E+12 -0.20 10621.61 /
N2H3<=>N2H2+H                                3.6E+47 -10.38
69015.60 ! 1 atm
  PLOG / 0.1 2.30E+43 -9.55 64474.84 /
  PLOG / 1.0 3.6E+47 -10.38 69015.60 /
  PLOG / 10.0 1.80E+45 -9.39 70148.30 /
N2H3+H<=>N2H2+H2                            2.40E+08 1.50 0.00

```

N2H3+O<=>NH2+HNO	3.00E+13	0.00	0.00
N2H3+O<=>N2H2+OH	1.70E+08	1.50	-645.84
N2H3+OH<=>N2H2+H2O	1.20E+06	2.00	-
1192.32			
N2H3+CH3<=>N2H2+CH4	8.20E+05	1.87	
1818.29			
N2H3+NH2<=>N2H2+NH3	9.20E+05	1.94	-
1152.58			
N2H3+HO2<=>N2H2+H2O2	2.90E+04	2.69	-1599.70

! Allen et al., Combustion and Flame (1997), Vol. 109, pp. 449-470

N2H3+M<=>NH2+NH+M	1.00E+16	0.00	
41700.00			
N2H3+H<=>NH+NH3	1.00E+11	0.00	
0.00			
N2H2+NH2<=>NH+N2H3	1.00E+11	0.50	
33800.00			
NH3+NH2<=>N2H3+H2	7.94E+11	0.50	
21600.00			
N2H2+N2H2<=>NNH+N2H3	1.00E+13	0.00	9940.00
N2H3+O<=>NNH+H2O	3.16E+11	0.50	0.00

!*****

! N2H4 mechanism-HPMECH

!
!
!

!*****

! Dean and Bozzelli, Chapter 2. Combustion Chemistry of Nitrogen, Gas-Phase Combustion Chemistry (2000), Gardiner ed., Springer

NH2+NH2<=>N2H4	5.6E+48	-11.30	
11883.48 ! 1 atm			
PLOG / 0.1	2.0E+46	-10.93	9995.64 /
PLOG / 1.0	5.6E+48	-11.30	11883.48 /
PLOG / 10.0	3.2E+49	-11.18	13989.92 /
N2H3+HO2<=>N2H4+O2	9.20E+05	1.94	
2126.31			
N2H4+H<=>N2H3+H2	9.60E+08	1.50	4838.84
N2H4+O<=>N2H3+OH	6.70E+08	1.50	2851.67
N2H4+OH<=>N2H3+H2O	4.80E+06	2.00	-
645.84			
N2H4+CH3<=>N2H3+CH4	3.30E+06	1.87	
5325.71			
N2H4+NH2<=>N2H3+NH3	3.70E+06	1.94	
1629.51			

! Allen et al., Combustion and Flame (1997), Vol. 109, pp. 449-470

N2H4+M<=>N2H3+H+M	1.00E+15	0.00	
63600.00			
N2H4+H<=>NH2+NH3	4.46E+09	0.00	3100.00
N2H4+NH<=>NH2+N2H3	1.00E+12	0.00	
1990.00			
N2H4+N2H2<=>N2H3+N2H3	2.50E+10	0.50	29800.00
N2H3+N2H2<=>N2H4+NNH	1.00E+13	0.00	9940.00

N2H4+O<=>N2H2+H2O 6.31E+13 0.00
1190.00
N2H4+HO2<=>N2H3+H2O2 3.98E+13 0.00 1990.00

!*****

!
!
! NO3 mechanism-HPMECH
!
!

!*****

! Mueller et al., International Journal of Chemical Kinetics (1999), Vol. 31, pp. 705-724

NO2+O(+M)<=>NO3(+M) 1.33E+13 0.00
0.00
LOW/1.49E+28 -4.08

2470.00/
TROE/0.826 1E-90 3.191E+03/ !Exponential fit to Fc=0.79-0.00018*T
AR/0.75/

NO2+NO2<=>NO3+NO 9.64E+09 0.73 20900.00

! Bromly et al., Combustion Science and Technology (1996), Vol. 115, pp. 259-296

NO3+OH<=>HO2+NO2 1.38E+13 0.00 0.00

NO3+O<=>O2+NO2 1.02E+13 0.00
0.00

NO3+H<=>NO2+OH 6.00E+13 0.00
0.00

NO3+HO2<=>O2+NO2+OH 2.00E+12 0.00
0.00

NO3+NO3<=>NO2+NO2+O2 5.12E+11 0.00 4840.00

NO3+M<=>O2+NO+M 2.05E+08 1.00
12122.00

NO2/0.0/
NO3+NO2<=>O2+NO+NO2 3.25E+10 0.00
2960.00

NO2+O3<=>NO3+O2 7.23E+10 0.00
4870.00

!*****

!
!
! HNO3 mechanism-HPMECH
!
!

!*****

! Mueller et al., International Journal of Chemical Kinetics (1999), Vol. 31, pp. 705-724

NO2+OH(+M)<=>HNO3(+M) 2.41E+13 0.00 0.00

2350.00/

TROE/0.837 1E-90 1.657E+03/ !Exponential fit to Fc=0.725-0.00025*T
AR/0.75/

! Bromly et al., Combustion Science and Technology (1996), Vol. 115, pp. 259-296

HO2+NO+M<=>HNO3+M 2.23E+12 -3.50
2200.00
HNO3+OH<=>H2O+NO3 1.03E+10 0.00 -
1240.00
NO3+HO2<=>O2+HNO3 5.60E+11 0.00
0.00

!
!

!-----

!----- AJOUT DAGAUT -----

!

! H2+ O2 = OH+ OH 1.700E+13 0.0 47780.0 !
(MILLER 77)
! H+ HO2 = H2O+ O 3.010E+13 0.0 1721.0 !
(BAULCH 92)
! OH+ OH = H2O2 1.329E+16 -1.462 61.0 !
(JPL , 1BAR)
! CH4 = CH3+ H 2.132E+31 -5.30 104906.0 !
(COBOS T 90,1BAR)
! CH3+ CH3 = C2H6 2.393E+38 -7.581 11359.0 !
(WALTER90 1BAR)
! CH2+ OH = CH2O+ H 2.500E+13 0.0 0.0 !
(MILLER BOWMAN 89)
! CH2+ CH3 = C2H4+ H 4.000E+13 0.0 0.0 !
(WARNATZ 84)
! CH2+ C2H6 = CH3+ C2H5 6.500E+12 0.0 7911.0 !
(BOHLAND 85)
! CH3O+ C2H3 = CH2O+ C2H4 2.410E+13 0.0 0.0 !
(TSANG HAMPSON 86)
! CH3O+ C2H4 = CH2O+ C2H5 1.200E+11 0.0 7000.0 !
(TSANG HAMPSON 86)
! C2H6 = C2H5+ H 2.080E+38 -7.08 106507.0 !
(STEWART 88,1BAR)
! C2H5+ OH => CH3+ CH2O +H 2.409E+13 0.0 0.0 !
(TSANG HAMPSON 86)
! C2H5 = C2H4+ H 4.588E+25 -4.163 40479.0 !
(FIT FENG93,1BAR)
! C2H5+ C2H5 = C2H4+ C2H6 1.400E+12 0.0 0.0 !
(WARNATZ 84)
! C2H2+ H = C2H3 4.526E+14 -0.713 2688.0 !
(BAULCH 92,1BAR)
! C2H3+ HO2 => CH3+ CO +OH 3.000E+13 0.0 0.0 !
(TSANG HAMPSON 86)
! C2H3+ O = CH3+ CO 1.500E+13 0.0 0.0 !
(HEINEMANN 86)
! C2H2+ O2 = HCCO+ OH 2.000E+08 1.5 30100.0 !
(MILLER 92)

! CH2CO+ H	=	CH2CHO	1.000E+14	0.0	2500.0	!
(ESTIMEE94)						
!CH2CHO+ O2	=	OH+ CHOCHO	2.510E+11	0.00	14640.0	!
(MARINOV94)						
!CH2CHO+ HO2	=	CH2O+ HCO +OH	1.000E+13	0.00	0.0	!
(MARINOV94)						
!CHOCHO	=	CH2O+ CO	1.176E+16	-1.28	50937.0	!
(MARINOV94,1BAR)						
!CHOCHO	=	CO + CO +H2	6.519E+39	-7.703	67469.0	!
(MARINOV94,1BAR)						
!CHOCHO+ H	=	CH2O + HCO	1.000E+12	0.00	0.0	!
(84SAIT/KAKU)						
!CHOCHO+ O2	=	HCO + CO +HO2	6.300E+13	0.00	30000.0	!
(MARINOV94)						
!CH2CO+ O2	=	CH2O + CO2	2.000E+13	0.0	61500.0	!
(DAGAUT 90 C2H4/2)						
!CH2CO+ HO2	=	CH2O + CO +OH	6.000E+11	0.0	12738.0	!
(PILLING 90)						
!CH2CO+ OH	=	HCO + CH2O	2.040E+11	0.0	0.0	!
(BAULCH92 2%)						
!CH2CO+ CH3	=	HCCO + CH4	7.500E+12	0.0	13000.0	!
(HIDAKA94)						
!CH2CO+ CH2	=	HCCO + CH3	1.000E+12	0.0	0.0	!
(HIDAKA82)						
!CH2CO+ CH2	=	C2H4 + CO	3.600E+13	0.0	11000.0	!
(HIDAKA94)						
!HCCO+ OH	=	HCO + CO +H	1.000E+13	0.0	0.0	!
(MILLER 82)						
!CH3OH	=	CH3 + OH	1.565E+46	-9.28	103522.0	!
(TSANG 87 1BAR)						
!CH3CHO	=	CH3 + HCO	9.586E+14	0.0	74180.0	!
(FIT)						
!CH3CHO+ HCO	=	CH3CO +CH2O	7.800E+13	0.0	8440.0	!
(=C2H6)						
!C2H4O1-2	=	CH4 + CO	1.210E+13	0.0	57200.0	!
(LIFSHITZ 83)						
!C2H4O1-2+ H	=	C2H3 + H2O	5.000E+09	0.0	5000.0	!
(LIFSHITZ 83)						
!C2H4O1-2+ H	=	C2H4 + OH	9.510E+10	0.0	5000.0	!
(LIFSHITZ 83)						
!CH3OCH3	=	CH3O + CH3	1.380E+52	-10.9	96640.0	!
(LLNL 1BAR97)						
!CH3OCH2+ HO2	=>	CH2O + CH3O +OH	1.000E+13	0.0	0.0	!
(ESTD)						
!CH3OCH2+ CH3	=>	C2H5 + CH3O	1.000E+11	0.0	0.0	!
(=CH2CO)						
!CH3OCH2O2 + HO2	=	CH3OCH2O2H + O2		6.800E+11	0.0	-
1270.0 ! (CH3O2*2)						
!CH3OCH2O2 + HO2	=	CH3OCHO+ O2 +H2O	5.400E+11	0.0	-1270.0	
! (CH3O2 >)						
!CH3OCH2O2H	=>	CH3O+ CH2O +OH	4.000E+15	0.0	42900.0	
! (CH3O2 92BAU/COB)						
!OCH2OCHO	=>	CH2O+ HOCO	1.000E+14	0.0	15000.0	
! (90COWART)						
!CH3 + O2	=	CH3O2	3.250E+26	-4.686	4292.0	!
(94BAU/COB 1BAR)						
!CH3O2 + HO2	=>	CH2O+ H2O +O2	1.800E+10	0.0	-1431.0	!
(92WAL/DAG)						

!CH3O2+CH3OCH2 ! (=CH3+CH3O2)	=	CH3O+ CH3OCH2O	8.170E+12	0.0	-906.0	
!CH3O2H+ H (77SLERM/WARNECK)	=	CH3O+ H2O	8.200E+10	0.0	1860.0	!
!CH3O2H+ O (90VAG/RAVI)	=	CH3O2+ OH	1.000E+12	0.0	3000.0	!
!CH3O2H+ OH (92ATK/BAU)	=	CH3O2+ H2O	1.800E+12	0.0	-378.0	!
!HO2CHO (LLNL)	=>	HOCO + OH	6.000E+14	0.0	37000.0	!
!HOCO + OH (LLNL)	=>	HO2CHO	3.290E+06	2.25	-2775.0	!
! CH2O+ OH (TSANG HAMPSON 86)	=	HOCHO + H	4.450E+07	1.18	-447.0	!
!HOCHO + M (82HSU/SHA)	=	CO + H2O + M	2.300E+13	0.0	50000.0	!
!HOCHO + M (82HSU/SHA)	=	CO2+ H2 + M	1.500E+16	0.0	57000.0	!
!HOCHO + OH (92ATK/BAU)	=	HOCO+ H2O	2.710E+11	0.0	0.0	!
!CH3OCH3 + HOCO ! (=CH3+CH3OCH3)	=	CH3OCH2 +HOCHO	0.106E+00	4.214	7527.0	
!CH2O + HOCO (=CH3+CH2O)	=	HCO +HOCHO	4.090E+12	0.0	8843.0	!
!HO2CHO (83DEV/PRI)	=>	CO2 + H2O	2.140E+11	0.0	28347.0	!
!HO2CHO + CH2O (STARK/CH3CO3H)	=>	HOCHO +HOCHO	2.000E+08	0.0	10000.0	!
! O2 + CH2OH (94STAR/WAD)	=>	HOCH2O2	8.320E+11	0.0	0.0	!
!HO2 + CH2O (82VEY/RAY)	=>	HOCH2O2	2.000E+18	-3.0	320.0	!
!HOCH2O2+CH3OCH2 (CH3O2+CH3)	=>	HOCH2O + CH2O +CH3O	8.170E+12	0.0	-906.0	!
!HOCH2O2+ HCO (HC3O+HCO TSA/HAM)	=>	HOCH2O + HOCO	3.000E+13	0.0	0.0	!
!HOCH2O + O2 (94STAR/WAD)	=>	HOCHO + HO2	4.300E+10	0.0	1076.0	!
!CH3OCH2O + M ! (CH3O+M>)	=	CH3OCHO+ H + M	7.000E+15	0.0	22773.0	
!CH3OCH2O + H ! (CH3O+H)	=	CH3OCHO+ H2	2.000E+13	0.0	0.0	
!CH3OCH2O + O ! (CH3O+O)	=	CH3OCHO+ OH	1.000E+13	0.0	0.0	
!CH3OCH2O + OH ! (CH3O+OH)	=	CH3OCHO+ H2O	1.000E+13	0.0	0.0	
!CH3OCH2O + HO2 ! (CH3O+HO2)	=	CH3OCHO+ H2O2	2.000E+11	0.0	0.0	
!CH3OCHO (MACET)	=	CH3OH+ CO	4.500E+16	0.0	88600.0	!
!CH3CO2 + M (CH3CO/89WILK)	=	CH3O+ CO + M	8.640E+15	0.0	14400.0	!
!CH2OCHO+ M (CH3CO/89WILK)	=	HCO+ CH2O + M	8.640E+15	0.0	14400.0	!
!CH3OCH3 + CH2OCHO ! (=CH3+CH3OCH3)	=	CH3OCH2+CH3OCHO	0.106E+00	4.214	7527.0	
!CH3OCH3 + CH3CO2 ! (=CH3+CH3OCH3)	=	CH3OCH2+CH3OCHO	0.106E+00	4.214	7527.0	

CH3 + NO	+M =	CH3NO+	M	2.060E+27	-3.5	0.0	!
(BCH3OCH2OMLY)						
CH3NO2	=	CH3+	NO2	1.800E+16	0.0	59000.0	!
(DOUGHTY96)							
CH3O + NO2	=	CH2O+	HONO	6.020E+12	0.0	2285.0	!
(BCH3OCH2OMLY)						
CH3O + NO2	+M =	CH3ONO2+	M	1.400E+30	-4.5	0.0	!
(BCH3OCH2OMLY)						
CH2CHO+ NO2	=	CH2O +	HCO + NO	8.900E+12	0.0	-159.0	!
(91BAR/SAN)						
CH3O + NO	=	CH2O +	HNO	1.000E+13	-0.583	-230.0	! (FIT
NIST 28/4/00<)							
CH3O2+ NO	=	CH3O+	NO2	5.540E+11	0.0	-1192.0	!
(99SCHOLTENS)							
CH3NO2+ O	=	H2CNO2+	OH	1.510E+13	0.0	5350.0	!
(SALTER77)						
CH3NO2+ OH	=	H2CNO2+	H2O	1.490E+13	0.0	5740.0	!
(TRICOT 81)						
CH3NO2+ H	=	H2CNO2+	H2	7.500E+12	0.0	10000.0	!
(BCH3OCH2OMLY)						
CH3NO2+ H	=	HONO+	CH3	3.270E+12	0.0	3730.0	!
(BCH3OCH2OMLY)						
CH3NO2+ H	=	CH3NO+	OH	1.400E+12	0.0	3730.0	!
(BCH3OCH2OMLY)						
CH3NO2+ CH3	=	H2CNO2+	CH4	7.080E+11	0.0	11140.0	!
(BCH3OCH2OMLY)						
CH3NO2+ CH3O	=	H2CNO2+CH3OH		3.000E+11	0.0	7000.0	!
(alzueta99/BALDWIN)							
CH3NO2+ C2H5	=	H2CNO2+ C2H6		3.000E+11	0.0	11700.0	!
(BALDWIN)						
CH3NO2+ HO2	=	H2CNO2+ H2O2		1.500E+11	0.0	15000.0	!
(BALDWIN)						
H2CNO2	=	CH2O+	NO	1.000E+13	0.0	36000.0	!
(BCH3OCH2OMLY)						
H2CNO2+ HONO	=	CH3NO2+	NO2	1.000E+12	0.0	0.0	!
(BCH3OCH2OMLY)						
CH3O + NO	+M =	CH3ONO+	M	2.700E+27	-3.5	0.0	!
(BCH3OCH2OMLY)						
CH3NO2	=	CH3ONO		2.900E+14	0.0	67000.0	!
(BCH3OCH2OMLY)						
CH3OCH2+ NO2	=	CH3OCH2O+	NO	3.000E+13	0.0	0.0	!
! (81YAM/SLA	*2)						
CH3OCH2O + NO2	=	CH3OCHO+	HONO	6.020E+12	0.0	1285.0	!
! (CH3O+NO2 E<)						
CH3OCH2O + NO	=	CH3OCHO+	HNO	2.600E+14	-0.7	0.0	!
! (92ATK/BAU	*2)						
CH3OCH2O2 + NO	=	CH3OCH2O+	NO2	3.500E+12	0.0	-	!
1192.0 ! (99SCHOLTENS >>)						
CH3OCH3 + NO	=	CH3OCH2+	HNO	1.000E+14	0.0	43400.0	!
(63MCK/WOJ)							
NO2+ HCO	=	CO+	NO + OH	0.945E+13	0.0	-430.0	!
(88TIMONEN;B.R.)							
CH3OCH3 + NO2	=	CH3OCH2+	HONO	9.000E+12	0.0	17600.0	!
(=HO2+CH3OCH3 >)							
H2NO+ NO	=	HNO +	HNO	2.000E+07	2.0	13000.0	!
(GLARBORG94)							

HONO+ CH3 = NO2 + CH4 2.140E+17 0.0 19975.0 !
 (97ZHA/BAU)
 HONO+ CH3OCH2O2 = NO2 +CH3OCH2O2H 2.140E+17 0.0
 19975.0 ! (=CH3+HONO)
 HONO+ CH3O2 = NO2+CH3O2H 2.140E+17 0.0 19975.0 !
 (=CH3+HONO)
 C2H5+ HONO = C2H6+ NO2 8.100E+05 1.87 5504.0 ! (
 =ch3/DEAN97)
 C2H3+ HONO = C2H4+ NO2 8.100E+05 1.87 5504.0 ! (
 =ch3/DEAN97)
 CH3O+ HONO = CH3OH+ NO2 8.100E+05 1.87 5504.0 ! (
 =ch3/DEAN97)
 HNO+ HO2 = NO+ H2O2 4.000E+12 0.0 0.0 !
 (28/4/00)
 CH3O + HNO = CH3OH+ NO 3.160E+13 0.0 0.0 !
 (88HE/SAN)

!
 !*****
 !*****pentane+NO coupling*****
 !*****

!
 !NC5H12+NO2=C5H11-1+HONO 1.32E+14 0.0
 31100 !
 !NC5H12+NO2=C5H11-2+HONO 3.48E+13 0.0
 28100 !
 !NC5H12+NO2=C5H11-3+HONO 3.48E+13 0.0
 28100 !

!
 !
 C5H11O-1+NO=PC4H9CHO+HNO +8.01E+11 0 0 !\Analogy of CH3O + NO=
 CH2O+HNO\REF:Kinet. Catal.\Zaslono, I.S.; Mukoseev, Yu.K.; Tyurin, A.N.
 C5H11O-2+NO=NC3H7COCH3+HNO +8.01E+11 0 0 !\Analogy of CH3O + NO=
 CH2O+HNO\REF:Kinet. Catal.\Zaslono, I.S.; Mukoseev, Yu.K.; Tyurin, A.N.
 C5H11O-3+NO=C2H5COC2H5+HNO +8.01E+11 0 0 !\Analogy of CH3O + NO=
 CH2O+HNO\REF:Kinet. Catal.\Zaslono, I.S.; Mukoseev, Yu.K.; Tyurin, A.N.

!
 C5H11O-1+O2=PC4H9CHO+HO2 +6.024E+10 0 1648 !\Analogy of Analogy with
 CH3CH2O + O2=CH3CHO + HO2\REF:J. Phys. Chem. Ref. Data; Baulch, D.L.;
 Cobos, C.J.; Cox, R.A.; Esser, C.; Frank, P.; Just, Th.; Kerr, J.A.;
 Pilling, M.J.; Troe, J.; Walker, R.W.; Warnatz, J.
 C5H11O-2+O2=NC3H7COCH3+HO2 +6.024E+10 0 1648 !\Analogy of Analogy with
 CH3CH2O + O2=CH3CHO + HO2\REF:J. Phys. Chem. Ref. Data; Baulch, D.L.;
 Cobos, C.J.; Cox, R.A.; Esser, C.; Frank, P.; Just, Th.; Kerr, J.A.;
 Pilling, M.J.; Troe, J.; Walker, R.W.; Warnatz, J.
 C5H11O-3+O2=C2H5COC2H5+HO2 +6.024E+10 0 1648 !\Analogy of Analogy with
 CH3CH2O + O2=CH3CHO + HO2\REF:J. Phys. Chem. Ref. Data; Baulch, D.L.;
 Cobos, C.J.; Cox, R.A.; Esser, C.; Frank, P.; Just, Th.; Kerr, J.A.;
 Pilling, M.J.; Troe, J.; Walker, R.W.; Warnatz, J.

!
 !
 C5H11O-1+M=PC4H9CHO+H+M +8.895E+10 0.75 21052 !\Analogy of n-
 C3H7O=C2H5CHO + H\REF:Int. J. Chem. Kinet.\Rate constant estimation for
 C-1 to C-4 alkyl and alkoxy radical decomposition
 C5H11O-2+M=NC3H7COCH3+H+M +8.895E+10 0.75 21052 !\Analogy of n-
 C3H7O=C2H5CHO + H\REF:Int. J. Chem. Kinet.\Rate constant estimation for
 C-1 to C-4 alkyl and alkoxy radical decomposition

C5H11O-3+M=C2H5COC2H5+H+M +8.895E+10 0.75 21052 !\Analogy of n-
C3H7O=C2H5CHO + H\REF:Int. J. Chem. Kinet.\Rate constant estimation for
C-1 to C-4 alkyl and alkoxy radical decomposition

```
!
!
!-----
!--- R + NO2 = RO + NO
!-----
C5H11-1+NO2=C5H11O-1+NO          4.00E+13  -0.2  0    ! ANDERLOHR
C5H11-2+NO2=C5H11O-2+NO          4.00E+13  -0.2  0    !
C5H11-3+NO2=C5H11O-3+NO          4.00E+13  -0.2  0    !
!
!CH3+NO2=NO+CH3O                  1.4E15    0.0    0.0
!SRI05*100 (PRINCE)
C2H5+NO2=NO+C2H5O                 4.00E13   -0.2  0
NC3H7+NO2=NO+NC3H7O               4.00E+13  -0.2  0
IC3H7+NO2=NO+IC3H7O               4.00E+13  -0.2  0
PC4H9+NO2=NO+PC4H9O               4.00E+13  -0.2  0
SC4H9+NO2=NO+SC4H9O               4.00E+13  -0.2  0
!
!-----
!--- RO2 + NO = RO + NO2
!-----
C5H11O2-1+NO=C5H11O-1+NO2        2.53E12   0.00  -358  !
C5H11O2-2+NO=C5H11O-2+NO2        2.53E12   0.00  -358  !
C5H11O2-3+NO=C5H11O-3+NO2        2.53E12   0.00  -358
!
!CH3O2+NO=CH3O+NO2                2.53E12   0.00  -358
C2H5O2+NO=C2H5O+NO2               2.53E12   0.00  -358
IC3H7O2+NO=IC3H7O+NO2             2.53E12   0.00  -358
NC3H7O2+NO=NC3H7O+NO2             2.53E12   0.00  -358
PC4H9O2+NO=PC4H9O+NO2             2.53E12   0.00  -358
SC4H9O2+NO=SC4H9O+NO2             2.53E12   0.00  -358
!
!
!
!-----
!--- OOQOOH+NO=OH+2CH2O+OLEFIN+NO2 (mec PFR_Tol_NOx)
!-----
!
C5H10OOH1-2O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358  !ORIGINAL
C5H10OOH1-2O2+NO=OH+2CH2O+CH2+C2H4+NO2 Modified 1206
C5H10OOH1-3O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
C5H10OOH1-4O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
C5H10OOH1-5O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
!
C5H10OOH2-1O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
C5H10OOH2-3O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
C5H10OOH2-4O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
C5H10OOH2-5O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
!
C5H10OOH3-1O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
C5H10OOH3-2O2+NO=OH+2CH2O+C3H6+NO2  4.70E12   0.0  -358
!
AC5H10OOH-AO2+NO=OH+2CH2O+C3H6+NO2  4.70E+12   0.00  -358.00
AC5H10OOH-BO2+NO=OH+2CH2O+C3H6+NO2  4.70E+12   0.00  -358.00
AC5H10OOH-CO2+NO=OH+2CH2O+C3H6+NO2  4.70E+12   0.00  -358.00
AC5H10OOH-DO2+NO=OH+2CH2O+C3H6+NO2  4.70E+12   0.00  -358.00
```

```

!
BC5H10OOH-AO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
BC5H10OOH-CO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
BC5H10OOH-DO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
!
CC5H10OOH-AO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
CC5H10OOH-BO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
CC5H10OOH-DO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
!
DC5H10OOH-AO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
DC5H10OOH-BO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
DC5H10OOH-CO2+NO=OH+2CH2O+C3H6+NO2      4.70E+12  0.00  -358.00
!
!-----
!--- ALDEHYDE + NO2 = R1 + CO + HONO
!-----
!
CH3CHO+NO2=CH3+CO+HONO                    8.35E-11  6.68  8300
C2H5CHO+NO2=C2H5+CO+HONO                    8.35E-11  6.68  8300
NC3H7CHO+NO2=NC3H7+CO+HONO                  8.35E-11  6.68  8300
IC3H7CHO+NO2=IC3H7+CO+HONO                  8.35E-11  6.68  8300
PC4H9CHO+NO2=PC4H9+CO+HONO                  8.35E-11  6.68  8300
!
!
!CH2O+NO=HCO+HNO                           1.02E13      0.0    40670
HNO+NO2=HNO2+NO                             3.0E11      0.0    1988 !
!HNO+CH3O=CH3OH+NO                          3.16E13      0.0     0.0 !
!
!-----
!--- .Y + NO2=acrolein+R+NO
!-----
!
C4H71-3+NO2=CH3+C2H3CHO+NO                  2.35E+13    0.0     0.0 !
C5H91-3+NO2=C2H5+C2H3CHO+NO                  2.35E+13    0.0     0.0 !
C3H5-A+NO2=H+C2H3CHO+NO                      2.35E+13    0.0     0.0 !
Modified 1206
!
!-----
!--- NO2 + RH=>R.+HONO
!-----
!
!Abstraction of primary H:                    2.2E+13      0.0    31100 !
!Abstraction of secondary H:                  5.8E+12      0.0    28100
!
!Abstraction of tertiary H:                  9.3E+13      0.0    25800
!
!
C4H10+NO2=PC4H9+HONO                         2.2E13      0.0    31100
C4H10+NO2=SC4H9+HONO                         5.8E12      0.0    28100
IC4H10+NO2=IC4H9+HONO                       2.2E13      0.0    31100
IC4H10+NO2=TC4H9+HONO                       9.3E+13     0.0    25800 !
Modified 1206
NC5H12+NO2=C5H11-1+HONO                      2.2E13      0.0    31100 !
Modified 1206
NC5H12+NO2=C5H11-2+HONO                      5.8E12      0.0    31100 !
Modified 1206
NC5H12+NO2=C5H11-3+HONO                      5.8E12      0.0    31100 !
Modified 1206

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!
!
!-----
!--- R.+HNO=> NO + RH
!same kinetics as CH3+HNO=NO+CH4 1.47E11/0.76/349
!-----
!
!CH3+HNO=NO+CH4          1.47E11      0.76      349 !
C2H5+HNO=NO+C2H6        1.47E11      0.76      349 !
NC3H7+HNO=NO+C3H8       1.47E11      0.76      349 !
IC3H7+HNO=NO+C3H8       1.47E11      0.76      349 !
PC4H9+HNO=NO+C4H10      1.47E11      0.76      349 !
SC4H9+HNO=NO+C4H10      1.47E11      0.76      349 !
!
C5H11-1+HNO=NO+NC5H12   1.47E11      0.76      349 !
C5H11-2+HNO=NO+NC5H12   1.47E11      0.76      349 !
C5H11-3+HNO=NO+NC5H12   1.47E11      0.76      349 !
!
!-----
!---R'.+NO2=compound
!Fall off Parameter Fc =0.183
!-----
!
C2H5NO2 (+M)=C2H5+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
NC3H7NO2 (+M)=NC3H7+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
IC3H7NO2 (+M)=IC3H7+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
PC4H9NO2 (+M)=PC4H9+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
SC4H9NO2 (+M)=SC4H9+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
!
C5H11-1NO2 (+M)=C5H11-1+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
C5H11-2NO2 (+M)=C5H11-2+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
C5H11-3NO2 (+M)=C5H11-3+NO2 (+M) 1.8E+16      0.0      58500.0 !
      Low /1.3E+17 0.0 42000./
!
!-----
!\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

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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
!-----

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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:

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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
!-----

!++++
!++++
!++++
!\END_KINETICS_MODULE: \H2_O2
!++++
!++++
!++++
!++++
!++++
!++++
!\KINETICS_MODULE: \C1
!\MODCOMMENTS:
!\MODWARNINGS:
!\MODSUBMECHS: CO, CH2O, CH4,
!++++
!++++
!++++
!-----

!\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

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!=====
=====

!

!\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/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950 !\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

!=====

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!

!\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
!

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!\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?
!

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!\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??
!
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!\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:
!-----
-----

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!

!\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 /


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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

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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 /

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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.

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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
C2H300<=>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
C2H300<=>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
C2H300<=>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 /

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 /

DUP
CHOCHO+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:

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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:

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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:

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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: GUPTA 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
!-----
!-----
!-----
!-----

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!\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: RRKM/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
\N \EA
!

\A

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

!=====

=====

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!=====
=====
!\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

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!-----

!

!\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?
CH3OCHO+OH<=>CH3OCO+H2O
+1.5800000E+007 +1.8000000E+000 +9.3400000E+002 !\AUTHOR: !\REF:ANOLOGY
TO PROPANE !\COMMENT: WARNING: POOR ANALOGY?
CH3OCHO+OH<=>CH2OCHO+H2O
+5.2700000E+009 +9.7000000E-001 +1.5860000E+003 !\AUTHOR: !\REF:ANOLOGY
TO PROPANE !\COMMENT: WARNING: POOR ANALOGY?
CH3OCHO+HO2<=>CH3OCO+H2O2
+4.8200000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:CURRAN
ESTIMATE TSANG '88 PRIMARY H !\COMMENT: WARNING: POOR ANALOGY?
CH3OCHO+HO2<=>CH2OCHO+H2O2
+2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:CURRAN
ESTIMATE TSANG '88 PRIMARY H !\COMMENT: WARNING: POOR ANALOGY?
CH3OCHO+O<=>CH3OCO+OH
+2.7550000E+005 +2.4500000E+000 +2.8300000E+003 !\AUTHOR: !\REF:TSANG,
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:
CH3OCHO+O<=>CH2OCHO+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?

CH3OCHO+H<=>CH3OCO+H2
 +6.5000000E+005 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:TSANG,
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:
 CH3OCHO+H<=>CH2OCHO+H2
 +6.6500000E+005 +2.5400000E+000 +6.7560000E+003 !\AUTHOR: !\REF:TSANG,
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:
 CH3OCHO+CH3<=>CH3OCO+CH4 +7.5500000E-
 001 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.
 CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:
 CH3OCHO+CH3<=>CH2OCHO+CH4 +4.5200000E-
 001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.
 CHEM. REF. DATA 17, 887 (1988) !\COMMENT: WARNING:
 CH3OCHO+CH3O<=>CH3OCO+CH3OH
 +5.4800000E+011 +0.0000000E+000 +5.0000000E+003 !\AUTHOR:
 !\REF:ESTIMATE !\COMMENT: WARNING: HOW WERE THESE ESTIMATED
 CH3OCHO+CH3O<=>CH2OCHO+CH3OH
 +2.1700000E+011 +0.0000000E+000 +6.4580000E+003 !\AUTHOR:
 !\REF:ESTIMATE !\COMMENT: WARNING: HOW WERE THESE ESTIMATED
 CH3OCHO+CH3O2<=>CH3OCO+CH3O2H
 +4.8200000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:ANOLOGY
 WITH HO2 !\COMMENT: WARNING: IS ANALOGY DATED?
 CH3OCHO+CH3O2<=>CH2OCHO+CH3O2H
 +2.3800000E+004 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:ANOLOGY
 WITH HO2 !\COMMENT: WARNING: IS ANALOGY DATED?
 CH3OCHO+HCO<=>CH3OCO+CH2O
 +5.4000000E+006 +1.9000000E+000 +1.7010000E+004 !\AUTHOR: !\REF:TSANG,
 W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
 CH3OCHO+HCO<=>CH2OCHO+CH2O
 +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
 !

CH3OCO<=>CH2OCHO
 +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

$C_3H_8 + NC_3H_7O_2 \rightleftharpoons IC_3H_7 + NC_3H_7O_2H$
+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:
 $C_3H_8 + CH_3CO_3 \rightleftharpoons IC_3H_7 + CH_3CO_3H$
+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:
 $C_3H_8 + O_2CHO \rightleftharpoons IC_3H_7 + HO_2CHO$
+1.4750000E+004 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:ANALOGY
TO $C_2H_6 + HO_2$!\COMMENT:
 $C_3H_8 + IC_3H_7O_2 \rightleftharpoons IC_3H_7 + IC_3H_7O_2H$
+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:
 $C_3H_8 + O_2 \rightleftharpoons NC_3H_7 + HO_2$
+6.0000000E+013 +0.0000000E+000 +5.2290000E+004 !\AUTHOR: !\REF:
ANALOGY WITH $C_4H_{10} + O_2 \rightleftharpoons PC_4H_9 + HO_2$!\COMMENT:
 $C_3H_8 + H \rightleftharpoons NC_3H_7 + H_2$
+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.
 $C_3H_8 + O \rightleftharpoons NC_3H_7 + OH$
+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:
 $C_3H_8 + OH \rightleftharpoons NC_3H_7 + H_2O$
+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:
 $C_3H_8 + HO_2 \rightleftharpoons NC_3H_7 + H_2O_2$
+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:
 $C_3H_8 + CH_3 \rightleftharpoons NC_3H_7 + CH_4$ +9.0400000E-
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:TSANG, W. J. PHYS.
CHEM. REF. DATA 17, 887 (1988) !\COMMENT:
 $C_3H_8 + C_2H_3 \rightleftharpoons NC_3H_7 + C_2H_4$
+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
 $C_3H_8 + C_2H_5 \rightleftharpoons NC_3H_7 + C_2H_6$
+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
 $C_3H_8 + C_3H_5-A \rightleftharpoons NC_3H_7 + C_3H_6$
+7.9400000E+011 +0.0000000E+000 +2.0500000E+004 !\AUTHOR: !\REF:DAGAUT
ET AL., CST 71, 111(1990) !\COMMENT:
 $C_3H_8 + CH_3O \rightleftharpoons NC_3H_7 + CH_3OH$
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:DRYER
ESTIMATE !\COMMENT:
 $C_3H_8 + CH_3O_2 \rightleftharpoons NC_3H_7 + CH_3O_2H$
+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
 $C_3H_8 + C_2H_5O_2 \rightleftharpoons NC_3H_7 + C_2H_5O_2H$
+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

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

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```

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

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```

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:
NC3H7O2+CH2O<=>NC3H7O2H+HCO
+5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY
TO CH2O+HO2 !\COMMENT:
NC3H7O2+CH4<=>NC3H7O2H+CH3
+1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:ANALOGY
TO CH4+HO2 !\COMMENT:
NC3H7O2+CH3OH<=>NC3H7O2H+CH2OH
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:ANALOGY
TO CH3OH+HO2 !\COMMENT:
NC3H7O2+CH3CHO<=>NC3H7O2H+CH3CO
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF
CH2O+HO2 !\COMMENT:
NC3H7O2+C2H4<=>NC3H7O2H+C2H3
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H4+HO2 !\COMMENT:

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NC3H7O2+C2H6<=>NC3H7O2H+C2H5
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE !\COMMENT:
NC3H7O2+C2H3CHO<=>NC3H7O2H+C2H3CO
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF
CH2O+HO2 !\COMMENT:
NC3H7O2+C2H5CHO<=>NC3H7O2H+C2H5CO
+2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE !\COMMENT:
!=====
=====
!\ENDSUBSPECIES: \NC3H7O2H
!=====
=====
!

!\REACTIONCLASS: \RO2_R_PRODUCTS \A
\N \EA
!

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

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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 /

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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 /

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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?

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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:

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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 /

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 /

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:
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 /
C3H5-A+CH3O2<=>AC4H7OOH
+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 /

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
!!=====
=====
!!\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<=>TQC3H5OHIQ-I 2.56E+12 -0.13 34360 !\AUTHOR: !\ C ZHOU
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!TQC3H5OHIQ-I<=>HO2CHO+CH3CHO+OH 5.819E+05 2.40 22790 !\AUTHOR: !\ C ZHOU
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!TQC3H5OHIQ-I<=>C3KET12+HO2 1.829E+10 0.790 15100 !\AUTHOR: !\ C ZHOU
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!TQC3H5OHIO2<=>TQC3H5OHIQ-P 5.69E+08 7.80E-01 21850 !\AUTHOR: !\ C ZHOU
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!TQC3H5OHIQ-P<=>C2H3COHOOH+HO2 1.83E+10 7.90E-01 15100 !\AUTHOR: !\ C
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION

!\COMMENT:

!TQC3H5OHIQ-P<=>C2H3OOH+HOCHO+OH 5.38E+11 0.070 24800 !\AUTHOR: !\ C ZHOU
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:

!TQC3H5OHIQ-P<=>COHOHCY(COC)+OH 2.28E+08 1.29E+00 9890 !\AUTHOR: !\ C
ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION

!\COMMENT:

!TQC3H5OHIQ-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<=>CHOCOHCH2OOH+OH 1.2E+10 0.35 15700 !\AUTHOR: !\ C ZHOU
ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION !\COMMENT:
!CHOCOHCH2OOH=>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 \A
\N \EA
!

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 /

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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.

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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

!\MODSUBMECHS:

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

!\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:ANALOGY
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:

$C_4H_{10} + C_3H_5 - A \rightleftharpoons PC_4H_9 + C_3H_6$
+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:

$C_4H_{10} + NC_3H_7O_2 \rightleftharpoons PC_4H_9 + NC_3H_7O_2H$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C₂H₆+HO₂ !\COMMENT:

$C_4H_{10} + IC_3H_7O_2 \rightleftharpoons PC_4H_9 + IC_3H_7O_2H$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C₂H₆+HO₂ !\COMMENT:

$C_4H_{10} + PC_4H_9 \rightleftharpoons SC_4H_9 + C_4H_{10}$
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:
WESTBROOK AND PITZ ESTIMATE (1983) !\COMMENT:

$C_4H_{10} + PC_4H_9O_2 \rightleftharpoons PC_4H_9 + PC_4H_9O_2H$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C₂H₆+HO₂ !\COMMENT:

$C_4H_{10} + SC_4H_9O_2 \rightleftharpoons PC_4H_9 + SC_4H_9O_2H$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C₂H₆+HO₂ !\COMMENT:

$C_4H_{10} + IC_4H_9O_2 \rightleftharpoons PC_4H_9 + IC_4H_9O_2H$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C₂H₆+HO₂ !\COMMENT:

$C_4H_{10} + TC_4H_9O_2 \rightleftharpoons PC_4H_9 + TC_4H_9O_2H$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C₂H₆+HO₂ !\COMMENT:

$C_4H_{10} + H \rightleftharpoons SC_4H_9 + H_2$
+2.6000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:TSANG,
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:

$C_4H_{10} + O_2 \rightleftharpoons SC_4H_9 + HO_2$
+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:

$C_4H_{10} + O \rightleftharpoons SC_4H_9 + OH$
+5.6200000E+013 +0.0000000E+000 +5.2000000E+003 !\AUTHOR:
!\REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705 (1983)
!\COMMENT:

$C_4H_{10} + OH \rightleftharpoons SC_4H_9 + H_2O$
+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:

$C_4H_{10} + HO_2 \rightleftharpoons SC_4H_9 + H_2O_2$
+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:

$C_4H_{10} + CH_3 \rightleftharpoons SC_4H_9 + CH_4$
+3.0200000E+000 +3.4600000E+000 +5.4810000E+003 !\AUTHOR: !\REF:TSANG,
W. J. PHYS. CHEM. REF. DATA 17, 887 (1988) !\COMMENT:

$C_4H_{10} + CH_3O \rightleftharpoons SC_4H_9 + CH_3OH$
+6.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:DRYER
ESTIMATE !\COMMENT:

$C_4H_{10} + CH_3O_2 \rightleftharpoons SC_4H_9 + CH_3O_2H$
+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

$C_4H_{10} + O_2CHO \rightleftharpoons SC_4H_9 + HO_2CHO$
+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
J. Curran International Journal of Chemical Kinetics (2006) 38: 250-275.
!\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:

$PC4H9O2+CH4 \rightleftharpoons PC4H9O2H+CH3$
+1.1200000E+013 +0.0000000E+000 +2.4640000E+004 !\AUTHOR: !\REF:ANALOGY
TO CH4+HO2 !\COMMENT:
 $PC4H9O2+CH3OH \rightleftharpoons PC4H9O2H+CH2OH$
+6.3000000E+012 +0.0000000E+000 +1.9360000E+004 !\AUTHOR: !\REF:ANALOGY
TO CH3OH+HO2 !\COMMENT:
 $PC4H9O2+CH2O \rightleftharpoons PC4H9O2H+HCO$
+5.6000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:ANALOGY
TO CH2O+HO2 !\COMMENT:
 $PC4H9O2+C2H6 \rightleftharpoons PC4H9O2H+C2H5$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE !\COMMENT:
 $PC4H9O2+CH3CHO \rightleftharpoons PC4H9O2H+CH3CO$
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF
CH2O+HO2 !\COMMENT:
 $PC4H9O2+C2H4 \rightleftharpoons PC4H9O2H+C2H3$
+1.1300000E+013 +0.0000000E+000 +3.0430000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H4+HO2 !\COMMENT:
 $PC4H9O2+C3H6 \rightleftharpoons PC4H9O2H+C3H5-A$ +5.3500000E-
002 +4.2070000E+000 +1.3288100E+004 !\AUTHOR: !\REF:ANALOGY TO C3H6+HO2
!\COMMENT:
 $PC4H9O2+C2H5CHO \rightleftharpoons PC4H9O2H+C2H5CO$
+2.0000000E+011 +0.0000000E+000 +9.5000000E+003 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE !\COMMENT:
 $PC4H9O2+C2H3CHO \rightleftharpoons PC4H9O2H+C2H3CO$
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:HALF OF
CH2O+HO2 !\COMMENT:
 $PC4H9O2+C3H8 \rightleftharpoons PC4H9O2H+NC3H7$
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:
 $PC4H9O2+C3H8 \rightleftharpoons PC4H9O2H+IC3H7$
+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
!

$PC4H9O2+CH3 \rightleftharpoons PC4H9O+CH3O$
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
 $PC4H9O2+C2H5 \rightleftharpoons PC4H9O+C2H5O$
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
 $PC4H9O2+IC3H7 \rightleftharpoons PC4H9O+IC3H7O$
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
 $PC4H9O2+NC3H7 \rightleftharpoons PC4H9O+NC3H7O$
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
 $PC4H9O2+C3H5-A \rightleftharpoons PC4H9O+C3H5O$
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
 $PC4H9O2+PC4H9 \rightleftharpoons PC4H9O+PC4H9O$
+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
!

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```

PC4H9O2H<=>PC4H9O+OH
+1.5000000E+016 +0.0000000E+000 +4.2500000E+004    !\AUTHOR:
!\REF:ESTIMATE !\COMMENT:
!

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```

!\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:

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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:
!-----

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!\REACTIONCLASS: \QOOH+O2_PRODUCTS \A
\N \EA
!

 $C_4H_8OOH_1-2+O_2 \rightleftharpoons C_4H_8OOH_1-2O_2$
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_1-3+O_2 \rightleftharpoons C_4H_8OOH_1-3O_2$
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_1-4+O_2 \rightleftharpoons C_4H_8OOH_1-4O_2$
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_2-1+O_2 \rightleftharpoons C_4H_8OOH_2-1O_2$
+3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_2-3+O_2 \rightleftharpoons C_4H_8OOH_2-3O_2$
+1.7440000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_2-4+O_2 \rightleftharpoons C_4H_8OOH_2-4O_2$
+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
!

 $C_4H_8OOH_1-2O_2 \rightleftharpoons C_4H_7_2-1OOH+HO_2$
+2.5400000E+010 +8.0400000E-001 +3.0098500E+004 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_1-3O_2 \rightleftharpoons C_4H_7_1-4OOH+HO_2$
+5.1300000E+009 +1.0000000E+000 +3.0400000E+004 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_1-3O_2 \rightleftharpoons C_4H_7_2-1OOH+HO_2$
+2.5400000E+010 +8.0400000E-001 +3.0098500E+004 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_1-4O_2 \rightleftharpoons C_4H_7_1-4OOH+HO_2$
+1.4400000E+007 +1.3800000E+000 +2.8900000E+004 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_2-3O_2 \rightleftharpoons C_4H_7_1-3OOH+HO_2$
+5.1300000E+009 +1.0000000E+000 +3.0400000E+004 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_2-4O_2 \rightleftharpoons C_4H_7_1-3OOH+HO_2$
+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
!

 $C_4H_8OOH_1-2O_2 \rightleftharpoons C_4H_7_1-3,4OOH$
+1.4400000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:Miyoshi
A/2 compared to R+O2 080415A !\COMMENT:
 $C_4H_8OOH_1-2O_2 \rightleftharpoons C_4H_7_2-3,4OOH$
+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:OEHLSCHLAEGER 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:OEHLSCHLAEGER 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:OEHLSCHLAEGER 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:

$\text{IC4H10} + \text{C2H5} \rightleftharpoons \text{IC4H9} + \text{C2H6}$
+1.5100000E+012 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:ALLARA
AND SHAW ANALOG !\COMMENT:

$\text{IC4H10} + \text{HO2} \rightleftharpoons \text{IC4H9} + \text{H2O2}$
+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:

$\text{IC4H10} + \text{O} \rightleftharpoons \text{IC4H9} + \text{OH}$
+4.0460000E+007 +2.0340000E+000 +5.1360000E+003 !\AUTHOR: !\REF:NIST
STANDARD REFERENCE DATABASE 17 -2Q98 !\COMMENT:

$\text{IC4H10} + \text{CH3O} \rightleftharpoons \text{IC4H9} + \text{CH3OH}$
+4.8000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:ANALOGY
TO C3H8+CH3O !\COMMENT:

$\text{IC4H10} + \text{O2} \rightleftharpoons \text{IC4H9} + \text{HO2}$
+9.0000000E+013 +0.0000000E+000 +5.2290000E+004 !\AUTHOR: !\REF:
ANALOGY WITH C4H10+O2<=>PC4H9+HO2 !\COMMENT:

$\text{IC4H10} + \text{CH3O2} \rightleftharpoons \text{IC4H9} + \text{CH3O2H}$
+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:

$\text{IC4H10} + \text{C2H5O2} \rightleftharpoons \text{IC4H9} + \text{C2H5O2H}$
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:SCOTT
AND WALKER C&F 129(4) 365--377 2002 (*1.5) !\COMMENT:

$\text{IC4H10} + \text{CH3CO3} \rightleftharpoons \text{IC4H9} + \text{CH3CO3H}$
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{NC3H7O2} \rightleftharpoons \text{IC4H9} + \text{NC3H7O2H}$
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{IC3H7O2} \rightleftharpoons \text{IC4H9} + \text{IC3H7O2H}$
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{IC4H9O2} \rightleftharpoons \text{IC4H9} + \text{IC4H9O2H}$
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{TC4H9O2} \rightleftharpoons \text{IC4H9} + \text{TC4H9O2H}$
+2.5500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{O2CHO} \rightleftharpoons \text{IC4H9} + \text{HO2CHO}$
+2.5200000E+013 +0.0000000E+000 +2.0440000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{SC4H9O2} \rightleftharpoons \text{IC4H9} + \text{SC4H9O2H}$
+2.2500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{SC4H9O2} \rightleftharpoons \text{TC4H9} + \text{SC4H9O2H}$
+2.8000000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:WALKER,
R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988
!\COMMENT:

$\text{IC4H10} + \text{PC4H9O2} \rightleftharpoons \text{IC4H9} + \text{PC4H9O2H}$
+2.2500000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:ANALOGY
TO C2H6+HO2 !\COMMENT:

$\text{IC4H10} + \text{H} \rightleftharpoons \text{TC4H9} + \text{H2}$
+6.0200000E+005 +2.4000000E+000 +2.5830000E+003 !\AUTHOR: !\REF:TSANG,
J. PHYS. CHEM. REF. DATA 19, 1-68 (1990) !\COMMENT:

$\text{IC4H10} + \text{CH3} \rightleftharpoons \text{TC4H9} + \text{CH4}$ +9.0400000E-
001 +3.4600000E+000 +4.5980000E+003 !\AUTHOR: !\REF:TSANG, J. PHYS.
CHEM. REF. DATA 19, 1-68 (1990) !\COMMENT:

IC4H10+OH<=>TC4H9+H2O
+2.9250000E+004 +2.5310000E+000 -1.6590000E+003 !\AUTHOR: !\REF:JOE
MICHAELS SYMP. PAPER 2008. !\COMMENT:
IC4H10+C2H5<=>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:

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!
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!\REACTIONCLASS:  \R_ISOMERISATION                \A
\N                \EA
!
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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:
!
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!\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:

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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:

!=====

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!\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+H2O2 +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+H2O2 +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
 \N \EA

\A

!

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<=>IC4H9O2H+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<=>IC4H7OOCH3

+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 /

IC4H7OOCH3<=>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
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 /

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
!

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!\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 /

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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 /

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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 /

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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+H2O2 +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+H2O2 +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+H2O2 +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+H2O2 +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_ABSORPTION \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+H2O +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

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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) 905-917
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) 905-917
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) 905-917
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, 2549-2556 !\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, 2549-2556 !\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, 2549-2556 !\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, 2549-2556 !\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+H2O +7.8200000E-
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF:Judit Zador,Stephen
J. Klippenstein,and James A. Miller J. Phys. Chem. A 2011, 115,
10218◆C10225 !\COMMENT: *2
C4H8-2+HO2<=>C4H71-3+H2O +6.9000000E-
001 +4.0000000E+000 +1.2103000E+004 !\AUTHOR: !\REF:Judit Zador,Stephen
J. Klippenstein,and James A. Miller J. Phys. Chem. A 2011, 115,
10218◆C10225 !\COMMENT: *2
C4H8-1+HO2<=>C4H71-4+H2O
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:ANALOGY
WITH C4H10+HO2<=>PC4H9+H2O
C4H8-1+HO2<=>C4H71-1+H2O
+9.5700000E+002 +3.0590000E+000 +2.0798600E+004 !\AUTHOR: !\REF:ANALOGY
WITH C3H6+HO2
C4H8-1+HO2<=>C4H71-2+H2O
+1.5600000E+004 +2.8200000E+000 +2.4427900E+004 !\AUTHOR: !\REF:ANALOGY
WITH C3H6+HO2
C4H8-2+HO2<=>C4H72-2+H2O
+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
C4H8-2+O2<=>C4H71-3+HO2
+2.0000000E+014 +0.0000000E+000 +3.9390000E+004 !\AUTHOR: !\REF:IN
ARAMCO !*5
C4H8-1+O2<=>C4H71-1+HO2
+2.0000000E+013 +0.0000000E+000 +6.2270000E+004 !\AUTHOR: !\REF:
ANALOGY WITH C3H6+O2
C4H8-1+O2<=>C4H71-2+HO2
+1.0000000E+013 +0.0000000E+000 +5.8770000E+004 !\AUTHOR: !\REF:
ANALOGY WITH C3H6+O2
C4H8-2+O2<=>C4H72-2+HO2
+2.0000000E+013 +0.0000000E+000 +5.8770000E+004 !\AUTHOR: !\REF:
ANALOGY WITH C3H6+O2 !*2
C4H8-1+O2<=>C4H71-4+HO2
+6.0000000E+013 +0.0000000E+000 +5.2340000E+004 !\AUTHOR: !\REF:
ANALOGY WITH C4H10+O2<=>PC4H9+HO2
C4H8-1+CH3<=>C4H71-3+CH4
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:IN
ARAMCO (TSANG '91)
C4H8-1+CH3<=>C4H71-4+CH4 +4.5200000E-
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:IN ARAMCO (TSANG
'91)
C4H8-2+CH3<=>C4H71-3+CH4
+7.1400000E+000 +3.5700000E+000 +7.6420000E+003 !\AUTHOR: !\REF:IN
ARAMCO (TSANG '91)
C4H8-1+CH3<=>C4H71-1+CH4
+1.3480000E+000 +3.5000000E+000 +1.2850000E+004 !\AUTHOR: !\REF:ANALOGY
WITH C3H6+CH3
C4H8-1+CH3<=>C4H71-2+CH4 +8.4000000E-
001 +3.5000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:ANALOGY WITH
C3H6+CH3
C4H8-2+CH3<=>C4H72-2+CH4
+1.6800000E+000 +3.5000000E+000 +1.1660000E+004 !\AUTHOR: !\REF:ANALOGY
WITH C3H6+CH3 !*2
C4H8-1+CH3O2<=>C4H71-3+CH3O2H
+2.7000000E+004 +7.0000000E-001 +5.8840000E+003 !\AUTHOR: !\REF:IN
ARAMCO (TSANG '91)
C4H8-1+CH3O2<=>C4H71-4+CH3O2H
+2.3800000E+003 +2.5500000E+000 +1.6490000E+004 !\AUTHOR: !\REF:IN
ARAMCO (TSANG '91)
C4H8-1+CH3O<=>C4H71-3+CH3OH
+4.0000000E+001 +2.9000000E+000 +8.6090000E+003 !\AUTHOR: !\REF:IN
ARAMCO (TSANG '91)

C4H8-1+CH3O<=>C4H71-4+CH3OH
+2.1700000E+011 +0.0000000E+000 +6.4580000E+003 !\AUTHOR: !\REF:IN
ARAMCO (TSANG '91)

C4H8-2+CH3O<=>C4H71-3+CH3OH
+1.8000000E+001 +2.9500000E+000 +1.1990000E+004 !\AUTHOR: !\REF:IN
ARAMCO (ESTIMATE)

C4H8-1+CH3CO3<=>C4H71-3+CH3CO3H
+1.0000000E+011 +0.0000000E+000 +8.0000000E+003 !\AUTHOR: !\REF:IN
ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))

C4H8-1+C3H5-A<=>C4H71-3+C3H6
+7.9000000E+010 +0.0000000E+000 +1.2400000E+004 !\AUTHOR: !\REF:IN
ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))

C4H8-1+C2H5O2<=>C4H71-3+C2H5O2H
+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 +5.6200000E-
012 +7.1900000E+000 +3.6200822E+004 !\AUTHOR: !\REF:YANG CALCULATIONS
C4H71-3<=>C4H72-2 +6.7600000E-
023 +1.0210000E+001 +4.1574211E+004 !\AUTHOR: !\REF:YANG CALCULATIONS

!

!\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 /

C4H72-100H<=>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<=>C4H72-1OOCH3
 +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: 250C275, 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: 250C275, 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: 250C275, 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: 250C275, 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: 250C275, 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: 250C275, 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:
C4H71-4O2+C2H3CHO<=>C4H71-4OOH+C2H3CO
+2.8000000E+012 +0.0000000E+000 +1.3600000E+004 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+C3H8<=>C4H71-4OOH+NC3H7
+1.7000000E+013 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+C3H8<=>C4H71-4OOH+IC3H7
+2.0000000E+012 +0.0000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+CH3<=>C4H7O1-4+CH3O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+C2H5<=>C4H7O1-4+C2H5O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+IC3H7<=>C4H7O1-4+IC3H7O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+NC3H7<=>C4H7O1-4+NC3H7O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+C3H5-A<=>C4H7O1-4+C3H5O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+PC4H9<=>C4H7O1-4+PC4H9O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+SC4H9<=>C4H7O1-4+SC4H9O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+C4H71-3<=>C4H7O1-4+C4H71-O
+7.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4OOH<=>C4H7O1-4+OH
+1.5000000E+016 +0.0000000E+000 +4.2500000E+004 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+CH3O2=>C4H7O1-4+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H71-4O2+CH3CO3=>C4H7O1-4+CH3CO2+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:

$C_4H_7-4O_2+C_2H_5O_2 \Rightarrow C_4H_7O_1-4+C_2H_5O+O_2$
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_7-4O_2+NC_3H_7O_2 \Rightarrow C_4H_7O_1-4+NC_3H_7O+O_2$
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_7-4O_2+IC_3H_7O_2 \Rightarrow C_4H_7O_1-4+IC_3H_7O+O_2$
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_7-4O_2+C_4H_7-4O_2 \Rightarrow C_4H_7O_1-4+C_4H_7O_1-4+O_2$
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_7-4O_2+SC_4H_9O_2 \Rightarrow C_4H_7O_1-4+SC_4H_9O+O_2$
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_7-4O_2 \rightleftharpoons C_4H_6-3OOH_4$
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_6-3OOH_4 \rightleftharpoons C_2H_3CHOCH_2+OH$
+1.7100000E+009 +1.0600000E+000 +1.0900000E+004 !\AUTHOR: !\REF:
!\COMMENT:
 $C_4H_6-3OOH_4 \rightleftharpoons C_4H_6O_2_5+OH$
+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:

C4H6O25+CH3O2<=>CH2CHCHCHO+CH3O2H
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR: !\REF:
!\COMMENT:
C4H61-3OOH4+HO2<=>C4H6O1-3OOH4+OH
+4.1000000E+003 +2.7400000E+000 +1.1444000E+003 !\AUTHOR: !\REF:ANALOGY
TO C4H71-3+HO2 ADDITION, FOLLOWED BY WDM
C4H61-3OOH4+HO2<=>C4H6O2-1OOH4+OH
+4.1000000E+003 +2.7400000E+000 +1.1444000E+003 !\AUTHOR: !\REF:ANALOGY
TO C4H71-3+HO2 ADDITION, FOLLOWED BY WDM
C4H6O1-3OOH4<=>C2H3CHO+CH2O+OH
+6.7000000E+039 -8.3800000E+000 +2.2782000E+004 !\AUTHOR: !\REF:ANALOGY
TO C4H71-3+HO2 ADDITION, FOLLOWED BY WDM
C4H6O1-3OOH4<=>C2H3+HO2CH2CHO
+2.6700000E+034 -6.6300000E+000 +2.2672000E+004 !\AUTHOR: !\REF:ANALOGY
TO C4H71-3+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 /

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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 /

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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 /

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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 \A
\N \EA
!

C4H71-1OH+H<=>PC4H8OH-1
+4.2679497E+012 +4.9275069E-001 +4.4445766E+003 !\AUTHOR: !\REF:J.
ZA?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? 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?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C4H71-2OH+H<=>SC4H8OH-2
+1.4000000E+008 +1.5155021E+000 +2.1884142E+002 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C2H5COCH3+H<=>SC4H8OH-2
+7.0000000E+007 +1.8013421E+000 +1.3223122E+004 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C4H8-1+OH<=>SC4H8OH-1
+7.0000000E+005 +1.8018819E+000 -3.2902438E+003 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526 !\COMMENT !*2*0.25
C2H3OH+C2H5<=>SC4H8OH-1
+6.4000000E+006 +1.6708958E+000 +1.0270243E+004 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C4H8-2+OH<=>SC4H8OH-3
+1.4000000E+006 +1.8018819E+000 -3.2902438E+003 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526 !\COMMENT !*2*0.25*2
SC3H5OH+CH3<=>SC4H8OH-3
+6.4000000E+006 +1.6708958E+000 +1.0270243E+004 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C2H5COCH3+H<=>SC4H9O
+2.7000000E+007 +1.7563257E+000 +6.2061519E+003 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C2H5CHO+CH3<=>SC4H9O
+1.2000000E+004 +2.2838256E+000 +7.9781023E+003 !\AUTHOR: !\REF:J.

ZA?? DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34
(2013) 519?C526
C4H71-4OH+OH<=>C4H64,2-1OH+H2O
+2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: !\REF:ANALOGY
WITH C4H8-1+OH

C4H71-4OH+HO2<=>C4H64,2-1OH+H2O2 +3.9100000E-
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF:ANALOGY WITH C4H8-
1+OH
!

!\REACTIONCLASS: \PC4H8OH-2_O2_PRODUCTS \A
\N \EA
!

PC4H8OH-2+O2<=>PC4H8OH-2O2
+3.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: H.
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PC4H8OH-2O2<=>SQC4H8OP
+2.9100000E+012 -2.2600000E-001 +2.2300000E+004 !\AUTHOR: !\REF: H.
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PC4H8OH-2O2<=>C4H72-1OH+HO2
+3.6400000E+014 -7.1100000E-001 +3.2710000E+004 !\AUTHOR: !\REF: H.
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PC4H8OH-2O2<=>C4H71-1OH+HO2
+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+H2O +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+H2O +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+H2O +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) 2028-2055
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) 2028-2055
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) 2028-2055

$C_4H_5OH-13 \rightleftharpoons C_2H_3+CH_2CHO$
+2.8160000E+024 -2.3810000E+000 +9.0130000E+004 !\AUTHOR: !\REF:S.M.
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028-2055
 $NC_4KET21OH+OH \rightleftharpoons C_2H_4COCH_2OH+H_2O$
+8.4500000E+011 +0.0000000E+000 -2.2800000E+002 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+HO_2 \rightleftharpoons C_2H_4COCH_2OH+H_2O_2$
+2.0000000E+011 +0.0000000E+000 +8.6980000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+O \rightleftharpoons C_2H_4COCH_2OH+OH$
+3.0700000E+013 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+H \rightleftharpoons C_2H_4COCH_2OH+H_2$
+4.4600000E+006 +2.0000000E+000 +3.2000000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+O_2 \rightleftharpoons C_2H_4COCH_2OH+HO_2$
+1.5500000E+013 +0.0000000E+000 +4.1970000E+004 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+CH_3 \rightleftharpoons C_2H_4COCH_2OH+CH_4$
+1.7400000E+000 +3.4600000E+000 +3.6800000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+CH_3O \rightleftharpoons C_2H_4COCH_2OH+CH_3OH$
+1.4500000E+011 +0.0000000E+000 +2.7710000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+CH_3O_2 \rightleftharpoons C_2H_4COCH_2OH+CH_3O_2H$
+2.0000000E+012 +0.0000000E+000 +1.5250000E+004 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+C_2H_3 \rightleftharpoons C_2H_4COCH_2OH+C_2H_4$
+3.0000000E+011 +0.0000000E+000 +3.4000000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $NC_4KET21OH+C_2H_5 \rightleftharpoons C_2H_4COCH_2OH+C_2H_6$
+3.0000000E+010 +0.0000000E+000 +8.6000000E+003 !\AUTHOR: !\REF:ANALOGY
WITH C₂H₅COCH₃ REACTIONS
 $C_2H_4COCH_2OH \rightleftharpoons CH_3CHCO+CH_2OH$
+9.4400000E+029 -4.9300000E+000 +3.8330000E+004 !\AUTHOR: !\REF:ANALOGY
WITH SC₄H₉ \rightleftharpoons C₃H₆+CH₃
PC₄H₈OH-2O₂ \rightleftharpoons SQC₄H₇OHP-4
+1.4390000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:SHARMA
SQC₄H₇OHP-4 \rightleftharpoons CY(CCCO)COH+OH
+2.4400000E+009 +7.8000000E-001 +1.8000000E+004 !\AUTHOR: !\REF:VILLANO
(FROM KUIWEN'S MECH)
SQC₄H₇OHP-4 \rightarrow OH+HOCH₂CHO+C₂H₄
+3.0800000E+008 +1.5000000E+000 +2.3500000E+004 !\AUTHOR: !\REF:VILLANO
(FROM KUIWEN'S MECH)
CY(CCCO)COH+H \rightarrow C₂H₄+HOCH₂CO+H₂
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CY(CCCO)COH+O \rightarrow C₂H₄+HOCH₂CO+OH
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CY(CCCO)COH+OH \rightarrow C₂H₄+HOCH₂CO+H₂O
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CY(CCCO)COH+HO₂ \rightarrow 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.
SC4H8OH-1O2<=>PQC4H8OS
+9.3000000E+010 -3.6000000E-002 +2.2890000E+004 !\AUTHOR: !\REF: H.
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
SC4H8OH-1O2<=>NC4KET12OH+OH
+1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PQC4H8OS=>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.
PQC4H8OS=>C2H5+HO2CH2CHO
+2.6700000E+034 -6.6300000E+000 +2.2672000E+004 !\AUTHOR: !\REF: H.
SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
SC4H8OH-1O2<=>C4H71-2OH+HO2
+2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR:
!\REF:DIFFERENT FROM IC4H8 SYSTEM (ANALOGY WITH PC4H8OH-2 SYSTEM)
SC4H8OH-1O2<=>PQC4H7OHS-3
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:SHARMA
PQC4H7OHS-3<=>CCY(COCC)OH+OH
+2.5900000E+009 +6.9000000E-001 +1.6000000E+004 !\AUTHOR: !\REF:VILLANO
(FROM KUIWEN'S MECH)
PQC4H7OHS-3=>OH+CH2O+SC3H5OH
+1.2300000E+009 +1.3000000E+000 +2.4900000E+004 !\AUTHOR: !\REF:VILLANO
(FROM KUIWEN'S MECH)
C4H71-2OH+OH<=>C4H63,1-2OH+H2O
+2.0200000E+006 +2.2000000E+000 -4.3720000E+002 !\AUTHOR: !\REF:ANALOGY
WITH C4H8-1+OH
C4H71-2OH+HO2<=>C4H63,1-2OH+H2O +3.9100000E-
001 +3.9700000E+000 +1.1702000E+004 !\AUTHOR: !\REF:ANALOGY WITH C4H8-
1+OH
C4H63,1-2OH<=>C4H612+OH
+7.0350000E+016 -1.0120000E+000 +3.6070000E+004 !\AUTHOR: !\REF:S.M.
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028-2055
NC4KET12OH+H<=>C2H5CHOHCO+H2
+1.0000000E+005 +2.5800000E+000 +1.2200000E+003 !\AUTHOR: !\REF:M.
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265-286.

$\text{NC4KET12OH+OH} \rightleftharpoons \text{C2H5CHOHCO+H2O}$
+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.

$\text{NC4KET12OH+O2} \rightleftharpoons \text{C2H5CHOHCO+HO2}$
+9.0300000E+013 +0.0000000E+000 +4.3320000E+004 !\AUTHOR: !\REF:M.
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265 C286.

$\text{NC4KET12OH+C2H3} \rightleftharpoons \text{C2H5CHOHCO+C2H4}$
+3.2560000E+005 +2.0000000E+000 +3.9656900E+003 !\AUTHOR: !\REF:M.
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265 C286.

$\text{NC4KET12OH+C2H5O} \rightleftharpoons \text{C2H5CHOHCO+C2H5OH}$
+6.0300000E+011 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:M.
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265 C286.

$\text{C2H5CHOHCO} \rightleftharpoons \text{C3H6OH1-1+CO}$
+5.7800000E+014 +0.0000000E+000 +1.6843510E+004 !\AUTHOR: !\REF:M.
PELUCCHI ET AL. COMBUSTION AND FLAME (2015) 162(2) 265 C286.

$\text{C3H6OH1-1} \rightleftharpoons \text{C2H5CHO+H}$
+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.

$\text{C2H3OH+CH3} \rightleftharpoons \text{C3H6OH1-1}$
+2.0400000E+040 -8.2500000E+000 +2.4214000E+004 !\AUTHOR: !\REF:ANALOGY
WITH $\text{C2H4+CH3} \rightleftharpoons \text{NC3H7}$
DUP

$\text{C2H3OH+CH3} \rightleftharpoons \text{C3H6OH1-1}$
+1.6600000E+021 -3.1700000E+000 +1.0241000E+004 !\AUTHOR: !\REF:ANALOGY
WITH $\text{C2H4+CH3} \rightleftharpoons \text{NC3H7}$
DUP

$\text{CCY(COCC)OH+H} \Rightarrow \text{OH+C2H3COCH3+H2}$
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+O} \Rightarrow \text{OH+C2H3COCH3+OH}$
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+OH} \Rightarrow \text{OH+C2H3COCH3+H2O}$
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+HO2} \Rightarrow \text{OH+C2H3COCH3+H2O2}$
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE

CCY (COCC) OH+CH3=>OH+C2H3COCH3+CH4
+2.0000000E+011 +0.0000000E+000 +1.0000000E+004 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CCY (COCC) OH+CH3O2=>OH+C2H3COCH3+CH3O2H
+1.0000000E+013 +0.0000000E+000 +1.9000000E+004 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CCY (COCC) OH+H=>OH+SC3H5CHO+H2
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CCY (COCC) OH+O=>OH+SC3H5CHO+OH
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CCY (COCC) OH+OH=>OH+SC3H5CHO+H2O
+5.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CCY (COCC) OH+HO2=>OH+SC3H5CHO+H2O2
+1.0000000E+013 +0.0000000E+000 +1.5000000E+004 !\AUTHOR:
!\REF:WESTBROOK ESTIMATE
CCY (COCC) OH+CH3=>OH+SC3H5CHO+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.
 C4H7O2-1,3OOH=>C3KET12+CH2O+OH
 +5.3600000E+012 -8.0000000E-002 +1.0790000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 C4H7O2-1,3OOH=>HO2CH2CHO+CH3CHO+OH
 +6.7000000E+039 -8.3800000E+000 +2.2782000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 PQC4H7OHS-3O2<=>NC4KET24OH-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<=>CHOCHO+OH +1.4600000E-
 003 +4.7300000E+000 +1.7270000E+003 !\AUTHOR: !\REF:ANALOGY WITH
 C2H5OH+OH<=>C2H5O+H2O
 HOCHCHO+OH<=>CHOCHO+H2O +5.8100000E-
 003 +4.2800000E+000 -3.5600000E+003 !\AUTHOR: !\REF:ANALOGY WITH
 C2H5OH+OH<=>C2H5O+H2O
 HOCHCHO+H<=>CHOCHO+H2
 +9.4500000E+002 +3.1400000E+000 +8.7011000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H5OH+OH<=>C2H5O+H2O
 HOCHCHO+HO2<=>CHOCHO+H2O2 +6.4700000E-
 007 +5.3000000E+000 +1.0533100E+004 !\AUTHOR: !\REF:ANALOGY WITH
 C2H5OH+OH<=>C2H5O+H2O
 HOCHCHO+CH3<=>CHOCHO+CH4
 +2.0350000E+000 +3.5700000E+000 +7.7210000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H5OH+OH<=>C2H5O+H2O
 HOCHCHO+CH3O2<=>CHOCHO+CH3O2H +3.2360000E-
 007 +5.3000000E+000 +1.0533100E+004 !\AUTHOR: !\REF:ANALOGY WITH
 C2H5OH+OH<=>C2H5O+H2O
 C4H6OHOOH1-3-4=>CH2O+PC3H4OH-3+OH
 +1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:Miyoshi
 A/2 compared to R+O2
 C4H6OHOOH2-2-1=>CH2O+PC3H4OH-1+OH
 +1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:Miyoshi
 A/2 compared to R+O2
 NC4KET24OH-3=>CH2O+CH3COCHOH+OH
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:Miyoshi
 A/2 compared to R+O2

$\text{PC3H4OH-3} \rightleftharpoons \text{C2H3CHO+H}$
 +5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{PC3H4OH-3} \rightleftharpoons \text{C3H5O}$
 +5.4800000E+045 -1.1630000E+001 +4.4328000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{PC3H4OH-3} \rightleftharpoons \text{CH2CCH2OH}$
 +2.6500000E+036 -8.8600000E+000 +5.1019000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{PC3H4OH-3+O2} \rightleftharpoons \text{C2H3CHO+HO2}$
 +5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{PC3H4OH-1} \rightleftharpoons \text{CH3CHCO+H}$
 +5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{PC3H4OH-1} \rightleftharpoons \text{PC3H4OH-2}$
 +2.6500000E+036 -8.8600000E+000 +5.1019000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{PC3H4OH-1+O2} \rightleftharpoons \text{CH3CHCO+HO2}$
 +5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{CH3COCHOH} \rightleftharpoons \text{CH3COCHO+H}$
 +5.6900000E+052 -1.3380000E+001 +4.5049000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{CH3COCHOH} \rightleftharpoons \text{CH3COCH2O}$
 +5.4800000E+045 -1.1630000E+001 +4.4328000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 $\text{CH3COCHOH+O2} \rightleftharpoons \text{CH3COCHO+HO2}$
 +5.2600000E+017 -1.6380000E+000 +8.6900000E+002 !\AUTHOR: !\REF:ANALOGY
 WITH SC2H4OH REACTIONS
 !

!\REACTIONCLASS: \SC4H8OH-3_O2_PRODUCTS \A
 \N \EA
 !

$\text{SC4H8OH-3+O2} \rightleftharpoons \text{SC4H8OH-3O2}$
 +3.6000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SC4H8OH-3O2} \rightleftharpoons \text{SQC4H8OS}$
 +2.9100000E+012 -2.2600000E-001 +2.2300000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SC4H8OH-3O2} \rightleftharpoons \text{C4H71-3OH+HO2}$
 +3.6400000E+014 -7.1100000E-001 +3.2710000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SC4H8OH-3O2} \rightleftharpoons \text{C4H72-2OH+HO2}$
 +2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SQC4H8OS} \rightleftharpoons \text{CH3CHO+CH3CHO+OH}$
 +2.6800000E+013 -8.0000000E-002 +1.0790000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974. !\COMMENT: !*5
 $\text{SC4H8OH-3O2} \rightleftharpoons \text{NC4KET23OH+OH}$
 +1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SC4H8OH-3O2} \rightleftharpoons \text{SQC4H7OHS-4}$
 +1.4390000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:SHARMA

$\text{SQC4H7OHS-4} \rightleftharpoons \text{CCY (COCC) OH+OH}$
 $+2.4400000\text{E}+009 +7.8000000\text{E}-001 +1.8000000\text{E}+004$!\AUTHOR: !\REF:VILLANO
(FROM KUIWEN'S MECH)

$\text{SQC4H7OHS-4} \rightleftharpoons \text{OH+CH3CHO+C2H3OH}$
 $+3.0800000\text{E}+008 +1.5000000\text{E}+000 +2.3500000\text{E}+004$!\AUTHOR: !\REF:VILLANO
(FROM KUIWEN'S MECH)

$\text{C4H71-3OH+OH} \rightleftharpoons \text{C4H63,1-3OH+H2O}$
 $+2.0200000\text{E}+006 +2.2000000\text{E}+000 -4.3720000\text{E}+002$!\AUTHOR: \REF:ANALOGY
WITH C4H8-1+OH

$\text{C4H71-3OH+HO2} \rightleftharpoons \text{C4H63,1-3OH+H2O2}$ $+3.9100000\text{E}-$
 $001 +3.9700000\text{E}+000 +1.1702000\text{E}+004$!\AUTHOR: \REF:ANALOGY WITH C4H8-
1+OH

$\text{C4H72-2OH+OH} \rightleftharpoons \text{C4H63,1-3OH+H2O}$
 $+2.0200000\text{E}+006 +2.2000000\text{E}+000 -4.3720000\text{E}+002$!\AUTHOR: \REF:ANALOGY
WITH C4H8-1+OH

$\text{C4H72-2OH+HO2} \rightleftharpoons \text{C4H63,1-3OH+H2O2}$ $+3.9100000\text{E}-$
 $001 +3.9700000\text{E}+000 +1.1702000\text{E}+004$!\AUTHOR: \REF:ANALOGY WITH C4H8-
1+OH

$\text{C4H63,1-3OH} \rightleftharpoons \text{C4H6+OH}$
 $+7.0350000\text{E}+016 -1.0120000\text{E}+000 +3.6070000\text{E}+004$!\AUTHOR: !\REF:S.M.
SARATHY ET AL. / COMBUSTION AND FLAME 159 (2012) 2028-2055

$\text{NC4KET23OH+OH} \rightleftharpoons \text{CH3COCOCH3+H2O}$
 $+8.4500000\text{E}+011 +0.0000000\text{E}+000 -2.2800000\text{E}+002$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+HO2} \rightleftharpoons \text{CH3COCOCH3+H2O2}$
 $+2.0000000\text{E}+011 +0.0000000\text{E}+000 +8.6980000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+O} \rightleftharpoons \text{CH3COCOCH3+OH}$
 $+3.0700000\text{E}+013 +0.0000000\text{E}+000 +3.4000000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+H} \rightleftharpoons \text{CH3COCOCH3+H2}$
 $+4.4600000\text{E}+006 +2.0000000\text{E}+000 +3.2000000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+O2} \rightleftharpoons \text{CH3COCOCH3+HO2}$
 $+1.5500000\text{E}+013 +0.0000000\text{E}+000 +4.1970000\text{E}+004$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+CH3} \rightleftharpoons \text{CH3COCOCH3+CH4}$
 $+1.7400000\text{E}+000 +3.4600000\text{E}+000 +3.6800000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+CH3O} \rightleftharpoons \text{CH3COCOCH3+CH3OH}$
 $+1.4500000\text{E}+011 +0.0000000\text{E}+000 +2.7710000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+CH3O2} \rightleftharpoons \text{CH3COCOCH3+CH3O2H}$
 $+2.0000000\text{E}+012 +0.0000000\text{E}+000 +1.5250000\text{E}+004$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+C2H3} \rightleftharpoons \text{CH3COCOCH3+C2H4}$
 $+3.0000000\text{E}+011 +0.0000000\text{E}+000 +3.4000000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{NC4KET23OH+C2H5} \rightleftharpoons \text{CH3COCOCH3+C2H6}$
 $+3.0000000\text{E}+010 +0.0000000\text{E}+000 +8.6000000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{CH3COHCO+CH3} \rightleftharpoons \text{CH3COCOCH3}$
 $+1.2300000\text{E}+011 +0.0000000\text{E}+000 +7.8000000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{CH3COHCO+OH} \rightleftharpoons \text{SC2H4OH+CO2}$
 $+1.7300000\text{E}+012 +0.0000000\text{E}+000 -1.0100000\text{E}+003$!\AUTHOR: !\REF:ANALOGY
WITH C2H5COCH3 REACTIONS

$\text{CH}_3\text{COHCO} + \text{H} \rightleftharpoons \text{SC}_2\text{H}_4\text{OH} + \text{CO}$
 +4.4000000E+012 +0.0000000E+000 +1.4590000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H5COCH3 REACTIONS
 $\text{SQC}_4\text{H}_7\text{OHS}-4 + \text{O}_2 \rightleftharpoons \text{SQC}_4\text{H}_7\text{OHS}-4\text{O}_2$
 +3.4330000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:MIYOSHI
 A/2 COMPARED TO R+O2
 $\text{SQC}_4\text{H}_7\text{OHS}-4\text{O}_2 \rightleftharpoons \text{NC}_4\text{KET}24\text{OH}-3 + \text{OH}$
 +5.7900000E+001 +2.9000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:MIYOSHI
 A/2 COMPARED TO R+O2
 $\text{SQC}_4\text{H}_7\text{OHS}-4\text{O}_2 \rightleftharpoons \text{C}_4\text{H}_7\text{O}_2-1,3\text{OOH}$
 +9.3000000E+010 -3.6000000E-002 +2.2890000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SQC}_4\text{H}_7\text{OHS}-4\text{O}_2 \rightleftharpoons \text{C}_4\text{H}_6\text{OHOOH}1-2-3 + \text{HO}_2$
 +2.4400000E+013 -2.5300000E-001 +3.2590000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{SQC}_4\text{H}_7\text{OHS}-4\text{O}_2 \rightleftharpoons \text{NC}_4\text{KET}13\text{OH}-2 + \text{OH}$
 +1.4900000E+009 +1.0900000E-001 +4.1390000E+004 !\AUTHOR: !\REF: H.
 SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 $\text{C}_4\text{H}_6\text{OHOOH}1-2-3 \rightleftharpoons \text{CH}_2\text{COHCHO} + \text{CH}_3 + \text{OH}$
 +1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:MIYOSHI
 A/2 COMPARED TO R+O2
 $\text{C}_4\text{H}_6\text{OHOOH}1-2-3 \rightleftharpoons \text{CH}_3\text{CHO} + \text{SC}_2\text{H}_2\text{OH} + \text{OH}$
 +1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:MIYOSHI
 A/2 COMPARED TO R+O2
 $\text{SC}_2\text{H}_2\text{OH} + \text{HCO} \rightleftharpoons \text{CH}_2\text{COHCHO}$
 +1.8100000E+013 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{H} \rightleftharpoons \text{CH}_2\text{COHCO} + \text{H}_2$
 +1.3400000E+013 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{O} \rightleftharpoons \text{CH}_2\text{COHCO} + \text{OH}$
 +5.9400000E+012 +0.0000000E+000 +1.8680000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{OH} \rightleftharpoons \text{CH}_2\text{COHCO} + \text{H}_2\text{O}$
 +9.2400000E+006 +1.5000000E+000 -9.6200000E+002 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{O}_2 \rightleftharpoons \text{CH}_2\text{COHCO} + \text{HO}_2$
 +1.0050000E+013 +0.0000000E+000 +4.0700000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{HO}_2 \rightleftharpoons \text{CH}_2\text{COHCO} + \text{H}_2\text{O}_2$
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{CH}_3 \rightleftharpoons \text{CH}_2\text{COHCO} + \text{CH}_4$
 +2.6080000E+006 +1.7800000E+000 +5.9110000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{C}_2\text{H}_3 \rightleftharpoons \text{CH}_2\text{COHCO} + \text{C}_2\text{H}_4$
 +1.7400000E+012 +0.0000000E+000 +8.4400000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_2\text{COHCO} + \text{CH}_3\text{OH}$
 +1.0000000E+012 +0.0000000E+000 +3.3000000E+003 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{CH}_2\text{COHCHO} + \text{CH}_3\text{O}_2 \rightleftharpoons \text{CH}_2\text{COHCO} + \text{CH}_3\text{O}_2\text{H}$
 +3.0100000E+012 +0.0000000E+000 +1.1920000E+004 !\AUTHOR: !\REF:ANALOGY
 WITH C2H3CHO REACTIONS
 $\text{SC}_2\text{H}_2\text{OH} + \text{CO} \rightleftharpoons \text{CH}_2\text{COHCO}$
 +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 UNCLER 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
 \N \EA

\A

!

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 \A
\N \EA
!

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_O2 \A
\N \EA
!

CH3CHCOCH3+O2<=>CH3CHOOCOCH3
+1.0000000E+011 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF: CURRAN
AND GAFFURI, 1995 !\COMMENT:
CH3CHOOCOCH3<=>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:

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!-----
!\ENDSUBMECH: \C2H5COCH3
!-----
!-----

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!\END_KINETICS_MODULE: \C4

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!+++++
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!+++++
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!\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:
!-----
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!

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

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NC5H12<=>NC3H7+C2H5
+5.2030000E+024 -2.0710000E+000 +8.8080000E+004 !\AUTHOR: JB !\REF: A.
W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014), 101-110 !\COMMENT:
HPL ESTIMATED BY JB, AND PRESSURE DEPENDENT RATE CONSTANTS CALCULATED
USIN

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PLOG / +1.0000000E-002
+1.1800000E+096 -2.3170000E+001 +1.2604600E+005 /
PLOG / +1.0000000E-001
+1.8550000E+089 -2.0900000E+001 +1.2563000E+005 /
PLOG / +1.0000000E+000
+3.5500000E+076 -1.7020000E+001 +1.2045800E+005 /
PLOG / +2.0000000E+000
+3.4750000E+071 -1.5540000E+001 +1.1785400E+005 /
PLOG / +5.0000000E+000
+2.1600000E+064 -1.3430000E+001 +1.1381500E+005 /
PLOG / +1.0000000E+001
+4.5500000E+058 -1.1790000E+001 +1.1045600E+005 /
PLOG / +2.0000000E+001
+1.0200000E+053 -1.0150000E+001 +1.0699600E+005 /
PLOG / +5.0000000E+001
+9.0000000E+045 -8.1300000E+000 +1.0253800E+005 /
NC5H12<=>PC4H9+CH3
+1.4510000E+022 -1.5220000E+000 +8.9100000E+004 !\AUTHOR: JB !\REF: A.
W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014), 101-110 !\COMMENT:
HPL ESTIMATED BY JB, AND PRESSURE DEPENDENT RATE CONSTANTS CALCULATED
USIN
PLOG / +1.0000000E-002
+7.0900000E+092 -2.2460000E+001 +1.2623500E+005 /
PLOG / +1.0000000E-001
+4.8300000E+086 -2.0360000E+001 +1.2633100E+005 /
PLOG / +1.0000000E+000
+3.2400000E+074 -1.6630000E+001 +1.2164000E+005 /
PLOG / +2.0000000E+000
+4.0300000E+069 -1.5180000E+001 +1.1914200E+005 /
PLOG / +5.0000000E+000
+3.0000000E+062 -1.3090000E+001 +1.1519900E+005 /
PLOG / +1.0000000E+001
+6.4700000E+056 -1.1440000E+001 +1.1187500E+005 /
PLOG / +2.0000000E+001
+1.3600000E+051 -9.8000000E+000 +1.0841800E+005 /
PLOG / +5.0000000E+001
+9.7400000E+043 -7.7500000E+000 +1.0392300E+005 /
NC5H12<=>C5H11-1+H
+4.2050000E+017 -3.9000000E-001 +1.0118000E+005 !\AUTHOR: JB !\REF: A.
W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014), 101-110 !\COMMENT:
HPL ESTIMATED BY JB, AND PRESSURE DEPENDENT RATE CONSTANTS CALCULATED
USIN
PLOG / +1.0000000E-002
+1.9900000E+074 -1.7750000E+001 +1.2479800E+005 /
PLOG / +1.0000000E-001
+5.7200000E+076 -1.8010000E+001 +1.3110600E+005 /
PLOG / +1.0000000E+000
+4.4200000E+072 -1.6460000E+001 +1.3294200E+005 /
PLOG / +2.0000000E+000
+4.5600000E+069 -1.5520000E+001 +1.3214800E+005 /
PLOG / +5.0000000E+000
+2.6400000E+064 -1.3920000E+001 +1.3002600E+005 /
PLOG / +1.0000000E+001
+3.8000000E+059 -1.2480000E+001 +1.2764800E+005 /
PLOG / +2.0000000E+001
+1.4400000E+054 -1.0890000E+001 +1.2470700E+005 /
PLOG / +5.0000000E+001
+3.2800000E+046 -8.6700000E+000 +1.2024100E+005 /

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NC5H12<=>C5H11-2+H
+2.4930000E+018 -6.3200000E-001 +9.7930000E+004 !\AUTHOR: JB !\REF: A.
W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014), 101-110 !\COMMENT:
HPL ESTIMATED BY JB, AND PRESSURE DEPENDENT RATE CONSTANTS CALCULATED
USIN

PLOG / +1.0000000E-002
+6.9300000E+079 -1.9240000E+001 +1.2571600E+005 /
PLOG / +1.0000000E-001
+7.6900000E+079 -1.8830000E+001 +1.3042500E+005 /
PLOG / +1.0000000E+000
+2.3400000E+073 -1.6630000E+001 +1.3041200E+005 /
PLOG / +2.0000000E+000
+5.6400000E+069 -1.5520000E+001 +1.2908700E+005 /
PLOG / +5.0000000E+000
+6.7700000E+063 -1.3740000E+001 +1.2635300E+005 /
PLOG / +1.0000000E+001
+4.3000000E+058 -1.2210000E+001 +1.2362200E+005 /
PLOG / +2.0000000E+001
+1.0600000E+053 -1.0570000E+001 +1.2045100E+005 /
PLOG / +5.0000000E+001
+2.5000000E+045 -8.3600000E+000 +1.1588300E+005 /

NC5H12<=>C5H11-3+H
+1.2570000E+018 -6.3300000E-001 +9.7930000E+004 !\AUTHOR: JB !\REF: A.
W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014), 101-110 !\COMMENT:
HPL ESTIMATED BY JB, AND PRESSURE DEPENDENT RATE CONSTANTS CALCULATED
USIN

PLOG / +1.0000000E-002
+3.4900000E+079 -1.9240000E+001 +1.2571600E+005 /
PLOG / +1.0000000E-001
+3.8800000E+079 -1.8840000E+001 +1.3042500E+005 /
PLOG / +1.0000000E+000
+1.1800000E+073 -1.6630000E+001 +1.3041200E+005 /
PLOG / +2.0000000E+000
+2.8400000E+069 -1.5520000E+001 +1.2908700E+005 /
PLOG / +5.0000000E+000
+3.4100000E+063 -1.3740000E+001 +1.2635300E+005 /
PLOG / +1.0000000E+001
+2.1700000E+058 -1.2210000E+001 +1.2362200E+005 /
PLOG / +2.0000000E+001
+5.3200000E+052 -1.0570000E+001 +1.2045100E+005 /
PLOG / +5.0000000E+001
+1.2600000E+045 -8.3600000E+000 +1.1588300E+005 /

!

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

!NC5H12+O2<=>C5H11-1+HO2
+4.2000000E+013 +0.0000000E+000 +5.2800000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT: MODIFIED FOR PENTANE 2
NC5H12+O2<=>C5H11-1+HO2
+2.1000000E+016 +0.0000000E+000 +4.9000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT: (X500)

NC5H12+O<=>C5H11-1+OH
+1.1300000E+014 +0.0000000E+000 +7.8500000E+003 !\AUTHOR: JB !\REF: J.

V. MICHAEL, D. G. KEIL, R. B. KLEMM, INT. J. CHEM. KINET., 15, 1983, 705-719 !\COMMENT:
NC5H12+H<=>C5H11-1+H2
+3.4900000E+005 +2.6900000E+000 +6.4500000E+003 !\AUTHOR: JB !\REF: W. TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951 !\COMMENT: APPEARS TO HAVE BEEN SLIGHTLY MODIFIED FROM THAT STATED IN ORIGINAL SOURCE
NC5H12+OH<=>C5H11-1+H2O
+2.7320000E+007 +1.8130000E+000 +8.6840000E+002 !\AUTHOR: JB !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060 !\COMMENT:
NC5H12+HO2<=>C5H11-1+H2O2
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: JB !\REF: J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M. SIMMIE, J. PHYS. CHEM. A, 112, 2008, 7047-7054 !\COMMENT:
NC5H12+CH3<=>C5H11-1+CH4 +9.0400000E-001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: JB !\REF: W. TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951 !\COMMENT:
NC5H12+CH3O<=>C5H11-1+CH3OH
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT: SEEMS TO BE AN ESTIMATE FROM FRED DRYER. UNKNOWN SOURCE OR YEAR
NC5H12+CH3O2<=>C5H11-1+CH3O2H
+1.3860000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT: IT APPEARS THIS COMES FROM ABSTRACTION BY HO2 AS RECOMMENDED IN J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M.
NC5H12+C2H5<=>C5H11-1+C2H6
+1.0000000E+011 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT:
NC5H12+C2H3<=>C5H11-1+C2H4
+1.0000000E+012 +0.0000000E+000 +1.8000000E+004 !\AUTHOR: JB !\REF: K. M. SUNDARAM, G. F. FROMENT, IND. ENG. CHEM. FUNDAM., 17, 1978, 174-182 !\COMMENT:
NC5H12+O2CHO<=>C5H11-1+HO2CHO
+1.3860000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT:
!NC5H12+O2<=>C5H11-2+HO2
+2.8000000E+013 +0.0000000E+000 +5.0160000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT: MODIFIED FOR PENTANE 1
NC5H12+O2<=>C5H11-2+HO2
+1.4000000E+016 +0.0000000E+000 +4.90000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT: (X500)
!
!NC5H12+O2<=>C5H11-3+HO2
+1.4000000E+013 +0.0000000E+000 +5.0160000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT: MODIFIED FOR PENTANE 2
NC5H12+O2<=>C5H11-3+HO2
+7.0000000E+015 +0.0000000E+000 +4.90000E+004 !\AUTHOR: JB !\REF: WARNING NO REFERENCE !\COMMENT: (X500)
!
NC5H12+O<=>C5H11-2+OH
+5.6200000E+013 +0.0000000E+000 +5.2000000E+003 !\AUTHOR: JB !\REF: J. V. MICHAEL, D. G. KEIL, R. B. KLEMM, INT. J. CHEM. KINET., 15, 1983, 705-719 !\COMMENT:
NC5H12+O<=>C5H11-3+OH
+2.8100000E+013 +0.0000000E+000 +5.2000000E+003 !\AUTHOR: JB !\REF: J. V. MICHAEL, D. G. KEIL, R. B. KLEMM, INT. J. CHEM. KINET., 15, 1983, 705-719 !\COMMENT:

NC5H12+H<=>C5H11-2+H2
+2.6000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: JB !\REF: W.
TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951 !\COMMENT:
NC5H12+H<=>C5H11-3+H2
+1.3000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: JB !\REF: W.
TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951 !\COMMENT:
NC5H12+OH<=>C5H11-2+H2O
+1.4110000E+010 +9.3500000E-001 +5.0470000E+002 !\AUTHOR: JB !\REF: R.
SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060
!\COMMENT:
NC5H12+OH<=>C5H11-3+H2O
+5.7210000E+006 +1.8110000E+000 -1.0155000E+003 !\AUTHOR: JB !\REF: R.
SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060
!\COMMENT:
NC5H12+HO2<=>C5H11-2+H2O2
+1.2640000E+002 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: JB !\REF: J.
AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M. SIMMIE, J. PHYS.
CHEM. A, 112, 2008, 7047-7054 !\COMMENT:
NC5H12+HO2<=>C5H11-3+H2O2
+6.3200000E+001 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: JB !\REF: J.
AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M. SIMMIE, J. PHYS.
CHEM. A, 112, 2008, 7047-7054 !\COMMENT:
NC5H12+CH3<=>C5H11-2+CH4
+1.6800000E+005 +2.1330000E+000 +7.5740000E+003 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT: NOT FROM SAME REFERENCE AS FOR PRIMARY
SITE. DIFFERS FROM RECOMMENDATION IN THAT REFERENCE BY UP TO FACTOR OF 2.
NC5H12+CH3<=>C5H11-3+CH4
+8.4000000E+004 +2.1330000E+000 +7.5740000E+003 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT: NOT FROM SAME REFERENCE AS FOR PRIMARY
SITE. DIFFERS FROM RECOMMENDATION IN THAT REFERENCE BY UP TO FACTOR OF 2.
NC5H12+CH3O<=>C5H11-2+CH3OH
+2.2000000E+011 +0.0000000E+000 +5.0000000E+003 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+CH3O<=>C5H11-3+CH3OH
+1.1000000E+011 +0.0000000E+000 +5.0000000E+003 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+CH3O2<=>C5H11-2+CH3O2H
+2.0370000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT: IT APPEARS THIS COMES FROM ABSTRACTION BY
HO2 AS RECOMMENDED IN J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER,
J. M.
NC5H12+CH3O2<=>C5H11-3+CH3O2H
+1.0190000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT: IT APPEARS THIS COMES FROM ABSTRACTION BY
HO2 AS RECOMMENDED IN J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER,
J. M.
NC5H12+C2H5<=>C5H11-2+C2H6
+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C2H5<=>C5H11-3+C2H6
+5.0000000E+010 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C2H3<=>C5H11-2+C2H4
+8.0000000E+011 +0.0000000E+000 +1.6800000E+004 !\AUTHOR: JB !\REF: K.
M. SUNDARAM, G. F. FROMENT, IND. ENG. CHEM. FUNDAM., 17, 1978, 174-182
!\COMMENT:
NC5H12+C2H3<=>C5H11-3+C2H4
+4.0000000E+011 +0.0000000E+000 +1.6800000E+004 !\AUTHOR: JB !\REF: K.

M. SUNDARAM, G. F. FROMENT, IND. ENG. CHEM. FUNDAM., 17, 1978, 174-182

!\COMMENT:

NC5H12+O2CHO<=>C5H11-2+HO2CHO

+2.0370000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: JB !\REF:

WARNING NO REFERENCE !\COMMENT:

NC5H12+O2CHO<=>C5H11-3+HO2CHO

+1.0190000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: JB !\REF:

WARNING NO REFERENCE !\COMMENT:

NC5H12+C5H11-1<=>C5H11-2+NC5H12

+1.0000000E+011 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: JB !\REF:

WARNING NO REFERENCE !\COMMENT:

NC5H12+C5H11-1<=>C5H11-3+NC5H12

+5.0000000E+010 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: JB !\REF:

WARNING NO REFERENCE !\COMMENT:

NC5H12+C5H11-2<=>C5H11-3+NC5H12

+5.0000000E+010 +0.0000000E+000 +1.2300000E+004 !\AUTHOR: JB !\REF:

WARNING NO REFERENCE !\COMMENT:

!

!\REACTIONCLASS: \RADICAL_BETA_SCISSION

\A

\N \EA

!

C5H11-1<=>C2H4+NC3H7

+3.2360000E+012 +3.2300000E-001 +2.8808400E+004 !\AUTHOR: JB !\REF: A.

COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26

!\COMMENT:

PLOG / +1.0000000E-001

+4.4100000E+003 +2.1920000E+000 +1.8827000E+004 /

PLOG / +1.0000000E+000

+8.0600000E+020 -2.6280000E+000 +2.9232000E+004 /

PLOG / +1.0000000E+001

+2.1700000E+028 -4.5780000E+000 +3.4864000E+004 /

PLOG / +1.0000000E+002

+6.4700000E+024 -3.3830000E+000 +3.4388000E+004 /

PLOG / +1.0000000E+003

+2.3400000E+017 -1.1230000E+000 +3.1176000E+004 /

C5H11-1<=>H+C5H10-1

+2.0420000E+010 +9.5000000E-001 +3.3810200E+004 !\AUTHOR: JB !\REF: A.

COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26

!\COMMENT:

PLOG / +1.0000000E-001 +3.2400000E-

014 +7.0220000E+000 +1.5354000E+004 /

PLOG / +1.0000000E+000

+5.1000000E+012 -4.0200000E-001 +2.9991000E+004 /

PLOG / +1.0000000E+001

+4.0700000E+027 -4.4830000E+000 +3.9814000E+004 /

PLOG / +1.0000000E+002

+1.0200000E+026 -3.7940000E+000 +4.0806000E+004 /

PLOG / +1.0000000E+003

+6.5200000E+016 -9.8700000E-001 +3.6957000E+004 /

C5H11-2<=>C3H6+C2H5

+4.0740000E+012 +2.7200000E-001 +2.9140300E+004 !\AUTHOR: JB !\REF: A.

COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26

!\COMMENT:

PLOG / +1.0000000E-001

+8.5400000E+025 -4.2410000E+000 +3.1303000E+004 /

PLOG / +1.0000000E+000
+2.3400000E+031 -5.5810000E+000 +3.5992000E+004 /
PLOG / +1.0000000E+001
+4.6300000E+028 -4.5920000E+000 +3.6186000E+004 /
PLOG / +1.0000000E+002
+3.7700000E+020 -2.1080000E+000 +3.2927000E+004 /
PLOG / +1.0000000E+003
+3.5600000E+014 -3.0100000E-001 +3.0124000E+004 /
C5H11-2<=>C5H10-1+H
+2.2390000E+008 +1.5170000E+000 +3.4750200E+004 !\AUTHOR: JB !\REF: A.
COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26
!\COMMENT:
PLOG / +1.0000000E-001
+8.2600000E+010 -1.1800000E-001 +2.9715000E+004 /
PLOG / +1.0000000E+000
+6.9200000E+026 -4.4560000E+000 +3.9997000E+004 /
PLOG / +1.0000000E+001
+3.8100000E+029 -4.9690000E+000 +4.3662000E+004 /
PLOG / +1.0000000E+002
+4.2200000E+020 -2.1600000E+000 +4.0523000E+004 /
PLOG / +1.0000000E+003
+5.0500000E+011 +5.2600000E-001 +3.6461000E+004 /
C5H11-2<=>C5H10-2+H
+2.7100000E+009 +1.1930000E+000 +3.4513500E+004 !\AUTHOR: JB !\REF: A.
COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26
!\COMMENT:
PLOG / +1.0000000E-001
+2.7970000E+013 -8.3300000E-001 +3.0422700E+004 /
PLOG / +1.0000000E+000
+9.9220000E+027 -4.7750000E+000 +3.9987000E+004 /
PLOG / +1.0000000E+001
+8.5040000E+029 -5.0630000E+000 +4.3150600E+004 /
PLOG / +1.0000000E+002
+1.0260000E+021 -2.2750000E+000 +3.9953200E+004 /
PLOG / +1.0000000E+003
+3.1410000E+012 +2.8700000E-001 +3.6068200E+004 /
C5H11-3<=>C4H8-1+CH3
+2.9510000E+010 +9.2800000E-001 +3.0048500E+004 !\AUTHOR: JB !\REF: A.
COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26
!\COMMENT:
PLOG / +1.0000000E-001
+1.3100000E+016 -1.1370000E+000 +2.9671000E+004 /
PLOG / +1.0000000E+000
+1.8500000E+025 -3.6430000E+000 +3.5787000E+004 /
PLOG / +1.0000000E+001
+1.0100000E+024 -3.1300000E+000 +3.6363000E+004 /
PLOG / +1.0000000E+002
+1.9800000E+016 -7.9300000E-001 +3.3017000E+004 /
PLOG / +1.0000000E+003
+2.1000000E+011 +6.8500000E-001 +3.0583000E+004 /
C5H11-3<=>C5H10-2+H
+1.2740000E+009 +1.3300000E+000 +3.4417900E+004 !\AUTHOR: JB !\REF: A.
COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26
!\COMMENT:
PLOG / +1.0000000E-001
+5.1190000E+006 +1.5110000E+000 +2.9138700E+004 /
PLOG / +1.0000000E+000
+4.0680000E+022 -2.9490000E+000 +3.8765500E+004 /

PLOG / +1.0000000E+001
+2.2980000E+025 -3.5690000E+000 +4.1777200E+004 /
PLOG / +1.0000000E+002
+8.1040000E+016 -9.8300000E-001 +3.8322300E+004 /
PLOG / +1.0000000E+003
+1.2140000E+010 +1.0470000E+000 +3.5008700E+004 /
!

!\REACTIONCLASS: \R+O2<=>E+HO2 \A
\N \EA
!

C5H11-1+O2<=>C5H10-1+HO2 +8.3700000E-
001 +3.5900000E+000 +1.1960000E+004 !\AUTHOR: JB !\REF: J. D. DESAIN,
S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107,
2003, 4415-4427 !\COMMENT: PROPYL ANALOGY
C5H11-2+O2<=>C5H10-1+HO2 +5.3500000E-
001 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: JB !\REF: J. D. DESAIN,
S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107,
2003, 4415-4427 !\COMMENT: PROPYL ANALOGY
C5H11-2+O2<=>C5H10-2+HO2
+1.0700000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: JB !\REF: J.
D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS.
CHEM. A, 107, 2003, 4415-4427 !\COMMENT: PROPYL ANALOGY
C5H11-3+O2<=>C5H10-2+HO2
+2.1400000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: JB !\REF: J.
D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS.
CHEM. A, 107, 2003, 4415-4427 !\COMMENT: PROPYL ANALOGY
!

!\REACTIONCLASS: \RADICAL_ISOMERISATION \A
\N \EA
!

C5H11-1<=>C5H11-2
+1.1480000E+001 +3.0330000E+000 +1.5313400E+004 !\AUTHOR: JB !\REF: A.
COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26
!\COMMENT:
PLOG / +1.0000000E-001
+1.6100000E+010 -1.2800000E-001 +1.6305000E+004 /
PLOG / +1.0000000E+000
+2.8800000E+017 -2.0730000E+000 +2.1414000E+004 /
PLOG / +1.0000000E+001
+5.0900000E+018 -2.2840000E+000 +2.3337000E+004 /
PLOG / +1.0000000E+002
+1.3800000E+014 -8.3800000E-001 +2.1871000E+004 /
PLOG / +1.0000000E+003
+1.6000000E+008 +9.5400000E-001 +1.9221000E+004 /
C5H11-1<=>C5H11-3 +3.8900000E-
012 +6.8430000E+000 +1.8781000E+004 !\AUTHOR: JB !\REF: A. COMANDINI,
I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26 !\COMMENT:
PLOG / +1.0000000E-001 +6.0800000E-
015 +6.8760000E+000 +1.1901000E+004 /
PLOG / +1.0000000E+000
+7.6800000E+007 +6.6700000E-001 +2.5012000E+004 /
PLOG / +1.0000000E+001
+1.2600000E+019 -2.3500000E+000 +3.2938000E+004 /

PLOG / +1.0000000E+002
+1.1600000E+016 -1.2560000E+000 +3.3072000E+004 /
PLOG / +1.0000000E+003
+6.0600000E+006 +1.5700000E+000 +2.9120000E+004 /
C5H11-2<=>C5H11-3
+2.7540000E+010 +7.1200000E-001 +4.1872300E+004 !\AUTHOR: JB !\REF: A.
COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26
!\COMMENT:
PLOG / +1.0000000E-001 +4.8000000E-
004 +3.7250000E+000 +2.8298000E+004 /
PLOG / +1.0000000E+000
+3.4100000E+022 -3.5170000E+000 +4.2976000E+004 /
PLOG / +1.0000000E+001
+1.5700000E+032 -6.0050000E+000 +5.0425000E+004 /
PLOG / +1.0000000E+002
+3.1200000E+024 -3.5140000E+000 +4.8305000E+004 /
PLOG / +1.0000000E+003
+1.5900000E+014 -4.0400000E-001 +4.3709000E+004 /
!

!\REACTIONCLASS: \R+O2<=>RO2 \A
\N \EA
!

C5H11-1+O2<=>C5H11O2-1
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT:
C5H11-2+O2<=>C5H11O2-2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT:
C5H11-3+O2<=>C5H11O2-3
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF: A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT:
!

!\REACTIONCLASS: \R+R'O2<=>RO+R'O \A
\N \EA
!

C5H11-1+HO2<=>C5H11O-1+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-2+HO2<=>C5H11O-2+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-3+HO2<=>C5H11O-3+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-1+CH3O2<=>C5H11O-1+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-2+CH3O2<=>C5H11O-2+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC

ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-3+CH3O2<=>C5H11O-3+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-1+C5H11O2-1<=>C5H11O-1+C5H11O-1
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-1+C5H11O2-2<=>C5H11O-1+C5H11O-2
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-1+C5H11O2-3<=>C5H11O-1+C5H11O-3
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-2+C5H11O2-1<=>C5H11O-2+C5H11O-1
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-2+C5H11O2-2<=>C5H11O-2+C5H11O-2
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-2+C5H11O2-3<=>C5H11O-2+C5H11O-3
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-3+C5H11O2-1<=>C5H11O-3+C5H11O-1
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-3+C5H11O2-2<=>C5H11O-3+C5H11O-2
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2
C5H11-3+C5H11O2-3<=>C5H11O-3+C5H11O-3
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: JB !\REF: HJC
ESTIMATE BASED ON CH3+HO2<=>PRODUCTS !\COMMENT: REF IS WHAT IS WRITTEN
FOR REACTIONS OF C2H5 WITH HO2 AND CH3O2

!

!\REACTIONCLASS: \RO2<=>QOOH \A
\N \EA
!

C5H11O2-1<=>C5H10OOH1-2
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-1<=>C5H10OOH1-3
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-1<=>C5H10OOH1-4
+3.7180000E+006 +1.2000000E+000 +1.6600000E+004 !\AUTHOR: JB !\REF: S.

SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-1<=>C5H10OOH1-5
+2.9410000E+005 +1.5000000E+000 +1.9900000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-2<=>C5H10OOH2-1
+7.2900000E+008 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-2<=>C5H10OOH2-3
+1.7160000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-2<=>C5H10OOH2-4
+7.0330000E+010 +2.0000000E-001 +1.9500000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-2<=>C5H10OOH2-5
+6.1700000E+005 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-3<=>C5H10OOH3-1
+2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-3<=>C5H10OOH3-2
+3.4320000E+009 +9.0000000E-001 +3.0500000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-1<=>PC4H9CHO+OH
+1.9840000E+009 +1.2000000E+000 +3.9700000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-2<=>NC3H7COCH3+OH
+5.3000000E+009 +1.0000000E+000 +3.8500000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
C5H11O2-3<=>C2H5COC2H5+OH
+5.3000000E+009 +1.0000000E+000 +3.8500000E+004 !\AUTHOR: JB !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM. A, 114, 2010, 5689-5701
!\COMMENT:
!
!

!\REACTIONCLASS: \RO2<=>E+HO2 \A
\N \EA
!

C5H11O2-1<=>C5H10-1+HO2
+3.8700000E+007 +1.5800000E+000 +2.8500000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT:
C5H11O2-2<=>C5H10-1+HO2
+3.6050000E+009 +1.1300000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT:
C5H11O2-2<=>C5H10-2+HO2
+5.1400000E+009 +1.0100000E+000 +2.9362000E+004 !\AUTHOR: JB !\REF: S.

M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT:
C5H11O2-3<=>C5H10-2+HO2
+7.2000000E+010 +7.3000000E-001 +3.0883000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT:
!

!\REACTIONCLASS: \RO2+HO2<=>RO2H+O2 \A
\N \EA
!

C5H11O2H-1+O2<=>C5H11O2-1+HO2
+3.7460000E+013 -7.9100000E-001 +3.3620000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H11O2H-2+O2<=>C5H11O2-2+HO2
+4.3800000E+013 -8.1200000E-001 +3.3640000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H11O2H-3+O2<=>C5H11O2-3+HO2
+4.3800000E+013 -8.1200000E-001 +3.3640000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+H2O2<=>RO2H+HO2 \A
\N \EA
!

C5H11O2H-1+HO2<=>C5H11O2-1+H2O2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H11O2H-2+HO2<=>C5H11O2-2+H2O2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H11O2H-3+HO2<=>C5H11O2-3+H2O2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+F<=>RO2H+R' \A
\N \EA
!

!\SITE: \PRIMARY
NC5H12+C5H11O2-1<=>C5H11-1+C5H11O2H-1
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C5H11O2-2<=>C5H11-1+C5H11O2H-2
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C5H11O2-3<=>C5H11-1+C5H11O2H-3
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
!\SITE: \SECONDARY
NC5H12+C5H11O2-1<=>C5H11-2+C5H11O2H-1
+8.0640000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:

NC5H12+C5H11O2-2<=>C5H11-2+C5H11O2H-2
+8.0640000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C5H11O2-3<=>C5H11-2+C5H11O2H-3
+8.0640000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C5H11O2-1<=>C5H11-3+C5H11O2H-1
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C5H11O2-2<=>C5H11-3+C5H11O2H-2
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5H12+C5H11O2-3<=>C5H11-3+C5H11O2H-3
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:

!

!\REACTIONCLASS: \RO2+CH3O2<=>RO+CH3O+O2 \A
\N \EA

!

C5H11O2-1+CH3O2=>C5H11O-1+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD
C5H11O2-2+CH3O2=>C5H11O-2+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD
C5H11O2-3+CH3O2=>C5H11O-3+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

!

!\REACTIONCLASS: \RO2+R'O2<=>RO+R'O+O2 \A
\N \EA

!

C5H11O2-1+C5H11O2-1=>C5H11O-1+C5H11O-1+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB
C5H11O2-1+C5H11O2-2=>C5H11O-1+C5H11O-2+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB
C5H11O2-1+C5H11O2-3=>C5H11O-1+C5H11O-3+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB
C5H11O2-2+C5H11O2-2=>C5H11O-2+C5H11O-2+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB
C5H11O2-2+C5H11O2-3=>C5H11O-2+C5H11O-3+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB
C5H11O2-3+C5H11O2-3=>C5H11O-3+C5H11O-3+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB

!

!\REACTIONCLASS: \RO2+R'O2<=>R<=>O+R'OH+O2 \A
\N \EA

!

C5H11O2-1+CH3O2=>PC4H9CHO+CH3OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-1+CH3O2=>NC5H11OH+CH2O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-2+CH3O2=>NC3H7COCH3+CH3OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-3+CH3O2=>C2H5COC2H5+CH3OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-1+C2H5O2=>PC4H9CHO+C2H5OH+O2
+3.5000000E+015 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-1+C2H5O2=>NC5H11OH+CH3CHO+O2
+3.5000000E+015 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-2+C2H5O2=>NC3H7COCH3+C2H5OH+O2
+3.5000000E+015 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-3+C2H5O2=>C2H5COC2H5+C2H5OH+O2
+3.5000000E+015 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

C5H11O2-1+C5H11O2-1=>PC4H9CHO+NC5H11OH+O2
+3.5000000E+015 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC. FARAD

!

!\REACTIONCLASS: \RO2H<=>RO+OH \A
\N \EA
!

C5H11O2H-1<=>C5H11O-1+OH
+7.3030000E+018 -8.9000000E-001 +4.5630000E+004 !\AUTHOR: JB !\REF:
ESTIMATED BY JB BY USING REVERSE OF CH3O2H<=>CH3O+OH FOR REVERSE OF THIS
REACTION AND DERIVING FORWARD FROM THERMOCHEMISTRY !\COMMENT:

C5H11O2H-2<=>C5H11O-2+OH
+4.2320000E+020 -1.4000000E+000 +4.5750000E+004 !\AUTHOR: JB !\REF:
ESTIMATED BY JB BY USING REVERSE OF CH3O2H<=>CH3O+OH FOR REVERSE OF THIS
REACTION AND DERIVING FORWARD FROM THERMOCHEMISTRY !\COMMENT:

C5H11O2H-3<=>C5H11O-3+OH
+1.4220000E+020 -1.3400000E+000 +4.5690000E+004 !\AUTHOR: JB !\REF:
ESTIMATED BY JB BY USING REVERSE OF CH3O2H<=>CH3O+OH FOR REVERSE OF THIS
REACTION AND DERIVING FORWARD FROM THERMOCHEMISTRY !\COMMENT:

!

!\REACTIONCLASS: \RO2H+OH<=>R<=>O+H2O+OH \A
\N \EA

!

C5H11O2H-1+OH=>PC4H9CHO+H2O+OH
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED TO BE 1E+12 PER H-ATOM BY JB !\COMMENT: ONLY ABSTRACTIONS BY OH
ARE CONSIDERED FOR NOW AS THIS IS EXPECTED TO BE THE DOMINANT ABTRACTOR
AT LOW

C5H11O2H-2+OH=>NC3H7COCH3+H2O+OH
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED TO BE 1E+12 PER H-ATOM BY JB !\COMMENT: ONLY ABSTRACTIONS BY OH
ARE CONSIDERED FOR NOW AS THIS IS EXPECTED TO BE THE DOMINANT ABSTRACTOR
AT LOW

C5H11O2H-3+OH=>C2H5COC2H5+H2O+OH
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED TO BE 1E+12 PER H-ATOM BY JB !\COMMENT: ONLY ABSTRACTIONS BY OH
ARE CONSIDERED FOR NOW AS THIS IS EXPECTED TO BE THE DOMINANT ABSTRACTOR
AT LOW

!

!\REACTIONCLASS: \RO_DECOMPOSITION \A
\N \EA

!

CH2O+PC4H9<=>C5H11O-1
+5.0000000E+010 +0.0000000E+000 +3.4570000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:

CH3CHO+NC3H7<=>C5H11O-2
+3.3300000E+010 +0.0000000E+000 +6.3970000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:

C2H5+C2H5CHO<=>C5H11O-3
+1.6700000E+010 +0.0000000E+000 +6.1930000E+003 !\AUTHOR: JB !\REF: H.
J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275 !\COMMENT:

!

!\REACTIONCLASS: \QOOH<=>CETH+OH \A
\N \EA

!

C5H10OOH1-2<=>C5H10O1-2+OH
+4.6670000E+012 +2.5000000E-001 +1.2840000E+004 !\AUTHOR: JB !\REF:
NEWLY CALCULATED BY JB !\COMMENT:

PLOG / +1.0000000E-002

+3.9000000E+007 -1.9000000E-001 +1.8710000E+003 /

PLOG / +1.0000000E-001

+3.1200000E+015 -2.1900000E+000 +5.9780000E+003 /

PLOG / +1.0000000E+000
 +3.2400000E+024 -4.4800000E+000 +1.1337000E+004 /
 PLOG / +2.0000000E+000
 +7.6000000E+026 -5.0600000E+000 +1.2972000E+004 /
 PLOG / +5.0000000E+000
 +1.8000000E+029 -5.5900000E+000 +1.4912000E+004 /
 PLOG / +1.0000000E+001
 +1.5200000E+030 -5.7300000E+000 +1.6062000E+004 /
 PLOG / +2.0000000E+001
 +1.3200000E+030 -5.5700000E+000 +1.6802000E+004 /
 PLOG / +5.0000000E+001
 +2.4600000E+028 -4.8900000E+000 +1.7020000E+004 /
 PLOG / +1.0000000E+002
 +1.1500000E+026 -4.0900000E+000 +1.6650000E+004 /
 C5H10OOH1-3<=>C5H10O1-3+OH
 +1.2750000E+005 +1.8300000E+000 +1.4460000E+004 !\AUTHOR: JB !\REF:
 NEWLY CALCULATED BY JB !\COMMENT:
 PLOG / +1.0000000E-002
 +4.2400000E+040 -9.5700000E+000 +2.5269000E+004 /
 PLOG / +1.0000000E-001
 +2.4300000E+026 -4.8700000E+000 +2.1713000E+004 /
 PLOG / +1.0000000E+000
 +2.9000000E+012 -4.8000000E-001 +1.6944000E+004 /
 PLOG / +2.0000000E+000
 +3.6800000E+010 +1.1000000E-001 +1.6258000E+004 /
 PLOG / +5.0000000E+000
 +1.7100000E+009 +5.2000000E-001 +1.5773000E+004 /
 PLOG / +1.0000000E+001
 +5.6100000E+008 +6.8000000E-001 +1.5596000E+004 /
 PLOG / +2.0000000E+001
 +3.1500000E+008 +7.5000000E-001 +1.5504000E+004 /
 PLOG / +5.0000000E+001
 +2.2100000E+008 +8.0000000E-001 +1.5448000E+004 /
 PLOG / +1.0000000E+002
 +1.9600000E+008 +8.2000000E-001 +1.5429000E+004 /
 C5H10OOH1-4<=>C5H10O1-4+OH
 +4.7280000E+005 +1.2400000E+000 +8.1300000E+003 !\AUTHOR: JB !\REF:
 NEWLY CALCULATED BY JB !\COMMENT:
 PLOG / +1.0000000E-002
 +1.4700000E+018 -3.0600000E+000 +1.0191000E+004 /
 PLOG / +1.0000000E-001
 +2.8000000E+014 -1.5900000E+000 +1.0655000E+004 /
 PLOG / +1.0000000E+000
 +5.9700000E+009 -7.0000000E-002 +9.3770000E+003 /
 PLOG / +2.0000000E+000
 +2.0600000E+009 +8.0000000E-002 +9.2360000E+003 /
 PLOG / +5.0000000E+000
 +1.0400000E+009 +1.8000000E-001 +9.1440000E+003 /
 PLOG / +1.0000000E+001
 +8.2000000E+008 +2.1000000E-001 +9.1120000E+003 /
 PLOG / +2.0000000E+001
 +7.2800000E+008 +2.3000000E-001 +9.0960000E+003 /
 PLOG / +5.0000000E+001
 +6.7700000E+008 +2.4000000E-001 +9.0860000E+003 /
 PLOG / +1.0000000E+002
 +6.6100000E+008 +2.4000000E-001 +9.0830000E+003 /

C5H10OOH1-5<=>C5H10O1-5+OH

+2.3140000E+004 +1.3100000E+000 +8.5500000E+003 !\AUTHOR: JB !\REF:
NEWLY CALCULATED BY JB !\COMMENT:

PLOG / +1.0000000E-002
+1.3300000E+012 -1.1900000E+000 +1.0872000E+004 /
PLOG / +1.0000000E-001
+1.8600000E+008 +6.0000000E-002 +9.7600000E+003 /
PLOG / +1.0000000E+000
+4.6800000E+007 +2.6000000E-001 +9.5740000E+003 /
PLOG / +2.0000000E+000
+4.3200000E+007 +2.7000000E-001 +9.5630000E+003 /
PLOG / +5.0000000E+000
+4.1100000E+007 +2.7000000E-001 +9.5560000E+003 /
PLOG / +1.0000000E+001
+4.0400000E+007 +2.8000000E-001 +9.5540000E+003 /
PLOG / +2.0000000E+001
+4.0100000E+007 +2.8000000E-001 +9.5530000E+003 /
PLOG / +5.0000000E+001
+3.9900000E+007 +2.8000000E-001 +9.5520000E+003 /
PLOG / +1.0000000E+002
+3.9800000E+007 +2.8000000E-001 +9.5520000E+003 /

C5H10OOH2-1<=>C5H10O1-2+OH

+2.5670000E+009 +1.0400000E+000 +1.1340000E+004 !\AUTHOR: JB !\REF:
NEWLY CALCULATED BY JB !\COMMENT:

PLOG / +1.0000000E-002
+2.8000000E+005 +5.2000000E-001 +1.2890000E+003 /
PLOG / +1.0000000E-001
+6.6200000E+015 -2.2000000E+000 +6.8790000E+003 /
PLOG / +1.0000000E+000
+1.9500000E+025 -4.6000000E+000 +1.3023000E+004 /
PLOG / +2.0000000E+000
+4.9900000E+026 -4.8800000E+000 +1.4402000E+004 /
PLOG / +5.0000000E+000
+5.5500000E+026 -4.7100000E+000 +1.5465000E+004 /
PLOG / +1.0000000E+001
+2.0700000E+025 -4.1600000E+000 +1.5596000E+004 /
PLOG / +2.0000000E+001
+8.1300000E+022 -3.3300000E+000 +1.5213000E+004 /
PLOG / +5.0000000E+001
+1.5400000E+019 -2.1000000E+000 +1.4271000E+004 /
PLOG / +1.0000000E+002
+5.3600000E+016 -1.3100000E+000 +1.3545000E+004 /

C5H10OOH2-3<=>C5H10O2-3+OH

+4.6630000E+008 +1.0900000E+000 +9.8500000E+003 !\AUTHOR: JB !\REF:
NEWLY CALCULATED BY JB !\COMMENT:

PLOG / +1.0000000E-002 +7.3800000E-
002 +2.4900000E+000 -1.6120000E+003 /
PLOG / +1.0000000E-002
+8.8200000E+002 +1.3300000E+000 +9.0400000E+002 /
PLOG / +1.0000000E-001
+2.8700000E+009 -2.9000000E-001 +4.0450000E+003 /
PLOG / +1.0000000E-001
+4.3800000E+012 -1.1600000E+000 +6.8120000E+003 /
PLOG / +1.0000000E+000
+2.1100000E+018 -2.5100000E+000 +9.9890000E+003 /
PLOG / +1.0000000E+000
+5.1100000E+013 -1.0800000E+000 +9.5220000E+003 /

PLOG / +2.0000000E+000
 +7.9900000E+018 -2.5500000E+000 +1.1002000E+004 /
 PLOG / +2.0000000E+000
 +1.0500000E+012 -4.8000000E-001 +9.3190000E+003 /
 PLOG / +5.0000000E+000
 +3.7400000E+017 -1.9800000E+000 +1.1395000E+004 /
 PLOG / +5.0000000E+000
 +4.7600000E+009 +3.0000000E-001 +8.7910000E+003 /
 PLOG / +1.0000000E+001
 +2.2300000E+015 -1.2100000E+000 +1.1062000E+004 /
 PLOG / +1.0000000E+001
 +2.1700000E+008 +7.4000000E-001 +8.4300000E+003 /
 PLOG / +2.0000000E+001
 +5.5300000E+012 -3.5000000E-001 +1.0430000E+004 /
 PLOG / +2.0000000E+001
 +2.9200000E+007 +1.0200000E+000 +8.1810000E+003 /
 PLOG / +5.0000000E+001
 +5.7100000E+009 +6.2000000E-001 +9.5720000E+003 /
 PLOG / +5.0000000E+001
 +7.1200000E+006 +1.2200000E+000 +8.0010000E+003 /
 PLOG / +1.0000000E+002
 +1.6900000E+008 +1.1100000E+000 +9.0990000E+003 /
 PLOG / +1.0000000E+002
 +4.2600000E+006 +1.2900000E+000 +7.9340000E+003 /
 C5H10OOH2-4<=>C5H10O2-4+OH
 +3.8350000E+006 +1.2600000E+000 +1.4970000E+004 !\AUTHOR: JB !\REF:
 NEWLY CALCULATED BY JB !\COMMENT:
 PLOG / +1.0000000E-002
 +1.5700000E+032 -7.0300000E+000 +2.2485000E+004 /
 PLOG / +1.0000000E-002
 +1.1400000E+036 -8.1900000E+000 +2.3953000E+004 /
 PLOG / +1.0000000E-001
 +2.9100000E+016 -1.9500000E+000 +1.7872000E+004 /
 PLOG / +1.0000000E-001
 +2.2400000E+020 -3.0800000E+000 +1.9618000E+004 /
 PLOG / +1.0000000E+000
 +3.4800000E+006 +1.1700000E+000 +1.4400000E+004 /
 PLOG / +1.0000000E+000
 +2.8600000E+007 +9.7000000E-001 +1.5137000E+004 /
 PLOG / +2.0000000E+000
 +3.3300000E+005 +1.4800000E+000 +1.4031000E+004 /
 PLOG / +2.0000000E+000
 +7.1100000E+005 +1.4700000E+000 +1.4555000E+004 /
 PLOG / +5.0000000E+000
 +7.1800000E+004 +1.6900000E+000 +1.3788000E+004 /
 PLOG / +5.0000000E+000
 +5.6400000E+004 +1.8200000E+000 +1.4153000E+004 /
 PLOG / +1.0000000E+001
 +4.2000000E+004 +1.7600000E+000 +1.3704000E+004 /
 PLOG / +1.0000000E+001
 +2.2700000E+004 +1.9400000E+000 +1.4008000E+004 /
 PLOG / +2.0000000E+001
 +3.2000000E+004 +1.8000000E+000 +1.3660000E+004 /
 PLOG / +2.0000000E+001
 +1.4200000E+004 +2.0000000E+000 +1.3933000E+004 /
 PLOG / +5.0000000E+001
 +2.7100000E+004 +1.8200000E+000 +1.3634000E+004 /

PLOG / +5.0000000E+001
 +1.0700000E+004 +2.0400000E+000 +1.3887000E+004 /
 PLOG / +1.0000000E+002
 +2.5700000E+004 +1.8300000E+000 +1.3625000E+004 /
 PLOG / +1.0000000E+002
 +9.7100000E+003 +2.0600000E+000 +1.3872000E+004 /
 C5H10OOH2-5<=>C5H10O1-4+OH
 +3.7850000E+005 +1.2800000E+000 +1.0220000E+004 !\AUTHOR: JB !\REF:
 NEWLY CALCULATED BY JB !\COMMENT:
 PLOG / +1.0000000E-002
 +2.5200000E+020 -3.6200000E+000 +1.3849000E+004 /
 PLOG / +1.0000000E-001
 +1.0900000E+012 -8.2000000E-001 +1.1988000E+004 /
 PLOG / +1.0000000E+000
 +9.1900000E+007 +4.8000000E-001 +1.0691000E+004 /
 PLOG / +2.0000000E+000
 +4.3900000E+007 +5.8000000E-001 +1.0585000E+004 /
 PLOG / +5.0000000E+000
 +2.7700000E+007 +6.4000000E-001 +1.0518000E+004 /
 PLOG / +1.0000000E+001
 +2.3700000E+007 +6.6000000E-001 +1.0496000E+004 /
 PLOG / +2.0000000E+001
 +2.1900000E+007 +6.7000000E-001 +1.0484000E+004 /
 PLOG / +5.0000000E+001
 +2.0900000E+007 +6.8000000E-001 +1.0477000E+004 /
 PLOG / +1.0000000E+002
 +2.0600000E+007 +6.8000000E-001 +1.0475000E+004 /
 C5H10OOH3-1<=>C5H10O1-3+OH
 +2.3980000E+006 +1.5200000E+000 +1.7240000E+004 !\AUTHOR: JB !\REF:
 NEWLY CALCULATED BY JB !\COMMENT:
 PLOG / +1.0000000E-002
 +2.6300000E+042 -9.9900000E+000 +2.8572000E+004 /
 PLOG / +1.0000000E-001
 +4.2800000E+025 -4.5600000E+000 +2.3726000E+004 /
 PLOG / +1.0000000E+000
 +1.0200000E+012 -2.9000000E-001 +1.8930000E+004 /
 PLOG / +2.0000000E+000
 +1.7600000E+010 +2.6000000E-001 +1.8283000E+004 /
 PLOG / +5.0000000E+000
 +1.0400000E+009 +6.4000000E-001 +1.7830000E+004 /
 PLOG / +1.0000000E+001
 +3.7500000E+008 +7.8000000E-001 +1.7665000E+004 /
 PLOG / +2.0000000E+001
 +2.2100000E+008 +8.5000000E-001 +1.7580000E+004 /
 PLOG / +5.0000000E+001
 +1.6000000E+008 +9.0000000E-001 +1.7528000E+004 /
 PLOG / +1.0000000E+002
 +1.4300000E+008 +9.1000000E-001 +1.7510000E+004 /
 C5H10OOH3-2<=>C5H10O2-3+OH
 +2.8140000E+009 +3.5000000E-001 +9.8600000E+003 !\AUTHOR: JB !\REF:
 NEWLY CALCULATED BY JB !\COMMENT:
 PLOG / +1.0000000E-002
 +7.3700000E+008 -3.9000000E-001 +4.6870000E+003 /
 PLOG / +1.0000000E-002
 +1.5700000E+000 +2.1000000E+000 -8.4100000E+002 /
 PLOG / +1.0000000E-001
 +3.6200000E+014 -1.6700000E+000 +9.2950000E+003 /

PLOG / +1.0000000E-001
+3.2500000E+010 -5.9000000E-001 +4.8370000E+003 /
PLOG / +1.0000000E+000
+5.6000000E+010 -2.2000000E-001 +9.4490000E+003 /
PLOG / +1.0000000E+000
+3.9300000E+017 -2.2800000E+000 +1.0081000E+004 /
PLOG / +2.0000000E+000
+2.0800000E+009 +2.5000000E-001 +9.1040000E+003 /
PLOG / +2.0000000E+000
+3.2200000E+017 -2.1200000E+000 +1.0773000E+004 /
PLOG / +5.0000000E+000
+1.1800000E+008 +6.6000000E-001 +8.7690000E+003 /
PLOG / +5.0000000E+000
+4.6300000E+015 -1.4200000E+000 +1.0845000E+004 /
PLOG / +1.0000000E+001
+3.6100000E+007 +8.3000000E-001 +8.6230000E+003 /
PLOG / +1.0000000E+001
+3.3400000E+013 -6.9000000E-001 +1.0443000E+004 /
PLOG / +2.0000000E+001
+1.8800000E+007 +9.2000000E-001 +8.5420000E+003 /
PLOG / +2.0000000E+001
+2.4700000E+011 +1.0000000E-002 +9.9050000E+003 /
PLOG / +5.0000000E+001
+1.2500000E+007 +9.8000000E-001 +8.4900000E+003 /
PLOG / +5.0000000E+001
+1.9100000E+009 +6.9000000E-001 +9.3010000E+003 /
PLOG / +1.0000000E+002
+1.0800000E+007 +1.0000000E+000 +8.4720000E+003 /
PLOG / +1.0000000E+002
+2.0700000E+008 +1.0000000E+000 +9.0090000E+003 /

!

!\REACTIONCLASS: \QOOH<=>E+HO2 \A
\N \EA

!

C5H10OOH1-2<=>C5H10-1+HO2
+1.0400000E+010 +9.4000000E-001 +1.5100000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH2-1<=>C5H10-1+HO2
+2.2100000E+012 +2.3000000E-001 +1.5600000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH2-3<=>C5H10-2+HO2
+4.5430000E+010 +7.5100000E-001 +1.5100000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH3-2<=>C5H10-2+HO2
+4.0660000E+010 +6.7800000E-001 +1.5034000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:

!

!\REACTIONCLASS: \QOOH_DECOMPOSITION \A
\N \EA

!

C5H10OOH1-3=>OH+CH2O+C4H8-1
+9.1000000E+008 +1.4000000E+000 +2.5500000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH2-4=>OH+CH3CHO+C3H6
+1.1800000E+009 +1.2000000E+000 +2.2700000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH3-1=>OH+C2H5CHO+C2H4
+3.0960000E+018 -1.7300000E+000 +2.6820000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH1-2<=>C2H5+AC3H5OOH
+2.4100000E+010 +1.0200000E+000 +2.8200000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH1-4<=>C3H6+C2H4O2H
+5.0800000E+011 +7.0000000E-001 +2.8700000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
C5H10OOH2-5<=>C2H4+C3H6OOH2-1
+6.8600000E+013 +1.0000000E-001 +2.9000000E+004 !\AUTHOR: JB !\REF:S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
116, 2012, 5068-5089 !\COMMENT:
!

!\REACTIONCLASS: \QOOH+O2<=>O2QOOH \A
\N \EA
!

C5H10OOH1-2+O2<=>C5H10OOH1-2O2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR
MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W.
H. GREEN, S. J
C5H10OOH1-3+O2<=>C5H10OOH1-3O2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR
MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W.
H. GREEN, S. J
C5H10OOH1-4+O2<=>C5H10OOH1-4O2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR
MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W.
H. GREEN, S. J
C5H10OOH1-5+O2<=>C5H10OOH1-5O2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR
MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W.
H. GREEN, S. J
C5H10OOH2-1+O2<=>C5H10OOH2-1O2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR
MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W.
H. GREEN, S. J
C5H10OOH2-3+O2<=>C5H10OOH2-3O2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR

MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W. H. GREEN, S. J

C5H10OOH2-4+O2<=>C5H10OOH2-4O2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR

MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W. H. GREEN, S. J

C5H10OOH2-5+O2<=>C5H10OOH2-5O2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR

MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W. H. GREEN, S. J

C5H10OOH3-1+O2<=>C5H10OOH3-1O2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR

MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W. H. GREEN, S. J

C5H10OOH3-2+O2<=>C5H10OOH3-2O2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: JB !\REF:A.
MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74 !\COMMENT: A-FACTOR

MULTIPLIED BY 0.45 BASED ON THEORETICAL RESULTS FROM C. F. GOLDSMITH, W. H. GREEN, S. J

!

!\REACTIONCLASS: \O2QOOH<=>EROOH+HO2 \A

\N \EA

!

C5H10OOH1-2O2<=>C5H92-1OOH+HO2

+5.1400000E+009 +1.0100000E+000 +2.9362000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH1-3O2<=>C5H92-1OOH+HO2

+3.6000000E+010 +7.3000000E-001 +2.9883000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH1-3O2<=>C5H92-5OOH+HO2

+3.6000000E+010 +7.3000000E-001 +2.9883000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH1-4O2<=>C5H91-5OOH+HO2

+3.6050000E+009 +1.1300000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH1-4O2<=>C5H92-5OOH+HO2

+5.1400000E+009 +1.0100000E+000 +2.9362000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH1-5O2<=>C5H91-5OOH+HO2

+3.8700000E+007 +1.5800000E+000 +2.8500000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH2-3O2<=>C5H92-4OOH+HO2

+3.6000000E+010 +7.3000000E-001 +2.9883000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2

C5H10OOH2-4O2<=>C5H92-4OOH+HO2

+5.1400000E+009 +1.0100000E+000 +2.9362000E+004 !\AUTHOR: JB !\REF: S.

M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2
C5H10OOH2-4O2<=>C5H91-4OOH+HO2
+3.6050000E+009 +1.1300000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2
C5H10OOH2-5O2<=>C5H91-4OOH+HO2
+3.8700000E+007 +1.5800000E+000 +2.8500000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2
C5H10OOH3-1O2<=>C5H91-3OOH+HO2
+3.8700000E+007 +1.5800000E+000 +2.8500000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2
C5H10OOH3-2O2<=>C5H91-3OOH+HO2
+3.6050000E+009 +1.1300000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF: S.
M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A,
115, 2011, 13425-13442 !\COMMENT: ANALOGY TO REACTION CLASS RO2<=>E+HO2
!

!\REACTIONCLASS: \O2QOOH<=>P(OOH)2 \A
\N \EA
!

C5H10OOH1-2O2<=>C5H93-1,2OOH
+1.7160000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-2O2<=>C5H92-4,5OOH
+7.0330000E+010 +2.0000000E-001 +1.8500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-2O2<=>C5H91-4,5OOH
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-3O2<=>C5H92-1,3OOH
+3.4320000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-3O2<=>C5H92-3,5OOH
+3.4320000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-3O2<=>C5H91-3,5OOH
+2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-4O2<=>C5H92-1,4OOH
+7.0330000E+010 +2.0000000E-001 +1.8500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-4O2<=>C5H93-1,4OOH
+1.7160000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-4O2<=>C5H91-2,5OOH
+7.2900000E+008 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10OOH1-5O2<=>C5H92-1,5OOH
+3.7180000E+006 +1.2000000E+000 +1.6600000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
DUP
C5H10OOH1-5O2<=>C5H93-1,5OOH
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H1000H1-502<=>C5H92-1,500H
 +4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 DUP
 C5H1000H2-102<=>C5H93-1,200H
 +1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-102<=>C5H92-4,500H
 +3.7180000E+006 +1.2000000E+000 +1.6600000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-102<=>C5H91-4,500H
 +2.9410000E+005 +1.5000000E+000 +1.9900000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-302<=>C5H91-2,300H
 +2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-302<=>C5H92-3,400H
 +3.4320000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-302<=>C5H91-3,400H
 +2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-402<=>C5H91-2,400H
 +1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 DUP
 C5H1000H2-402<=>C5H93-2,400H
 +1.7160000E+009 +9.0000000E-001 +2.9500000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-402<=>C5H91-2,400H
 +7.2900000E+008 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 DUP
 C5H1000H2-502<=>C5H91-2,500H
 +2.9410000E+005 +1.5000000E+000 +1.9900000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-502<=>C5H93-1,400H
 +1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H2-502<=>C5H92-1,400H
 +4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H3-102<=>C5H92-1,300H
 +4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H3-102<=>C5H92-3,500H
 +3.7180000E+006 +1.2000000E+000 +1.6600000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H3-102<=>C5H91-3,500H
 +2.9410000E+005 +1.5000000E+000 +1.9900000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H3-202<=>C5H91-2,300H
 +7.2900000E+008 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H1000H3-202<=>C5H92-3,400H
 +7.0330000E+010 +2.0000000E-001 +1.8500000E+004 !\AUTHOR: JB !\REF:
 WARNING NO REFERENCE !\COMMENT:

C5H10OOH3-2O2<=>C5H91-3,4OOH
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: JB !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \O2QOOH<=>KET+OH \A
\N \EA
!

C5H10OOH1-2O2<=>NC5KET12+OH
+2.4410000E+007 +1.6000000E+000 +2.7900000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH1-3O2<=>NC5KET13+OH
+1.0980000E+004 +2.4000000E+000 +1.9900000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH1-4O2<=>NC5KET14+OH
+1.2560000E+003 +2.2000000E+000 +1.7400000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH1-5O2<=>NC5KET15+OH
+1.1150000E+003 +1.8000000E+000 +1.6600000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH2-1O2<=>NC5KET21+OH
+2.7630000E+008 +1.2000000E+000 +2.5700000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH2-3O2<=>NC5KET23+OH
+1.7480000E+008 +1.7000000E+000 +2.6000000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH2-4O2<=>NC5KET24+OH
+1.7540000E+002 +3.1000000E+000 +1.7500000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH2-5O2<=>NC5KET25+OH
+3.7680000E+002 +2.2000000E+000 +1.5300000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH3-1O2<=>NC5KET31+OH
+5.7860000E+001 +2.9000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
C5H10OOH3-2O2<=>NC5KET32+OH
+1.7480000E+008 +1.7000000E+000 +2.6000000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
!

!\REACTIONCLASS: \O2QOOH+O2Q'OOH<=>O<=>QOOH+OHQ'OOH+O2 \A
\N \EA
!

C5H10OOH1-3O2+C5H10OOH1-3O2=>NC5KET31+C5H10OOH1-3OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.
C5H10OOH1-3O2+C5H10OOH2-4O2=>NC5KET31+C5H10OOH2-4OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.
C5H10OOH1-3O2+C5H10OOH2-4O2=>NC5KET24+C5H10OOH1-3OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS

REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J. CHEM. SOC.

C5H10OOH1-3O2+C5H10OOH3-1O2=>NC5KET31+C5H10OOH3-1OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.

C5H10OOH1-3O2+C5H10OOH3-1O2=>NC5KET13+C5H10OOH1-3OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.

C5H10OOH2-4O2+C5H10OOH2-4O2=>NC5KET24+C5H10OOH2-4OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.

C5H10OOH2-4O2+C5H10OOH3-1O2=>NC5KET24+C5H10OOH3-1OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.

C5H10OOH2-4O2+C5H10OOH3-1O2=>NC5KET13+C5H10OOH2-4OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.

C5H10OOH3-1O2+C5H10OOH3-1O2=>NC5KET13+C5H10OOH3-1OH+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: JB !\REF:
!\COMMENT: SAME RATE CONSTANT AS CH3O2+CH3O2=>CH3O+CH3O+O2 WHICH IS
REFERENCED AS P. D. LIGHTFOOT, P. ROUSSEL, F. CARALP, R. LESCLAUX, J.
CHEM. SOC.

!

!\REACTIONCLASS: \P(OOH)2_DECOMPOSITION \A
\N \EA

!

C5H91-3,4OOH=>C3KET12+C2H4+OH
+3.0960000E+018 -1.7300000E+000 +2.6820000E+004 !\AUTHOR: !\REF:

WARNING NO REFERENCE !\COMMENT:

C5H91-3,5OOH=>C3KET13+C2H4+OH
+3.0960000E+018 -1.7300000E+000 +2.6820000E+004 !\AUTHOR: !\REF:

WARNING NO REFERENCE !\COMMENT:

C5H91-4,5OOH=>AC3H5OOH+C2H4+HO2
+6.8600000E+013 +1.0000000E-001 +2.9000000E+004 !\AUTHOR: !\REF:

WARNING NO REFERENCE !\COMMENT:

C5H92-1,4OOH=>AC3H5OOH+CH3CHO+OH
+2.4100000E+010 +1.0200000E+000 +2.8200000E+004 !\AUTHOR: !\REF:

WARNING NO REFERENCE !\COMMENT:

C5H92-1,5OOH<=>AC3H5OOH+C2H4O2H
+2.4100000E+010 +1.0200000E+000 +2.8200000E+004 !\AUTHOR: !\REF:

WARNING NO REFERENCE !\COMMENT:

C5H92-4,5OOH=>HO2CH2CHO+C3H6+OH
+1.1800000E+009 +1.2000000E+000 +2.2700000E+004 !\AUTHOR: !\REF:

WARNING NO REFERENCE !\COMMENT:

C5H93-1,4OOH=>CH2O+C4H71-3OOH+OH
+9.1000000E+008 +1.4000000E+000 +2.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,5OOH=>CH2O+C4H71-4OOH+OH
+1.8200000E+009 +1.4000000E+000 +2.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \KET_DECOMPOSITION \A
\N \EA
!

NC5KET12<=>NC5KET12O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET13<=>NC5KET13O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET14<=>NC5KET14O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET15<=>NC5KET15O+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET21<=>NC5KET21O+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET23<=>NC5KET23O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET24<=>NC5KET24O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET25<=>NC5KET25O+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET31<=>NC5KET31O+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET32<=>NC5KET32O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5KET12O<=>NC3H7CHO+HCO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET13O<=>C2H5CHO+CH2CHO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET14O<=>CH3CHO+CH2CH2CHO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET15O<=>CH2O+C3H6CHO-1
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET21O<=>CH2O+NC3H7CO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471

NC5KET23O<=>C2H5CHO+CH3CO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET24O<=>CH3CHO+CH3COCH2
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET25O<=>CH2O+CH2CH2COCH3
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET31O<=>C2H5COCH2+CH2O
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
NC5KET32O<=>CH3CHO+C2H5CO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
!

!\REACTIONCLASS: \KORCEK \A
\N \EA
!

NC5KET13<=>NC5CYCPER13
+2.1000000E+008 +0.0000000E+000 +2.8000000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
NC5KET24<=>NC5CYCPER24
+2.1000000E+008 +0.0000000E+000 +2.8000000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
NC5KET31<=>NC5CYCPER31
+2.1000000E+008 +0.0000000E+000 +2.8000000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
NC5CYCPER13<=>HOCHO+C2H5COCH3
+3.4000000E+013 +0.0000000E+000 +3.4400000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
NC5CYCPER13<=>CH3COOH+C2H5CHO
+3.7000000E+013 +0.0000000E+000 +3.6800000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
NC5CYCPER24<=>CH3COOH+CH3COCH3
+3.4000000E+013 +0.0000000E+000 +3.4400000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
NC5CYCPER31<=>C2H5COOH+CH3CHO
+3.4000000E+013 +0.0000000E+000 +3.4400000E+004 !\AUTHOR: JB !\REF: A.
JALAN ET AL., J. AM. CHEM. SOC., 2013, 135, 11100-11114 !\COMMENT:
!

!\REACTIONCLASS: \OHQOOH_DECOMPOSITION \A
\N \EA
!

C5H10OOH1-3OH=>CH2O+SC4H8OH-1+OH
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: JB !\REF: H.
J. CURRAN, P. GAFFURI, W. J. PITZ, C. K. WESTBROOK, COMBUST. FLAME, 1998,
114, 149-177 !\COMMENT: ASSUMED TO BE THE SAME AS SIMPLE FISSION OF O-O
BOND
C5H10OOH2-4OH=>CH3CHO+C3H6OH2-1+OH
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: JB !\REF: H.
J. CURRAN, P. GAFFURI, W. J. PITZ, C. K. WESTBROOK, COMBUST. FLAME, 1998,
114, 149-177 !\COMMENT: ASSUMED TO BE THE SAME AS SIMPLE FISSION OF O-O
BOND

C5H10OOH3-1OH=>C2H5CHO+PC2H4OH+OH
+1.0000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: JB !\REF: H.
J. CURRAN, P. GAFFURI, W. J. PITZ, C. K. WESTBROOK, COMBUST. FLAME, 1998,
114, 149-177 !\COMMENT: ASSUMED TO BE THE SAME AS SIMPLE FISSION OF O-O
BOND

!

!\REACTIONCLASS: \DIONE \A
\N \EA

!

NC5KET13+OH=>NC5DIONE13+OH+H2O
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED TO BE 1E+12 PER H-ATOM BY JB !\COMMENT: ONLY ABSTRACTIONS BY OH
ARE CONSIDERED FOR NOW AS THIS IS EXPECTED TO BE THE DOMINANT ABTRACTOR
AT LOW

NC5KET24+OH=>NC5DIONE24+OH+H2O
+1.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED TO BE 1E+12 PER H-ATOM BY JB !\COMMENT: ONLY ABSTRACTIONS BY OH
ARE CONSIDERED FOR NOW AS THIS IS EXPECTED TO BE THE DOMINANT ABSTRACTOR
AT LOW

NC5KET31+OH=>NC5DIONE13+OH+H2O
+2.0000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: JB !\REF:
ESTIMATED TO BE 1E+12 PER H-ATOM BY JB !\COMMENT: ONLY ABSTRACTIONS BY OH
ARE CONSIDERED FOR NOW AS THIS IS EXPECTED TO BE THE DOMINANT ABSTRACTOR
AT LOW

!

!\REACTIONCLASS: \P(OOH)2<=>EROOH+HO2 \A
\N \EA

!

C5H91-2,3OOH<=>C5H91-3OOH+HO2
+2.2100000E+012 +2.3000000E-001 +1.5600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-2,4OOH<=>C5H91-4OOH+HO2
+2.2100000E+012 +2.3000000E-001 +1.5600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-2,5OOH<=>C5H91-5OOH+HO2
+2.2100000E+012 +2.3000000E-001 +1.5600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,3OOH<=>C5H91-3OOH+HO2
+1.0400000E+010 +9.4000000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,3OOH<=>C5H92-1OOH+HO2
+4.0660000E+010 +6.7800000E-001 +1.5034000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,4OOH<=>C5H91-4OOH+HO2
+1.0400000E+010 +9.4000000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,5OOH<=>C5H91-5OOH+HO2
+1.0400000E+010 +9.4000000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-3,4OOH<=>C5H92-4OOH+HO2
+4.0660000E+010 +6.7800000E-001 +1.5034000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H92-3,5OOH<=>C5H92-5OOH+HO2
+4.0660000E+010 +6.7800000E-001 +1.5034000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,2OOH<=>C5H92-1OOH+HO2
+4.5430000E+010 +7.5100000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,4OOH<=>C5H92-5OOH+HO2
+4.5430000E+010 +7.5100000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-2,4OOH<=>C5H92-4OOH+HO2
+9.0860000E+010 +7.5100000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \EROOH_DECOMPOSITION \A
\N \EA
!

C5H91-3OOH=>C2H5CHO+C2H3+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-3OOH=>C2H3CHO+C2H5+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-4OOH=>CH3CHO+C3H5-A+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-4OOH=>SC3H5CHO+CH3+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-5OOH=>CH2O+C4H71-4+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1OOH=>CH2O+C4H71-1+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-4OOH=>CH3CHO+C3H5-S+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-4OOH=>SC3H5CHO+CH3+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-5OOH=>CH2O+C4H71-3+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \P(OOH)2<=>CETH-OOH+OH \A
\N \EA
!

C5H91-2,3OOH<=>C5H901-2OOH-3+OH
+5.8000000E+010 +4.3000000E-001 +1.0700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-2,3OOH<=>C5H901-3OOH-2+OH
+1.0150000E+010 +4.6000000E-001 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H91-2,4OOH<=>C5H9O1-2OOH-4+OH
+5.8000000E+010 +4.3000000E-001 +1.0700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-2,4OOH<=>C5H9O1-4OOH-2+OH
+1.2400000E+009 +3.5000000E-001 +1.1200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-2,5OOH<=>C5H9O1-2OOH-5+OH
+5.8000000E+010 +4.3000000E-001 +1.0700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-2,5OOH<=>C5H9O1-5OOH-2+OH
+1.4450000E+007 +7.6000000E-001 +1.1300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-3,4OOH<=>C5H9O1-3OOH-4+OH
+1.0150000E+010 +4.6000000E-001 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-3,4OOH<=>C5H9O1-4OOH-3+OH
+1.2400000E+009 +3.5000000E-001 +1.1200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-3,5OOH<=>C5H9O1-3OOH-5+OH
+1.0150000E+010 +4.6000000E-001 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-3,5OOH<=>C5H9O1-5OOH-3+OH
+1.4450000E+007 +7.6000000E-001 +1.1300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-4,5OOH<=>C5H9O1-4OOH-5+OH
+1.2400000E+009 +3.5000000E-001 +1.1200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H91-4,5OOH<=>C5H9O1-5OOH-2+OH
+1.4450000E+007 +7.6000000E-001 +1.1300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,3OOH<=>C5H9O1-2OOH-3+OH
+3.6700000E+009 +9.3000000E-001 +1.0900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,3OOH<=>C5H9O2-3OOH-1+OH
+7.0400000E+009 +7.8400000E-001 +9.5910000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,4OOH<=>C5H9O1-2OOH-4+OH
+3.6700000E+009 +9.3000000E-001 +1.0900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,4OOH<=>C5H9O2-4OOH-1+OH
+1.3400000E+009 +7.0000000E-001 +1.6415000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,5OOH<=>C5H9O1-2OOH-5+OH
+3.6700000E+009 +9.3000000E-001 +1.0900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-1,5OOH<=>C5H9O1-4OOH-5+OH
+2.4100000E+007 +9.4000000E-001 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-3,4OOH<=>C5H9O2-3OOH-4+OH
+7.0400000E+009 +7.8400000E-001 +9.5910000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-3,4OOH<=>C5H9O2-4OOH-3+OH
+1.3400000E+009 +7.0000000E-001 +1.6415000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-3,5OOH<=>C5H9O2-3OOH-5+OH
+7.0400000E+009 +7.8400000E-001 +9.5910000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H92-3,5OOH<=>C5H9O1-4OOH-3+OH
+2.4100000E+007 +9.4000000E-001 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-4,5OOH<=>C5H9O2-4OOH-1+OH
+1.3400000E+009 +7.0000000E-001 +1.6415000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H92-4,5OOH<=>C5H9O1-4OOH-2+OH
+2.4100000E+007 +9.4000000E-001 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,2OOH<=>C5H9O1-3OOH-2+OH
+4.2250000E+008 +9.0000000E-001 +1.5300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,2OOH<=>C5H9O2-3OOH-1+OH
+2.4410000E+009 +9.0000000E-001 +9.4030000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,4OOH<=>C5H9O1-3OOH-4+OH
+4.2250000E+008 +9.0000000E-001 +1.5300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,4OOH<=>C5H9O2-3OOH-5+OH
+2.4410000E+009 +9.0000000E-001 +9.4030000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-1,5OOH<=>C5H9O1-3OOH-5+OH
+4.2250000E+008 +9.0000000E-001 +1.5300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H93-2,4OOH<=>C5H9O2-3OOH-4+OH
+4.8810000E+009 +9.0000000E-001 +9.4030000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \CETH-OOH_DECOMPOSITION \A
\N \EA
!

C5H9O1-2OOH-3=>C2H5CHO+CH2CHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-3OOH-2=>C2H5CHO+CH2CHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-3OOH-2=>CH2O+C3H6CHO-3+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-2OOH-4=>CH3CHO+C3H5O+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-4OOH-2=>CH2O+C3H6CHO-2+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-4OOH-2=>C3H6+OCH2CHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-2OOH-5<=>C5H9O1-2O-5+OH
+4.1510000E+019 -1.3100000E+000 +4.5700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-5OOH-2=>CH2O+C3H6CHO-1+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H9O1-5OOH-2=>C2H4+CH2OCH2CHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-3OOH-4=>CH3CHO+CH2CH2CHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-4OOH-3=>C2H4+C2H4OCHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-3OOH-5=>CH2O+C4H7O1-4+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-5OOH-3<=>CH2CH2OCH2CH2CHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O1-4OOH-5=>CH2O+C3H6CHO-1+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O2-3OOH-1=>CH2O+C3H6CHO-3+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O2-4OOH-1=>CH2O+C3H6CHO-2+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O2-4OOH-3=>CH3CHO+CH3CHCHO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9O2-3OOH-5=>CH2O+C4H71-O+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \CETH_DECOMPOSITION \A
\N \EA
!

C5H10O1-2+OH=>CH2CO+NC3H7+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10O1-3+OH=>C2H4+C2H5CO+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10O1-4+OH=>CH3COCH2+C2H4+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10O1-5+OH=>CH2CH2CHO+C2H4+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10O2-3+OH=>CH3CHCO+C2H5+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10O2-4+OH=>CH3CO+C3H6+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H10O1-2+OH=>C2H3CHO+C2H5+H2O
+2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H10O1-3+OH=>HCO+C4H8-1+H2O
 +2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-4+OH=>CH2CHO+C3H6+H2O
 +2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-5+OH=>CH2O+C4H71-3+H2O
 +2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O2-3+OH=>C2H3COCH3+CH3+H2O
 +2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O2-4+OH=>CH3CHO+C3H5-S+H2O
 +2.2600000E+003 +2.7300000E+000 -4.6886000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-2+HO2=>CH2CO+NC3H7+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-3+HO2=>C2H4+C2H5CO+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-4+HO2=>CH3COCH2+C2H4+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-5+HO2=>CH2CH2CHO+C2H4+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O2-3+HO2=>CH3CHCO+C2H5+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O2-4+HO2=>CH3CO+C3H6+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-2+HO2=>C2H3CHO+C2H5+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-3+HO2=>HCO+C4H8-1+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-4+HO2=>CH2CHO+C3H6+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O1-5+HO2=>CH2O+C4H71-3+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O2-3+HO2=>C2H3COCH3+CH3+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H10O2-4+HO2=>CH3CHO+C3H5-S+H2O2
 +1.7200000E+001 +3.4600000E+000 +9.7333000E+003 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 !

!\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:
OCH2CHO<=>CH2O+HCO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H901-2O-5=>CH2O+CH2CHO+C2H4
+1.3260000E+021 -2.3490000E+000 +2.5084000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH2OCH2CHO<=>CH2O+CH2CHO
+1.6000000E+013 +0.0000000E+000 +2.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C2H4OCHO<=>CH3CHO+HCO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C4H701-4<=>CH2O+C3H5-A
+1.3260000E+021 -2.3490000E+000 +2.5084000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH2CH2OCH2CH2CHO=>CH2O+C2H4+CH2CHO
+1.6000000E+013 +0.0000000E+000 +2.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NC5DIONE13+OH=>CH3CHCO+CH2CHO+H2O
+2.3600000E+002 +3.1500000E+000 +3.0500000E+003 !\AUTHOR: JB !\REF:
PELUCCHI ET AL., COMBUST. FLAME, 162, 2015, 265-286 !\COMMENT: H-ATOM
ABSTRACTION FOLLOWED BY BETA-SCISSION
NC5DIONE24+OH=>CH2CO+CH3COCH2+H2O
+1.7200000E+005 +2.4000000E+000 +8.1500000E+002 !\AUTHOR: JB !\REF:
PELUCCHI ET AL., COMBUST. FLAME, 162, 2015, 265-286 !\COMMENT: H-ATOM
ABSTRACTION FOLLOWED BY BETA-SCISSION
!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: \IC5H12
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
!-----
!

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

IC5H12<=>IC3H7+C2H5

+1.4690000E+026 -2.6590000E+000 +8.6860000E+004 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE

PLOG / +1.0000000E-002
+4.0700000E+095 -2.3370000E+001 +1.2161400E+005 /
PLOG / +1.0000000E-001
+2.8000000E+090 -2.1550000E+001 +1.2233900E+005 /
PLOG / +1.0000000E+000
+8.5800000E+079 -1.8270000E+001 +1.1900100E+005 /
PLOG / +2.0000000E+000
+3.9600000E+075 -1.6970000E+001 +1.1701500E+005 /
PLOG / +5.0000000E+000
+1.4100000E+069 -1.5060000E+001 +1.1372300E+005 /
PLOG / +1.0000000E+001
+7.2900000E+063 -1.3510000E+001 +1.1081100E+005 /
PLOG / +2.0000000E+001
+2.4600000E+058 -1.1910000E+001 +1.0764500E+005 /
PLOG / +5.0000000E+001
+1.5500000E+051 -9.8300000E+000 +1.0329200E+005 /

IC5H12<=>SC4H9+CH3

+8.6940000E+023 -2.0190000E+000 +8.7290000E+004 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE

PLOG / +1.0000000E-002
+1.0500000E+093 -2.2640000E+001 +1.2164100E+005 /
PLOG / +1.0000000E-001
+1.3100000E+088 -2.0890000E+001 +1.2256300E+005 /
PLOG / +1.0000000E+000
+6.8000000E+077 -1.7670000E+001 +1.1942000E+005 /
PLOG / +2.0000000E+000
+3.5500000E+073 -1.6390000E+001 +1.1748400E+005 /
PLOG / +5.0000000E+000
+1.4300000E+067 -1.4490000E+001 +1.1424800E+005 /
PLOG / +1.0000000E+001
+7.8100000E+061 -1.2940000E+001 +1.1136500E+005 /
PLOG / +2.0000000E+001
+2.7000000E+056 -1.1350000E+001 +1.0821800E+005 /
PLOG / +5.0000000E+001
+1.6600000E+049 -9.2600000E+000 +1.0387100E+005 /

IC5H12<=>IC4H9+CH3

+1.0670000E+021 -1.4600000E+000 +8.9070000E+004 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE

PLOG / +1.0000000E-002
+2.9100000E+088 -2.1680000E+001 +1.2166600E+005 /
PLOG / +1.0000000E-001
+4.7900000E+084 -2.0230000E+001 +1.2342100E+005 /
PLOG / +1.0000000E+000
+2.4500000E+075 -1.7280000E+001 +1.2110800E+005 /
PLOG / +2.0000000E+000
+2.2100000E+071 -1.6050000E+001 +1.1939100E+005 /
PLOG / +5.0000000E+000
+1.5600000E+065 -1.4220000E+001 +1.1639700E+005 /

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PLOG / +1.0000000E+001
+1.1200000E+060 -1.2700000E+001 +1.1365100E+005 /
PLOG / +2.0000000E+001
+4.3500000E+054 -1.1120000E+001 +1.1059100E+005 /
PLOG / +5.0000000E+001
+2.4900000E+047 -9.0200000E+000 +1.0628200E+005 /
IC5H12<=>AC5H11+H
+5.0900000E+017 -4.1700000E-001 +1.0118000E+005 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE
PLOG / +1.0000000E-002
+8.0100000E+067 -1.6140000E+001 +1.1871200E+005 /
PLOG / +1.0000000E-001
+1.4800000E+072 -1.6920000E+001 +1.2562600E+005 /
PLOG / +1.0000000E+000
+7.2500000E+070 -1.6140000E+001 +1.2931900E+005 /
PLOG / +2.0000000E+000
+9.5700000E+068 -1.5500000E+001 +1.2939400E+005 /
PLOG / +5.0000000E+000
+2.1400000E+065 -1.4330000E+001 +1.2859200E+005 /
PLOG / +1.0000000E+001
+4.9600000E+061 -1.3210000E+001 +1.2726900E+005 /
PLOG / +2.0000000E+001
+2.3000000E+057 -1.1910000E+001 +1.2533400E+005 /
PLOG / +5.0000000E+001
+5.7000000E+050 -9.9500000E+000 +1.2193300E+005 /
IC5H12<=>BC5H11+H
+6.3420000E+018 -7.8400000E-001 +9.6250000E+004 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE
PLOG / +1.0000000E-002
+1.2400000E+077 -1.8650000E+001 +1.2036100E+005 /
PLOG / +1.0000000E-001
+1.4300000E+078 -1.8530000E+001 +1.2542400E+005 /
PLOG / +1.0000000E+000
+2.4800000E+073 -1.6810000E+001 +1.2665700E+005 /
PLOG / +2.0000000E+000
+3.3900000E+070 -1.5900000E+001 +1.2595100E+005 /
PLOG / +5.0000000E+000
+4.9000000E+065 -1.4410000E+001 +1.2415300E+005 /
PLOG / +1.0000000E+001
+1.9500000E+061 -1.3090000E+001 +1.2215000E+005 /
PLOG / +2.0000000E+001
+2.3100000E+056 -1.1630000E+001 +1.1964400E+005 /
PLOG / +5.0000000E+001
+2.0300000E+049 -9.5600000E+000 +1.1572900E+005 /
IC5H12<=>CC5H11+H
+1.7390000E+018 -6.8500000E-001 +9.7930000E+004 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE
PLOG / +1.0000000E-002
+7.6100000E+073 -1.7850000E+001 +1.1981700E+005 /
PLOG / +1.0000000E-001
+1.2200000E+076 -1.8050000E+001 +1.2558100E+005 /

```

PLOG / +1.0000000E+000
+3.0700000E+072 -1.6650000E+001 +1.2766300E+005 /
PLOG / +2.0000000E+000
+8.7900000E+069 -1.5820000E+001 +1.2721800E+005 /
PLOG / +5.0000000E+000
+3.0600000E+065 -1.4440000E+001 +1.2574700E+005 /
PLOG / +1.0000000E+001
+2.1100000E+061 -1.3180000E+001 +1.2396100E+005 /
PLOG / +2.0000000E+001
+3.7700000E+056 -1.1760000E+001 +1.2163400E+005 /
PLOG / +5.0000000E+001
+4.4000000E+049 -9.7300000E+000 +1.1787100E+005 /
IC5H12<=>DC5H11+H
+5.0610000E+017 -6.3300000E-001 +1.0118000E+005 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013) FOR N-PENTANE
PLOG / +1.0000000E-002
+7.9600000E+067 -1.6350000E+001 +1.1871200E+005 /
PLOG / +1.0000000E-001
+1.4800000E+072 -1.7130000E+001 +1.2562600E+005 /
PLOG / +1.0000000E+000
+7.2100000E+070 -1.6360000E+001 +1.2931900E+005 /
PLOG / +2.0000000E+000
+9.5100000E+068 -1.5710000E+001 +1.2939400E+005 /
PLOG / +5.0000000E+000
+2.1300000E+065 -1.4550000E+001 +1.2859200E+005 /
PLOG / +1.0000000E+001
+4.9400000E+061 -1.3430000E+001 +1.2726900E+005 /
PLOG / +2.0000000E+001
+2.2900000E+057 -1.2120000E+001 +1.2533400E+005 /
PLOG / +5.0000000E+001
+5.6600000E+050 -1.0170000E+001 +1.2193300E+005 /
!

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

!\SITE: \PRIMARY
IC5H12+O2<=>AC5H11+HO2
+4.2000000E+013 +0.0000000E+000 +5.2800000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+O2<=>DC5H11+HO2
+2.1000000E+013 +0.0000000E+000 +5.2800000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+O<=>AC5H11+OH
+1.1300000E+014 +0.0000000E+000 +7.8500000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+O<=>DC5H11+OH
+1.0460000E+006 +2.4240000E+000 +4.7660000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+H<=>AC5H11+H2
+3.4900000E+005 +2.6900000E+000 +6.4500000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+H<=>DC5H11+H2
+1.7450000E+005 +2.6900000E+000 +6.4500000E+003 !\AUTHOR: !\REF:
!\COMMENT:

IC5H12+OH<=>AC5H11+H2O
+3.3480000E+006 +2.0780000E+000 +3.7560000E+002 !\AUTHOR: !\REF:R.
SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060
IC5H12+OH<=>DC5H11+H2O
+1.3660000E+007 +1.8130000E+000 +8.6840000E+002 !\AUTHOR: !\REF:R.
SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060
IC5H12+HO2<=>AC5H11+H2O2
+4.0800000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+HO2<=>DC5H11+H2O2
+2.0400000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+CH3<=>AC5H11+CH4 +9.0400000E-
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF: !\COMMENT:
IC5H12+CH3<=>DC5H11+CH4 +4.5200000E-
001 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF: !\COMMENT:
IC5H12+CH3O<=>AC5H11+CH3OH
+3.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+CH3O<=>DC5H11+CH3OH
+1.5000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+CH3O2<=>AC5H11+CH3O2H
+1.3860000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+CH3O2<=>DC5H11+CH3O2H +6.9300000E-
001 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF: !\COMMENT:
IC5H12+C2H5<=>AC5H11+C2H6
+1.0000000E+011 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+C2H5<=>DC5H11+C2H6
+5.0000000E+010 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+C2H3<=>AC5H11+C2H4
+1.0000000E+012 +0.0000000E+000 +1.8000000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+C2H3<=>DC5H11+C2H4
+5.0000000E+011 +0.0000000E+000 +1.8000000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+O2CHO<=>AC5H11+HO2CHO
+1.6800000E+013 +0.0000000E+000 +2.0440000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+O2CHO<=>DC5H11+HO2CHO
+8.4000000E+012 +0.0000000E+000 +2.0440000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+AC5H11<=>DC5H11+IC5H12
+7.5000000E+010 +0.0000000E+000 +1.2300000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+BC5H11<=>DC5H11+IC5H12
+7.5000000E+010 +0.0000000E+000 +1.2300000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+CC5H11<=>DC5H11+IC5H12
+7.5000000E+010 +0.0000000E+000 +1.2300000E+004 !\AUTHOR: !\REF:
!\COMMENT:
!\SITE: \SECONDARY
IC5H12+O2<=>CC5H11+HO2
+1.4000000E+013 +0.0000000E+000 +5.0160000E+004 !\AUTHOR: !\REF:
!\COMMENT:

IC5H12+O<=>CC5H11+OH
 +5.9460000E+005 +2.4390000E+000 +2.8460000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+H<=>CC5H11+H2
 +1.3000000E+006 +2.4000000E+000 +4.4710000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+OH<=>CC5H11+H2O
 +7.0530000E+009 +9.3500000E-001 +5.0470000E+002 !\AUTHOR: !\REF:R.
 SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060

IC5H12+HO2<=>CC5H11+H2O2
 +6.3200000E+001 +3.3700000E+000 +1.3720000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+CH3<=>CC5H11+CH4
 +8.4000000E+004 +2.1330000E+000 +7.5740000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+CH3O<=>CC5H11+CH3OH
 +1.1000000E+011 +0.0000000E+000 +5.0000000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+CH3O2<=>CC5H11+CH3O2H
 +1.0190000E+001 +3.5800000E+000 +1.4810000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+C2H5<=>CC5H11+C2H6
 +5.0000000E+010 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+C2H3<=>CC5H11+C2H4
 +4.0000000E+011 +0.0000000E+000 +1.6800000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+O2CHO<=>CC5H11+HO2CHO
 +5.6000000E+012 +0.0000000E+000 +1.7690000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+AC5H11<=>CC5H11+IC5H12
 +5.0000000E+010 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+BC5H11<=>CC5H11+IC5H12
 +5.0000000E+010 +0.0000000E+000 +1.0400000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

!\SITE: \TERTIARY

IC5H12+O2<=>BC5H11+HO2
 +7.0000000E+012 +0.0000000E+000 +4.8000000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+O<=>BC5H11+OH
 +3.9680000E+005 +2.4010000E+000 +1.1500000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+H<=>BC5H11+H2
 +6.0200000E+005 +2.4000000E+000 +2.5830000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+OH<=>BC5H11+H2O
 +4.8440000E+006 +1.8400000E+000 -9.9960000E+002 !\AUTHOR: !\REF:R.
 SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060

IC5H12+HO2<=>BC5H11+H2O2
 +6.5040000E+002 +3.0100000E+000 +1.2090000E+004 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+CH3<=>BC5H11+CH4 +6.0100000E-010 +6.3600000E+000 +8.9300000E+002 !\AUTHOR: !\REF: !\COMMENT:

IC5H12+CH3O<=>BC5H11+CH3OH
 +1.9000000E+010 +0.0000000E+000 +2.8000000E+003 !\AUTHOR: !\REF:
 !\COMMENT:

IC5H12+CH3O2<=>BC5H11+CH3O2H
+2.6200000E+002 +3.1200000E+000 +1.1100000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+C2H5<=>BC5H11+C2H6
+1.0000000E+011 +0.0000000E+000 +7.9000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+C2H3<=>BC5H11+C2H4
+2.0000000E+011 +0.0000000E+000 +1.4300000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+O2CHO<=>BC5H11+HO2CHO
+1.5000000E+004 +2.5000000E+000 +1.2260000E+004 !\AUTHOR: !\REF:
!\COMMENT:
IC5H12+AC5H11<=>BC5H11+IC5H12
+2.5000000E+010 +0.0000000E+000 +7.9000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
!

!\REACTIONCLASS: \RADICAL_BETA_SCISSION \A
\N \EA
!

C3H6+C2H5<=>AC5H11
+1.4200000E+003 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H8-1+CH3<=>AC5H11
+1.8900000E+003 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H10+H<=>AC5H11
+6.2500000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:
!\COMMENT:
IC4H8+CH3<=>BC5H11
+4.4000000E+004 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H10+H<=>BC5H11
+1.0600000E+012 +5.1000000E-001 +1.2300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H10+H<=>BC5H11
+6.2500000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C4H8-2+CH3<=>CC5H11
+1.8900000E+003 +2.6700000E+000 +6.8500000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H10+H<=>CC5H11
+2.5000000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H10+H<=>CC5H11
+6.2500000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:
!\COMMENT:
C2H4+IC3H7<=>DC5H11
+8.8000000E+003 +2.4800000E+000 +6.1300000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H10+H<=>DC5H11
+2.5000000E+011 +5.1000000E-001 +2.6200000E+003 !\AUTHOR: !\REF:
!\COMMENT:
!

!\REACTIONCLASS: \R+O2<=>E+HO2 \A
\N \EA

!

AC5H11+O2<=>AC5H10+HO2 +8.3700000E-
001 +3.5900000E+000 +1.1960000E+004 !\AUTHOR: !\REF: !\COMMENT:
BC5H11+O2<=>AC5H10+HO2 +5.3500000E-
001 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF: !\COMMENT:
BC5H11+O2<=>BC5H10+HO2
+1.0700000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+O2<=>BC5H10+HO2
+1.0700000E+000 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+O2<=>CC5H10+HO2 +5.3500000E-
001 +3.7100000E+000 +9.3220000E+003 !\AUTHOR: !\REF: !\COMMENT:
DC5H11+O2<=>CC5H10+HO2 +8.3700000E-
001 +3.5900000E+000 +1.1960000E+004 !\AUTHOR: !\REF: !\COMMENT:
!

!\REACTIONCLASS: \RADICAL_ISOMERISATION \A
\N \EA
!

AC5H11<=>DC5H11
+3.0000000E+011 +0.0000000E+000 +2.1100000E+004 !\AUTHOR: !\REF:
!\COMMENT:
!

!\REACTIONCLASS: \R+O2<=>RO2 \A
\N \EA
!

AC5H11+O2<=>AC5H11O2
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
BC5H11+O2<=>BC5H11O2
+9.7560000E+011 +3.2500000E-001 -4.1730000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
CC5H11+O2<=>CC5H11O2
+3.4870000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
DC5H11+O2<=>DC5H11O2
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
!

!\REACTIONCLASS: \R+R'O2<=>RO+R'O \A
\N \EA
!

AC5H11+HO2<=>AC5H11O+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H11+HO2<=>BC5H11O+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+HO2<=>CC5H11O+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:

DC5H11+HO2<=>DC5H11O+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H11+CH3O2<=>AC5H11O+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H11+CH3O2<=>BC5H11O+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+CH3O2<=>CC5H11O+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
DC5H11+CH3O2<=>DC5H11O+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H11+AC5H11O2<=>AC5H11O+AC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H11+BC5H11O2<=>AC5H11O+BC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H11+CC5H11O2<=>AC5H11O+CC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
AC5H11+DC5H11O2<=>AC5H11O+DC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H11+AC5H11O2<=>BC5H11O+AC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H11+BC5H11O2<=>BC5H11O+BC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H11+CC5H11O2<=>BC5H11O+CC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
BC5H11+DC5H11O2<=>BC5H11O+DC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+AC5H11O2<=>CC5H11O+AC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+BC5H11O2<=>CC5H11O+BC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+CC5H11O2<=>CC5H11O+CC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
CC5H11+DC5H11O2<=>CC5H11O+DC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
DC5H11+AC5H11O2<=>DC5H11O+AC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
DC5H11+BC5H11O2<=>DC5H11O+BC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:

DC5H11+CC5H11O2<=>DC5H11O+CC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
DC5H11+DC5H11O2<=>DC5H11O+DC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
!\COMMENT:
!

!\REACTIONCLASS: \RO2<=>QOOH \A
\N \EA
!

AC5H11O2<=>AC5H10OOH-A
+4.9100000E+007 +1.3000000E+000 +2.1500000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
AC5H11O2<=>AC5H10OOH-B
+2.3090000E+009 +8.0000000E-001 +2.7100000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
AC5H11O2<=>AC5H10OOH-C
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
AC5H11O2<=>AC5H10OOH-D
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
BC5H11O2<=>BC5H10OOH-A
+3.0140000E+009 +1.2000000E+000 +3.3500000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
BC5H11O2<=>BC5H10OOH-C
+6.5130000E+009 +7.0000000E-001 +3.0100000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
BC5H11O2<=>BC5H10OOH-D
+1.5040000E+008 +1.1000000E+000 +2.1900000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
CC5H11O2<=>CC5H10OOH-A
+2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
CC5H11O2<=>CC5H10OOH-B
+7.4490000E+009 +6.0000000E-001 +2.7300000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
CC5H11O2<=>CC5H10OOH-D
+1.4580000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
DC5H11O2<=>DC5H10OOH-A
+2.4670000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
DC5H11O2<=>DC5H10OOH-B
+1.2310000E+007 +1.2000000E+000 +1.5400000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
DC5H11O2<=>DC5H10OOH-C
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF: S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
!

!\REACTIONCLASS: \RO2<=>E+HO2 \A
\N \EA
!

AC5H11O2<=>AC5H10+HO2
+1.2600000E+008 +1.3200000E+000 +2.8900000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2011, 115, 13425-13442
BC5H11O2<=>AC5H10+HO2
+2.4480000E+010 +8.9000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2011, 115, 13425-13442
BC5H11O2<=>BC5H10+HO2
+1.1240000E+011 +5.8000000E-001 +2.9600000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2011, 115, 13425-13442
CC5H11O2<=>BC5H10+HO2
+3.5000000E+010 +7.1000000E-001 +3.0100000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2011, 115, 13425-13442
CC5H11O2<=>CC5H10+HO2
+1.4760000E+009 +1.2100000E+000 +2.9800000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2011, 115, 13425-13442
DC5H11O2<=>CC5H10+HO2
+1.5180000E+007 +1.6600000E+000 +2.8400000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2011, 115, 13425-13442
!

!\REACTIONCLASS: \RO2+HO2<=>RO2H+O2 \A
\N \EA
!

AC5H11O2+HO2<=>AC5H11O2H+O2
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2+HO2<=>BC5H11O2H+O2
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H11O2+HO2<=>CC5H11O2H+O2
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H11O2+HO2<=>DC5H11O2H+O2
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+H2O2<=>RO2H+HO2 \A
\N \EA
!

AC5H11O2+H2O2<=>AC5H11O2H+HO2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2+H2O2<=>BC5H11O2H+HO2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H11O2+H2O2<=>CC5H11O2H+HO2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

DC5H11O2+H2O2<=>DC5H11O2H+HO2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+F<=>RO2H+R' \A
\N \EA
!

!\SITE: \PRIMARY

IC5H12+AC5H11O2<=>AC5H11+AC5H11O2H
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+BC5H11O2<=>AC5H11+BC5H11O2H
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+CC5H11O2<=>AC5H11+CC5H11O2H
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+DC5H11O2<=>AC5H11+DC5H11O2H
+1.2100000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+AC5H11O2<=>DC5H11+AC5H11O2H
+6.0480000E+012 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+BC5H11O2<=>DC5H11+BC5H11O2H
+6.0480000E+012 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+CC5H11O2<=>DC5H11+CC5H11O2H
+6.0480000E+012 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+DC5H11O2<=>DC5H11+DC5H11O2H
+6.0480000E+012 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

!\SITE: \SECONDARY

IC5H12+AC5H11O2<=>CC5H11+AC5H11O2H
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+BC5H11O2<=>CC5H11+BC5H11O2H
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+CC5H11O2<=>CC5H11+CC5H11O2H
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+DC5H11O2<=>CC5H11+DC5H11O2H
+4.0320000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

!\SITE: \TERTIARY

IC5H12+AC5H11O2<=>BC5H11+AC5H11O2H
+2.0160000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+BC5H11O2<=>BC5H11+BC5H11O2H
+2.0160000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+CC5H11O2<=>BC5H11+CC5H11O2H
+2.0160000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC5H12+DC5H11O2<=>BC5H11+DC5H11O2H
+2.0160000E+012 +0.0000000E+000 +1.6000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+CH3O2<=>RO+CH3O+O2 \A
\N \EA
!

AC5H11O2+CH3O2=>AC5H11O+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2+CH3O2=>BC5H11O+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H11O2+CH3O2=>CC5H11O+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H11O2+CH3O2=>DC5H11O+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+R'O2<=>RO+R'O+O2 \A
\N \EA
!

AC5H11O2+AC5H11O2=>AC5H11O+AC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H11O2+BC5H11O2=>AC5H11O+BC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H11O2+CC5H11O2=>AC5H11O+CC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H11O2+DC5H11O2=>AC5H11O+DC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2+BC5H11O2=>BC5H11O+BC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2+CC5H11O2=>BC5H11O+CC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2+DC5H11O2=>BC5H11O+DC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H11O2+CC5H11O2=>CC5H11O+CC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H11O2+DC5H11O2=>CC5H11O+DC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H11O2+DC5H11O2=>DC5H11O+DC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

!

!\REACTIONCLASS: \RO2H<=>RO+OH \A
\N \EA
!

AC5H11O2H<=>AC5H11O+OH
+3.0310000E+020 -1.4140000E+000 +4.6072100E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H11O2H<=>BC5H11O+OH
+8.6180000E+020 -1.6410000E+000 +4.5155600E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H11O2H<=>CC5H11O+OH
+1.1290000E+021 -1.5550000E+000 +4.5777400E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H11O2H<=>DC5H11O+OH
+3.5910000E+020 -1.4360000E+000 +4.6103700E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO_DECOMPOSITION \A
\N \EA
!

CH2O+SC4H9<=>AC5H11O
+5.0000000E+010 +0.0000000E+000 +2.3300000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C2H5+CH3COCH3<=>BC5H11O
+8.3300000E+009 +0.0000000E+000 +7.2400000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH3CHO+IC3H7<=>CC5H11O
+1.6650000E+010 +0.0000000E+000 +5.2300000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CH2O+IC4H9<=>DC5H11O
+5.0000000E+010 +0.0000000E+000 +2.3300000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \QOOH<=>CETH+OH \A
\N \EA
!

AC5H10OOH-A<=>A-AC5H10O+OH
+4.1000000E+010 +3.6000000E-001 +1.7200000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
AC5H10OOH-B<=>A-BC5H10O+OH
+7.1900000E+009 +8.8000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
AC5H10OOH-C<=>A-CC5H10O+OH
+1.7010000E+009 +7.3400000E-001 +1.4983000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
AC5H10OOH-D<=>A-DC5H10O+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089

BC5H10OOH-A<=>A-BC5H10O+OH
+1.0500000E+012 +1.5000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
BC5H10OOH-C<=>B-CC5H10O+OH
+4.2700000E+010 +5.2000000E-001 +8.8000000E+003 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
BC5H10OOH-D<=>B-DC5H10O+OH
+1.0300000E+010 +5.5000000E-001 +1.6200000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
CC5H10OOH-A<=>A-CC5H10O+OH
+3.7920000E+007 +1.5170000E+000 +1.6033000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
CC5H10OOH-B<=>B-CC5H10O+OH
+5.3600000E+010 +5.4000000E-001 +8.9000000E+003 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
CC5H10OOH-D<=>C-DC5H10O+OH
+1.5300000E+010 +6.4000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
DC5H10OOH-A<=>A-DC5H10O+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
DC5H10OOH-B<=>B-DC5H10O+OH
+2.8500000E+008 +9.2000000E-001 +1.3400000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
DC5H10OOH-C<=>C-DC5H10O+OH
+1.1200000E+010 +8.2000000E-001 +1.0900000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089

!

!\REACTIONCLASS: \QOOH<=>E+HO2

\A

\N

\EA

!

AC5H10OOH-B<=>AC5H10+HO2
+8.3800000E+009 +9.2000000E-001 +1.4500000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
BC5H10OOH-A<=>AC5H10+HO2
+3.8900000E+013 -1.5000000E-001 +1.5500000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
BC5H10OOH-C<=>BC5H10+HO2
+3.0100000E+011 +3.5000000E-001 +1.5200000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
CC5H10OOH-B<=>BC5H10+HO2
+9.7900000E+012 +4.0000000E-002 +1.5400000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089

CC5H10OOH-D<=>CC5H10+HO2
+6.8300000E+009 +9.2000000E-001 +1.5100000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
DC5H10OOH-C<=>CC5H10+HO2
+6.2400000E+010 +7.2000000E-001 +1.5000000E+004 !\AUTHOR: !\REF:S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
!

!\REACTIONCLASS: \QOOH_DECOMPOSITION \A
\N \EA
!

AC5H10OOH-C=>OH+CH2O+C4H8-2
+1.9600000E+009 +1.2000000E+000 +2.3400000E+004 !\AUTHOR: !\REF: S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
AC5H10OOH-A=>OH+CH2O+C4H8-1
+8.2830000E+013 -1.7000000E-001 +3.0090000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-D=>OH+CH3COCH3+C2H4
+1.1820000E+020 -2.0600000E+000 +2.4210000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-A=>OH+CH3CHO+C3H6
+3.5300000E+009 +1.2000000E+000 +2.1900000E+004 !\AUTHOR: !\REF: S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
DC5H10OOH-B=>OH+CH2O+IC4H8
+6.2700000E+008 +1.4000000E+000 +2.3600000E+004 !\AUTHOR: !\REF: S. M.
VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A
2012, 116, 5068-5089
!

!\REACTIONCLASS: \QOOH+O2<=>O2QOOH \A
\N \EA
!

AC5H10OOH-A+O2<=>AC5H10OOH-AO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
AC5H10OOH-B+O2<=>AC5H10OOH-BO2
+4.3900000E+011 +3.2500000E-001 -4.1730000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
AC5H10OOH-C+O2<=>AC5H10OOH-CO2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
AC5H10OOH-D+O2<=>AC5H10OOH-DO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
BC5H10OOH-A+O2<=>BC5H10OOH-AO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
BC5H10OOH-C+O2<=>BC5H10OOH-CO2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45

BC5H10OOH-D+O2<=>BC5H10OOH-DO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
CC5H10OOH-A+O2<=>CC5H10OOH-AO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
CC5H10OOH-B+O2<=>CC5H10OOH-BO2
+4.3900000E+011 +3.2500000E-001 -4.1730000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
CC5H10OOH-D+O2<=>CC5H10OOH-DO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
DC5H10OOH-A+O2<=>DC5H10OOH-AO2
+3.0890000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
DC5H10OOH-B+O2<=>DC5H10OOH-BO2
+4.3900000E+011 +3.2500000E-001 -4.1730000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
DC5H10OOH-C+O2<=>DC5H10OOH-CO2
+1.5690000E+014 -8.1600000E-001 -5.3650000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.45
!

!\REACTIONCLASS: \O2QOOH<=>EROOH+HO2 \A
\N \EA
!

AC5H10OOH-AO2<=>C5H9A-AOOH+HO2
+1.2600000E+008 +1.3200000E+000 +2.8900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-BO2<=>C5H9A-AOOH+HO2
+2.4480000E+010 +8.9000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-BO2<=>C5H9B-AOOH+HO2
+1.1240000E+011 +5.8000000E-001 +2.9600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-CO2<=>C5H9B-AOOH+HO2
+3.5000000E+010 +7.1000000E-001 +3.0100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-CO2<=>C5H9C-AOOH+HO2
+1.4760000E+009 +1.2100000E+000 +2.9800000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-DO2<=>C5H9C-AOOH+HO2
+1.5180000E+007 +1.6600000E+000 +2.8400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-CO2<=>C5H9C-BOOH+HO2
+1.4760000E+009 +1.2100000E+000 +2.9800000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-DO2<=>C5H9C-BOOH+HO2
+1.5180000E+007 +1.6600000E+000 +2.8400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-AO2<=>C5H9A-COOH+HO2
+1.2600000E+008 +1.3200000E+000 +2.8900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-BO2<=>C5H9A-COOH+HO2
+2.4480000E+010 +8.9000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

DC5H10OOH-AO2<=>C5H9A-DOOH+HO2
+1.2600000E+008 +1.3200000E+000 +2.8900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-BO2<=>C5H9A-DOOH+HO2
+2.4480000E+010 +8.9000000E-001 +2.9500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-BO2<=>C5H9B-DOOH+HO2
+1.1240000E+011 +5.8000000E-001 +2.9600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-CO2<=>C5H9B-DOOH+HO2
+3.5000000E+010 +7.1000000E-001 +3.0100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \O2QOOH<=>P(OOH)2 \A
\N \EA
!

AC5H10OOH-AO2<=>C5H9B-A, AOOH
+2.3090000E+009 +8.0000000E-001 +2.7100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-AO2<=>C5H9C-A, AOOH
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-AO2<=>C5H9D-A, AOOH
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-BO2<=>C5H9A-A, BOOH
+3.0140000E+009 +1.2000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-BO2<=>C5H9C-A, BOOH
+6.5130000E+009 +7.0000000E-001 +3.0100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-BO2<=>C5H9D-A, BOOH
+1.5040000E+008 +1.1000000E+000 +2.1900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-CO2<=>C5H9A-A, COOH
+2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-CO2<=>C5H9B-A, COOH
+7.4490000E+009 +6.0000000E-001 +2.7300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-CO2<=>C5H9D-A, COOH
+1.4580000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-DO2<=>C5H9A-A, DOOH
+2.4670000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-DO2<=>C5H9B-A, DOOH
+1.2310000E+007 +1.2000000E+000 +1.5400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
AC5H10OOH-DO2<=>C5H9C-A, DOOH
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-AO2<=>C5H9A-A, BOOH
+4.9100000E+007 +1.3000000E+000 +2.1500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

BC5H10OOH-AO2<=>C5H9C-A, BOOH
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-AO2<=>C5H9D-A, BOOH
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-CO2<=>C5H9A-B, COOH
+2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-CO2<=>C5H9D-B, COOH
+1.4580000E+009 +1.1000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-DO2<=>C5H9A-B, DOOH
+2.4670000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
BC5H10OOH-DO2<=>C5H9C-B, DOOH
+4.0090000E+008 +1.1000000E+000 +3.0100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-AO2<=>C5H9A-A, COOH
+4.9100000E+007 +1.3000000E+000 +2.1500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-AO2<=>C5H9B-A, COOH
+2.3090000E+009 +8.0000000E-001 +2.7100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-AO2<=>C5H9D-A, COOH
+1.2330000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-BO2<=>C5H9A-B, COOH
+3.0140000E+009 +1.2000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-BO2<=>C5H9D-B, COOH
+1.5040000E+008 +1.1000000E+000 +2.1900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-DO2<=>C5H9A-C, DOOH
+2.4670000E+006 +1.5000000E+000 +2.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
CC5H10OOH-DO2<=>C5H9B-C, DOOH
+1.2310000E+007 +1.2000000E+000 +1.5400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-AO2<=>C5H9A-A, DOOH
+4.9100000E+007 +1.3000000E+000 +2.1500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-AO2<=>C5H9B-A, DOOH
+2.3090000E+009 +8.0000000E-001 +2.7100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-AO2<=>C5H9C-A, DOOH
+1.3600000E+007 +1.3000000E+000 +1.8200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-BO2<=>C5H9A-B, DOOH
+3.0140000E+009 +1.2000000E+000 +3.3500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-BO2<=>C5H9C-B, DOOH
+6.5130000E+009 +7.0000000E-001 +3.0100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
DC5H10OOH-CO2<=>C5H9A-C, DOOH
+2.8770000E+007 +1.4000000E+000 +2.0800000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

DC5H10OOH-CO2<=>C5H9B-C, DOOH
+7.4490000E+009 +6.0000000E-001 +2.7300000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \O2QOOH<=>KET+OH \A
\N \EA
!

AC5H10OOH-AO2<=>IC5KETAA+OH
+5.1880000E+004 +1.9000000E+000 +1.8800000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
AC5H10OOH-BO2<=>IC5KETAB+OH
+2.4410000E+007 +1.6000000E+000 +2.7900000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
AC5H10OOH-CO2<=>IC5KETAC+OH
+1.0980000E+004 +2.4000000E+000 +1.9900000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
AC5H10OOH-DO2<=>IC5KETAD+OH
+4.7660000E+003 +1.7000000E+000 +1.6600000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
CC5H10OOH-AO2<=>IC5KETCA+OH
+5.7860000E+001 +2.9000000E+000 +1.7000000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
CC5H10OOH-BO2<=>IC5KETCB+OH
+1.7470000E+008 +1.7000000E+000 +2.6000000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
CC5H10OOH-DO2<=>IC5KETCD+OH
+2.7630000E+008 +1.2000000E+000 +2.5700000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
DC5H10OOH-AO2<=>IC5KETDA+OH
+4.7660000E+003 +1.7000000E+000 +1.6600000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
DC5H10OOH-BO2<=>IC5KETDB+OH
+1.0980000E+004 +2.4000000E+000 +1.9900000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
DC5H10OOH-CO2<=>IC5KETDC+OH
+2.4410000E+007 +1.6000000E+000 +2.7900000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
!

!\REACTIONCLASS: \P(OOH)2_DECOMPOSITION \A
\N \EA
!

C5H9A-A, COOH=>AC4H7OOH+CH2O+OH
+1.9780000E+008 +1.5210000E+000 +2.1890000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-A, DOOH<=>AC3H5OOH+C2H4O2H
+1.9780000E+008 +1.5210000E+000 +2.1890000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-C, DOOH=>C3H6+HO2CH2CHO+OH
+3.5300000E+009 +1.2000000E+000 +2.1900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A, AOOH=>C4H72-1OOH+CH2O+OH
+1.9600000E+009 +1.2000000E+000 +2.3400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H9D-A, AOOH=>AC3H5OOH+C2H4+HO2
+1.9780000E+008 +1.5210000E+000 +2.1890000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-A, BOOH=>IC3H5O+C2H4+HO2
+1.9600000E+009 +1.2000000E+000 +2.3400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!\WARNING: KPS \MISCELLANEOUS REACTION. WHERE DO WE PUT THIS??
!

!\REACTIONCLASS: \KET_DECOMPOSITION \A
\N \EA
!

IC5KETAA<=>IC5KETAAO+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETAB<=>IC5KETABO+OH
+6.0000000E+015 +0.0000000E+000 +4.1200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETAC<=>IC5KETACO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETAD<=>IC5KETADO+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETCA<=>IC5KETCAO+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETCB<=>IC5KETCBO+OH
+6.0000000E+015 +0.0000000E+000 +4.1200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETCD<=>IC5KETCDO+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETDA<=>IC5KETDAO+OH
+1.5000000E+016 +0.0000000E+000 +4.2000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETDB<=>IC5KETDBO+OH
+6.0000000E+015 +0.0000000E+000 +4.1200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETDC<=>IC5KETDCO+OH
+1.0500000E+016 +0.0000000E+000 +4.1600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC5KETAAO<=>CH2O+C3H6CHO-3
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETABO<=>C2H5COCH3+HCO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETACO<=>CH3CHO+CH3CHCHO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETADO<=>CH2O+IC3H6CHO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETCAO<=>CH2O+CH3CHCOCH3
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471

IC5KETCBO<=>CH3COCH3+CH3CO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETCDO<=>CH2O+IC3H7CO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETDAO<=>CH2O+C3H6CHO-2
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETDBO<=>CH3COCH3+CH2CHO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471
IC5KETDCO<=>IC3H7CHO+HCO
+2.9000000E+012 +3.8000000E-001 +1.1080000E+004 !\AUTHOR: !\REF:O.
HERBINET ET AL. COMBUST. FLAME 2012, 159, 3455-3471

!

!\REACTIONCLASS: \P(OOH)2<=>EROOH+HO2 \A
\N \EA

!

C5H9A-A,BOOH<=>C5H9A-AOOH+HO2
+3.8900000E+013 -1.5000000E-001 +1.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-B,COOH<=>C5H9A-COOH+HO2
+3.8900000E+013 -1.5000000E-001 +1.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-B,DOOH<=>C5H9A-DOOH+HO2
+3.8900000E+013 -1.5000000E-001 +1.5500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A,AOOH<=>C5H9A-AOOH+HO2
+1.6760000E+010 +9.2000000E-001 +1.4500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A,COOH<=>C5H9A-COOH+HO2
+8.3800000E+009 +9.2000000E-001 +1.4500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A,COOH<=>C5H9B-AOOH+HO2
+9.7900000E+012 +4.0000000E-002 +1.5400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A,DOOH<=>C5H9A-DOOH+HO2
+8.3800000E+009 +9.2000000E-001 +1.4500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-C,DOOH<=>C5H9B-DOOH+HO2
+9.7900000E+012 +4.0000000E-002 +1.5400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A,BOOH<=>C5H9B-AOOH+HO2
+3.0100000E+011 +3.5000000E-001 +1.5200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A,DOOH<=>C5H9C-AOOH+HO2
+6.2400000E+010 +7.2000000E-001 +1.5000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-B,DOOH<=>C5H9B-DOOH+HO2
+3.0100000E+011 +3.5000000E-001 +1.5200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-B,DOOH<=>C5H9C-BOOH+HO2
+6.2400000E+010 +7.2000000E-001 +1.5000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H9D-A, COOH<=>C5H9C-AOOH+HO2
+6.8300000E+009 +9.2000000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-B, COOH<=>C5H9C-BOOH+HO2
+6.8300000E+009 +9.2000000E-001 +1.5100000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \EROOH_DECOMPOSITION \A
\N \EA
!

C5H9A-AOOH=>CH2O+C4H71-2+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-COOH=>CH3CHO+C3H5-T+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-DOOH=>CH2O+IC4H7+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-AOOH=>CH2O+C4H72-2+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-DOOH=>CH2O+IC4H7+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-AOOH=>CH2O+C4H71-3+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-BOOH=>CH3COCH3+C2H3+OH
+6.0000000E+015 +0.0000000E+000 +4.2200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \P(OOH)2<=>CETH-OOH+OH \A
\N \EA
!

C5H9A-A, BOOH<=>C5H9OA-AOOH-B+OH
+4.1000000E+010 +3.6000000E-001 +1.7200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-A, BOOH<=>C5H9OA-BOOH-A+OH
+1.0500000E+012 +1.5000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-A, COOH<=>C5H9OA-AOOH-C+OH
+4.1000000E+010 +3.6000000E-001 +1.7200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-A, COOH<=>C5H9OA-COOH-A+OH
+3.7920000E+007 +1.5170000E+000 +1.6033000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-A, DOOH<=>C5H9OA-AOOH-D+OH
+4.1000000E+010 +3.6000000E-001 +1.7200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-A, DOOH<=>C5H9OA-DOOH-A+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H9A-B, COOH<=>C5H9OA-BOOH-C+OH
+1.0500000E+012 +1.5000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-B, COOH<=>C5H9OA-COOH-B+OH
+3.7920000E+007 +1.5170000E+000 +1.6033000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-B, DOOH<=>C5H9OA-BOOH-D+OH
+1.0500000E+012 +1.5000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-B, DOOH<=>C5H9OA-DOOH-B+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-C, DOOH<=>C5H9OA-COOH-D+OH
+3.7920000E+007 +1.5170000E+000 +1.6033000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9A-C, DOOH<=>C5H9OA-DOOH-C+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A, AOOH<=>C5H9OA-BOOH-A+OH
+7.1900000E+009 +8.8000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A, COOH<=>C5H9OA-BOOH-C+OH
+7.1900000E+009 +8.8000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A, COOH<=>C5H9OB-COOH-A+OH
+5.3600000E+010 +5.4000000E-001 +8.9000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A, DOOH<=>C5H9OA-BOOH-D+OH
+7.1900000E+009 +8.8000000E-001 +9.6000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-A, DOOH<=>C5H9OB-DOOH-A+OH
+2.8500000E+008 +9.2000000E-001 +1.3400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-C, DOOH<=>C5H9OB-COOH-D+OH
+5.3600000E+010 +5.4000000E-001 +8.9000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9B-C, DOOH<=>C5H9OB-DOOH-C+OH
+2.8500000E+008 +9.2000000E-001 +1.3400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A, AOOH<=>C5H9OA-COOH-A+OH
+1.7010000E+009 +7.3400000E-001 +1.4983000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A, BOOH<=>C5H9OA-COOH-B+OH
+1.7010000E+009 +7.3400000E-001 +1.4983000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A, BOOH<=>C5H9OB-COOH-A+OH
+4.2700000E+010 +5.2000000E-001 +8.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A, DOOH<=>C5H9OA-COOH-D+OH
+1.7010000E+009 +7.3400000E-001 +1.4983000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-A, DOOH<=>C5H9OC-DOOH-A+OH
+1.1200000E+010 +8.2000000E-001 +1.0900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9C-B, DOOH<=>C5H9OB-COOH-D+OH
+4.2700000E+010 +5.2000000E-001 +8.8000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H9C-B, DOOH<=>C5H9OC-DOOH-B+OH
+1.1200000E+010 +8.2000000E-001 +1.0900000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-A, AOOH<=>C5H9OA-DOOH-A+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-A, BOOH<=>C5H9OA-DOOH-B+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-A, BOOH<=>C5H9OB-DOOH-A+OH
+1.0300000E+010 +5.5000000E-001 +1.6200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-A, COOH<=>C5H9OA-DOOH-C+OH
+5.2000000E+008 +6.7000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-A, COOH<=>C5H9OC-DOOH-A+OH
+1.5300000E+010 +6.4000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-B, COOH<=>C5H9OB-DOOH-C+OH
+1.0300000E+010 +5.5000000E-001 +1.6200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9D-B, COOH<=>C5H9OC-DOOH-B+OH
+1.5300000E+010 +6.4000000E-001 +1.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \CETH-OOH_DECOMPOSITION \A
\N \EA
!

C5H9OA-AOOH-B=>CH2O+C2H5COCH2+OH
+6.0000000E+015 +0.0000000E+000 +4.2200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-BOOH-A=>CH2O+C2H5COCH2+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-AOOH-C=>CH3CHO+C3H5O+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-COOH-A=>CH2O+C4H71-O+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-AOOH-D=>CH2O+AC3H5OCH2+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-DOOH-A=>CH2O+C4H7O1-4+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-BOOH-C=>CH3CHO+CH3COCH2+OH
+1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-COOH-B=>CH3CHO+CH3COCH2+OH
+6.0000000E+015 +0.0000000E+000 +4.2200000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C5H9OA-BOOH-D=>CH2O+IC4H7O+OH
+1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

C5H9OA-DOOH-B<=>CH3COCH2OCH2CH2+OH
 +6.0000000E+015 +0.0000000E+000 +4.2200000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OA-COOH-D=>CH2O+IC3H6CHO+OH
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OA-DOOH-C=>CH2O+IC3H6CHO+OH
 +1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OB-COOH-A=>CH2O+CH3CHCOCH3+OH
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OB-DOOH-A=>CH2O+CH2CH2COCH3+OH
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OB-COOH-D=>CH2O+TC3H6CHO+OH
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OB-DOOH-C=>CH3COCH3+CH2CHO+OH
 +1.0500000E+016 +0.0000000E+000 +4.2600000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OC-DOOH-A=>CH2O+C4H7O2-1+OH
 +1.5000000E+016 +0.0000000E+000 +4.3000000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C5H9OC-DOOH-B=>CH3COCH3+CH2CHO+OH
 +6.0000000E+015 +0.0000000E+000 +4.2200000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 !\WARNING: KPS \MISC
 CH3COCH2OCH2CH2=>CH2O+C2H4+CH3CO
 +1.6000000E+013 +0.0000000E+000 +2.5500000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 !

!\REACTIONCLASS: \CETH_DECOMPOSITION \A
 \N \EA
 !

A-AC5H10O+OH=>CH2O+C4H71-2+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 A-BC5H10O+OH=>IC3H5CHO+CH3+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 A-CC5H10O+OH=>C3H6+CH3CO+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 A-DC5H10O+OH=>C3H6+CH2CHO+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 B-CC5H10O+OH=>IC3H5COCH3+H+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 B-DC5H10O+OH=>IC4H8+HCO+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 C-DC5H10O+OH=>CH2CO+IC3H7+H2O
 +2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:

A-AC5H100+OH=>C2H3CHO+C2H5+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-BC5H100+OH=>CH2O+C4H72-2+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-CC5H100+OH=>C3H5-T+CH3CHO+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-DC5H100+OH=>CH3CHCHO+C2H4+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
B-CC5H100+OH=>IC3H5CHO+CH3+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
B-DC5H100+OH=>CH3COCH3+C2H3+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C-DC5H100+OH=>SC3H5CHO+CH3+H2O
+2.5000000E+012 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-AC5H100+HO2=>CH2O+C4H71-2+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-BC5H100+HO2=>IC3H5CHO+CH3+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-CC5H100+HO2=>C3H6+CH3CO+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-DC5H100+HO2=>C3H6+CH2CHO+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
B-CC5H100+HO2=>IC3H5COCH3+H+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
B-DC5H100+HO2=>IC4H8+HCO+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C-DC5H100+HO2=>CH2CO+IC3H7+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-AC5H100+HO2=>C2H3CHO+C2H5+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-BC5H100+HO2=>CH2O+C4H72-2+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-CC5H100+HO2=>C3H5-T+CH3CHO+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
A-DC5H100+HO2=>CH3CHCHO+C2H4+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
B-CC5H100+HO2=>IC3H5CHO+CH3+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

B-DC5H10O+HO2=>CH3COCH3+C2H3+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
C-DC5H10O+HO2=>SC3H5CHO+CH3+H2O2
+5.0000000E+012 +0.0000000E+000 +1.7700000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

!=====
=====

!\SUBSPECIES: \IC3H5COCH3

!=====
=====

!

!\REACTIONCLASS: \MISC \A
\N \EA

!

IC3H5COCH3<=>IC3H5CO+CH3
+1.9030000E+022 -1.7520000E+000 +8.3625500E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3<=>C3H5-T+CH3CO
+6.0700000E+024 -2.2100000E+000 +9.6960000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+OH<=>IC3H5COCH2+H2O
+5.1000000E+011 +0.0000000E+000 +1.1920000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+O<=>IC3H5COCH2+OH
+5.0000000E+012 +0.0000000E+000 +5.9620000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+H<=>IC3H5COCH2+H2
+9.3000000E+012 +0.0000000E+000 +6.3570000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+CH3<=>IC3H5COCH2+CH4
+1.6200000E+011 +0.0000000E+000 +9.6300000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+HO2<=>IC3H5COCH2+H2O2
+8.5000000E+012 +0.0000000E+000 +2.0460000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+O2<=>IC3H5COCH2+HO2
+6.0000000E+013 +0.0000000E+000 +4.6000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH2<=>C3H5-T+CH2CO
+5.9720000E+014 +1.8800000E-001 +5.1272000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+OH<=>AC3H4COCH3+H2O
+3.1200000E+006 +2.0000000E+000 -2.9800000E+002 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+O<=>AC3H4COCH3+OH
+6.0300000E+010 +7.0000000E-001 +7.6330000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+H<=>AC3H4COCH3+H2
+1.7300000E+005 +2.5000000E+000 +2.4920000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
IC3H5COCH3+CH3<=>AC3H4COCH3+CH4
+2.2100000E+000 +3.5000000E+000 +5.6750000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

IC3H5COCH3+HO2<=>AC3H4COCH3+H2O2
 +9.6400000E+003 +2.6000000E+000 +1.3910000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 IC3H5COCH3+O2<=>AC3H4COCH3+HO2
 +6.0300000E+013 +0.0000000E+000 +4.7590000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 AC3H4COCH3<=>C3H4-A+CH3CO
 +1.4000000E+013 +0.0000000E+000 +6.0000000E+004 !\AUTHOR: !\REF:
 WARNING NO REFERENCE !\COMMENT:
 !=====

!\SUBSPECIES: \IC3H5COCH3
 !=====

!-----
 !-----
 !\ENDSUBMECH: \IC5H12
 !-----
 !-----
 !-----
 !\SUBMECH: \NEOC5H12
 !\MECHCOMMENTS:
 !\MECHWARNINGS: THE SPECIES IC4H6Q2-II DOES NOT APPEAR TO HAVE ANY
 FORMATION PATHWAY IN C0-C4 OR PENTANE PARTS OF C5 MODULE, JB, CAN YOU
 EXPLAIN?
 !-----
 !-----
 !-----
 !-----

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

NEOC5H12<=>TC4H9+CH3
 +1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: JB 7
 /10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
 CONSTANTS CALCULATED BY BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
 MILLE
 PLOG / +1.0000000E-002
 +2.5700000E+105 -2.6530000E+001 +1.2382600E+005 /
 PLOG / +1.0000000E-001
 +1.6000000E+101 -2.4970000E+001 +1.2457500E+005 /
 PLOG / +3.0000000E-001
 +8.9400000E+097 -2.3870000E+001 +1.2419000E+005 /
 PLOG / +1.0000000E+000
 +2.3600000E+093 -2.2400000E+001 +1.2310200E+005 /
 PLOG / +2.0000000E+000
 +1.7900000E+090 -2.1410000E+001 +1.2214000E+005 /
 PLOG / +5.0000000E+000
 +4.0000000E+085 -1.9970000E+001 +1.2047500E+005 /
 PLOG / +1.0000000E+001
 +4.9900000E+081 -1.8770000E+001 +1.1891300E+005 /
 PLOG / +2.0000000E+001
 +3.1000000E+077 -1.7490000E+001 +1.1709500E+005 /
 PLOG / +5.0000000E+001
 +3.5500000E+071 -1.5710000E+001 +1.1433700E+005 /

PLOG / +1.0000000E+002
+7.5700000E+066 -1.4320000E+001 +1.1204100E+005 /
NEOC5H12<=>NEOC5H11+H
+1.0000000E+000 +1.0000000E+000 +1.0000000E+000 !\AUTHOR: !\REF: JB 7
/10 /2013 !\COMMENT: !PRESSURE DEPENDENT UNIMOLECULAR DECOMPOSITION RATE
CONSTANTS CALCULATED BY BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLE
PLOG / +1.0000000E-002
+1.0200000E+082 -2.0610000E+001 +1.2368700E+005 /
PLOG / +1.0000000E-001
+8.0200000E+083 -2.0760000E+001 +1.2766000E+005 /
PLOG / +3.0000000E-001
+2.9300000E+083 -2.0440000E+001 +1.2899800E+005 /
PLOG / +1.0000000E+000
+7.7400000E+081 -1.9790000E+001 +1.2993100E+005 /
PLOG / +2.0000000E+000
+2.9000000E+080 -1.9260000E+001 +1.3019100E+005 /
PLOG / +5.0000000E+000
+9.0400000E+077 -1.8400000E+001 +1.3016200E+005 /
PLOG / +1.0000000E+001
+3.4400000E+075 -1.7600000E+001 +1.2979200E+005 /
PLOG / +2.0000000E+001
+4.1700000E+072 -1.6670000E+001 +1.2906300E+005 /
PLOG / +5.0000000E+001
+9.6200000E+067 -1.5220000E+001 +1.2749400E+005 /
PLOG / +1.0000000E+002
+8.7600000E+063 -1.3990000E+001 +1.2585800E+005 /
!

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

!\SITE: \PRIMARY
NEOC5H12+O2<=>NEOC5H11+HO2
+8.4000000E+013 +0.0000000E+000 +5.2800000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+O<=>NEOC5H11+OH
+2.2600000E+014 +0.0000000E+000 +7.8500000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+H<=>NEOC5H11+H2
+6.9800000E+005 +2.6900000E+000 +6.4500000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+OH<=>NEOC5H11+H2O
+6.5670000E+007 +1.7630000E+000 +7.4320000E+002 !\AUTHOR: !\REF: R.
SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060
NEOC5H12+HO2<=>NEOC5H11+H2O2
+8.1600000E+001 +3.5900000E+000 +1.7160000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+CH3<=>NEOC5H11+CH4
+1.8080000E+000 +3.6500000E+000 +7.1540000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+CH3O<=>NEOC5H11+CH3OH
+6.0000000E+011 +0.0000000E+000 +7.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+CH3O2<=>NEOC5H11+CH3O2H
+2.7720000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

NEOC5H12+C2H5<=>NEOC5H11+C2H6
+2.0000000E+011 +0.0000000E+000 +1.3400000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+C2H3<=>NEOC5H11+C2H4
+2.0000000E+012 +0.0000000E+000 +1.8000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+O2CHO<=>NEOC5H11+HO2CHO
+2.7720000E+000 +3.9700000E+000 +1.8280000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+IC4H6OH<=>NEOC5H11+IC4H7OH
+9.4000000E+002 +3.3000000E+000 +1.9840000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+IC4H7O<=>NEOC5H11+IC4H7OH
+5.4000000E+011 +0.0000000E+000 +4.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+TC3H6CHO<=>NEOC5H11+IC3H7CHO
+9.4000000E+002 +3.3000000E+000 +1.9840000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H12+CH2CCH2OH<=>NEOC5H11+C3H5OH
+1.5900000E+012 +0.0000000E+000 +2.0500000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:

!

!\REACTIONCLASS: \RADICAL_BETA_SCISSION \A
\N \EA

!

NEOC5H11<=>IC4H8+CH3
+3.6520000E+018 -1.3370000E+000 +3.3461500E+004 !\AUTHOR: !\REF:H. J.
CURRAN INT. J. CHEM. KIN. 2006, 38, 4, 250-275 !\COMMENT: !ADDITION
DIRECTION ESTIMATE USED FROM REFERENCE. DECOMPOSITION K FROM THERMO. P
DEPENDENCE TREATED USING QRRK /MSC.

PLOG / +1.0000000E-002
+2.7500000E+032 -6.6600000E+000 +3.1143000E+004 /
PLOG / +1.0000000E-001
+2.6500000E+037 -7.6800000E+000 +3.6912000E+004 /
PLOG / +1.0000000E+000
+6.5300000E+039 -7.9800000E+000 +4.1554000E+004 /
PLOG / +2.0000000E+000
+1.0500000E+040 -7.9400000E+000 +4.2640000E+004 /
PLOG / +5.0000000E+000
+1.1900000E+040 -7.8300000E+000 +4.3859000E+004 /
PLOG / +1.0000000E+001
+1.1300000E+040 -7.7500000E+000 +4.4627000E+004 /
PLOG / +2.0000000E+001
+1.1500000E+040 -7.6900000E+000 +4.5269000E+004 /
PLOG / +5.0000000E+001
+1.4400000E+040 -7.6600000E+000 +4.5920000E+004 /
PLOG / +1.0000000E+002
+1.8100000E+040 -7.6700000E+000 +4.6255000E+004 /

!

!\REACTIONCLASS: \R+O2<=>RO2 \A
\N \EA

!

NEOC5H11+O2<=>NEOC5H11O2
+6.8650000E+016 -1.6270000E+000 +1.9870000E+002 !\AUTHOR: !\REF:A.
MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !\COMMENT:
!

!\REACTIONCLASS: \R+R'O2<=>RO+R'O \A
\N \EA
!

NEOC5H11+HO2<=>NEOC5H11O+OH
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H11+CH3O2<=>NEOC5H11O+CH3O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
NEOC5H11+NEOC5H11O2<=>NEOC5H11O+NEOC5H11O
+9.0000000E+012 +0.0000000E+000 -1.0000000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2<=>QOOH \A
\N \EA
!

NEOC5H11O2<=>NEOC5H10OOH
+1.1980000E+009 +1.2000000E+000 +2.1600000E+004 !\AUTHOR: !\REF:S.
SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701
!

!\REACTIONCLASS: \RO2+HO2<=>RO2H+O2 \A
\N \EA
!

NEOC5H11O2+HO2<=>NEOC5H11O2H+O2
+1.7500000E+010 +0.0000000E+000 -3.2750000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+H2O2<=>RO2H+HO2 \A
\N \EA
!

NEOC5H11O2+H2O2<=>NEOC5H11O2H+HO2
+2.4000000E+012 +0.0000000E+000 +1.0000000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+F<=>RO2H+R' \A
\N \EA
!

!\SITE: \PRIMARY
NEOC5H12+NEOC5H11O2<=>NEOC5H11+NEOC5H11O2H
+2.4190000E+013 +0.0000000E+000 +2.0430000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+CH3O2<=>RO+CH3O+O2 \A
\N \EA
!

NEOC5H11O2+CH3O2=>NEOC5H11O+CH3O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2+R'O2<=>RO+R'O+O2 \A
\N \EA
!

NEOC5H11O2+NEOC5H11O2=>NEOC5H11O+NEOC5H11O+O2
+1.4000000E+016 -1.6100000E+000 +1.8600000E+003 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO2H<=>RO+OH \A
\N \EA
!

NEOC5H11O2H<=>NEOC5H11O+OH
+2.0940000E+017 -4.0000000E-001 +4.5110000E+004 !\AUTHOR: !\REF:
WARNING NO REFERENCE !\COMMENT:
!

!\REACTIONCLASS: \RO_DECOMPOSITION \A
\N \EA
!

END