


```
!+++++
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!\SPECIES_MODULE: \H2_O2
!\MODSUBMECHS: \H2 \O2 \H2O \H2O2
!+++++
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!-----
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!\SUBMECH: \H2
!-----
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!\PYROSPEC:
H2 H
!-----
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!-----
!\SUBMECH: \O2
!-----
-----
!\PYROSPEC:
O2 O
!-----
-----
!-----
!\SUBMECH: \H2O
!-----
-----
!\PYROSPEC:
H2O OH OHV
!-----
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!-----
!\SUBMECH: \H2O2
!-----
-----
!\PYROSPEC:
H2O2 HO2
!-----
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!+++++
+++++
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!\END_SPECIES_MODULE: \H2_O2
!+++++
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!+++++
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!\SPECIES_MODULE: \C1
!\MODSUBMECHS: \CO \CH4 \CH3OH \CH2O
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!+++++
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!-----
-----
!\SUBMECH: \CO
!-----
-----
!\PYROSPEC:
CO CO2
!\OXIDSPEC:
HOCO
!-----
-----
!-----
!\SUBMECH: \CH4
!-----
-----
!\PYROSPEC:
CH4 CH3 CH2 CH2(S) C CH CHV
!\OXIDSPEC:
CH3O2H CH3O2 CH2O2H
!-----
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!-----
!\SUBMECH: \CH3OH
!-----
-----
!\PYROSPEC:
CH3OH CH3O CH2OH
!\OXIDSPEC:
!-----
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!-----
!\SUBMECH: \CH2O
!-----
-----
!\PYROSPEC:
CH2O HCO HCOH
!\OXIDSPEC:
HO2CHO HOCH2O2H HOCH2O2 OCH2O2H HOCH2O O2CHO HOCHO OCHO
!-----
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!+++++
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!\END_SPECIES_MODULE: \C1
!+++++
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!+++++
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!\SPECIES_MODULE: \C2
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!\MODSUBMECHS: \C2H6 \CH3CHO \CH2CO \C2H4 \C2H2 \C2H5OH \CH3OCH3 \CH3OCHO
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!\SUBMECH: \C2H6

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!\PYROSPEC:

C2H6 C2H5

!\OXIDSPEC:

C2H5O2H C2H5O2

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!-----

!\SUBMECH: \C2H4

!-----

!\PYROSPEC:

C2H4 C2H3

!\OXIDSPEC:

CHOCHO C2H3OOH C2H3OO CHCHO

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!\SUBMECH: \C2H2

!-----

!\PYROSPEC:

C2H2 C2H H2CC

!\OXIDSPEC:

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!\SUBMECH: \C2H5OH

!-----

!\PYROSPEC:

C2H5OH C2H5O PC2H4OH SC2H4OH

!\OXIDSPEC:

O2C2H4OH C2H4O2H C2H4O1-2 C2H3O1-2

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!\SUBMECH: \CH3CHO

!-----

!\PYROSPEC:

CH3CHO CH3CO CH2CHO

!\OXIDSPEC:

O2CH2CHO HO2CH2CO

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!\SUBMECH: \C2H3OH
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!\PYROSPEC:
C2H3OH C2H2OH
!\OXIDSPEC:
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!-----
-----
!\SUBMECH: \CH2CO
!-----
-----
!\PYROSPEC:
CH2CO HCCO HCCOH
!\OXIDSPEC:
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!-----
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!\SUBMECH: \ACID
!-----
-----
!\PYROSPEC:
!\OXIDSPEC:
CH3CO3H CH3CO3 CH3CO2
!-----
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!-----
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!\SUBMECH: \CH3OCH3
!-----
-----
!\PYROSPEC:
CH3OCH3 CH3OCH2
!\OXIDSPEC:
CH3OCH2O2H CH3OCH2O2 CH2OCH2O2H O2CH2OCH2O2H HO2CH2OCHO OCH2OCHO HOCH2OCO
CH3OCH2O
!-----
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!-----
-----
!\SUBMECH: \CH3OCHO
!-----
-----
!\PYROSPEC:
CH3OCHO CH3OCO CH2OCHO
!\OXIDSPEC:
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!+++++
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!\END_SPECIES_MODULE: \C2
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!+++++
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!\SPECIES_MODULE: \C3
!\MODSUBMECHS: \CH3COCH3 \C2H3CHO \C2H5CHO \C3H8 \C3H6 \C3H4-A \C3H4-P
!+++++
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!\SUBMECH: \C3H8
!-----
-----
!\PYROSPEC:
C3H8 IC3H7 NC3H7
!\OXIDSPEC:
NC3H7O2H NC3H7O2 IC3H7O2H IC3H7O2 NC3H7O IC3H7O C3H6OOH1-2 C3H6OOH1-3
C3H6OOH2-1 C3H6OOH1-2O2 C3H6OOH1-3O2 C3H6OOH2-1O2 C3KET12 C3KET13 C3H51-
2,3OOH C3H52-1,3OOH C3H5O1-2OOH-3 C3H5O1-3OOH-2 C3H6O1-2 C3H6O1-3
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!\SUBMECH: \C3H6
!-----
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!\PYROSPEC:
C3H6 C3H5-A C3H5-S C3H5-T CC3H6
!\OXIDSPEC:
C3H5O CH2CHOCH2 CH3CHCHO AC4H7OOH C3H6OH1-2 CH3CHCO AC3H5OOH
C3H6OH2-1 HOC3H6O2
SC3H5OH IC3H5OH C3H5OH CH2CCH2OH
!-----
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!-----
-----
!\SUBMECH: \C3H4-A\C3H4-P
!-----
-----
!\PYROSPEC:
C3H4-P C3H4-A C3H3 CC3H4 C3H2 H2CCC(S) C3H2(S) C3H2C
!\OXIDSPEC:
PC3H4OH-2 SC3H4OH C3H3O C3H3O2H C2HCHO
!-----
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!-----
-----
!\SUBMECH: \C2H5CHO
!-----
-----
!\PYROSPEC:
C2H5CHO C2H5CO CH2CH2CHO C2H3CHO C2H3CO
!\OXIDSPEC:
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!\SUBMECH: \CH3COCH3
!-----
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!\PYROSPEC:
CH3COCH3 CH3COCH2
!\OXIDSPEC:
CH3COCH2O2 CH3COCH2O C3KET21
!-----
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!+++++
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!\END_SPECIES_MODULE: \C3
!+++++
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!+++++
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!\SPECIES_MODULE: \C4
!\MODSUBMECHS: \C4H10 \IC4H10 \IC4H8 \C4H8-1 \C4H8-2 \C4H6 \C4H612 \C4H6-
2 \C4H4 \C4H2 \NC3H7CHO \C2H5COCH3
!+++++
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!-----
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!\SUBMECH: \C4H10
!-----
-----
!\PYROSPEC:
C4H10 PC4H9 SC4H9
!\OXIDSPEC:
PC4H9O SC4H9O PC4H9O2 SC4H9O2 PC4H9O2H SC4H9O2H
C4H8OOH1-2 C4H8OOH1-3 C4H8OOH1-4 C4H8OOH2-1 C4H8OOH2-3 C4H8OOH2-4
C4H8O1-2 C4H8O1-3 C4H8O1-4 C4H8O2-3
C4H8OOH1-2O2 C4H8OOH1-3O2 C4H8OOH1-4O2 C4H8OOH2-1O2 C4H8OOH2-3O2
C4H8OOH2-4O2
C4H71-2,4OOH C4H72-1,3OOH C4H72-1,4OOH C4H71-2,3OOH
C4H7O1-3OOH-4 C4H7O1-3OOH-2
C4H7O1-2OOH-4 C4H7O1-4OOH-2 C4H7O1-2OOH-3 C4H7O2-3OOH-1 C4H72-1OOH
NC4KET12 NC4KET13 NC4KET14 NC4KET21 NC4KET23 NC4KET24
C4H71-3OOH C4H71-3,4OOH C4H72-3,4OOH HO2CH2CHO
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!-----
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!\SUBMECH: \IC4H10
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!\PYROSPEC:
IC4H10 IC4H9 TC4H9
!\OXIDSPEC:

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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
 !-----

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 !\SUBMECH: \IC4H8
 !-----

 !\PYROSPEC:
 IC4H8 IC4H7 IC4H7-I1
 !\OXIDSPEC:
 IC4H7O2 IC4H6OOH-I CCYCCOOC-T1 C2CYCOOC-I1 IC4H7O CVCYCCOC CCYC2OCO
 CCYCCOOC-I2
 CHOIC3H6O IC3H5OOCH2 CCYCCO-T1
 IC4H8OH-IT IC4H8OH-TI IC4H7OH IC4H8OH IC4H6OH
 TQJC4H8OH TQC4H8OI QC4H7OHP TQC4H7OHI CCY(CCO)COH C2CY(COC)OH IQJC4H8OH
 IC3H6OHCHO IQC4H8OT IQC4H7OHT
 CCY(CCO)OH CH2COHCH2OOH
 TC3H6OH
 TQC4H7OHIO2 TQC4H7OHTO2 TQC4H7OHIQ-I TQC4H7OHIQ-P
 IC3H5COHQ CH2CQCOHQ IC3H5Q COHQCYC(COC) QCYC(CCO)OH HOCOCQ(CH3)2
 IQC4H7OHTO2 IQC4H8OTQ-I IQC4H7OHTQ-P CHOC(CH3)OHCH2Q CO(CH2OOH)2
 CH3COCHO IC3H5OCH2 IC4H7OOCH3 IC4H7OOIC4H7
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 !\SUBMECH: \C4H8-1\C4H8-2
 !-----

 !\PYROSPEC:
 C4H8-1 C4H8-2 C4H71-1 C4H71-2 C4H71-3 C4H71-4 C4H72-2
 !\OXIDSPEC:
 C4H71-O PC4H8OH-2 SC4H8OH-1 SC4H8OH-3
 C4H71-3OH C4H71-4OH C4H71-1OH C4H71-2OH C4H72-1OH C4H72-2OH
 SQC4H8OP PQC4H8OS
 PQC4H7OHS-3
 NC4KET12OH SQC4H7OHS-4
 SQC4H8OS NC4KET23OH SC4H8OH-3O2 CCY(COCC)OH
 C4H7O2-1 C4H6-1 AC3H5OCH2 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
 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		

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!\SUBMECH: \C4H6\C4H612\C4H6-2\C4H4\C4H2

!-----

!\PYROSPEC:

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

!\OXIDSPEC:

C4H6O25 C2H3CHOCH2 C4H4O C4H6O23 CH2CHCHCHO H2C4O

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!\SUBMECH: \NC3H7CHO

!-----

!\PYROSPEC:

NC3H7CHO NC3H7CO C3H6CHO-1 C3H6CHO-2 C3H6CHO-3 SC3H5CHO SC3H5CO

!\OXIDSPEC:

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!-----

!\SUBMECH: \C2H5COCH3

!-----

!\PYROSPEC:

C2H5COCH3 C2H5COCH2 CH2CH2COCH3 CH3CHCOCH3 C2H3COCH3

!\OXIDSPEC:

CH3CHOOCOCH3 CH2CHOOHCOCH3

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!\SUBMECH: \C2H5CHCO

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!\PYROSPEC:

C2H5CHCO

!\OXIDSPEC:

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!+++++
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!\END_SPECIES_MODULE: \C4
!+++++
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!+++++
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!\SPECIES_MODULE: \C5
!\MODSUBMECHS: \NC5H12 \IC5H12 \NEOC5H12 \AC5H10 \BC5H10 \CC5H10 \B13DE2M
\TC4H8CHO \PC4H8CHO-1\PC4H8CHO-2\PC4H8CHO-3 \C5H9O12-5\C5H9O13-5\C5H9O14-
5\C5H9O23-1\C5H9O23-5\C5H9O24-1\NC3H7COCH3\C2H5COC2H5
!+++++
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!-----
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!\SUBMECH: \NC5H12
!-----
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!\PYROSPEC:
NC5H12 C5H11-1 C5H11-2 C5H11-3
!\OXIDSPEC:
C5H11O2H-1 C5H11O2H-2 C5H11O2H-3 C5H11O2-1 C5H11O2-2 C5H11O2-3 C5H11O-1
C5H11O-2 C5H11O-3 C5H10OOH1-2 C5H10OOH1-3 C5H10OOH1-4 C5H10OOH1-5
C5H10OOH2-1 C5H10OOH2-3 C5H10OOH2-4 C5H10OOH2-5 C5H10OOH3-1 C5H10OOH3-2
C5H10O1-2 C5H10O1-3 C5H10O1-4
C5H10O1-5 C5H10O2-3 C5H10O2-4 C5H10OOH1-2O2 C5H10OOH1-3O2 C5H10OOH1-4O2
C5H10OOH1-5O2 C5H10OOH2-1O2 C5H10OOH2-3O2 C5H10OOH2-4O2 C5H10OOH2-5O2
C5H10OOH3-1O2 C5H10OOH3-2O2 C5H91-2,3OOH C5H91-2,4OOH C5H91-2,5OOH C5H91-
3,4OOH C5H91-3,5OOH
C5H91-4,5OOH C5H92-1,3OOH C5H92-1,4OOH C5H92-1,5OOH C5H92-3,4OOH C5H92-
3,5OOH C5H92-4,5OOH C5H93-1,2OOH C5H93-1,4OOH C5H93-1,5OOH C5H93-2,4OOH
C5H91-3OOH C5H91-4OOH C5H91-5OOH C5H92-1OOH C5H92-4OOH C5H92-5OOH C5H9O1-
2OOH-3 C5H9O1-2OOH-4
C5H9O1-2OOH-5 C5H9O1-3OOH-2 C5H9O1-3OOH-4 C5H9O1-3OOH-5 C5H9O1-4OOH-2
C5H9O1-4OOH-3 C5H9O1-4OOH-5 C5H9O1-5OOH-2 C5H9O1-5OOH-3 C5H9O2-3OOH-1
C5H9O2-3OOH-4 C5H9O2-3OOH-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
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!-----
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!\SUBMECH: \IC5H12
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!\PYROSPEC:
IC5H12 AC5H11 BC5H11 CC5H11 DC5H11
!\OXIDSPEC:
AC5H9O-A2 AC5H11O2H BC5H11O2H CC5H11O2H DC5H11O2H AC5H11O2 BC5H11O2
CC5H11O2 DC5H11O2 AC5H11O BC5H11O CC5H11O DC5H11O AC5H10OOH-A AC5H10OOH-B
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AC5H1000H-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 AC5H100H BC5H100H CC5H100H AO2C5H100H BO2C5H100H CO2C5H100H
IC3H5COCH3 IC3H5COCH2 AC3H4COCH3

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!\SUBMECH: \NEOC5H12

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!\PYROSPEC:

NEOC5H12 NEOC5H11

!\OXIDSPEC:

NEOC5H11O2H NEOC5H11O2 NEOC5H11O NEOC5H1000H NEO-C5H100 NEOC5H1000H-O2

NEOC5H9Q2 NEOC5KET NEOC5KETOX NEOC5KEJOL IC4H6Q2-II NEOC5H9O-OH

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

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!\PYROSPEC:

C5H10-1 C5H10-2 C5H81-3 C5H91-3 C5H91-4 C5H91-5 C5H92-4 C5H92-5

!\OXIDSPEC:

C5H9O1-3 C5H9O2-4

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!-----

!\SUBMECH: \CC5H10\BC5H10

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!\PYROSPEC:

BC5H10 CC5H10 CC5H9-A CC5H9-B

!\OXIDSPEC:

AC5H9O-C CC5H9O-B

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!\SUBMECH: \AC5H10
!-----

!\PYROSPEC:
AC5H10 AC5H9-A2 AC5H9-C AC5H9-D
!\OXIDSPEC:
B2E2M1OJ
!-----

!-----

!\SUBMECH: \B13DE2M
!-----

!\PYROSPEC:
B13DE2M B13DE2MJ B12DE3M
!\OXIDSPEC:
B2E3M1OJ
!-----

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!\SUBMECH: \TC4H8CHO
!-----

!\PYROSPEC:
TC4H8CHO
!\OXIDSPEC:
O2C4H8CHO O2HC4H8CO
!-----

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

!\PYROSPEC:

!\OXIDSPEC:
PC4H8CHO-1O2 PC4H8CHO-2O2 PC4H8CHO-3O2 PC4H8CHO-4O2 C4H7CHO-2 C4H7CHO-3
C4H7CHO-4
!-----

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

!\OXIDSPEC:
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!\SUBMECH: \NC3H7COCH3\C2H5COC2H5
!-----
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!\PYROSPEC:
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
!-----
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!\SUBMECH: \NC5H11OH
!-----
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!\PYROSPEC:
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
!-----
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!+++++
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!\END_SPECIES_MODULE: \C5
!+++++
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!+++++
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!\SPECIES_MODULE: \C6
!\MODSUBMECHS: \NC6H14 \C6H12-1\C6H12-2\C6H12-3 \NC5H11CHO
\C6H10D13\C6H10D24 \C6H10-15
!+++++
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!-----
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!\SUBMECH: \NC6H14
!-----
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!\PYROSPEC:
NC6H14          C6H13-1          C6H13-2          C6H13-3
!\OXIDSPEC:
C6H13OOH-1
C6H13OOH-2          C6H13OOH-3          C6H13O2-1          C6H13O2-2
C6H13O2-3          C6H13O-1          C6H13O-2          C6H13O-3
C6H12OOH1-2          C6H12OOH1-3          C6H12OOH1-4          C6H12OOH1-5
C6H12OOH2-1          C6H12OOH2-3          C6H12OOH2-4          C6H12OOH2-5
C6H12OOH2-6          C6H12OOH3-1          C6H12OOH3-2          C6H12OOH3-4
C6H12OOH3-5          C6H12OOH3-6          C6H12O1-2          C6H12O1-3
C6H12O1-4          C6H12O1-5          C6H12O2-3          C6H12O2-4
C6H12O2-5          C6H12O3-4          C6H12OOH1-2O2          C6H12OOH1-3O2
C6H12OOH1-4O2          C6H12OOH1-5O2          C6H12OOH2-1O2          C6H12OOH2-3O2
C6H12OOH2-4O2          C6H12OOH2-5O2          C6H12OOH2-6O2          C6H12OOH3-1O2

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C6H12OOH3-2O2	C6H12OOH3-4O2	C6H12OOH3-5O2	C6H12OOH3-6O2
C6H11-1D3OOH	C6H11-1D4OOH	C6H11-1D5OOH	C6H11-1D6OOH
C6H11-2D1OOH	C6H11-2D4OOH	C6H11-2D5OOH	C6H11-2D6OOH
C6H11-3D1OOH	C6H11-3D2OOH	C6H11Q12-3	C6H11Q12-4
C6H11Q12-5	C6H11Q12-6	C6H11Q13-2	C6H11Q13-4
C6H11Q13-5	C6H11Q13-6	C6H11Q14-2	C6H11Q14-3
C6H11Q14-5	C6H11Q14-6	C6H11Q15-2	C6H11Q15-3
C6H11Q15-4	C6H11Q15-6	C6H11Q23-1	C6H11Q23-4
C6H11Q23-5	C6H11Q23-6	C6H11Q24-1	C6H11Q24-3
C6H11Q24-5	C6H11Q24-6	C6H11Q25-1	C6H11Q25-3
C6H11Q34-1	C6H11Q34-2	C6KET12	C6KET13
C6KET14	C6KET15	C6KET21	C6KET23
C6KET24	C6KET25	C6KET26	C6KET31
C6KET32	C6KET34	C6KET35	C6KET36
C5H91-1	C6H11O12-3OOH	C6H11O12-4OOH	C6H11O12-5OOH
C6H11O12-6OOH	C6H11O13-2OOH	C6H11O13-4OOH	C6H11O13-5OOH
C6H11O13-6OOH	C6H11O14-2OOH	C6H11O14-3OOH	C6H11O14-5OOH
C6H11O14-6OOH	C6H11O15-2OOH	C6H11O15-3OOH	C6H11O15-4OOH
C6H11O15-6OOH	C6H11O23-1OOH	C6H11O23-4OOH	C6H11O23-5OOH
C6H11O23-6OOH	C6H11O24-1OOH	C6H11O24-3OOH	C6H11O24-5OOH
C6H11O24-6OOH	C6H11O25-1OOH	C6H11O25-3OOH	C6H11O34-1OOH
C6H11O34-2OOH	C4H7O12-4	C4H7O13-4	C4H7O23-1
C5H9O12-5	C5H9O13-5	C5H9O14-5	C5H9O23-1
C5H9O23-5	C5H9O24-1	AC3H5CHO	
PC4H9CO	C6KET120	C6KET130	C6KET140
C6KET150	C6KET210	C6KET230	C6KET240
C6KET250	C6KET260	C6KET310	C6KET320
C6KET340	C6KET350	C6KET360	C6H12OOH1-2O
C6H12OOH1-3O	C6H12OOH1-4O	C6H12OOH1-5O	C6H12OOH2-1O
C6H12OOH2-3O	C6H12OOH2-4O	C6H12OOH2-5O	C6H12OOH2-6O
C6H12OOH3-1O	C6H12OOH3-2O	C6H12OOH3-4O	C6H12OOH3-5O
C6H12OOH3-6O	NC5H11CHO	C6Y2	CH3COOH

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!\SUBMECH: \C6H12-1\C6H12-2\C6H12-3

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!\PYROSPEC:

C6H12-1	C6H12-2	C6H12-3	C6H111-3
C6H111-4	C6H111-5	C6H111-6	C6H112-4
C6H112-5	C6H112-6	C6H113-1	

!\OXIDSPEC:

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C6H12OH-1J2			
C6H12OH-2J1	C6H12OH-2J3	C6H12OH-3J2	C6H12OH-3J4
C6H12OH-1O2-2	C6H12OH-2O2-1	C6H12OH-2O2-3	C6H12OH-3O2-2
C6H12OH-3O2-4	PC4H9CHO		
PC4H8CHO-1	PC4H8CHO-2	PC4H8CHO-3	PC4H8CHO-4
C6H11-1D3O	C6H11-1D4O	C6H11-1D5O	
C6H11-1D6O	C6H11-2D1O	C6H11-2D4O	C6H11-2D5O
C6H11-2D6O	C6H11-3D1O	C6H11-3D2O	

!-----

!\SUBMECH: \NC5H11CHO

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!\PYROSPEC:
NC5H11CO          NC5H10CHO-1      NC5H10CHO-2      NC5H10CHO-3
NC5H10CHO-4      NC5H10CHO-5
!\OXIDSPEC:
!-----
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!-----
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!\SUBMECH: \C6H10D13\C6H10D24
!-----
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!\PYROSPEC:
C6H10D13 C6H10D24
!\OXIDSPEC:
!-----
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!-----
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!\SUBMECH: \C6H101-5
!-----
-----
!\PYROSPEC:
C6H101-5 C6H9-A
!\OXIDSPEC:
!-----
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!+++++
!+++++
!+++++
!\END_SPECIES_MODULE: \C6
!+++++
!+++++
!+++++
!\SPECIES_MODULE: \C7
!\MODSUBMECHS: \NC7H16 \C7H14-1\C7H14-2\C7H14-3 \H15DE25DM
!+++++
!+++++
!-----
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!\SUBMECH: \NC7H16
!-----
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!\PYROSPEC:
NC7H16          C7H15-1          C7H15-2          C7H15-3
C7H15-4
!\OXIDSPEC:
C7H15OOH-1      C7H15OOH-2      C7H15OOH-3      C7H15OOH-4
C7H15-1O2      C7H15-2O2      C7H15-3O2      C7H15-4O2
C7H15-1O      C7H15-2O      C7H15-3O      C7H15-4O
C7H14OOH1-2    C7H14OOH1-3    C7H14OOH1-4    C7H14OOH1-5
C7H14OOH2-1    C7H14OOH2-3    C7H14OOH2-4    C7H14OOH2-5
C7H14OOH2-6    C7H14OOH3-1    C7H14OOH3-2    C7H14OOH3-4

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C7H1400H3-5	C7H1400H3-6	C7H1400H3-7	C7H1400H4-1
C7H1400H4-2	C7H1400H4-3	C7H1401-2	C7H1401-3
C7H1401-4	C7H1401-5	C7H1402-3	C7H1402-4
C7H1402-5	C7H1402-6	C7H1403-4	C7H1403-5
C7H1400H1-202	C7H1400H1-302	C7H1400H1-402	C7H1400H1-502
C7H1400H2-102	C7H1400H2-302	C7H1400H2-402	C7H1400H2-502
C7H1400H2-602	C7H1400H3-102	C7H1400H3-202	C7H1400H3-402
C7H1400H3-502	C7H1400H3-602	C7H1400H3-702	C7H1400H4-102
C7H1400H4-202	C7H1400H4-302	C7H13Q12-3	C7H13Q12-4
C7H13Q12-5	C7H13Q12-6	C7H13Q13-2	C7H13Q13-4
C7H13Q13-5	C7H13Q13-6	C7H13Q13-7	C7H13Q14-2
C7H13Q14-3	C7H13Q14-5	C7H13Q14-6	C7H13Q14-7
C7H13Q15-2	C7H13Q15-3	C7H13Q15-4	C7H13Q15-6
C7H13Q15-7	C7H13Q23-1	C7H13Q23-4	C7H13Q23-5
C7H13Q23-6	C7H13Q23-7	C7H13Q24-1	C7H13Q24-3
C7H13Q24-5	C7H13Q24-6	C7H13Q24-7	C7H13Q25-1
C7H13Q25-3	C7H13Q25-4	C7H13Q25-6	C7H13Q25-7
C7H13Q26-1	C7H13Q26-3	C7H13Q26-4	C7H13Q34-1
C7H13Q34-2	C7H13Q34-5	C7H13Q34-6	C7H13Q34-7
C7H13Q35-1	C7H13Q35-2	C7H13Q35-4	C7KET12
C7KET13	C7KET14	C7KET15	C7KET21
C7KET23	C7KET24	C7KET25	C7KET26
C7KET31	C7KET32	C7KET34	C7KET35
C7KET36	C7KET37	C7KET41	C7KET42
C7KET43	C7H13-1D300H	C7H13-1D400H	C7H13-1D500H
C7H13-1D600H	C7H13-2D100H	C7H13-2D400H	C7H13-2D500H
C7H13-2D600H	C7H13-2D700H	C7H13-3D100H	C7H13-3D200H
C7H13-3D500H	C7H13-3D600H	C7H13-3D700H	C7H13012-300H
C7H13012-400H	C7H13012-500H	C7H13012-600H	C7H13013-200H
C7H13013-400H	C7H13013-500H	C7H13013-600H	C7H13013-700H
C7H13014-200H	C7H13014-300H	C7H13014-500H	C7H13014-600H
C7H13014-700H	C7H13015-200H	C7H13015-300H	C7H13015-400H
C7H13015-600H	C7H13015-700H	C7H13023-100H	C7H13023-400H
C7H13023-500H	C7H13023-600H	C7H13023-700H	C7H13024-100H
C7H13024-300H	C7H13024-500H	C7H13024-600H	C7H13024-700H
C7H13025-100H	C7H13025-300H	C7H13025-400H	C7H13025-600H
C7H13025-700H	C7H13026-100H	C7H13026-300H	C7H13026-400H
C7H13034-100H	C7H13034-200H	C7H13034-500H	C7H13034-600H
C7H13034-700H	C7H13035-100H	C7H13035-200H	C7H13035-400H
C7KET120	C7KET130	C7KET140	C7KET150
C7KET210	C7KET230	C7KET240	C7KET250
C7KET260	C7KET310	C7KET320	C7KET340
C7KET350	C7KET360	C7KET370	C7KET410
C7KET420	C7KET430	C7Y24	C7Y13
C7Y35	C7H1400H1-20	C7H1400H1-30	C7H1400H1-40
C7H1400H1-50	C7H1400H2-10	C7H1400H2-30	C7H1400H2-40
C7H1400H2-50	C7H1400H2-60	C7H1400H3-10	C7H1400H3-20
C7H1400H3-40	C7H1400H3-50	C7H1400H3-60	C7H1400H3-70
C7H1400H4-10	C7H1400H4-20	C7H1400H4-30	
C6H11013-6	C6H11014-6	C6H11015-6	C6H11023-1
C6H11023-6	C6H11024-1	C6H11024-6	C6H11034-1
C6Y2-1J	C6Y3-6J	C6Y3-1J	

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!\SUBMECH: \C7H14-1\C7H14-2\C7H14-3

!-----

!\PYROSPEC:

C7H14-1	C7H14-2	C7H14-3	
C7H131-3	C7H131-4	C7H131-5	C7H131-6
C7H131-7	C7H132-4	C7H132-5	C7H132-6
C7H132-7	C7H133-1	C7H133-5	C7H133-6
C7H133-7			

!\OXIDSPEC:

C7H13-1D3O	C7H13-2D4O	C7H13-3D5O	
C7H14OH-1J2	C7H14OH-2J1	C7H14OH-2J3	
C7H14OH-3J2	C7H14OH-3J4	C7H14OH-4J3	
C7H14OH-1O2-2	C7H14OH-2O2-1	C7H14OH-2O2-3	
C7H14OH-3O2-2	C7H14OH-3O2-4	C7H14OH-4O2-3	
C5D2Y1	C5D2Y1-1R	C3Y1-3OR	C4Y1-3OR
C6D2Y1	C6D2Y1-1R		

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!\END_SPECIES_MODULE: \C7

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!\SPECIES_MODULE: \C8

!\MODSUBMECHS: \H15DE25DM

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!\SUBMECH: \H15DE25DM

!-----

!\PYROSPEC:

H15DE25DM	H15DE25DM-S
H15DE25DM-A	

!\OXIDSPEC:

H15DE25DM-AO H15DE25DM-SO H15DE2M-T IC4H7CHO

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!\END_SPECIES_MODULE: \C8

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!\SPECIES_MODULE: \AROMATIC

!\MODSUBMECHS: \CORE_TO_AROMATIC_LINKERS \C6H6 \C6H5OH \C5H6

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!\SUBMECH: \CORE_TO_AROMATIC_LINKERS
!-----
-----
!\PYROSPEC:
L-C6H4 C-C6H4 C6H3 C6H2
!\OXIDSPEC:
!-----
-----
!-----
-----
!\SUBMECH: \C6H6
!-----
-----
!\PYROSPEC:
C6H6 FULVENE C6H5
!\OXIDSPEC:
C6H5OO C6H5OOH
!-----
-----
!-----
-----
!\SUBMECH: \C6H5OH
!-----
-----
!\PYROSPEC:
C6H5OH C6H5O C6H4OH
!\OXIDSPEC:
OC6H4OH O-C6H4O2 P-C6H4O2 O-OC6H5OJ P-OC6H5OJ P-C6H3O2
!-----
-----
!-----
-----
!\SUBMECH: \C5H6
!-----
-----
!\PYROSPEC:
C5H6 C5H5 C5H6-L C#CCVCCJ C5H7 CVCCJCVC CVCCVCCJ
!\OXIDSPEC:
CVCCJCVCOH HOCVCCVO CVCCVCCOH OC5H7O OC4H6O OC4H5O O2CCHOOJ HOCVCCJVO
C5H5OH C5H5O C5H4OH C5H4O C5H3O CJVCCVCCVO CVCCVCCJVO CJVCCVO
!VINYL KETENE (CALLED C4H4O IN AROMATIC CHEMISTRY) SHOULD BE RENAMED AND
PLACED HERE
!-----
-----
!+++++
+++++
+++++
!\END_SPECIES_MODULE: \AROMATIC
!+++++
+++++
+++++
END
!\END_SPECIES_LIST

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!\START_KINETICS_INPUT

REACTIONS

!++++++
++++++
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!\KINETICS_MODULE: \H2_O2

!\MODSUBMECHS:

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

!-----

!\SUBMECH: \H2

!-----

!_____

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!_____

H2+M<=>H+H+M 4.577E+019 -1.400
104400.0 !\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
H2/ 2.50/ H2O/ 12.00/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.83/ CH4/ 2.00/ C2H6/
3.00/

!_____

!\REACTIONCLASS: \ABSTRACTION \A \N

\EA

!_____

!\SITE: \UNDEF

H2+O<=>H+OH 5.080E+004 2.670
6292.0 !\AUTHOR: AK !\REF: SUTHERLAND ET AL., 21ST SYMPOSIUM, P. 929
(1986)

H2+OH<=>H+H2O 4.380E+013 0.000
6990.0 !\AUTHOR: AK !\REF: LAM ET AL. SUBMITTED IJCK

!-----

!\ENDSUBMECH: \H2

!-----

!-----

!\SUBMECH: \O2

!-----

!_____

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!_____

O+O+M<=>O2+M 6.165E+015 -0.500
0.0 !\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
H2/ 2.50/ H2O/ 12.00/ AR/ 0.83/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.83/ CH4/ 2.00/
C2H6/ 3.00/
!

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
\EA
!

O2+H<=>O+OH 1.040E+014 0.000
15286.0 !\AUTHOR: AK !\REF: HONG ET AL. PROC. OF THE COMB. INST. 33
(2011) 309;§C316

!\ENDSUBMECH: \O2

!\SUBMECH: \H2O

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

H+OH+M<=>H2O+M 3.500E+022 -2.000
0.0 !\AUTHOR: AK !\REF: LI IJCK 36: 566;§C575, 2004
H2/ 0.73/ H2O/ 3.65/ CH4/ 2.00/ C2H6/ 3.00/ AR/ 0.38/
!

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

O+H2O<=>OH+OH 6.70E+07 1.704
14986.8 !\AUTHOR: AK !\REF: SUTHERLAND ET AL., 23RD SYMPOSIUM, P. 51
(1990)
!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N
\EA
!

O+H+M<=>OH+M 4.714E+018 -1.000
0.0 !\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
H2/ 2.50/ H2O/ 12.00/ AR/ 0.75/ CO/ 1.50/ CO2/ 2.00/ HE/ 0.75/ CH4/ 2.00/
C2H6/ 3.00/
!

!\SUBSPECIES: \OHV

!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION
!

H+O+M<=>OHV+M 1.500E+013 0.000
5975.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
H2/ 1.00/ H2O/ 6.50/ O2/ 0.40/ N2/ 0.40/ AR/ 0.35/

!

!\REACTIONCLASS: \DEACTIVATION
!

OHV+H2O<=>OH+H2O 5.930E+012 0.500
-860.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+H2<=>OH+H2 2.950E+012 0.500
-444.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+N2<=>OH+N2 1.080E+011 0.500
-1242.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+OH<=>OH+OH 6.010E+012 0.500
-764.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+H<=>OH+H 1.310E+012 0.500
-167.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+AR<=>OH+AR 1.690E+012 0.000
4135.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV<=>OH 1.450E+006 0.000
0.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+O2<=>OH+O2 2.100E+012 0.500
-478.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+CO2<=>OH+CO2 2.750E+012 0.500
-968.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+CO<=>OH+CO 3.230E+012 0.500
-787.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010
OHV+CH4<=>OH+CH4 3.360E+012 0.500
-635.0 !\AUTHOR: AK !\REF:KATHROTIA ET AL. COMB & FLAME 2010

!=====
=====

!\ENDSUBSPECIES: \OHV

!=====
=====

!-----

!\ENDSUBMECH: \H2O

!-----

!-----

!\SUBMECH: \H2O2

!-----

!

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

!

H2O2 (+M) <=>OH+OH (+M) 2.000E+012 0.900
48749.0 !\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601 (2011)

LOW/ 2.490E+024 -2.300
48749.0/
TROE/ 4.300E-001 1.000E-030 1.000E+030/
H2O/ 7.65/ CO2/ 1.60/ N2/ 1.50/ O2/ 1.20/ HE/ 0.65/ H2O2/ 7.70/ H2/ 3.70/
CO/ 2.80/
!

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

H2O2+H<=>H2O+OH 2.410E+013 0.000
3970.0 !\AUTHOR: AK !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
H2O2+H<=>H2+HO2 2.150E+010 1.000
6000.0 !\AUTHOR: AK !\REF: ELLINGSON J. PHYS. CHEM. (2007) 111, (51),
13554-13566
H2O2+O<=>OH+HO2 9.550E+006 2.000
3970.0 !\AUTHOR: AK !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
H2O2+OH<=>H2O+HO2 1.740E+012 0.000
318.0 !\AUTHOR: AK !\REF: HONG ET AL. J. PHYS. CHEM. A 114 (2010) 5718-
5727
DUP
H2O2+OH<=>H2O+HO2 7.590E+013 0.000
7269.0
DUP
!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

HO2+H<=>OH+OH 7.079E+013 0.0000
295.0 !\AUTHOR:
HO2+H<=>H2+O2 1.1402E+010 1.0827
553.78 !\AUTHOR: AK !\REF:MICHAEL SUTHERLAND 2000
HO2+O<=>OH+O2 3.250E+013 0.0000
0.0000 !\AUTHOR: AK !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA,
21:411 (1992)
OH+HO2<=>H2O+O2 7.00E+12 0.0000
-1092.96 !\AUTHOR: !\REF: hong pci 2013 1015C
DUP
OH+HO2<=>H2O+O2 4.50E+14 0.0000
10929.6
DUP
HO2+HO2<=>H2O2+O2 1.00E+14 0.0000
11040.8832 !\AUTHOR: AK !\REF: hong pci 2013, kapel 2002
DUP
HO2+HO2<=>H2O2+O2 1.90E+11 0.0000
-1408.9248
DUP
!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N
\EA
!

H+O2 (+M) <=> HO2 (+M) 4.650E+012 0.440
0.0 !\AUTHOR: AK !\REF:FERNANDES PCCP 2008 !COMMENT: Efficiencis of
AR and HE derived from seperated reactions, otherwise lead to error in
flame extinction simulation

LOW/ 1.737E+019 -1.230
0.0/

TROE/ 6.700E-001 1.000E-030 1.000E+030 1.000E+030/
H2/ 1.30/ CO/ 1.90/ CO2/ 3.80/ HE/ 0.64/ H2O/ 10.00/ AR/ 0.50/ CH4/ 2.00/
C2H6/ 3.00/

!-----

!\ENDSUBMECH: \H2O2

!-----

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

!\END_KINETICS_MODULE: \H2_O2

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

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

!\KINETICS_MODULE: \C1

!\MODSUBMECHS: CO, CH2O, CH4,

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

!-----

!\SUBMECH: \CO

!-----

!

!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N
\EA

!-----

CO+O (+M) <=> CO2 (+M) 1.362E+010 0.000
2384.0 !\AUTHOR: !\REF: MEULLER 99 * 0.76

LOW/ 1.173E+024 -2.790
4191.0/

H2/ 2.00/ H2O/ 12.00/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.70/ HE/ 0.70/

!-----

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA

!-----

CO+OH <=> CO2+H 7.015E+004 2.053
-355.7 !\AUTHOR: !\REF: JOSHI AND WANG IJCK (2006), 38, (1), 57-73.

DUP

CO+OH <=> CO2+H 5.757E+012 -0.664
331.8

DUP

```

!
-----
!\REACTIONCLASS: \RADICAL_ADDITION\HO2          \A          \N
\EA
!
-----
CO+HO2<=>CO2+OH                                1.570E+005      2.180
17940.0 !\AUTHOR: !\REF: YOU ET AL. J. PHYS. CHEM. A 2007, 111, 4031-4042
!
-----
!\REACTIONCLASS: \R+O2                          \A          \N
\EA
!
-----
CO+O2<=>CO2+O                                  1.119E+012      0.000
47700.0 !\AUTHOR: !\REF: 86TSA/ HAM * 0.44
!=====
=====
!\SUBSPECIES: \CO2
!=====
=====
!
-----
!\REACTIONCLASS: \RADICAL_ADIDTION\H
!
-----
H+CO2<=>OCHO                                    7.500E+013      0.000
29000.0 !\AUTHOR: !\REF: CURRAN ESTIMATE
!=====
=====
!\ENDSUBSPECIES: \CO2
!=====
=====
!
=====
!\SUBSPECIES: \HOCO
!=====
=====
HOCO<=>CO+OH                                    6.300E+032      -5.960
32470.0 !\AUTHOR: !\REF: JOHN R. BARKER CALCULATION 7/ 3/ 2013
PLOG/      0.0010      1.550E-008      2.930      8768.0/
PLOG/      0.0030      1.770E+003      0.340      18076.0/
PLOG/      0.0296      2.020E+013     -1.870      22755.0/
PLOG/      0.0987      1.680E+018     -3.050      24323.0/
PLOG/      0.2961      2.500E+024     -4.630      27067.0/
PLOG/      0.9869      4.540E+026     -5.120      27572.0/
PLOG/      2.9607      7.120E+028     -5.600      28535.0/
PLOG/      9.8690      5.480E+029     -5.700      28899.0/
PLOG/     29.6070      9.890E+031     -6.190      30518.0/
PLOG/     98.6900      5.740E+033     -6.530      32068.0/
PLOG/    296.0700      2.610E+033     -6.290      32231.0/
PLOG/   986.9000      6.300E+032     -5.960      32470.0/
HOCO<=>CO2+H                                    1.897E+038      -8.047
34240.0 !\AUTHOR: !\REF: JOHN R. BARKER CALCULATION 7/ 3/ 2013
PLOG/      0.0010      4.758E+018     -3.817      17676.0/
PLOG/      0.0030      2.225E+020     -4.149      19037.0/
PLOG/      0.0099      7.564E+021     -4.434      20325.0/
PLOG/      0.0296      9.107E+024     -5.189      22419.0/

```


PLOG/	0.0987	3.144E+029	-6.376	25233.0/
PLOG/	0.2961	1.150E+032	-7.037	26662.0/
PLOG/	0.9869	1.069E+036	-8.107	29064.0/
PLOG/	2.9607	2.438E+036	-8.153	29336.0/
PLOG/	9.8690	6.663E+035	-7.919	29217.0/
PLOG/	29.6070	1.723E+038	-8.506	31273.0/
PLOG/	98.6900	3.007E+041	-9.290	33966.0/
PLOG/	296.0700	6.767E+036	-7.832	31613.0/
PLOG/	986.9000	1.897E+038	-8.047	34240.0/

!=====

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!\ENDUBSPECIES: \HOCO

!=====

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!-----

!\ENDSUBMECH: \CO

!-----

!-----

!\SUBMECH: \CH4

!-----

!-----

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!-----

CH3+H(+M)<=>CH4(+M)	1.270E+016	-0.630
383.0 !\AUTHOR: !\REF: GRI MECHANISM		
LOW/	2.477E+033	-4.760
2440.0/		
TROE/ 7.830E-001 7.400E+001 2.941E+003 6.964E+003/		
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/		
3.00/ HE/ 0.70/		

!-----

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!-----

CH4+H<=>CH3+H2	6.140E+005	2.500
9587.0 !\AUTHOR: !\REF: BAULCH, D.L.; ET AL., J. PHYS. CHEM. REF. DATA (2005)		
CH4+O<=>CH3+OH	1.020E+009	1.500
8600.0 !\AUTHOR: !\REF: !REF:GRI 3.0		
CH4+OH<=>CH3+H2O	5.830E+004	2.600
2190.0 !\AUTHOR: !\REF: CURRAN ESTIMATE, FIT TO NIST DATABASE		
CH4+HO2<=>CH3+H2O2	1.130E+001	3.740
21010.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
CH4+CH3O2<=>CH3+CH3O2H	9.600E-001	3.770
17810.0 !\AUTHOR: !\REF: NEW FIT FROM HJC		
CH3+HO2<=>CH4+O2	1.160E+005	2.230
-3022.0 !\AUTHOR: !\REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279;§C286		

!

!\REACTIONCLASS: \RADICAL_ADDITION\CH2 \A \N
\EA
!

CH4+CH2<=>CH3+CH3 2.460E+006 2.000
8270.0 !\AUTHOR: !\REF: GRI 3.0

!=====

!\SUBSPECIES: \CH2 (S)
!=====

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!

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

CH2 (S) +N2<=>CH2+N2 1.500E+013 0.000
600.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +AR<=>CH2+AR 9.000E+012 0.000
600.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +H2O<=>CH2+H2O 3.000E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +CO<=>CH2+CO 9.000E+012 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +CO2<=>CH2+CO2 7.000E+012 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
!

!\REACTIONCLASS: \RADICAL_RECOMBINATIONS \A \N
\EA
!

CH2 (S) +O2=>H+OH+CO 2.800E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +O2<=>CO+H2O 1.200E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +O<=>CO+H2 1.500E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +O<=>HCO+H 1.500E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +H2<=>CH3+H 7.000E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +H<=>CH+H2 3.000E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +OH<=>CH2O+H 3.000E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2 (S) +CO2<=>CH2O+CO 1.400E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0

!=====

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!\ENDSUBSPECIES: \CH2 (S)
!=====

=====

!=====

=====

!\SUBSPECIES: \CH2

!=====
=====
CH2+H(+M)<=>CH3(+M) 2.500E+016 -0.800
0.0 !\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000
LOW/ 3.200E+027 -3.140
1230.0/
TROE/ 6.800E-001 7.800E+001 1.995E+003 5.590E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/
!

!\REACTIONCLASS: \RADICAL_RECOMBINATIONS \A \N
\EA
!

CH2+O2<=>HCO+OH 1.060E+013 0.000
1500.0 !\AUTHOR: !\REF: GRI 3.0
CH2+O2=>CO2+H+H 2.640E+012 0.000
1500.0 !\AUTHOR: !\REF: GRI 3.0
CH2+O=>CO+H+H 5.000E+013 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
CH2+H<=>CH+H2 3.000E+013 0.000
0.0 !\AUTHOR: !\REF: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION,
SAN ANTONIO (1985)
CH2+OH<=>CH+H2O 1.130E+007 2.000
3000.0 !\AUTHOR: !\REF: GRI 3.0

!=====
=====
!\ENDSUBSPECIES: \CH2

!\SUBSPECIES: \CHV

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

CHV+AR<=>CH+AR 4.000E+011 0.500
0.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
65-75 (1987)
CHV+H2O<=>CH+H2O 5.300E+013 0.000
0.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
65-75 (1987)
CHV+CO<=>CH+CO 2.440E+012 0.500
0.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
65-75 (1987)
CHV+CO2<=>CH+CO2 2.410E-001 4.300
-1694.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
67, 65-75 (1987)
CHV+O2<=>CH+O2 2.480E+006 2.140
-1720.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
67, 65-75 (1987)

CHV+H2<=>CH+H2	1.470E+014	0.000
1361.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)		
CHV+CH4<=>CH+CH4	1.730E+013	0.000
167.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)		
CHV<=>CH	1.860E+006	0.000
0.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)		
CHV+N2<=>CH+N2	3.030E+002	3.400
-381.0 !\AUTHOR: !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)		
C+H+M<=>CHV+M	6.000E+014	0.000
6940.0 !\AUTHOR: !\REF:KATHROTIA ET AL. COMB & FLAME 2010		
!		

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

CH+O2<=>CO+OHV	4.040E+013	0.000
0.0 !\AUTHOR: !\REF:KATHROTIA ET AL. COMB & FLAME 2010		
CH+O2<=>HCO+O	3.300E+013	0.000
0.0 !\AUTHOR: !\REF: GRI 3.0		
CH+O<=>CO+H	5.700E+013	0.000
0.0 !\AUTHOR: !\REF: MESSING ET AL., J. CHEM. PHYS. 74, 3874 (1981)		
CH+H<=>C+H2	1.100E+014	0.000
0.0 !\AUTHOR: !\REF: GRI 3.0		
CH+OH<=>HCO+H	3.000E+013	0.000
0.0 !\AUTHOR: !\REF: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)		
CH+H2O<=>H+CH2O	1.774E+016	-1.220
23.8 !\AUTHOR: !\REF:BERGEAT ET AL., CHEM. PHYS. LETT. 480, 21 (2009)		
CH+CO2<=>HCO+CO	1.700E+012	0.000
685.0 !\AUTHOR: !\REF: BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB. P. 73, 1982		

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!=====
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```
!\ENDSUBSPECIES: \CHV
```

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!=====
```

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!=====
```

```
!\SUBSPECIES: \C
```

```
!=====
```

C+OH<=>CO+H	5.000E+013	0.000
0.0 !\AUTHOR: !\REF: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)		

C+O2<=>CO+O	5.000E+013	0.000
0.0 !\AUTHOR: !\REF: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION, SAN ANTONIO (1985)		

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!=====
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```
!\ENDSUBSPECIES: \C
```

```
!=====
```

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=====
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!=====
=====
!\SUBSPECIES: \CH3
!=====
=====
!

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

CH3+O2 (+M) <=> CH3O2 (+M) 7.812E+009 0.900
0.0 !\AUTHOR: !\REF: R.X. FERNANDES ET AL., J. PHYS. CHEM. A, (2006)
110:4442-4449.

LOW/ 6.850E+024 -3.000
0.0/

TROE/ 6.000E-001 1.000E+003 7.000E+001 1.700E+003/
CH3+O2 <=> CH3O+O 7.546E+012 0.000
28320.0 !\AUTHOR: !\REF: N. K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109,
7902-7914 (2005)

CH3+O2 <=> CH2O+OH 2.641E+000 3.283
8105.0 !\AUTHOR: !\REF: PERSONAL COMMUNICATION, STEVE KLIPPENSTEIN
!

!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N
\EA
!

CH3+O <=> CH2O+H 5.540E+013 0.050
-136.0 !\AUTHOR: !\REF: HARDING AND KLIPPENSTEIN 2B04, 30TH SYMP 2004.
!

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA
!

CH3+OH <=> CH2(S)+H2O 4.936E+014 -0.669
-445.8 !\AUTHOR: !\REF: FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-
3950

PLOG/ 0.0100 4.936E+014 -0.669 -445.8/
PLOG/ 0.1000 1.207E+015 -0.778 -175.6/
PLOG/ 1.0000 5.282E+017 -1.518 1772.0/
PLOG/ 10.0000 4.788E+023 -3.155 7003.0/
PLOG/ 100.0000 8.433E+019 -1.962 8244.0/

CH3+OH <=> CH2O+H2 3.502E+005 1.441
-3244.0 !\AUTHOR: !\REF: FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-
3950

PLOG/ 0.0100 3.502E+005 1.441 -3244.0/
PLOG/ 0.1000 8.854E+005 1.327 -2975.0/
PLOG/ 1.0000 1.650E+007 0.973 -2010.0/
PLOG/ 10.0000 5.374E+009 0.287 280.0/
PLOG/ 100.0000 9.494E+018 -2.199 9769.0/

CH3+OH <=> CH2OH+H 1.621E+010 0.965
3210.0 !\AUTHOR: !\REF: FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-
3950

PLOG/ 0.0100 1.621E+010 0.965 3214.0/
PLOG/ 0.1000 1.807E+010 0.950 3247.0/
PLOG/ 1.0000 4.686E+010 0.833 3566.0/

PLOG/	10.0000	1.525E+013	0.134	5641.0/	
PLOG/	100.0000	3.590E+014	-0.186	8601.0/	
CH3+OH<=>H+CH3O				1.186E+009	1.016
11940.0 !\AUTHOR:	!\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950				
PLOG/	0.0100	1.186E+009	1.016	11940.0/	
PLOG/	0.1000	1.188E+009	1.016	11940.0/	
PLOG/	1.0000	1.230E+009	1.011	11950.0/	
PLOG/	10.0000	1.798E+009	0.965	12060.0/	
PLOG/	100.0000	5.242E+010	0.551	13070.0/	
CH3+OH<=>HCOH+H2				8.674E+008	0.787
-3046.0 !\AUTHOR:	!\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950				
PLOG/	0.0100	8.674E+008	0.787	-3046.0/	
PLOG/	0.1000	3.115E+009	0.630	-2669.0/	
PLOG/	1.0000	1.557E+011	0.156	-1368.0/	
PLOG/	10.0000	1.704E+021	-2.641	6412.0/	
PLOG/	100.0000	7.250E+020	-2.402	9639.0/	
CH3+OH<=>CH2+H2O				4.293E+004	2.568
3997.8 !\AUTHOR:	!\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-3950				

!

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

```
CH3+HO2<=>CH3O+OH           1.000E+012   0.269
-687.5 !\AUTHOR: !\REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009)
279;§C286
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!=====
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```
!\ENDSUBSPECIES: \CH3
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!=====
=====

```
!\SUBSPECIES: \CH3O2
```

!=====
=====

!

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

```
CH3O2+O<=>CH3O+O2           3.600E+013   0.000
0.0 !\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991,
87(19), 3213--3220.
```

```
CH3O2+H<=>CH3O+OH           9.600E+013   0.000
0.0 !\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991,
87(19), 3213--3220.
```

```
CH3O2+OH<=>CH3OH+O2         6.000E+013   0.000
0.0 !\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991,
87(19), 3213--3220.
```

```
CH3O2+HO2<=>CH3O2H+O2       2.470E+011   0.000
-1570.0 !\AUTHOR: !\REF:LIGHTFOOT,P.D. ETAL., ATMOS. ENVIRON. PART A: 26,
1805-1961 (1992)
```

CH3O2+H2O2<=>CH3O2H+HO2 2.410E+012 0.000
9936.0 !\AUTHOR: !\REF:!REF:Tsang, W., J. Phys. Chem. Ref. Data 15, 1087
(1986)
CH3O2+CH3<=>CH3O+CH3O 5.080E+012 0.000
-1411.0 !\AUTHOR: !\REF:KEIFFER, M. ET AL., J. CHEM. SOC. FARADAY TRANS.
2: 84, 505 (1988)
CH3O2+CH3O2=>CH2O+CH3OH+O2 3.110E+014 -1.610
-1051.0 !\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991,
87(19), 3213--3220.
CH3O2+CH3O2=>O2+CH3O+CH3O 1.400E+016 -1.610
1860.0 !\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991,
87(19), 3213--3220.
!

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

H2+CH3O2<=>H+CH3O2H 1.500E+014 0.000
26030.0 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF.
DATA, VOL 15, 1986
!

!\REACTIONCLASS: \KHP_DECOMP \A \N
\EA
!

CH3O2H<=>CH3O+OH 6.310E+014 0.000
42300.0 !\AUTHOR: !\REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991,
87(19), 3213--3220.
CH2O2H<=>CH2O+OH 9.000E+014 0.000
1500.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!=====
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!\ENDSUBSPECIES: \CH3O2

!=====
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!\ENDSUBMECH: \CH4

!-----

!\SUBMECH: \CH3OH

!-----

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

CH3OH(+M)<=>CH3+OH(+M) 2.084E+018 -0.615
92540.6 !\AUTHOR: !\REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-
3950
LOW/ 1.500E+043 -6.995
97992.2/

TROE/ -4.748E-001 3.558E+004 1.116E+003 9.023E+003/
 CH3OH(+M)<=>CH2(S)+H2O(+M) 3.121E+018 -1.017
 91712.0 !\AUTHOR: !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-
 3950
 LOW/ 1.430E+047 -8.227
 99417.1/
 TROE/ 2.545E+000 3.290E+003 4.732E+004 4.711E+004/
 CH3OH(+M)<=>CH2OH+H(+M) 7.896E-003 5.038
 84467.4 !\AUTHOR: !\REF:FROM JASPER/ KLIPP,J.PHYS.CHEM A 111,19,3932-
 3950
 LOW/ 3.390E+042 -7.244
 105230.3/
 TROE/ -7.391E+001 3.705E+004 4.150E+004 5.220E+003/
 !

!\REACTIONCLASS: \RH_R_ABSTRACTIONS \A \N
 \EA
 !

CH3OH+H<=>CH3O+H2 1.990E+005 2.560
 10300.0 !\AUTHOR: !\REF:J. CHEM. PHYS. 134, 094302 (2011)
 CH3OH+H<=>CH2OH+H2 3.070E+005 2.550
 5440.0 !\AUTHOR: !\REF:J. CHEM. PHYS. 134, 094302 (2011)
 CH3OH+O<=>CH3O+OH 3.880E+004 2.500
 3080.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
 CH3OH+O<=>CH2OH+OH 3.880E+005 2.500
 3080.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
 CH3OH+OH<=>CH3O+H2O 1.500E+002 3.030
 -763.0 !\AUTHOR: !\REF:XU ET AL. PROC 31 2007 159-166
 CH3OH+OH<=>CH2OH+H2O 3.080E+004 2.650
 -806.7 !\AUTHOR: !\REF:XU ET AL. PROC 31 2007 159-166
 CH3OH+O2<=>CH3O+HO2 3.580E+004 2.270
 42764.5 !\AUTHOR: !\REF:S. J. Klippenstein, L. B. Harding, M. J. Davis,
 A. S. Tomlin, R. T. Skodje, PCI, 33 (2011) 351-357
 CH3OH+O2<=>CH2OH+HO2 3.580E+005 2.270
 42764.5 !\AUTHOR: !\REF:S. J. Klippenstein, L. B. Harding, M. J. Davis, A.
 S. Tomlin, R. T. Skodje, PCI, 33 (2011) 351-357
 CH3OH+HO2<=>CH3O+H2O2 1.220E+012 0.000
 20070.7 !\AUTHOR: !\REF: M. Altarawneh, A. H. Al-Muhtaseb, B. Z.
 Dlugogorski, E. M. Kennedy, J. C. Mackie, J. Comp. Chem. 32 (2011) 1725-
 1733
 CH3OH+HO2<=>CH2OH+H2O2 3.260E+013 0.000
 18782.2 !\AUTHOR: !\REF: M. Altarawneh, A. H. Al-Muhtaseb, B. Z.
 Dlugogorski, E. M. Kennedy, J. C. Mackie, J. Comp. Chem. 32 (2011) 1725-
 1733
 CH3OH+CH3<=>CH2OH+CH4 2.130E-001 3.953
 7055.1 !\AUTHOR: !\REF:I. M. Alecu, D. G. Truhlar, J. Phys. Chem. A, 115
 (2011) 14599-14611
 CH3OH+CH3<=>CH3O+CH4 3.220E+003 2.425
 8579.5 !\AUTHOR: !\REF:I. M. Alecu, D. G. Truhlar, J. Phys. Chem. A, 115
 (2011) 14599-14611
 CH3OH+HCO<=>CH2OH+CH2O 9.630E+003 2.900
 13110.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
 CH3OH+CH3O<=>CH2OH+CH3OH 3.000E+011 0.000
 4074.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
 CH3OH+CH3O2<=>CH2OH+CH3O2H 1.810E+012 0.000
 13710.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)

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!\SUBSPECIES: \CH2OH
!=====
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!

!\REACTIONCLASS: \R_R_ABSTRACTIONS \A \N
\EA
!

CH2OH+O2<=>CH2O+HO2 1.510E+015 -1.000
0.0 !\AUTHOR: !\REF:GROTHER, H. H. ET AL., J. PHYS. CHEM. 92: 4028
(1988).
DUP
CH2OH+O2<=>CH2O+HO2 2.410E+014 0.000
5017.0
DUP
CH2OH+H<=>CH2O+H2 6.000E+012 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH2OH+HO2<=>CH2O+H2O2 1.200E+013 0.000
0.0 !\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991).
CH2OH+HCO<=>CH2O+CH2O 1.800E+014 0.000
0.0 !\AUTHOR: !\REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998)
CH2OH+HCO<=>CH3OH+CO 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:
CH2OH+CH3O<=>CH2O+CH3OH 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991).
CH2OH+OH<=>H2O+CH2O 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH2OH+O<=>OH+CH2O 4.200E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH2OH+CH2OH<=>CH2O+CH3OH 3.000E+012 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!

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

CH2OH+HO2<=>HOCH2O+OH 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

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

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

!\REACTIONCLASS: \R_R_ABSTRACTIONS \A \N
\EA
!

CH3O+O2<=>CH2O+HO2	4.380E-019	9.500
-5501.0 !\AUTHOR: !\REF:WANTUCK, P.J. E AL. J. PHYS. CHEM. 91, 4653 (1987)		
CH3O+H<=>CH2O+H2	2.000E+013	0.000
0.0 !\AUTHOR: !\REF:HOYERMANN ET AL., 18TH SYMPOSIUM		
CH3O+HO2<=>CH2O+H2O2	3.010E+011	0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
CH3O+CH3<=>CH2O+CH4	1.200E+013	0.000
0.0 !\AUTHOR: !\REF: NO REFERENCE		
CH3O+CH3O<=>CH3OH+CH2O	6.030E+013	0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		

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!\ENDSUBSPECIES: \CH3O

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!\SUBSPECIES: \HCOH

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!=====
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!\REACTIONCLASS: \LUMPED_BIMOLECULAR	\A	\N
\EA		

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HCOH+O2=>CO2+H+OH	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:MARINOV 1996		
HCOH+O2<=>CO2+H2O	3.000E+013	0.000
0.0 !\AUTHOR: !\REF:MARINOV 1996		
HCOH+O=>CO2+H+H	5.000E+013	0.000
0.0 !\AUTHOR: !\REF:MARINOV 1996		
HCOH+O=>CO+OH+H	3.000E+013	0.000
0.0 !\AUTHOR: !\REF:MARINOV 1996		
HCOH+H<=>CH2O+H	2.000E+014	0.000
0.0 !\AUTHOR: !\REF:MARINOV 1996		
HCOH+OH<=>HCO+H2O	2.000E+013	0.000
0.0 !\AUTHOR: !\REF:MARINOV 1996		

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!\ENDSUBSPECIES: \CH3O

!=====
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!\ENDSUBMECH: \CH3OH

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!-----

!\SUBMECH: \CH2O

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

HCO+H(+M)<=>CH2O(+M) 1.090E+012 0.480
-260.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
LOW/ 1.350E+024 -2.570
1425.0/
TROE/ 7.824E-001 2.710E+002 2.755E+003 6.570E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/
CO+H2(+M)<=>CH2O(+M) 4.300E+007 1.500
79600.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
LOW/ 5.070E+027 -3.420
84348.0/
TROE/ 9.320E-001 1.970E+002 1.540E+003 1.030E+004/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/
!

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

CH2O+O2<=>HCO+HO2 8.070E+015 0.000
53420.0 !\AUTHOR: !\REF: N. K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109,
7902-7914 (2005)
CH2O+O<=>HCO+OH 6.260E+009 1.150
2260.0 !\AUTHOR: !\REF: CURRAN FIT TO NIST DATABASE
CH2O+H<=>HCO+H2 5.740E+007 1.900
2740.0 !\AUTHOR: !\REF: IRDAM ET AL., IJCK 1993, 25, 285
CH2O+OH<=>HCO+H2O 7.820E+007 1.630
-1055.0 !\AUTHOR: !\REF: V. VASUDEVAN ET AL. IJCK. 37: 98--109 (2005).
CH2O+HO2<=>HCO+H2O2 1.880E+004 2.700
11520.0 !\AUTHOR: !\REF: J. PHYS. CHEM. A 109, 12027-12035, 2005
CH2O+CH3<=>HCO+CH4 3.830E+001 3.360
4312.0 !\AUTHOR: !\REF: BAULCH ET AL. JOURNAL OF PHYSICAL AND CHEMICAL
REFERENCE DATA, 34, 3, 757-1397 2005
CH2O+O2CHO<=>HCO+HO2CHO 1.990E+012 0.000
11660.0 !\AUTHOR: !\REF: ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986
CH2O+OCHO<=>HCO+HOCHO 5.600E+012 0.000
13600.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
CH2O+CH3O<=>HCO+CH3OH 6.620E+011 0.000
2294.0 !\AUTHOR: !\REF:FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998).
CH2O+CH3O2<=>HCO+CH3O2H 1.990E+012 0.000
11660.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N
\EA
!

HCO+M<=>H+CO+M 5.700E+011 0.660
14870.0 !\AUTHOR: !\REF: LI ET AL. IJCK 2007
H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/
!

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!\REACTIONCLASS: \R_R_ABSTRACTION          \A          \N
\EA
!
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HCO+O2<=>CO+HO2                          7.580E+012      0.000
410.0 !\AUTHOR: !\REF:TIMONEN ET AL., JPC, 92:651 (1988)
HCO+O<=>CO+OH                              3.020E+013      0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
HCO+H<=>CO+H2                              7.340E+013      0.000
0.0 !\AUTHOR: !\REF:TIMONEN ET AL., JPC, 92:651 (1988)
HCO+OH<=>CO+H2O                            3.011E+013      0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
HCO+CH3<=>CH4+CO                           2.650E+013      0.000
0.0 !\AUTHOR: !\REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987)
HCO+HCO<=>CH2O+CO                          1.800E+013      0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
!
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!\REACTIONCLASS: \LUMPED_BIMOLECULAR        \A          \N
\EA
!
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HCO+O<=>CO2+H                              3.000E+013      0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
HCO+HO2=>CO2+H+OH                          3.000E+013      0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
HCO+HCO=>H2+CO+CO                          3.000E+012      0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
!
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!\REACTIONCLASS: \RADICAL_ADDITION\H        \A          \N
\EA
!
-----
CH2O+H(+M)<=>CH2OH(+M)                      5.400E+011      0.454
3600.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
LOW/                                         1.270E+032      -4.820
6530.0/
TROE/ 7.187E-001 1.030E+002 1.291E+003 4.160E+003/
H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/
CH3O(+M)<=>CH2O+H(+M)                       6.800E+013      0.000
26170.0 !\AUTHOR: !\REF:HIPPLER ET AL. PCCP. 3: 3450--2458 (2001).
LOW/                                        1.867E+025      -3.000
24307.0/
TROE/ 9.000E-001 2.500E+003 1.300E+003 1.000E+099/
H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/
!
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!\REACTIONCLASS: \RADICAL_ADDITION\OH        \A          \N
\EA
!
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CH2O+OH<=>HOCH2O 4.500E+015 -1.100
0.0 !\AUTHOR: !\REF:26TH INTL. COMBUSTION SYMP. P 497--504.
HOCH2O<=>HOCHO+H 1.000E+014 0.000
14900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!

!\REACTIONCLASS: \RADICAL_ADDITION\HO2 \A \N
\EA

!

CH2O+HO2<=>OCH2O2H 1.500E+011 0.000
11900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
OCH2O2H<=>HOCH2O2 3.000E+011 0.000
8600.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
HOCH2O2+HO2<=>HOCH2O2H+O2 3.500E+010 0.000
-3275.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
HOCH2O+OH<=>HOCH2O2H 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!

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

!

HCO+O2<=>O2CHO 1.200E+011 0.000
-1100.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!

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!\SUBSPECIES: \HOCHO

!

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!

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

!

HOCHO<=>CO+H2O 2.450E+012 0.000
60470.0 !\AUTHOR: !\REF:BLAKE ET AL. J. CHEM. SOC. B: 10, 1923 (1971)
HOCHO<=>CO2+H2 2.950E+009 0.000
48520.0 !\AUTHOR: !\REF:BLAKE ET AL. J. CHEM. SOC. B: 10, 1923 (1971)

!

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

!

OCHO+HO2<=>HOCHO+O2 3.500E+010 0.000
-3275.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
OCHO+H2O2<=>HOCHO+HO2 2.400E+012 0.000
10000.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!

!\REACTIONCLASS: \LUMPED_BIMOLECULAR \A \N
\EA

!

HOCHO+H=>H2+CO2+H	4.240E+006	2.100
4868.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		
HOCHO+H=>H2+CO+OH	6.030E+013	-0.350
2988.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		
HOCHO+O=>CO+OH+OH	1.770E+018	-1.900
2975.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		
HOCHO+OH=>H2O+CO2+H	2.620E+006	2.060
916.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		
HOCHO+OH=>H2O+CO+OH	1.850E+007	1.510
-962.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		
HOCHO+CH3=>CH4+CO+OH	3.900E-007	5.800
2200.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		
HOCHO+HO2=>H2O2+CO+OH	1.000E+012	0.000
11920.0 !\AUTHOR: !\REF:MARINOV ESTIMATE		

!

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!\REACTIONCLASS: \RADICAL_ADDITION\OH      \A      \N
\EA
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!

OCHO+OH<=>HO2CHO	2.000E+013	0.000
0.0 !\AUTHOR: !\REF:WKM ESTIMATE		

!=====

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!\ENDSUBSPECIES: \HOCHO

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!\ENDSUBMECH: \CH2O

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!\END_KINETICS_MODULE: \C1

!+++++

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!\KINETICS_MODULE: \C2

!+++++

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!\MODSUBMECHS:

!+++++

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!-----

!\SUBMECH: \C2H6

!-----

!

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

$\text{CH}_3 + \text{CH}_3 (+M) \rightleftharpoons \text{C}_2\text{H}_6 (+M)$ 2.277E+015 -0.690
 174.9 !\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003)
 LOW/ 8.054E+031 -3.750
 981.6/
 TROE/ 0.000E+000 5.700E+002 1.000E+030 1.000E+030/
 H2O/ 5.00/ CO/ 2.00/ CO2/ 3.00/
 $\text{C}_2\text{H}_5 + \text{H} (+M) \rightleftharpoons \text{C}_2\text{H}_6 (+M)$ 5.210E+017 -0.990
 1580.0 !\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003)
 LOW/ 1.990E+041 -7.080
 6685.0/
 TROE/ 8.420E-001 1.250E+002 2.219E+003 6.882E+003/
 H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
 3.00/ HE/ 0.70/
 !

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

$\text{C}_2\text{H}_6 + \text{O}_2 \rightleftharpoons \text{C}_2\text{H}_5 + \text{HO}_2$ 6.030E+013 0.000
 51870.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
 (1992)
 $\text{C}_2\text{H}_6 + \text{O} \rightleftharpoons \text{C}_2\text{H}_5 + \text{OH}$ 3.550E+006 2.400
 5830.0 !\AUTHOR: !\REF:MIYOSHI, A. ET AL., CHEM. PHYS. LETT. 204, 241-247
 (1993)
 $\text{C}_2\text{H}_6 + \text{H} \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}_2$ 1.150E+008 1.900
 7530.0 !\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003)
 $\text{C}_2\text{H}_6 + \text{OH} \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}_2\text{O}$ 1.480E+007 1.900
 950.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE
 $\text{C}_2\text{H}_6 + \text{HO}_2 \rightleftharpoons \text{C}_2\text{H}_5 + \text{H}_2\text{O}_2$ 3.460E+001 3.610
 16920.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054.
 $\text{C}_2\text{H}_6 + \text{CH} \rightleftharpoons \text{C}_2\text{H}_5 + \text{CH}_2$ 1.100E+014 0.000
 -260.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
 15:1087 (1986)
 $\text{C}_2\text{H}_6 + \text{CH}_2 (\text{S}) \rightleftharpoons \text{C}_2\text{H}_5 + \text{CH}_3$ 1.200E+014 0.000
 0.0 !\AUTHOR: !\REF:MECHANISM AND MODELING OF NITROGEN CHEMISTRY IN
 COMBUSTION, WSS/ CI, AUTUMN 1988
 $\text{C}_2\text{H}_6 + \text{CH}_3 \rightleftharpoons \text{C}_2\text{H}_5 + \text{CH}_4$ 5.550E-004 4.720
 3231.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
 15:1087 (1986)
 $\text{C}_2\text{H}_6 + \text{CH}_3\text{O} \rightleftharpoons \text{C}_2\text{H}_5 + \text{CH}_3\text{OH}$ 2.410E+011 0.000
 7090.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
 15:1087 (1986)
 $\text{C}_2\text{H}_6 + \text{CH}_3\text{O}_2 \rightleftharpoons \text{C}_2\text{H}_5 + \text{CH}_3\text{O}_2\text{H}$ 1.940E+001 3.640
 17100.0 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995;§C1003
 $\text{C}_2\text{H}_6 + \text{C}_2\text{H}_5\text{O}_2 \rightleftharpoons \text{C}_2\text{H}_5 + \text{C}_2\text{H}_5\text{O}_2\text{H}$ 8.600E+000 3.760
 17200.0 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995;§C1003
 !

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

$\text{C}_2\text{H}_4 + \text{H} (+M) \rightleftharpoons \text{C}_2\text{H}_5 (+M)$ 9.569E+008 1.463
 1355.0 !\AUTHOR: !\REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202

LOW/ 1.419E+039 -6.642
5769.0/
TROE/ -5.690E-001 2.990E+002 -9.147E+003 1.524E+002/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/
!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

C2H5+H<=>C2H4+H2 2.000E+012 0.000
0.0 !\AUTHOR: !\REF: CURRAN: FIT TO PRATT/ WOOD 84 AND PRATT/ VELDMAN 76
C2H4+C2H4<=>C2H5+C2H3 4.820E+014 0.000
71530.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
C2H5+CH3<=>CH4+C2H4 1.180E+004 2.450
-2921.0 !\AUTHOR: !\REF:ZHU, R.S. ET AL., J. CHEM. PHYS. 120:6566:6573
(2004)
!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA
!

C2H5+O<=>CH3CHO+H 1.100E+014 0.000
0.0 !\AUTHOR: !\REF:GRI 3.0
C2H5+HO2<=>C2H5O+OH 1.100E+013 0.000
0.0 !\AUTHOR: !\REF:CURRAN. BASED ON CH3+HO2<=>PRODUCTS
C2H5+CH3O2<=>C2H5O+CH3O 8.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:CURRAN. BASED ON CH3+HO2<=>PRODUCTS
!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA
!

CH3+CH3<=>H+C2H5 4.740E+012 0.105
10664.3 !\AUTHOR: !\REF:STEWART ET AL C&F 1989
PLOG/ 0.0100 4.740E+012 0.105 10664.3/
PLOG/ 0.1000 2.570E+013 -0.096 11406.1/
PLOG/ 1.0000 3.100E+014 -0.362 13372.5/
PLOG/ 10.0000 2.150E+010 0.885 13532.5/
PLOG/ 100.0000 1.032E+002 3.230 11236.1/
!

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

C2H5+O2<=>C2H5O2 3.398E+053 -13.900
9279.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;SC4427
PLOG/ 0.0400 3.398E+053 -13.900 9279.0/
PLOG/ 1.0000 9.362E+059 -15.280 14240.0/
PLOG/ 10.0000 1.262E+060 -14.910 16240.0/
!

C2H5+O2<=>C2H4O2H 2.103E+034 -9.010
5444.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 2.103E+034 -9.010 5444.0/
PLOG/ 1.0000 4.884E+033 -8.310 7710.0/
PLOG/ 10.0000 1.705E+045 -11.490 14590.0/

C2H5+O2<=>C2H4+HO2 2.094E+009 0.490
-391.4 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 2.094E+009 0.490 -391.4/
PLOG/ 1.0000 1.843E+007 1.130 -720.6/
PLOG/ 10.0000 7.561E+014 -1.010 4749.0/

C2H5+O2<=>C2H4O1-2+OH 1.303E+003 1.930
-502.7 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 1.303E+003 1.930 -502.7/
PLOG/ 1.0000 2.438E+002 2.180 -62.5/
PLOG/ 10.0000 4.621E+009 0.150 5409.0/

C2H5+O2<=>CH3CHO+OH 4.908E-006 4.760
254.3 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 4.908E-006 4.760 254.3/
PLOG/ 1.0000 6.803E-002 3.570 2643.0/
PLOG/ 10.0000 8.265E+002 2.410 5285.0/

C2H4O2H<=>C2H5O2 2.653E-016 6.960
2396.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 2.653E-016 6.960 2396.0/
PLOG/ 1.0000 1.064E+041 -10.100 26030.0/
PLOG/ 10.0000 1.203E+036 -8.130 27020.0/

C2H5O2<=>CH3CHO+OH 1.237E+035 -9.420
36360.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 1.237E+035 -9.420 36360.0/
PLOG/ 1.0000 1.687E+036 -9.220 38700.0/
PLOG/ 10.0000 2.520E+041 -10.200 43710.0/

C2H5O2<=>C2H4+HO2 1.782E+032 -7.100
32840.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 1.782E+032 -7.100 32840.0/
PLOG/ 1.0000 2.701E+037 -8.470 35840.0/
PLOG/ 10.0000 1.980E+038 -8.460 37900.0/

C2H5O2<=>C2H4O1-2+OH 5.778E+045 -11.900
4112.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 5.778E+045 -11.900 4112.0/
PLOG/ 1.0000 1.916E+043 -10.750 42400.0/
PLOG/ 10.0000 3.965E+043 -10.460 45580.0/

C2H4O2H<=>C2H4O1-2+OH 8.959E+038 -9.400
20660.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 8.959E+038 -9.400 20660.0/
PLOG/ 1.0000 1.224E+037 -8.320 21460.0/
PLOG/ 10.0000 8.848E+030 -6.080 20660.0/

C2H4O2H<=>C2H4+HO2 3.918E+040 -10.200
22250.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 3.918E+040 -10.200 22250.0/
PLOG/ 1.0000 6.825E+040 -9.610 23840.0/
PLOG/ 10.0000 3.980E+034 -7.250 23250.0/

C2H4O2H<=>CH3CHO+OH 5.819E+026 -7.970
20860.0 !\AUTHOR: !\REF:John D. DeSain, J. Phys. Chem. A, 2003, 107 (22),
pp 4415;\\$C4427
PLOG/ 0.0400 5.819E+026 -7.970 20860.0/
PLOG/ 1.0000 5.520E+034 -9.880 26230.0/
PLOG/ 10.0000 1.188E+034 -9.020 29210.0/

!

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

!

H2+C2H5O2<=>H+C2H5O2H 1.500E+014 0.000
26030.0 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF.
DATA, VOL 15, 1986

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!\SUBSPECIES: \C2H5O2H

!=====

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!

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

!

C2H5O2+HO2<=>C2H5O2H+O2 1.750E+010 0.000
-3275.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
C2H5O2+CH2O<=>C2H5O2H+HCO 1.990E+012 0.000
11660.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
C2H5O2+CH4<=>C2H5O2H+CH3 1.810E+011 0.000
18480.0 !\AUTHOR: !\REF:BASED ON CH4+CH3O2
C2H5O2+CH3OH<=>C2H5O2H+CH2OH 1.810E+012 0.000
13710.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)

!

!\REACTIONCLASS: \KHP_DECOMP \A \N \EA

!

C2H5O2H<=>C2H5O+OH 6.310E+014 0.000
42300.0 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
995;\\$C1003

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!\ENDSUBSPECIES: \C2H5O2H
!
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!
=====
!\SUBSPECIES: C2H4O1-2
!
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!
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!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
-----
C2H4O1-2<=>CH3+HCO                        3.630E+013      0.000
57200.0 !\AUTHOR: !\REF:LIFSHITZ ET AL. 1983
C2H4O1-2<=>CH3CHO                          7.407E+012      0.000
53800.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE
!
-----
!\REACTIONCLASS: \RH_R_ABSTRACTION       \A                \N
\EA
!
-----
C2H4O1-2+H<=>C2H3O1-2+H2                  8.000E+013      0.000
9680.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984)
C2H4O1-2+OH<=>C2H3O1-2+H2O                1.780E+013      0.000
3610.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984)
C2H4O1-2+HO2<=>C2H3O1-2+H2O2              1.130E+013      0.000
30430.0 !\AUTHOR: !\REF:ANALOGY WITH ETHENE
C2H4O1-2+CH3<=>C2H3O1-2+CH4               1.070E+012      0.000
11830.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984)
C2H4O1-2+CH3O<=>C2H3O1-2+CH3OH            1.200E+011      0.000
6750.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984)
C2H4O1-2+CH3O2<=>C2H3O1-2+CH3O2H         1.130E+013      0.000
30430.0 !\AUTHOR: !\REF:ANALOGY WITH ETHENE
C2H4O1-2+C2H5O2<=>C2H3O1-2+C2H5O2H       1.130E+013      0.000
30430.0 !\AUTHOR: !\REF:ANALOGY WITH ETHENE
!
-----
!\REACTIONCLASS: \RADICAL_ISOMERISATION  \A                \N
\EA
!-----
-----
C2H3O1-2<=>CH3CO                          8.500E+014      0.000
14000.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984)
C2H3O1-2<=>CH2CHO                          1.000E+014      0.000
14000.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984)
!
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=====

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!\ENDSUBSPECIES: \C2H4O1-2

!=====
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!-----

!\ENDSUBMECH: \C2H6

!-----

!-----

!\SUBMECH: \C2H4

!-----

!

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!

C2H3+H(+M)<=>C2H4(+M) 6.080E+012 0.270

280.0 !\AUTHOR: !\REF:GRI 3.0

LOW/ 1.400E+030 -3.860

3320.0/

TROE/ 7.820E-001 2.075E+002 2.663E+003 6.095E+003/

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

3.00/ HE/ 0.70/

C2H4(+M)<=>H2+H2CC(+M) 8.000E+012 0.440

88770.0 !\AUTHOR: !\REF:GRI

LOW/ 7.000E+050 -9.310

99860.0/

TROE/ 7.345E-001 1.800E+002 1.035E+003 5.417E+003/

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

0.70/

!

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!

C2H4+O2<=>C2H3+HO2 4.220E+013 0.000

57623.1 !\AUTHOR: !\REF:CHECK EFFECT!!\!\!\!\!\

C2H4+H<=>C2H3+H2 5.070E+007 1.930

12950.0 !\AUTHOR: !\REF:KNYAZEV,V.D. ET AL.,J. PHYS. CHEM. 100, 11346-1135 (1996)

C2H4+OH<=>C2H3+H2O 2.230E+004 2.745

2215.5 !\AUTHOR: !\REF: FROM STANFORD

C2H4+CH3O<=>C2H3+CH3OH 1.200E+011 0.000

6750.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)

C2H4+CH3O2<=>C2H3+CH3O2H 8.590E+000 3.754

27132.0 !\AUTHOR: !\REF:FROM BILL PITZ'S SUGGESTION

C2H4+C2H5O2<=>C2H3+C2H5O2H 8.590E+000 3.754

27132.0 !\AUTHOR: !\REF:FROM BILL PITZ'S SUGGESTION

C2H4+CH3CO3<=>C2H3+CH3CO3H 1.130E+013 0.000

30430.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)

C2H4+CH3<=>C2H3+CH4 9.760E+002 2.947

15148.0 !\AUTHOR: !\REF:

DUP
C2H4+CH3<=>C2H3+CH4 8.130E-005 4.417
8835.8

DUP

!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA

!

C2H4+O<=>CH3+HCO 7.453E+006 1.880
183.0 !\AUTHOR: !\REF: BAULCH ET AL. JOURNAL OF PHYSICAL AND CHEMICAL
REFERENCE DATA: 34, 3, 757-1397 2005

C2H4+O<=>CH2CHO+H 6.098E+006 1.880
183.0 !\AUTHOR: !\REF: BAULCH ET AL. JOURNAL OF PHYSICAL AND CHEMICAL
REFERENCE DATA: 34, 3, 757-1397 2005

CH+CH4<=>C2H4+H 6.000E+013 0.000
0.0 !\AUTHOR: !\REF: BUTLER, FLEMING, GOSS, LIN, ACS SYMP. SER. 134
(1980).

CH2(S)+CH3<=>C2H4+H 2.000E+013 0.000
0.0 !\AUTHOR: !\REF: MARINOV ESTIMATE.

!

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA

!

C2H4+OH<=>CH3+CH2O 5.350E+000 2.920
-1732.7 !\AUTHOR: !\REF: SJK, J PHYS CHEM 110 2006 6960-6970

PLOG/ 0.0100 5.350E+000 2.920 -1732.7/

PLOG/ 0.0250 3.190E+001 2.710 -1172.3/

PLOG/ 0.1000 5.550E+002 2.360 -180.8/

PLOG/ 1.0000 1.780E+005 1.680 2060.5/

PLOG/ 10.0000 2.370E+009 0.560 6006.7/

PLOG/ 100.0000 2.760E+013 -0.500 11455.1/

C2H4+OH<=>CH3CHO+H 2.370E-007 5.300
-2050.6 !\AUTHOR: !\REF: SJK, J PHYS CHEM 110 2006 6960-6970

PLOG/ 0.0100 2.370E-007 5.300 -2050.6/

PLOG/ 0.0250 8.730E-005 4.570 -618.0/

PLOG/ 0.1000 4.030E-001 3.540 1881.7/

PLOG/ 1.0000 2.380E-002 3.910 1722.7/

PLOG/ 10.0000 8.250E+008 1.010 10507.3/

PLOG/ 100.0000 6.800E+009 0.810 13867.3/

C2H4+OH<=>C2H3OH+H 1.040E+004 2.600
4121.0 !\AUTHOR: !\REF: SJK, J PHYS CHEM 110 2006 6960-6970

PLOG/ 0.0100 1.040E+004 2.600 4121.0/

PLOG/ 0.0250 1.070E+004 2.600 4129.0/

PLOG/ 0.1000 1.520E+004 2.560 4238.3/

PLOG/ 1.0000 3.190E+005 2.190 5255.6/

PLOG/ 10.0000 1.940E+008 1.430 7828.8/

PLOG/ 100.0000 8.550E+010 0.750 11490.8/

C2H4+OH<=>PC2H4OH 1.740E+043 -10.461
7698.7 !\AUTHOR: !\REF: SJK, J PHYS CHEM 110 2006 6960-6970

PLOG/ 0.0100 1.740E+043 -10.461 7698.7/

PLOG/ 0.0250 3.250E+037 -8.629 5214.7/

PLOG/ 0.1000 1.840E+035 -7.750 4908.9/

PLOG/ 1.0000 2.560E+036 -7.752 6946.1/

PLOG/ 10.0000 3.700E+033 -6.573 7605.9/

PLOG/ 100.0000 1.120E+026 -4.101 5757.0/
!

!\REACTIONCLASS: \ALKENE_RO2_CYC_ETH_RO \A \N
\EA
!

C2H4+HO2<=>C2H4O1-2+OH 3.345E+012 0.000
17190.0 !\AUTHOR: !\REF:BAULCH AND COBOS
C2H4+CH3O2<=>C2H4O1-2+CH3O 2.820E+012 0.000
17110.0 !\AUTHOR: !\REF:PITZ ESTIMATE
C2H4+C2H5O2<=>C2H4O1-2+C2H5O 2.820E+012 0.000
17110.0 !\AUTHOR: !\REF:PITZ ESTIMATE

!=====
=====
!\SUBSPECIES: \C2H3
!=====
=====
!

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

C2H2+H(+M)<=>C2H3(+M) 1.710E+010 1.266
2709.0 !\AUTHOR: !\REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202
LOW/ 6.346E+031 -4.664
3780.0/
TROE/ 7.880E-001 -1.020E+004 1.000E-030/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/
!

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

C2H3+O2<=>C2H3OO 4.07E+27 -4.67 5222 ! !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.55E+24 -5.45 9662.0/
PLOG/1.000E-01 3.48E+56 -15.01 19160.0/
PLOG/3.160E-01 1.25E+64 -16.97 21290.0/
PLOG/1.000E+00 3.34E+61 -15.79 20150.0/
PLOG/3.160E+00 7.34E+53 -13.11 17300.0/
PLOG/1.000E+01 4.16E+48 -11.21 16000.0/
PLOG/3.160E+01 2.33E+43 -9.38 14810.0/
PLOG/1.000E+02 3.41E+39 -8.04 14360.0/
DUP

C2H3+O2<=>C2H3OO 4.07E+27 -4.67 5222 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.78E-09 4.15 -4707.0/
PLOG/1.000E-01 2.36E+22 -4.52 2839.0/
PLOG/3.160E-01 2.00E+26 -5.43 2725.0/
PLOG/1.000E+00 6.13E+28 -5.89 3154.0/
PLOG/3.160E+00 2.14E+29 -5.8 3520.0/
PLOG/1.000E+01 3.48E+28 -5.37 3636.0/
PLOG/3.160E+01 3.32E+27 -4.95 3610.0/
PLOG/1.000E+02 1.03E+27 -4.72 3680.0/

DUP

C2H3+O2<=>CHCHO+OH 2.84E+14 -0.8 7232 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 3.91E+11 -0.11 2131.0/
PLOG/1.000E-01 1.13E+09 0.55 46.0/
PLOG/3.160E-01 8.46E+08 0.56 0.7/
PLOG/1.000E+00 2.75E+14 -1.83 4.6/
PLOG/3.160E+00 2.58E+20 -2.84 7530.0/
PLOG/1.000E+01 9.18E+14 -2.26 -0.4/
PLOG/3.160E+01 6.11E+25 -4.21 13050.0/
PLOG/1.000E+02 1.65E+30 -5.35 18430.0/

DUP

C2H3+O2<=>CHCHO+OH 2.84E+14 -0.8 7232 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 9.91E+11 -0.66 -0.6/
PLOG/1.000E-01 6.94E+14 -1.16 4542.0/
PLOG/3.160E-01 2.79E+13 -0.72 3479.0/
PLOG/1.000E+00 4.99E+11 -0.14 1995.0/
PLOG/3.160E+00 2.35E+10 0.23 1573.0/
PLOG/1.000E+01 1.70E+14 -0.82 4450.0/
PLOG/3.160E+01 1.42E+11 0.05 3774.0/
PLOG/1.000E+02 3.17E+11 -0.02 5338.0/

DUP

C2H3+O2<=>CH2CHO+O 1.76E+12 0.15 4205 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 7.88E+20 -2.67 6742.0/
PLOG/1.000E-01 7.72E+20 -2.67 6713.0/
PLOG/3.160E-01 9.87E+20 -2.7 6724.0/
PLOG/1.000E+00 7.10E+20 -2.65 6489.0/
PLOG/3.160E+00 4.50E+20 -2.53 6406.0/
PLOG/1.000E+01 1.76E+23 -3.22 8697.0/
PLOG/3.160E+01 3.14E+25 -3.77 11530.0/
PLOG/1.000E+02 1.02E+26 -3.8 13910.0/

DUP

C2H3+O2<=>CH2CHO+O 1.76E+12 0.15 4205 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.36E+10 0.62 -277.6/
PLOG/1.000E-01 1.42E+10 0.62 -247.7/
PLOG/3.160E-01 1.66E+10 0.6 -162.5/
PLOG/1.000E+00 2.02E+10 0.58 38.4/
PLOG/3.160E+00 9.75E+09 0.67 248.0/
PLOG/1.000E+01 7.34E+09 0.72 778.1/
PLOG/3.160E+01 1.57E+09 0.92 1219.0/
PLOG/1.000E+02 7.85E+07 1.28 1401.0/

DUP

C2H3+O2<=>C2H2+HO2 6.49E+06 1.5 5218 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.08E+07 1.28 3322.0/
PLOG/1.000E-01 7.75E+06 1.33 3216.0/
PLOG/3.160E-01 1.21E+07 1.27 3311.0/
PLOG/1.000E+00 2.15E+07 1.19 3367.0/
PLOG/3.160E+00 1.13E+08 1 3695.0/
PLOG/1.000E+01 1.31E+11 0.12 5872.0/
PLOG/3.160E+01 1.19E+09 0.82 5617.0/
PLOG/1.000E+02 1.06E+17 -1.45 12230.0/

DUP

C2H3+O2<=>C2H2+HO2 6.49E+06 1.5 5218 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 4.76E+01 2.75 -796.4/
PLOG/1.000E-01 5.16E+01 2.73 -768.3/
PLOG/3.160E-01 5.55E+01 2.73 -658.5/
PLOG/1.000E+00 4.60E+01 2.76 -492.8/
PLOG/3.160E+00 3.75E+00 3.07 -601.0/
PLOG/1.000E+01 5.48E+00 3.07 85.7/
PLOG/3.160E+01 4.47E+08 0 955.0/
PLOG/1.000E+02 2.02E+01 2.94 1847.0/
DUP

!\DUP\PDEPP

C2H3+O2<=>CHOCHO+H 3.08E+12 -0.26 3277 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 4.79E+14 -1.03 912.0/
PLOG/1.000E-01 5.03E+14 -1.04 922.5/
PLOG/3.160E-01 6.43E+14 -1.07 982.9/
PLOG/1.000E+00 3.73E+15 -1.29 1441.0/
PLOG/3.160E+00 2.44E+18 -2.13 3234.0/
PLOG/1.000E+01 1.30E+15 -1.09 2393.0/
PLOG/3.160E+01 3.57E+33 -6.5 14910.0/
PLOG/1.000E+02 3.28E+31 -5.76 16250.0/
DUP

C2H3+O2<=>CHOCHO+H 3.08E+12 -0.26 3277 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 2.80E-04 4.04 -7019.0/
PLOG/1.000E-01 3.45E-04 4.01 -6978.0/
PLOG/3.160E-01 9.73E-04 3.89 -6768.0/
PLOG/1.000E+00 4.98E-01 3.15 -5496.0/
PLOG/3.160E+00 1.34E+05 1.67 -2931.0/
PLOG/1.000E+01 4.50E+15 -3.08 -4836.0/
PLOG/3.160E+01 3.84E+10 0.22 941.3/
PLOG/1.000E+02 2.75E+08 0.83 857.6/
DUP

C2H3+O2<=>CH2CO+OH 1.17E+03 2.43 7074 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 8.66E+02 2.41 6061.0/
PLOG/1.000E-01 8.91E+02 2.41 6078.0/
PLOG/3.160E-01 9.43E+02 2.4 6112.0/
PLOG/1.000E+00 1.06E+03 2.39 6180.0/
PLOG/3.160E+00 1.09E+03 2.38 6179.0/
PLOG/1.000E+01 1.39E+03 2.36 6074.0/
PLOG/3.160E+01 2.49E+06 1.42 8480.0/
PLOG/1.000E+02 1.66E+10 0.36 12010.0/
DUP

C2H3+O2<=>CH2CO+OH 1.17E+03 2.43 7074 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.82E-01 3.12 1331.0/
PLOG/1.000E-01 2.07E-01 3.11 1383.0/
PLOG/3.160E-01 2.71E-01 3.08 1496.0/
PLOG/1.000E+00 5.26E-01 3.01 1777.0/
PLOG/3.160E+00 1.37E+00 2.9 2225.0/
PLOG/1.000E+01 4.19E-01 2.93 2052.0/
PLOG/3.160E+01 1.19E-04 4.21 2043.0/
PLOG/1.000E+02 1.30E-03 3.97 3414.0/
DUP

C2H3+O2<=>CH2O+HCO 1.16E+16 -1.13 3791 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 2.49E+36 -7.6 12640.0/
PLOG/1.000E-01 2.43E+36 -7.6 12610.0/
PLOG/3.160E-01 1.95E+36 -7.57 12490.0/
PLOG/1.000E+00 2.73E+35 -7.32 11820.0/
PLOG/3.160E+00 1.43E+36 -7.47 12460.0/
PLOG/1.000E+01 5.18E+35 -7.2 13430.0/
PLOG/3.160E+01 3.19E+20 -2.57 5578.0/
PLOG/1.000E+02 2.73E+33 -6.28 16000.0/

DUP

C2H3+O2<=>CH2O+HCO 1.16E+16 -1.13 3791 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 4.54E+15 -1.28 515.3/
PLOG/1.000E-01 4.59E+15 -1.28 513.0/
PLOG/3.160E-01 4.81E+15 -1.29 520.6/
PLOG/1.000E+00 6.08E+15 -1.31 645.7/
PLOG/3.160E+00 9.45E+15 -1.36 1066.0/
PLOG/1.000E+01 2.56E+15 -1.18 1429.0/
PLOG/3.160E+01 1.03E+69 -19.23 14760.0/
PLOG/1.000E+02 4.21E+10 0.19 830.6/

DUP

C2H3+O2=>CH2O+H+CO 1.16E+16 -1.13 3791 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 5.82E+36 -7.6 12640.0/
PLOG/1.000E-01 5.66E+36 -7.6 12610.0/
PLOG/3.160E-01 4.55E+36 -7.57 12490.0/
PLOG/1.000E+00 6.36E+35 -7.32 11820.0/
PLOG/3.160E+00 3.35E+36 -7.47 12460.0/
PLOG/1.000E+01 1.21E+36 -7.2 13430.0/
PLOG/3.160E+01 7.43E+20 -2.57 5578.0/
PLOG/1.000E+02 6.36E+33 -6.28 16000.0/

DUP

C2H3+O2=>CH2O+H+CO 1.16E+16 -1.13 3791 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.06E+16 -1.28 515.3/
PLOG/1.000E-01 1.07E+16 -1.28 513.0/
PLOG/3.160E-01 1.13E+16 -1.29 520.6/
PLOG/1.000E+00 1.42E+16 -1.31 645.7/
PLOG/3.160E+00 2.20E+16 -1.36 1066.0/
PLOG/1.000E+01 5.98E+15 -1.18 1429.0/
PLOG/3.160E+01 2.39E+69 -19.23 14760.0/
PLOG/1.000E+02 9.81E+10 0.19 830.6/

DUP

C2H3+O2<=>CO+CH3O 3.09E+13 -0.89 3682 !\AUTHOR: !\REF: Goldsmith et
al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 8.19E+18 -2.66 3201.0/
PLOG/1.000E-01 4.06E+14 -1.32 885.8/
PLOG/3.160E-01 4.34E+14 -1.33 900.6/
PLOG/1.000E+00 1.03E+11 -0.33 -747.8/
PLOG/3.160E+00 1.89E+12 -3 -8995.0/
PLOG/1.000E+01 1.93E+24 -5.63 1.8/
PLOG/3.160E+01 1.10E+18 -2.22 5178.0/
PLOG/1.000E+02 5.79E+32 -6.45 16810.0/

DUP

C2H3+O2<=>CO+CH3O 3.09E+13 -0.89 3682 !\AUTHOR: !\REF: Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.29E+09 0.18 -1717.0/
PLOG/1.000E-01 5.99E+11 -2.93 -9564.0/
PLOG/3.160E-01 2.91E+11 -2.93 -10120.0/
PLOG/1.000E+00 5.77E+21 -3.54 4772.0/
PLOG/3.160E+00 4.99E+15 -1.62 1849.0/
PLOG/1.000E+01 9.33E+16 -1.96 3324.0/
PLOG/3.160E+01 1.02E+72 -20.69 15860.0/
PLOG/1.000E+02 1.10E+09 0.31 1024.0/
DUP

C2H3+O2<=>CO2+CH3 6.16E+13 -1.05 3743 !\AUTHOR: !\REF: Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 2.37E+35 -7.76 12630.0/
PLOG/1.000E-01 1.73E+35 -7.72 12520.0/
PLOG/3.160E-01 4.47E+34 -7.55 12140.0/
PLOG/1.000E+00 7.25E+31 -6.7 10440.0/
PLOG/3.160E+00 3.63E+35 -7.75 12830.0/
PLOG/1.000E+01 2.09E+35 -7.53 14050.0/
PLOG/3.160E+01 3.84E+18 -2.44 5408.0/
PLOG/1.000E+02 1.21E+32 -6.32 16190.0/
DUP

C2H3+O2<=>CO2+CH3 6.16E+13 -1.05 3743 !\AUTHOR: !\REF: Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 6.27E+13 -1.16 406.3/
PLOG/1.000E-01 6.24E+13 -1.16 401.4/
PLOG/3.160E-01 6.12E+13 -1.16 397.0/
PLOG/1.000E+00 5.32E+13 -1.14 446.7/
PLOG/3.160E+00 1.45E+14 -1.26 987.7/
PLOG/1.000E+01 5.02E+13 -1.11 1409.0/
PLOG/3.160E+01 1.40E+70 -20.11 15430.0/
PLOG/1.000E+02 9.21E+08 0.25 855.3/
DUP

C2H3OO<=>CHCHO+OH 5.89E+36 -7.1 51440 !\AUTHOR: !\REF: Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 3.64E+49 -12.13 67420.0/
PLOG/1.000E-01 1.44E+36 -9.92 41220.0/
PLOG/3.160E-01 4.18E+40 -10.53 43670.0/
PLOG/1.000E+00 3.79E+46 -10.72 51900.0/
PLOG/3.160E+00 1.60E+49 -11.24 54150.0/
PLOG/1.000E+01 2.38E+51 -11.64 56980.0/
PLOG/3.160E+01 2.00E+54 -12.22 61840.0/
PLOG/1.000E+02 9.54E+195 -52.27 163500.0/
DUP

C2H3OO<=>CHCHO+OH 5.89E+36 -7.1 51440 !\AUTHOR: !\REF: Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.17E+56 -14.81 60700.0/
PLOG/1.000E-01 2.32E+40 -9.39 50420.0/
PLOG/3.160E-01 1.61E+43 -9.99 50290.0/
PLOG/1.000E+00 2.33E+124 -36.77 70100.0/
PLOG/3.160E+00 1.88E+103 -29.49 65410.0/
PLOG/1.000E+01 5.96E+86 -23.81 62170.0/
PLOG/3.160E+01 1.51E+57 -13.94 55390.0/
PLOG/1.000E+02 1.79E+34 -6.4 50000.0/
DUP

C2H3OO<=>CH2CHO+O 1.22E+29 -4.71 42340 !\AUTHOR: !\REF:
 Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
 PLOG/1.000E-02 2.70E+180 -48.19 169300.0/
 PLOG/1.000E-01 3.90E+38 -8.69 42770.0/
 PLOG/3.160E-01 4.57E+47 -11.21 47050.0/
 PLOG/1.000E+00 7.62E+81 -21.28 65080.0/
 PLOG/3.160E+00 1.86E+68 -16.83 60680.0/
 PLOG/1.000E+01 2.02E+55 -12.69 55840.0/
 PLOG/3.160E+01 1.11E+53 -11.79 56690.0/
 PLOG/1.000E+02 4.30E+48 -10.31 56090.0/
 DUP

C2H3OO<=>CH2CHO+O 1.22E+29 -4.71 42340 !\AUTHOR: !\REF: Goldsmith
 et al, J. Phys. Chem. A 2015, 119, 7766-7779
 PLOG/1.000E-02 1.47E+30 -6.64 41110.0/
 PLOG/1.000E-01 9.65E-12 5.96 22890.0/
 PLOG/3.160E-01 3.95E+22 -3.71 36270.0/
 PLOG/1.000E+00 2.39E+33 -6.62 41280.0/
 PLOG/3.160E+00 6.37E+31 -5.96 41260.0/
 PLOG/1.000E+01 2.13E+29 -5.1 40710.0/
 PLOG/3.160E+01 4.66E+27 -4.5 40530.0/
 PLOG/1.000E+02 5.99E+25 -3.85 40120.0/
 DUP

C2H3OO<=>CHOCHO+H 4.72E+20 -2.69 32320 !\AUTHOR: !\REF: Goldsmith
 et al, J. Phys. Chem. A 2015, 119, 7766-7779
 PLOG/1.000E-02 6.41E+80 -22.2 51750.0/
 PLOG/1.000E-01 3.31E+65 -17.01 48090.0/
 PLOG/3.160E-01 5.98E+51 -12.62 43000.0/
 PLOG/1.000E+00 1.48E+44 -10.12 40790.0/
 PLOG/3.160E+00 1.26E+59 -14.33 51390.0/
 PLOG/1.000E+01 4.93E+26 -4.67 34320.0/
 PLOG/3.160E+01 2.06E+33 -6.38 39520.0/
 PLOG/1.000E+02 1.30E+32 -5.92 40660.0/
 DUP

C2H3OO<=>CHOCHO+H 4.72E+20 -2.69 32320 !\AUTHOR: !\REF: Goldsmith
 et al, J. Phys. Chem. A 2015, 119, 7766-7779
 PLOG/1.000E-02 1.19E+28 -6.01 28740.0/
 PLOG/1.000E-01 1.40E+25 -4.8 28940.0/
 PLOG/3.160E-01 2.91E+20 -3.29 27550.0/
 PLOG/1.000E+00 1.58E+19 -2.82 27620.0/
 PLOG/3.160E+00 1.93E+22 -3.54 29980.0/
 PLOG/1.000E+01 7.51E+29 -5.75 34490.0/
 PLOG/3.160E+01 7.14E+61 -16.16 43280.0/
 PLOG/1.000E+02 1.14E+19 -2.56 29670.0/
 DUP

C2H3OO<=>CH2CO+OH 1.55E+24 -3.87 49850 !\AUTHOR: !\REF: Goldsmith
 et al, J. Phys. Chem. A 2015, 119, 7766-7779
 PLOG/1.000E-02 1.15E+47 -12.28 75330.0/
 PLOG/1.000E-01 8.43E+09 -2.06 33720.0/
 PLOG/3.160E-01 6.06E+04 0.17 34220.0/
 PLOG/1.000E+00 1.51E+19 -3.61 43060.0/
 PLOG/3.160E+00 2.13E+33 -7.39 51610.0/
 PLOG/1.000E+01 4.44E+36 -7.99 54680.0/
 PLOG/3.160E+01 1.19E+37 -7.8 56460.0/
 PLOG/1.000E+02 9.08E+35 -7.21 57550.0/
 DUP

C2H3OO<=>CH2CO+OH 1.55E+24 -3.87 49850 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 2.31E+02 -0.73 25710.0/
PLOG/1.000E-01 1.83E-23 7.84 20190.0/
PLOG/3.160E-01 3.82E+63 -20.44 43420.0/
PLOG/1.000E+00 3.18E+27 -7.76 37230.0/
PLOG/3.160E+00 2.32E-05 3.47 31560.0/
PLOG/1.000E+01 1.06E-01 2.64 34160.0/
PLOG/3.160E+01 5.62E+02 1.7 36450.0/
PLOG/1.000E+02 1.11E+07 0.52 38670.0/
DUP

C2H3OO<=>CH2O+HCO 1.19E+20 -2.29 30170 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 1.66E+174 -55.52 60320.0/
PLOG/1.000E-01 9.03E+66 -17.25 48120.0/
PLOG/3.160E-01 1.82E+43 -9.87 37960.0/
PLOG/1.000E+00 8.64E+33 -6.88 34370.0/
PLOG/3.160E+00 7.29E+171 -43.53 191900.0/
PLOG/1.000E+01 1.03E+32 -6.06 35500.0/
PLOG/3.160E+01 1.85E+34 -6.57 38510.0/
PLOG/1.000E+02 5.70E+29 -5.19 36800.0/
DUP

C2H3OO<=>CH2O+HCO 1.19E+20 -2.29 30170 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 2.27E+35 -7.97 31280.0/
PLOG/1.000E-01 2.08E+26 -4.96 28780.0/
PLOG/3.160E-01 1.45E+20 -3.08 26630.0/
PLOG/1.000E+00 1.06E+130 -39.38 54700.0/
PLOG/3.160E+00 2.35E+34 -6.87 35700.0/
PLOG/1.000E+01 2.18E+175 -53.78 68500.0/
PLOG/3.160E+01 1.07E+185 -54.22 88990.0/
PLOG/1.000E+02 4.68E+02 1.81 18100.0/
DUP

C2H3OO=>CH2O+H+CO 1.19E+20 -2.29 30170 !\AUTHOR: !\REF:
Goldsmith et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 3.88E+174 -55.52 60320.0/
PLOG/1.000E-01 2.11E+67 -17.25 48120.0/
PLOG/3.160E-01 4.26E+43 -9.87 37960.0/
PLOG/1.000E+00 2.02E+34 -6.88 34370.0/
PLOG/3.160E+00 1.70E+172 -43.53 191900.0/
PLOG/1.000E+01 2.40E+32 -6.06 35500.0/
PLOG/3.160E+01 4.32E+34 -6.57 38510.0/
PLOG/1.000E+02 1.33E+30 -5.19 36800.0/
DUP

C2H3OO=>CH2O+H+CO 1.19E+20 -2.29 30170 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 5.29E+35 -7.97 31280.0/
PLOG/1.000E-01 4.85E+26 -4.96 28780.0/
PLOG/3.160E-01 3.37E+20 -3.08 26630.0/
PLOG/1.000E+00 2.46E+130 -39.38 54700.0/
PLOG/3.160E+00 5.49E+34 -6.87 35700.0/
PLOG/1.000E+01 5.09E+175 -53.78 68500.0/
PLOG/3.160E+01 2.49E+185 -54.22 88990.0/
PLOG/1.000E+02 1.09E+03 1.81 18100.0/
DUP

C2H3OO<=>CO+CH3O 1.16E-01 3.16 18420 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 5.20E+33 -7.92 31320.0/
PLOG/1.000E-01 1.26E+98 -27.09 64060.0/
PLOG/3.160E-01 1.80E+33 -7.27 33760.0/
PLOG/1.000E+00 3.83E+33 -7.2 35100.0/
PLOG/3.160E+00 1.28E+79 -19.61 74870.0/
PLOG/1.000E+01 4.07E+32 -6.62 37210.0/
PLOG/3.160E+01 6.86E+44 -10.04 47030.0/
PLOG/1.000E+02 1E-10 0.0 0.0/
!PLOG/1.000E+02 -1.07E+04 1.33 15620.0/
DUP

C2H3OO<=>CO+CH3O 1.16E-01 3.16 18420 !\AUTHOR: !\REF: Goldsmith
et al, J. Phys. Chem. A 2015, 119, 7766-7779
PLOG/1.000E-02 2.31E+129 -41.86 45850.0/
PLOG/1.000E-01 2.42E+28 -5.99 30540.0/
PLOG/3.160E-01 8.69E-50 16.63 -3900.0/
PLOG/1.000E+00 1.19E-39 13.61 -1317.0/
PLOG/3.160E+00 8.80E+86 -23.08 61010.0/
PLOG/1.000E+01 1.27E+03 1.44 18660.0/
PLOG/3.160E+01 1.97E+17 -2.23 28590.0/
PLOG/1.000E+02 3.25E+04 1.694 23327.6/
!PLOG/1.000E+02 1.16E-07 4.81 12010.0/
DUP

CHOCHO+OH=>HCO+CO+H2O 61329.9 2.65 -4586.4
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104.

!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA

!

C2H3+H<=>C2H2+H2 1.700E+014 0.000
0.0 !\AUTHOR: !\REF:86TSA/ HAM
C2H3+H<=>H2CC+H2 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:USC ESTIMATE
C2H3+OH<=>C2H2+H2O 3.011E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)
C2H3+CH3<=>CH4+C2H2 3.920E+011 0.000
0.0 !\AUTHOR: !\REF:Tsang, W.; Hampson, R.F., J. Phys. Chem. Ref. Data
15, 1087 (1986)
C2H3+C2H3<=>C2H2+C2H4 9.600E+011 0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986)

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!\ENDSUBSPECIES: \C2H3

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!\ENDSUBMECH: \C2H4

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!\SUBMECH: \C2H2

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

C2H+H(+M)<=>C2H2(+M) 1.000E+017 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0
LOW/ 3.750E+033 -4.800
1900.0/
TROE/ 6.460E-001 1.320E+002 1.315E+003 5.566E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/
C2H2(+M)<=>H2CC(+M) 8.000E+014 -0.520
50750.0 !\AUTHOR: !\REF:99 LAS/ WA
LOW/ 2.450E+015 -0.640
49700.0/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/
2.50/ C2H4/ 2.50/

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA

C2H2+O<=>CH2+CO 7.395E+008 1.280
2472.0 !\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706
C2H2+O<=>HCCO+H 2.958E+009 1.280
2472.0 !\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706
C2H2+HO2<=>CH2CO+OH 6.030E+009 0.000
7949.0 !\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706
C2H2+HCO<=>C2H3+CO 1.000E+007 2.000
6000.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
C2H2+CH2<=>C3H3+H 1.200E+013 0.000
6620.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
C2H2+CH2(S)<=>C3H3+H 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
C2H2+HCCO<=>C3H3+CO 1.000E+011 0.000
3000.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II

H2CC+H<=>C2H2+H 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
H2CC+OH<=>CH2CO+H 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
H2CC+O2<=>HCO+HCO 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA

C2H2+OH<=>C2H+H2O 2.632E+006 2.140
17060.0 !\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055

C2H2+OH<=>HCCOH+H		2.800E+005	2.280	
12420.0 !\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055				
PLOG/	0.0100	2.800E+005	2.280	12420.0/
PLOG/	0.0250	7.467E+005	2.160	12550.0/
PLOG/	0.1000	1.776E+006	2.040	12670.0/
PLOG/	1.0000	2.415E+006	2.000	12710.0/
PLOG/	10.0000	3.210E+006	1.970	12810.0/
PLOG/	100.0000	7.347E+006	1.890	13600.0/
C2H2+OH<=>CH2CO+H		1.578E+003	2.560	
-844.5 !\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055				
PLOG/	0.0100	1.578E+003	2.560	-844.5/
PLOG/	0.0250	1.518E+004	2.280	-292.1/
PLOG/	0.1000	3.017E+005	1.920	598.1/
PLOG/	1.0000	7.528E+006	1.550	2106.0/
PLOG/	10.0000	5.101E+006	1.650	3400.0/
PLOG/	100.0000	1.457E+004	2.450	4477.0/
C2H2+OH<=>CH3+CO		4.757E+005	1.680	
-329.8 !\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055				
PLOG/	0.0100	4.757E+005	1.680	-329.8/
PLOG/	0.0250	4.372E+006	1.400	226.5/
PLOG/	0.1000	7.648E+007	1.050	1115.0/
PLOG/	1.0000	1.277E+009	0.730	2579.0/
PLOG/	10.0000	4.312E+008	0.920	3736.0/
PLOG/	100.0000	8.250E+005	1.770	4697.0/
C2H2+OH<=>C2H2OH		3.913E+032	-7.126	
5824.0 !\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055				
PLOG/	0.0100	3.913E+032	-7.126	5824.0/
PLOG/	0.0250	1.067E+032	-6.847	5508.0/
PLOG/	0.1000	1.646E+032	-6.717	5822.0/
PLOG/	1.0000	1.387E+031	-6.087	6348.0/
PLOG/	10.0000	2.892E+029	-5.288	7055.0/
PLOG/	100.0000	1.367E+025	-3.754	6543.0/
H+HCCOH<=>H+CH2CO		1.000E+013	0.000	
0.0 !\AUTHOR: !\REF:GRI 2.11				

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!\SUBSPECIES: \C2H

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C2H+O2<=>CO2+CHV		2.170E+010	0.000	
0.0 !\AUTHOR: !\REF:DEVRIENDT, VAN LOOK, CEURSTERS, AND PEETERS, CHEM PHYS LETT. 261 (1996) 450, C2H+O2				
C2H+O2<=>HCO+CO		5.000E+013	0.000	
1500.0 !\AUTHOR: !\REF:GRI				
C2H+O<=>CO+CHV		6.200E+012	0.000	
0.0 !\AUTHOR: !\REF:OHV KATHROTIA ET AL. COMB & FLAME 2010				
C2H+O<=>CO+CH		5.000E+013	0.000	
0.0 !\AUTHOR: !\REF:GRI				
C2H+H2<=>H+C2H2		4.900E+005	2.500	
560.0 !\AUTHOR: !\REF:GRI				
C2H+OH<=>H+HCCO		2.000E+013	0.000	
0.0 !\AUTHOR: !\REF:GRI				

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!\SUBSPECIES: \C2H

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!\ENDSUBMECH: C2H2
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!-----
!\SUBMECH: \CH3CHO
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!\REACTIONCLASS: \UNIMOL          \A          \N
\EA
!
-----
CH3CHO (+M) <=> CH3+HCO (+M)          2.450E+022   -1.740
86355.0  !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO.
2, 2010
LOW/          1.030E+059   -11.300
95912.5/
TROE/  2.490E-003  7.181E+002  6.089E+000  3.780E+003/
CH3CHO (+M) <=> CH4+CO (+M)          2.720E+021   -1.740
86355.0  !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO.
2, 2010
LOW/          1.144E+058   -11.300
95912.5/
TROE/  2.490E-003  7.181E+002  6.089E+000  3.780E+003/
!
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!\REACTIONCLASS: \RH_ABSTRACTION  \A          \N
\EA
!
-----
CH3CHO+O2<=>CH3CO+HO2          3.010E+013    0.000
39150.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
(1992)
CH3CHO+O<=>CH3CO+OH          5.940E+012    0.000
1868.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE
CH3CHO+H<=>CH3CO+H2          1.310E+005    2.580
1220.0 !\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010
CH3CHO+OH<=>CH3CO+H2O          3.370E+012    0.000
-619.0 !\AUTHOR: !\REF:JUAN LI'S PHD THESIS
CH3CHO+HO2<=>CH3CO+H2O2          3.010E+012    0.000
11920.0 !\AUTHOR: !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA,
21:411 (1992)
CH3CHO+CH3<=>CH3CO+CH4          7.080E-004    4.580
1966.0 !\AUTHOR: !\REF: GUPTA ET AL., PROC COMBUST INST 31 (2007)
167;§C174
CH3CHO+CH3O2<=>CH3CO+CH3O2H          3.010E+012    0.000
11920.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
(1992)
CH3CHO+CH3CO3<=>CH3CO+CH3CO3H          3.010E+012    0.000
11920.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
(1992)
CH3CHO+H<=>CH2CHO+H2          2.720E+003    3.100
5210.0 !\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010

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CH3CHO+OH<=>CH2CHO+H2O 1.720E+005 2.400
815.0 !\AUTHOR: !\REF:TAYLOR ET AL. 1996
!

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA
!

CH3CHO+OH<=>CH3+HOCHO 3.000E+015 -1.076
0.0 !\AUTHOR: !\REF:TAYLOR ET AL. 1996

!=====
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!\SUBSPECIES: \CH3CO
!=====
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!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N
\EA
!

CH3CO(+M)<=>CH3+CO(+M) 1.070E+012 0.630
16900.0 !\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
LOW/ 5.650E+018 -0.970
14600.0/
TROE/ 6.290E-001 8.730E+009 5.520E+000 7.600E+007/
CH3CO(+M)<=>CH2CO+H(+M) 9.413E+007 1.917
44987.2 !\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
LOW/ 1.516E+051 -10.270
55390.0/
TROE/ 6.009E-001 8.103E+009 6.677E+002 5.000E+009/
!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

CH3CO+H<=>CH2CO+H2 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE
CH3CO+O<=>CH2CO+OH 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE
CH3CO+CH3<=>CH2CO+CH4 5.000E+013 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE
!

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

CH3CO+O2<=>CH3CO3 1.200E+011 0.000
-1100.0 !\AUTHOR: !\REF: CURRAN ESTIMATE
CH3CO3+HO2<=>CH3CO3H+O2 1.750E+010 0.000
-3275.0 !\AUTHOR: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
H2O2+CH3CO3<=>HO2+CH3CO3H 2.410E+012 0.000
9936.0 !\AUTHOR: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)

CH4+CH3CO3<=>CH3+CH3CO3H 1.810E+011 0.000
18480.0 !\AUTHOR: !\REF:BASED ON CH4+CH3O2

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!\ENDSUBSPECIES: \CH3CO

!=====
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!=====
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!\SUBSPECIES: \C2H3OH

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!=====
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!\REACTIONCLASS: \UNIMOL \A \N

\EA

!

C2H3OH<=>CH3CHO 7.420E+046 -10.560
67420.0 !\AUTHOR: !\REF:CHANGED PRODUCTS FROM CH3+HCO

PLOG/ 0.1000 7.420E+046 -10.560 67420.0/

PLOG/ 1.0000 4.420E+042 -9.090 67069.2/

PLOG/ 100.0000 2.900E+027 -4.350 61612.9/

!

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!

C2H3OH+O2<=>CH2CHO+HO2 5.310E+011 0.210

39830.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+O<=>CH2CHO+OH 1.875E+006 1.900

-860.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+H<=>CH2CHO+H2 1.480E+003 3.077

7220.0 !\AUTHOR: !\REF:ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608,

C2H3OH+OH<=>CH2CHO+H2O 3.330E+009 1.100

540.5 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+CH3<=>CH2CHO+CH4 2.030E-008 5.900

1052.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+CH3O2<=>CH2CHO+CH3O2H 3.400E+003 2.500

8922.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+H<=>C2H2OH+H2 2.470E+007 2.030

15200.0 !\AUTHOR: !\REF:ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-

1608,

!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N

\EA

!

C2H3OH+H<=>PC2H4OH 3.010E+008 1.577

3670.0 !\AUTHOR: !\REF:ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608,

C2H3OH+HO2<=>CH3CHO+HO2 1.490E+005 1.670

6810.0 !\AUTHOR: !\REF:DA SILVA BOZZELLI CHEMICAL PHYSICS LETTERS 483

(2009) 25-29

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!\ENDSUBSPECIES: \C2H3OH

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!=====
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!\SUBSPECIES: CH2CHO
!=====
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!\REACTIONCLASS: \RADICAL_DECOMPOSITION          \A          \N
\EA
!
-----
CH2CHO (+M) <=> CH2CO+H (+M)                      1.430E+015    -0.150
45600.0 !\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
LOW/                                              6.000E+029    -3.800
43423.9/
TROE/ 9.850E-001 3.930E+002 9.800E+009 5.000E+009/
CH2CHO (+M) <=> CH3+CO (+M)                        2.930E+012     0.290
40300.0 !\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781
LOW/                                              9.520E+033    -5.070
41300.0/
TROE/ 7.130E-017 1.150E+003 4.990E+009 1.790E+009/
!=====
=====
!\ENDSUBSPECIES: \CH2CHO
!=====
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!
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!\SUBSPECIES: \CH3CO3H
!=====
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!
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!\REACTIONCLASS: \UNIMOL                          \A          \N
\EA
!
-----
CH3CO3H <=> CH3CO2+OH                              5.010E+014     0.000
40150.0 !\AUTHOR: !\REF:SAHETCHIAN ET AL. 1992
!
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!\REACTIONCLASS: \RH_R_ABSTRACTION                \A          \N
\EA
!
-----
CH3CO3+CH2O <=> CH3CO3H+HCO                        1.990E+012     0.000
11660.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH2O
CH3CO3+C2H6 <=> CH3CO3H+C2H5                      1.700E+013     0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH2O
!
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!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION          \A          \N
\EA
!
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CH3CO2+M<=>CH3+CO2+M 4.400E+015 0.000
10500.0 !\AUTHOR: !\REF:ANALOGY TO CH3CO<=>CH3+CO
!

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

CH2CHO+O2<=>O2CH2CHO 1.580E+077 -21.900
19350.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A,
2003, 107 (19), 3778-3791

PLOG/ 0.0100 1.580E+077 -21.900 19350.0/
PLOG/ 0.1000 3.880E+069 -18.840 19240.0/
PLOG/ 1.0000 7.800E+059 -15.400 17650.0/
PLOG/ 10.0000 3.050E+050 -12.200 15630.0/

CH2CHO+O2<=>CH2CO+HO2 1.880E+005 2.370
23730.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A,
2003, 107 (19), 3778-3791

PLOG/ 0.0100 1.880E+005 2.370 23730.0/
PLOG/ 0.1000 1.880E+005 2.370 27370.0/
PLOG/ 1.0000 2.510E+005 2.330 23800.0/
PLOG/ 10.0000 7.050E+007 1.630 25290.0/

CH2CHO+O2=>CH2O+CO+OH 2.680E+017 -1.840
6530.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003,
107 (19), 3778-3791

PLOG/ 0.0100 2.680E+017 -1.840 6530.0/
PLOG/ 0.1000 1.520E+020 -2.580 8980.0/
PLOG/ 1.0000 1.650E+019 -2.220 10340.0/
PLOG/ 10.0000 8.953E+013 -0.600 10120.0/

CH2CHO+O2<=>HO2CH2CO 3.640E+065 -21.870
19020.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A,
2003, 107 (19), 3778-3791

PLOG/ 0.0100 3.640E+065 -21.870 19020.0/
PLOG/ 0.1000 3.640E+058 -19.000 19090.0/
PLOG/ 1.0000 6.650E+048 -15.550 17460.0/
PLOG/ 10.0000 4.800E+038 -12.140 14960.0/

O2CH2CHO<=>HO2CH2CO 8.270E+030 -6.650
24500.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A,
2003, 107 (19), 3778-3791

PLOG/ 0.0100 8.270E+030 -6.650 24500.0/
PLOG/ 0.1000 1.730E+026 -4.990 23760.0/
PLOG/ 1.0000 9.030E+019 -2.920 22170.0/
PLOG/ 10.0000 1.430E+016 -1.670 21210.0/

O2CH2CHO<=>CH2CO+HO2 2.050E+040 -13.310
52150.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A,
2003, 107 (19), 3778-3791

PLOG/ 0.0100 2.050E+040 -13.310 52150.0/
PLOG/ 0.1000 5.720E+045 -14.000 52200.0/
PLOG/ 1.0000 4.160E+055 -15.760 55080.0/
PLOG/ 10.0000 1.120E+061 -16.040 60010.0/

HO2CH2CO=>CO+CH2O+OH 2.360E+017 -2.950
8100.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003,
107 (19), 3778-3791

PLOG/ 0.0100 2.360E+017 -2.950 8100.0/
PLOG/ 0.1000 2.380E+018 -2.950 8100.0/
PLOG/ 1.0000 2.510E+019 -2.950 8110.0/
PLOG/ 10.0000 4.160E+020 -3.020 8240.0/

HO2CH2CO<=>CH2CO+HO2 1.120E+007 -3.760
21680.0 !\AUTHOR: !\REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A,
2003, 107 (19), 3778-3791
PLOG/ 0.0100 1.120E+007 -3.760 21680.0/
PLOG/ 0.1000 1.100E+008 -3.760 21680.0/
PLOG/ 1.0000 9.200E+008 -3.730 21630.0/
PLOG/ 10.0000 2.090E+009 -3.550 21220.0/

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!\ENDSUBSPECIES: \CH3CO3H

!=====
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!-----

!\ENDSUBMECH: \CH3CHO

!-----

!-----

!\SUBMECH: \CH2CO

!-----

CH2+CO (+M) <=> CH2CO (+M) 8.100E+011 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
LOW/ 2.690E+033 -5.110
7095.0/
TROE/ 5.907E-001 2.750E+002 1.226E+003 5.185E+003/
H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
3.00/ HE/ 0.70/
!

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!-----

CH2CO+H<=>HCCO+H2 1.401E+015 -0.171
8783.2 !\AUTHOR: !\REF:WKM (SEE COMMENTS AT BEGINNING OF FILE 15/ 09/
2011
CH2CO+O<=>HCCO+OH 1.000E+013 0.000
8000.0 !\AUTHOR: !\REF:WKM ESTIMATE
CH2CO+OH<=>HCCO+H2O 1.000E+013 0.000
2000.0 !\AUTHOR: !\REF:WKM ESTIMATE
!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N

\EA

!-----

CH2CO+H<=>CH3+CO 7.704E+013 -0.171
4183.2 !\AUTHOR: !\REF:WKM (SEE COMMENTS AT BEGINNING OF FILE 15/ 09/
2011
CH+CH2O<=>H+CH2CO 9.460E+013 0.000
-515.0 !\AUTHOR: !\REF:REG 2.11
CH2CO+O<=>CH2+CO2 1.750E+012 0.000
1350.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
CH2CO+OH<=>CH2OH+CO 2.000E+012 0.000
-1010.0 !\AUTHOR: !\REF:BROWN ET AL. CHEM. PHYS. LETT. 1989, 161, 491.

CH2CO+CH2(S)<=>C2H4+CO 1.600E+014 0.000
0.0 !\AUTHOR: !\REF:WKM CALCULATION
CH2CO+CH3<=>C2H5+CO 4.769E+004 2.312
9468.0 !\AUTHOR: !\REF:WKM CALCULATION

!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA

!

HCCO+OH=>H2+CO+CO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:WKM CALCULATION
HCCO+O=>H+CO+CO 8.000E+013 0.000
0.0 !\AUTHOR: !\REF:WKM CALCULATION

!=====

=====

!\SUBSPECIES: \HCCO

!=====

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!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION \A \N
\EA

!

CH+CO+M<=>HCCO+M 7.570E+022 -1.900
0.0 !\AUTHOR: !\REF:J. CHEM. PHYS. 108: 6709-6716 1998

!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA

!

HCCO+H<=>CH2(S)+CO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:GRI
HCCO+O2=>OH+CO+CO 1.910E+011 -0.020
1020.0 !\AUTHOR: !\REF:KLIPPENSTEIN 2002
HCCO+O2=>CO2+CO+H 4.780E+012 -0.142
1150.0 !\AUTHOR: !\REF:KLIPPENSTEIN 2002
CH+HCCO<=>CO+C2H2 5.000E+013 0.000
0.0 !\AUTHOR: !\REF:REG 2.11

!=====

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!\ENDSUBSPECIES: \HCCO

!=====

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!-----

!\ENDSUBMECH: \CH2CO

!-----

!-----

!\SUBMECH: \C2H5OH

!-----

!

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!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
-----
C2H5OH<=>C2H4+H2O                        3.410E+059   -14.200
83672.6 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO.
35, 2010
PLOG/      0.0010      3.410E+059   -14.200      83672.6/
PLOG/      0.0100      2.620E+057   -13.300      85262.2/
PLOG/      0.1000      1.650E+052   -11.500      84745.6/
PLOG/      1.0000      5.230E+043   -8.900       81506.7/
PLOG/     10.0000      4.590E+032   -5.600       76062.4/
PLOG/    100.0000      3.840E+020   -2.060       69465.5/
C2H5OH<=>CH3+CH2OH                        1.200E+054   -12.900
100005.7 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114,
NO. 35, 2010
PLOG/      0.0010      1.200E+054   -12.900     100005.7/
PLOG/      0.0100      5.180E+059   -14.000      99906.4/
PLOG/      0.1000      1.620E+066   -15.300     105390.5/
PLOG/      1.0000      5.550E+064   -14.500     106183.0/
PLOG/     10.0000      1.550E+058   -12.300     105768.0/
PLOG/    100.0000      1.780E+047    -8.960     101058.8/
C2H5OH<=>C2H5+OH                          8.100E+046   -11.300
111053.4 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114,
NO. 35, 2010
PLOG/      0.0010      8.100E+046   -11.300     111053.4/
PLOG/      0.0100      1.860E+056   -13.500     107238.4/
PLOG/      0.1000      4.650E+063   -15.000     109622.8/
PLOG/      1.0000      4.460E+065   -14.900     112345.0/
PLOG/     10.0000      2.790E+061   -13.400     113080.2/
PLOG/    100.0000      6.170E+051   -10.300     109940.7/
!
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!\REACTIONCLASS: \RH_R_ABSTRACTION        \A                \N
\EA
!
-----
C2H5OH+O<=>C2H5O+OH                       1.460E-003    4.730
1727.0 !\AUTHOR: !\REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703
C2H5OH+OH<=>C2H5O+H2O                     5.810E-003    4.280
-3560.0 !\AUTHOR: !\REF: SMB 04/ 09/ 2013
C2H5OH+H<=>C2H5O+H2                       9.450E+002    3.140
8701.1 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO.
35, 2010
C2H5OH+HO2<=>C2H5O+H2O2                   6.470E-007    5.300
10533.1 !\AUTHOR: !\REF: Mittal 2013
C2H5OH+CH3<=>C2H5O+CH4                     2.035E+000    3.570
7721.0 !\AUTHOR: !\REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599,
2004
C2H5OH+CH3O2<=>C2H5O+CH3O2H               3.236E-007    5.300
10533.1 !\AUTHOR: !\REF:ANAOLGY WITH C2H5OH+HO2
C2H5OH+C2H5<=>PC2H4OH+C2H6                 5.000E+010    0.000
13400.0 !\AUTHOR: !\REF:1/ 2 OF C4H10+C2H5
C2H5OH+O2<=>SC2H4OH+HO2                   1.500E+013    0.000
50150.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO.
35, 2010
C2H5OH+O<=>SC2H4OH+OH                      1.450E+005    2.470
876.0 !\AUTHOR: !\REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703

```

C2H5OH+H<=>SC2H4OH+H2	8.790E+004	2.680
2910.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010		
C2H5OH+OH<=>SC2H4OH+H2O	7.520E+004	2.490
-1474.1 !\AUTHOR: !\REF: SMB 04/ 09/ 2013		
C2H5OH+HO2<=>SC2H4OH+H2O2	2.450E-005	5.260
7475.1 !\AUTHOR: !\REF: Mittal 2013		
C2H5OH+CH3<=>SC2H4OH+CH4	1.993E+001	3.370
7634.0 !\AUTHOR: !\REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004		
C2H5OH+CH3O2<=>SC2H4OH+CH3O2H	1.225E-005	5.260
7475.1 !\AUTHOR: !\REF:ANAOLGY WITH C2H5OH+HO2		
C2H5OH+C2H5<=>SC2H4OH+C2H6	5.000E+010	0.000
10400.0 !\AUTHOR:		
C2H5OH+O2<=>PC2H4OH+HO2	2.000E+013	0.000
52800.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010		
C2H5OH+O<=>PC2H4OH+OH	9.690E+002	3.230
4658.0 !\AUTHOR: !\REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703		
C2H5OH+H<=>PC2H4OH+H2	5.310E+004	2.810
7490.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010		
C2H5OH+OH<=>PC2H4OH+H2O	3.760E+003	2.780
-1810.2 !\AUTHOR: !\AUTHOR: !\REF: SMB 04/ 09/ 2013		
C2H5OH+HO2<=>PC2H4OH+H2O2	3.986E-002	4.300
15333.0 !\AUTHOR: !\REF: Mittal 2013		
C2H5OH+CH3<=>PC2H4OH+CH4	3.300E+002	3.300
12290.0 !\AUTHOR: !\REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004		
C2H5OH+CH3O2<=>PC2H4OH+CH3O2H	1.995E-002	4.300
15333.0 !\AUTHOR: !\REF:ANAOLGY WITH C2H5OH+HO2		
!		

!\REACTIONCLASS: \RADICAL_DECOMPOSITION	\A	\N
\EA		
!		

SC2H4OH<=>CH3CHO+H	5.690E+052	-13.380
45049.0 !\AUTHOR: !\REF:WKM CALCULATION.		
PLOG/ 0.0010	5.690E+052	-13.380
PLOG/ 0.0100	3.290E+056	-14.120
PLOG/ 0.1000	8.580E+057	-14.160
PLOG/ 1.0000	5.360E+055	-13.150
PLOG/ 10.0000	1.660E+048	-10.640
PLOG/ 20.0000	8.260E+044	-9.590
PLOG/ 50.0000	1.010E+040	-8.060
PLOG/ 100.0000	1.100E+036	-6.840
SC2H4OH<=>C2H3OH+H	5.400E+046	-11.630
44323.0 !\AUTHOR: !\REF:WKM CALCULATION.		
PLOG/ 0.0010	5.400E+046	-11.630
PLOG/ 0.0100	1.210E+051	-12.550
PLOG/ 0.1000	2.870E+054	-13.150
PLOG/ 1.0000	3.790E+053	-12.510
PLOG/ 10.0000	6.330E+046	-10.200
PLOG/ 20.0000	3.870E+043	-9.170
PLOG/ 50.0000	5.080E+038	-7.650
PLOG/ 100.0000	5.120E+034	-6.410

SC2H4OH<=>C2H5O 5.480E+045 -11.630
 44328.0 !\AUTHOR: !\REF:WKM CALCULATION.
 PLOG/ 0.0010 5.480E+045 -11.630 44328.0/
 PLOG/ 0.0100 2.540E+049 -12.370 46445.0/
 PLOG/ 0.1000 1.650E+054 -13.400 50330.0/
 PLOG/ 1.0000 1.810E+055 -13.310 53132.0/
 PLOG/ 10.0000 4.580E+049 -11.320 52714.0/
 PLOG/ 20.0000 4.110E+046 -10.330 51834.0/
 PLOG/ 50.0000 6.680E+041 -8.830 50202.0/
 PLOG/ 100.0000 6.540E+037 -7.580 48697.0/
 SC2H4OH<=>PC2H4OH 2.650E+036 -8.860
 51019.0 !\AUTHOR: !\REF:WKM CALCULATION.
 PLOG/ 0.0010 2.650E+036 -8.860 51019.0/
 PLOG/ 0.0100 3.560E+037 -8.890 51114.0/
 PLOG/ 0.1000 4.140E+039 -9.190 51912.0/
 PLOG/ 1.0000 5.820E+044 -10.340 55296.0/
 PLOG/ 10.0000 4.260E+048 -11.060 59458.0/
 PLOG/ 20.0000 8.840E+047 -10.740 59901.0/
 PLOG/ 50.0000 2.230E+045 -9.840 59604.0/
 PLOG/ 100.0000 1.700E+042 -8.830 58737.0/
 CH3+CH2O<=>C2H5O 3.000E+011 0.000
 6336.0 !\AUTHOR: !\REF: CURRAN ESTIMATE
 CH3CHO+H<=>C2H5O 4.610E+007 1.710
 7090.0 !\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010
 !

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

C2H5O+O2<=>CH3CHO+HO2 4.280E+010 0.000
 1097.0 !\AUTHOR: !\REF: HARTMANN ET AL. 1990
 O2C2H4OH<=>PC2H4OH+O2 3.900E+016 -1.000
 30000.0 !\AUTHOR: !\REF:BASED ON C3H6OH+O2 REACTION
 O2C2H4OH=>OH+CH2O+CH2O 1.250E+011 0.000
 18900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
 SC2H4OH+O2<=>CH3CHO+HO2 5.260E+017 -1.638
 869.0 !\AUTHOR: !\REF:DA SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933
 PLOG/ 0.0100 5.260E+017 -1.637 838.0/
 PLOG/ 0.1000 5.260E+017 -1.637 838.0/
 PLOG/ 1.0000 5.280E+017 -1.638 839.0/
 PLOG/ 10.0000 1.540E+018 -1.771 1120.0/
 PLOG/ 100.0000 3.780E+020 -2.429 3090.0/
 SC2H4OH+O2<=>C2H3OH+HO2 5.512E+003 2.495
 -414.0 !\AUTHOR: !\REF:DA SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933
 PLOG/ 0.0100 5.120E+002 2.496 -414.0/
 PLOG/ 0.1000 5.330E+002 2.490 -402.0/
 PLOG/ 1.0000 7.620E+002 2.446 -296.0/
 PLOG/ 10.0000 8.920E+003 2.146 470.0/
 PLOG/ 100.0000 4.380E+005 1.699 2330.0/

!-----
 !\ENDSUBMECH: C2H5OH
 !-----
 !-----
 !-----
 !-----
 !\SUBMECH: \CH3OCH3

!

CH3OCH2+CH3O<=>CH3OCH3+CH2O 2.410E+013 0.000
0.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL
JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
CH3OCH2+CH2O<=>CH3OCH3+HCO 5.490E+003 2.800
5862.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
CH3OCH2+CH3CHO<=>CH3OCH3+CH3CO 1.260E+012 0.000
8499.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA
!

CH3OCH2<=>CH3+CH2O 8.03E+12 0.440284 26490.7
!\AUTHOR: !\REF:BURKE, CNF 2014
PLOG/ 1.00E-02 7.494E+23 -4.5152 25236.1/
PLOG/ 1.00E-01 6.921E+28 -5.7271 27494.9/
PLOG/ 1.00E+00 4.229E+29 -5.6103 28898.3/
PLOG/ 1.00E+01 6.608E+27 -4.7073 29735.2/
PLOG/ 1.00E+02 2.659E+29 -4.9358 31785.5/
!

!\REACTIONCLASS: \R_O2_PRODUCTS \A \N
\EA
!

CH3OCH2+O2<=>CH3OCH2O2 1.0 1.0 1.0
!\AUTHOR: !\REF:BURKE, CNF 2014
PLOG/ 1.000E-003 1.120E+018 -3.37 -4294./
PLOG/ 1.000E-002 1.330E+021 -3.95 -2615./
PLOG/ 1.000E+000 1.130E+028 -5.24 4088./
PLOG/ 2.000E+000 3.910E+027 -5.00 4512./
PLOG/ 1.000E+001 2.750E+024 -3.87 4290./
PLOG/ 2.000E+001 2.970E+022 -3.23 3781./
PLOG/ 5.000E+001 5.190E+019 -2.35 2908./
PLOG/ 1.000E+002 5.430E+017 -1.73 2210./
CH3OCH2+O2<=>CH2OCH2O2H 1.0 1.0 1.0
!\AUTHOR: !\REF:BURKE, CNF 2014
PLOG/ 1.000E-003 5.080E+020 -4.39 469./
PLOG/ 1.000E-002 5.470E+023 -4.96 2183./
PLOG/ 1.000E+000 2.810E+028 -5.63 7848./
PLOG/ 2.000E+000 5.190E+027 -5.33 8144./
PLOG/ 1.000E+001 9.670E+024 -4.36 8417./
PLOG/ 2.000E+001 4.080E+023 -3.90 8494./
PLOG/ 5.000E+001 5.080E+021 -3.28 8585./
PLOG/ 1.000E+002 1.620E+020 -2.81 8619./
CH3OCH2+O2=>CH2O+CH2O+OH 1.0 1.0 1.0
!\AUTHOR: !\REF:BURKE, CNF 2014
PLOG/ 1.000E-003 8.010E+021 -3.18 3067./
PLOG/ 1.000E-002 1.730E+023 -3.55 4050./
PLOG/ 1.000E+000 2.040E+031 -5.76 11594./
PLOG/ 2.000E+000 5.990E+031 -5.87 12710./
PLOG/ 1.000E+001 9.390E+030 -5.59 14517./
PLOG/ 2.000E+001 1.090E+030 -5.30 15051./

PLOG/ 5.000E+001 3.580E+028 -4.88 15664./
PLOG/ 1.000E+002 2.410E+027 -4.55 16107./
CH3OCH2O2<=>CH2OCH2O2H 1.0 1.0 1.0
!\AUTHOR: !\REF: BURKE, CNF 2014
PLOG/ 1.000E-003 1.940E+029 -6.99 22446./
PLOG/ 1.000E-002 4.070E+027 -6.16 21619./
PLOG/ 1.000E+000 2.520E+025 -4.76 22691./
PLOG/ 2.000E+000 5.970E+024 -4.48 22868./
PLOG/ 1.000E+001 4.440E+021 -3.38 22386./
PLOG/ 2.000E+001 4.520E+019 -2.74 21803./
PLOG/ 5.000E+001 5.720E+016 -1.82 20829./
PLOG/ 1.000E+002 3.700E+014 -1.13 20034./
CH3OCH2O2=>CH2O+CH2O+OH 1.0 1.0 1.0
!\AUTHOR: !\REF: BURKE, CNF 2014
PLOG/ 1.000E-003 2.060E+036 -8.32 33415./
PLOG/ 1.000E-002 2.070E+039 -8.86 35842./
PLOG/ 1.000E+000 1.120E+040 -8.42 39835./
PLOG/ 2.000E+000 9.720E+038 -8.04 39923./
PLOG/ 1.000E+001 6.280E+035 -6.97 39900./
PLOG/ 2.000E+001 1.600E+034 -6.46 39850./
PLOG/ 5.000E+001 8.320E+031 -5.75 39719./
PLOG/ 1.000E+002 1.220E+030 -5.20 39549./
CH2OCH2O2H=>CH2O+CH2O+OH 1.0 1.0 1.0
!\AUTHOR: !\REF: BURKE, CNF 2014
PLOG/ 1.000E-003 1.660E+023 -4.53 22243./
PLOG/ 1.000E-002 5.300E+025 -4.93 24158./
PLOG/ 1.000E+000 7.810E+022 -3.50 23156./
PLOG/ 2.000E+000 4.980E+022 -3.35 23062./
PLOG/ 1.000E+001 8.460E+022 -3.22 23559./
PLOG/ 2.000E+001 9.090E+022 -3.14 23899./
PLOG/ 5.000E+001 4.590E+022 -2.94 24262./
PLOG/ 1.000E+002 1.400E+022 -2.72 24407./
!

!\REACTIONCLASS: \QOOH_O2

\A

\N

\EA

!

CH2OCH2O2H+O2<=>O2CH2OCH2O2H 1.0 1.0 1.0
!\AUTHOR: !\REF: BURKE, CNF 2014
PLOG/ 1.000E-003 9.420E+012 -1.68 -4998./
PLOG/ 1.000E-002 8.160E+016 -2.50 -2753./
PLOG/ 1.000E+000 1.060E+022 -3.30 3389./
PLOG/ 2.000E+000 3.480E+020 -2.79 3131./
PLOG/ 1.000E+001 2.860E+016 -1.48 1873./
PLOG/ 2.000E+001 8.550E+014 -1.01 1312./
PLOG/ 5.000E+001 2.680E+013 -0.54 727./
PLOG/ 1.000E+002 4.870E+012 -0.32 428./
CH2OCH2O2H+O2<=>HO2CH2OCHO+OH 1.0 1.0 1.0
!\AUTHOR: !\REF: BURKE, CNF 2014
PLOG/ 1.000E-003 5.900E+020 -2.88 3234./
PLOG/ 1.000E-002 2.060E+023 -3.59 5116./
PLOG/ 1.000E+000 4.450E+029 -5.29 12791./
PLOG/ 2.000E+000 2.440E+028 -4.92 12891./
PLOG/ 1.000E+001 9.420E+023 -3.68 12049./
PLOG/ 2.000E+001 1.040E+022 -3.16 11505./
PLOG/ 5.000E+001 6.950E+019 -2.60 10861./
PLOG/ 1.000E+002 3.960E+018 -2.31 10500./

O2CH2OCH2O2H<=>HO2CH2OCHO+OH 1.0 1.0 1.0
!\AUTHOR: !\REF: BURKE, CNF 2014
PLOG/ 1.000E-003 9.050E+023 -4.88 18805./
PLOG/ 1.000E-002 6.840E+026 -5.32 22533./
PLOG/ 1.000E+000 5.070E+016 -1.81 21175./
PLOG/ 2.000E+000 2.660E+014 -1.11 20310./
PLOG/ 1.000E+001 1.690E+010 0.18 18604./
PLOG/ 2.000E+001 1.110E+009 0.54 18100./
PLOG/ 5.000E+001 1.070E+008 0.84 17661./
PLOG/ 1.000E+002 3.860E+007 0.98 17467./
!

!\REACTIONCLASS: \RO2_RO2_PRODUCTS \A \N
\EA
!

CH3OCH2O2+CH3OCH2O2=>O2+CH3OCH2O+CH3OCH2O 1.547E+023 -4.500
0.0 !\AUTHOR: !\REF: NIST FIT

!\SUBSPECIES: \CH3OCH2O2H

CH3OCH2O2+CH2O<=>CH3OCH2O2H+HCO 1.000E+012 0.000
11660.0 !\AUTHOR: !\REF: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF.
DATA, 15:1087 (1986)

CH3OCH2O2+CH3CHO<=>CH3OCH2O2H+CH3CO 2.800E+012 0.000
13600.0 !\AUTHOR: !\REF: S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.

CH3OCH2O+OH<=>CH3OCH2O2H 2.000E+013 0.000
0.0 !\AUTHOR: !\REF: S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL
JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.

!\ENDSUBSPECIES: \CH3OCH2O2H

!\SUBSPECIES: \HO2CH2OCHO

!\REACTIONCLASS: \KHP_UNIMOL \A \N
\EA
!

HO2CH2OCHO<=>OCH2OCHO+OH 5.000E+016 0.000
43000.0 !\AUTHOR: !\REF: K.A. SAHETCHIAN, R. RIGNY, J. TARDIEU DE
MALEISSYE, L. BATT, M. ANWAR KHAN, S. MATHEWS, SYMPOSIUM (INTERNATIONAL)
ON COMBUSTION, 24 (1992) 637-643.

!\ENDSUBSPECIES: \HO2CH2OCHO

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!=====
=====
!\SUBSPECIES: \OCH2OCHO
!=====
=====
CH2O+OCHO<=>OCH2OCHO                1.250E+011    0.000
11900.0 !\AUTHOR: !\REF: ESTIMATE WKM RECOMMENDATION 8/ 9/ 2010
OCH2OCHO<=>HOCH2OCO                1.000E+011    0.000
14000.0 !\AUTHOR: !\REF: ESTIMATE WKM RECOMMENDATION 8/ 9/ 2010
HOCH2OCO<=>CH2OH+CO2                1.117E+017   -1.526
20771.9 !\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                2.920E+018   -1.965
19619.0 !\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                1.000E+011    0.000
7960.0 !\AUTHOR: !\REF: S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
CH3OCH2O+O2<=>CH3OCHO+HO2          4.380E-019    9.500
-5501.0 !\AUTHOR: !\REF: WANTUCK, P.J. E AL. J. PHYS. CHEM. 91, 4653
(1987)
CH3OCH2O<=>CH3OCHO+H                3.300E+013    0.004
26136.3 !\AUTHOR: !\REF: HIPPLER ET AL. PCCP. 3: 3450--2458 (2001).
!=====
=====
!\ENDSUBSPECIES: \CH3OCH2O
!=====
-----
!\ENDSUBMECH: \CH3OCH3
!-----
-----
!\SUBMECH: \CH3OCHO
!-----
-----
!
-----
!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
-----

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CH3O+HCO<=>CH3OCHO	3.000E+013	0.000
0.0 !\AUTHOR: !\REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.		
CH3O+HCO<=>CH3OH+CO	9.000E+013	0.000
0.0 !\AUTHOR: !\REF:Friedrichs, G.; Davidson, D. F.; Hanson, R. K. Int J. Chem. Kinet. 2004, 36, 157.		
CH3+OCHO<=>CH3OCHO	1.000E+013	0.000
0.0 !\AUTHOR:		
CH2OCHO+H<=>CH3OCHO	1.000E+014	0.000
0.0 !\AUTHOR: !\REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.		
CH3OCO+H<=>CH3OCHO	1.000E+014	0.000
0.0 !\AUTHOR: !\REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.		

!

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

!

CH3OCHO+O2<=>CH3OCO+HO2	1.000E+013	0.000
49700.0 !\AUTHOR:		
CH3OCHO+O2<=>CH2OCHO+HO2	2.050E+013	0.000
52000.0 !\AUTHOR:		
CH3OCHO+OH<=>CH3OCO+H2O	1.580E+007	1.800
934.0 !\AUTHOR: !\REF:ANOLOGY TO PROPANE		
CH3OCHO+OH<=>CH2OCHO+H2O	5.270E+009	0.970
1586.0 !\AUTHOR: !\REF:ANOLOGY TO PROPANE		
CH3OCHO+HO2<=>CH3OCO+H2O2	4.820E+003	2.600
13910.0 !\AUTHOR: !\REF:CURRAN ESTIMATE TSANG '88 PRIMARY H		
CH3OCHO+HO2<=>CH2OCHO+H2O2	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:CURRAN ESTIMATE TSANG '88 PRIMARY H		
CH3OCHO+O<=>CH3OCO+OH	2.755E+005	2.450
2830.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+O<=>CH2OCHO+OH	9.800E+005	2.430
4750.0 !\AUTHOR: !\REF: FIT TO COHEN/ WESTBERG '86		
CH3OCHO+H<=>CH3OCO+H2	6.500E+005	2.400
4471.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+H<=>CH2OCHO+H2	6.650E+005	2.540
6756.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+CH3<=>CH3OCO+CH4	7.550E-001	3.460
5481.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+CH3<=>CH2OCHO+CH4	4.520E-001	3.650
7154.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+CH3O<=>CH3OCO+CH3OH	5.480E+011	0.000
5000.0 !\AUTHOR:		
CH3OCHO+CH3O<=>CH2OCHO+CH3OH	2.170E+011	0.000
6458.0 !\AUTHOR:		
CH3OCHO+CH3O2<=>CH3OCO+CH3O2H	4.820E+003	2.600
13910.0 !\AUTHOR: !\REF:ANOLOGY WITH HO2		
CH3OCHO+CH3O2<=>CH2OCHO+CH3O2H	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:ANOLOGY WITH HO2		
CH3OCHO+HCO<=>CH3OCO+CH2O	5.400E+006	1.900
17010.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3OCHO+HCO<=>CH2OCHO+CH2O	1.025E+005	2.500
18430.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		

!

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!\REACTIONCLASS: \RADICAL DECOMPOSITION          \A          \N
\EA
!
-----
CH3OCO<=>CH2OCHO                                1.629E+012    -0.180
40670.0
CH3OCO<=>CH3+CO2                                  8.691E+017    -1.810
13656.7
PLOG/          0.0500      9.720E+012    -1.310      9416.7/
PLOG/          1.0000      1.250E+016    -1.830     11340.8/
PLOG/         10.0000      1.040E+018    -2.100     12826.9/
PLOG/        100.0000      8.690E+017    -1.810     13656.7/
CH3OCO<=>CH3O+CO                                  8.691E+017    -1.810
13656.7
PLOG/          0.0500      1.030E+003     1.290     25401.0/
PLOG/          1.0000      4.090E+005     0.810     21969.1/
PLOG/         10.0000      9.020E+014    -1.720     21767.5/
PLOG/        100.0000      2.825E+022    -3.440     23592.4/
CH2O+HCO<=>CH2OCHO                                1.500E+011     0.000
11900.0
!-----
!-----
!\ENDSUBMECH: \CH3OCHO
!-----
!-----
!+++++
!+++++
!+++++
!\END_KINETICS_MODULE: \C2
!+++++
!+++++
!+++++
!\KINETICS_MODULE: \C3
!\MODSUBMECHS:
!+++++
!+++++
!+++++
!-----
!-----
!\SUBMECH: \C3H8
!-----
!-----
!

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!\REACTIONCLASS: \UNIMOL          \A          \N
\EA
!
-----
C3H8 (+M) <=>CH3+C2H5 (+M)                    1.290E+037    -5.840
97380.0      !\AUTHOR: !\REF:OEHSCHLAEGER ET AL., PROC COMB INST 30 (2005)
1119-1127
LOW/                                                5.640E+074    -15.740
98714.0/
TROE/  3.100E-001  5.000E+001  3.000E+003  9.000E+003/

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H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/
 3.00/ HE/ 0.70/
 NC3H7+H<=>C3H8 1.000E+014 0.000
 0.0 !\AUTHOR: !\REF:ESTIMATE
 IC3H7+H<=>C3H8 1.000E+014 0.000
 0.0 !\AUTHOR: !\REF:ESTIMATE
 !

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

C3H8+IC3H7<=>NC3H7+C3H8 3.000E+010 0.000
 12900.0 !\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F.
 L., AND GLASSMAN, I., TO BE PUBLISHED.
 C3H8+O2<=>IC3H7+HO2 2.000E+013 0.000
 49640.0 !\AUTHOR: !\REF: Ingham, T.; Walker, R.W.; Woolford, R.E., Symp.
 Int. Combust. Proc. 25, 767-774 (1994)
 C3H8+H<=>IC3H7+H2 1.300E+006 2.400
 4471.0 !\AUTHOR: !\REF:Tsang, W. Chemical kinetic data base for
 combustion chemistry. Part 3. Propane J. Phys. Chem. Ref. Data 17, 887
 (1988)
 C3H8+O<=>IC3H7+OH 5.490E+005 2.500
 3140.0 !\AUTHOR: !\REF:Tsang, W. Chemical kinetic data base for
 combustion chemistry. Part 3. Propane J. Phys. Chem. Ref. Data 17, 887
 (1988)
 C3H8+OH<=>IC3H7+H2O 4.670E+007 1.610
 -35.0 !\AUTHOR: !\REF: Droege, A. T. and Tully, F. P.: Hydrogen-atom
 abstraction from alkanes by OH. 3. Propane, J. Phys. Chem., 90,
 1949;§C1954
 C3H8+HO2<=>IC3H7+H2O2 6.320E+001 3.370
 13720.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054.
 C3H8+CH3<=>IC3H7+CH4 6.400E+004 2.170
 7520.0 !\AUTHOR: !\REF:FIT TO NIST DATABASE
 C3H8+C2H3<=>IC3H7+C2H4 1.000E+011 0.000
 10400.0 !\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F.
 L., AND GLASSMAN, I., TO BE PUBLISHED.
 C3H8+C2H5<=>IC3H7+C2H6 1.000E+011 0.000
 10400.0 !\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F.
 L., AND GLASSMAN, I., TO BE PUBLISHED.
 C3H8+C3H5-A<=>IC3H7+C3H6 7.940E+011 0.000
 16200.0 !\AUTHOR: !\REF:DAGAUT ET AL., CST 71, 111(1990)
 C3H8+CH3O<=>IC3H7+CH3OH 3.000E+011 0.000
 7000.0 !\AUTHOR: !\REF:DRYER ESTIMATE
 C3H8+CH3O2<=>IC3H7+CH3O2H 1.019E+001 3.580
 14810.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054.
 C3H8+C2H5O2<=>IC3H7+C2H5O2H 1.019E+001 3.580
 14810.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054.
 C3H8+NC3H7O2<=>IC3H7+NC3H7O2H 2.000E+012 0.000
 17000.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P.
 R. CHEMICAL SOCIETY, 1975
 C3H8+CH3CO3<=>IC3H7+CH3CO3H 2.000E+012 0.000
 17000.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P.
 R. CHEMICAL SOCIETY, 1975

C3H8+O2CHO<=>IC3H7+HO2CHO	1.475E+004	2.600
13910.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C3H8+IC3H7O2<=>IC3H7+IC3H7O2H	2.000E+012	0.000
17000.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
C3H8+O2<=>NC3H7+HO2	6.000E+013	0.000
52290.0 !\AUTHOR: !\REF: ANALOGY WITH C4H10+O2<=>PC4H9+HO2		
C3H8+H<=>NC3H7+H2	3.490E+005	2.690
6450.0 !\AUTHOR: !\REF:Curran estimate, 15% lower than Tsang, W., J. Phys. Chem. Ref. Data 17, 887 (1988)		
C3H8+O<=>NC3H7+OH	3.710E+006	2.400
5505.0 !\AUTHOR: !\REF:Tsang, W. Chemical kinetic data base for combustion chemistry. Part 3. Propane J. Phys. Chem. Ref. Data 17, 887 (1988)		
C3H8+OH<=>NC3H7+H2O	1.054E+010	0.970
1586.0 !\AUTHOR: !\REF: Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by OH. 3. Propane, J. Phys. Chem., 90, 1949;§C1954		
C3H8+HO2<=>NC3H7+H2O2	4.080E+001	3.590
17160.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C3H8+CH3<=>NC3H7+CH4	9.040E-001	3.650
7154.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
C3H8+C2H3<=>NC3H7+C2H4	1.000E+011	0.000
10400.0 !\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE PUBLISHED.		
C3H8+C2H5<=>NC3H7+C2H6	1.000E+011	0.000
10400.0 !\AUTHOR: !\REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L., AND GLASSMAN, I., TO BE PUBLISHED.		
C3H8+C3H5-A<=>NC3H7+C3H6	7.940E+011	0.000
20500.0 !\AUTHOR: !\REF:DAGAUT ET AL., CST 71, 111(1990)		
C3H8+CH3O<=>NC3H7+CH3OH	3.000E+011	0.000
7000.0 !\AUTHOR: !\REF:DRYER ESTIMATE		
C3H8+CH3O2<=>NC3H7+CH3O2H	1.386E+000	3.970
18280.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C3H8+C2H5O2<=>NC3H7+C2H5O2H	1.386E+000	3.970
18280.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C3H8+NC3H7O2<=>NC3H7+NC3H7O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C3H8+IC3H7O2<=>NC3H7+IC3H7O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C3H8+CH3CO3<=>NC3H7+CH3CO3H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C3H8+O2CHO<=>NC3H7+HO2CHO	5.520E+004	2.550
16480.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
!		

!\REACTIONCLASS: \R_R_RECOMBIN	\A	\N
\EA		
!		

IC3H7+H<=>C2H5+CH3	2.000E+013	0.000
0.0 !\AUTHOR: !\REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST		
IC3H7+OH<=>C3H6+H2O	2.410E+013	0.000
0.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		

IC3H7+O<=>CH3COCH3+H 4.818E+013 0.000
0.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
IC3H7+O<=>CH3CHO+CH3 4.818E+013 0.000
0.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
!

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

NC3H7+HO2<=>NC3H7O+OH 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING
NC3H7+CH3O2<=>NC3H7O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING
IC3H7+HO2<=>IC3H7O+OH 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING
IC3H7+CH3O2<=>IC3H7O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING

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

!\REACTIONCLASS: \R_BETA_SCISSION \A \N
\EA
!

C2H5+CH2O<=>NC3H7O 1.000E+011 0.000
3496.0 !\AUTHOR: !\REF: H.J. Curran, International Journal of Chemical
Kinetics (2006) 38: 250;§C275.
C2H5CHO+H<=>NC3H7O 4.000E+012 0.000
6260.0 !\AUTHOR: !\REF: H.J. Curran, International Journal of Chemical
Kinetics (2006) 38: 250;§C275.

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

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

!\REACTIONCLASS: \R_BETA_SCISSION \A \N
\EA
!

CH3+CH3CHO<=>IC3H7O 1.000E+011 0.000
9256.0 !\AUTHOR: !\REF: H.J. Curran, International Journal of Chemical
Kinetics (2006) 38: 250;§C275.
CH3COCH3+H<=>IC3H7O 2.000E+012 0.000
7270.0 !\AUTHOR: !\REF: H.J. Curran, International Journal of Chemical
Kinetics (2006) 38: 250;§C275.

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!
-----
!\REACTIONCLASS: \R_O2_PRODUCTS           \A           \N
\EA
!
-----
IC3H7O+O2<=>CH3COCH3+HO2                   9.090E+009      0.000
390.0 !\AUTHOR: !\REF:BALLA ET AL., CHEM. PHYSICS, 99, 323 (1985)
!=====
=====
!\ENDSUBSPECIES: \IC3H7O
!=====
=====
!
-----
!\REACTIONCLASS: \R+O2                     \A           \N
\EA
!
-----
NC3H7+O2<=>C3H6+HO2                         1.312E-009      5.660
3050.0 !\AUTHOR: !\REF: !J. D. DeSain, et al., J. Phys. Chem. A 108 (34)
(2004) 7127 - 7128
DUP
NC3H7+O2<=>C3H6+HO2                         8.047E+000      3.320
6470.0 !\AUTHOR: !\REF: !J. D. DeSain, et al., J. Phys. Chem. A 108 (34)
(2004) 7127 - 7128
DUP
NC3H7+O2<=>NC3H7O2       1.0E11  0.0  0.0           !\AUTHOR:
PLOG/ 0.01 9.2e+008 0.405 -4398.65/
PLOG/ 0.1 1.45e+014 -0.984 -1710.8/
PLOG/ 1 2.09e+013 -0.499 -938.423/
PLOG/ 10 1.15e+020 -2.42 2451.26/
PLOG/ 100 2.07e+016 -1.3 803.419/
IC3H7+O2<=>IC3H7O2       1.0E11  0.0  0.0           !\AUTHOR:
PLOG/ 0.01 7.33e+005 1.33 -6345.64/
PLOG/ 0.1 2.24e+011 -0.105 -3697.87/
PLOG/ 1 1.54e+018 -2.02 -498.567/
PLOG/ 10 6.74e+027 -4.85 3779.82/
PLOG/ 100 1.67e+029 -5.15 5036.45/
!
-----
!\REACTIONCLASS: \RO2_ALKENE_HO2           \A           \N
\EA
!
-----
IC3H7O2<=>C3H6+HO2                          1.224E+09       1.28
30000 !\AUTHOR: !\REF:
NC3H7O2<=>C3H6+HO2                          6.24E+08        1.25
29600 !\AUTHOR: !\REF: \VLN 2011
!
-----
!\REACTIONCLASS: \RO2_QOOH                 \A           \N
\EA
!
-----
NC3H7O2<=>C3H6OOH1-2                       4.090E+008      1.100
30100.0 !\AUTHOR: !\REF:Sharma

```

NC3H7O2<=>C3H6OOH1-3	3.566E+006	1.600
21000.0 !\AUTHOR: !\REF		
IC3H7O2<=>C3H6OOH2-1	2.917E+009	1.100
33500.0 !\AUTHOR: !\REF		
!		
!\REACTIONCLASS: \QOOH_PRODUCTS	\A	\N
\EA		
!		
C3H6OOH1-2<=>C3H6O1-2+OH	1.210E+009	1.050
11300.0 !\AUTHOR: !\REF:HIGH PRESSURE RATE RULES FOR ALKYL+O2 REACTIONS 2 VLN2012		
C3H6OOH1-3<=>C3H6O1-3+OH	2.640E+009	0.710
18500.0 !\AUTHOR: !\REF:HIGH PRESSURE RATE RULES FOR ALKYL+O2 REACTIONS 2 VLN2012		
C3H6OOH1-2<=>C3H6+HO2	2.340E+010	0.770
15300.0 !\AUTHOR: !\REF:Villano		
C3H6OOH1-3=>OH+CH2O+C2H4	2.890E+009	1.300
26700.0 !\AUTHOR: !\REF:Villano		
C3H6OOH2-1<=>C2H3OOH+CH3	8.560E+010	0.850
30700.0 !\AUTHOR: !\REF:Villano		
C3H6OOH1-2=>C2H4+CH2O+OH	1.310E+033	-7.010
48120.0 !\AUTHOR: !\REF:Villano		
!		
!\REACTIONCLASS: \QOOH_O2_O2QOOH	\A	\N
\EA		
!		
C3H6OOH1-2+O2<=>C3H6OOH1-2O2	1.744E+014	-0.816
-536.5 !\AUTHOR: !\REF:Miyoshi A/2 !\ 080415A		
C3H6OOH1-3+O2<=>C3H6OOH1-3O2	3.433E+016	-1.627
198.7 !\AUTHOR: !\REF:Miyoshi A/2 !\ 080415A		
C3H6OOH2-1+O2<=>C3H6OOH2-1O2	3.433E+016	-1.627
198.7 !\AUTHOR: !\REF:Miyoshi A/2 !\ 080415A		
!		
!\REACTIONCLASS: \O2QOOH_ISOMERISATION	\A	\N
\EA		
!		
C3H6OOH1-2O2<=>C3H51-2,3OOH	2.917E+009	1.100
33500.0 !\AUTHOR: !\REF: !\Analogy to 1st isomerisations		
C3H6OOH1-3O2<=>C3H52-1,3OOH	4.009E+008	1.100
30100.0 !\AUTHOR: !\REF: !\Analogy to 1st isomerisations		
C3H6OOH2-1O2<=>C3H51-2,3OOH	3.566E+006	1.600
21000.0 !\AUTHOR: !\REF: !\Analogy to 1st isomerisations		
C3H51-2,3OOH<=>AC3H5OOH+HO2	2.560E+013	-0.490
17770.0 !\AUTHOR: !\REF: BOZZELLI AND PITZ, 1993.		
C3H52-1,3OOH<=>AC3H5OOH+HO2	1.150E+014	-0.630
17250.0 !\AUTHOR: !\REF: BOZZELLI AND PITZ, 1993.		
C3H51-2,3OOH<=>C3H5O1-2OOH-3+OH	4.450E+009	0.860
10800.0 !\AUTHOR: !\REF:		
C3H51-2,3OOH<=>C3H5O1-3OOH-2+OH	2.640E+009	0.710
18500.0 !\AUTHOR: !\REF: !\Hydroperoxy cyclic ether formation		
C3H52-1,3OOH<=>C3H5O1-2OOH-3+OH	1.210E+009	1.050
11300.0 !\AUTHOR: !\REF: !\Hydroperoxy cyclic ether formation		

C3H5O1-2OOH-3=>CH2CHO+CH2O+OH	1.000E+016	0.000
43000.0 !\AUTHOR: !\REF:!\Hydroperoxy cyclic ether formation		
C3H5O1-3OOH-2=>CH2CHO+CH2O+OH	1.000E+016	0.000
43000.0 !\AUTHOR: !\REF:!\Hydroperoxy cyclic ether formation		

```
!\REACTIONCLASS: \O2QOOH_KHP          \A          \N
\EA
!
```

C3H6OOH1-2O2<=>C3KET12+OH	6.000E+011	0.000
26400.0 !\AUTHOR: !\REF:Sharma 080415A		
C3H6OOH1-3O2<=>C3KET13+OH	7.500E+010	0.000
21400.0 !\AUTHOR: !\REF:Sharma 080415A		
C3H6OOH2-1O2<=>C3KET21+OH	3.000E+011	0.000
23850.0 !\AUTHOR: !\REF:Sharma 080415A		

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

C3KET12=>CH3CHO+HCO+OH	9.500E+015	0.000
42540.0 !\AUTHOR: !\ C ZHOU !REF: ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION		
C3KET13=>CH2O+CH2CHO+OH	1.000E+016	0.000
43000.0 !\AUTHOR: !\REF: WARNING		
C3KET21=>CH2O+CH3CO+OH	1.000E+016	0.000
43000.0 !\AUTHOR: !\REF: WARNING		
C3KET21=>OH+CH2O+CO+CH3	1.59E+20	-1.5
42879.46 !\AUTHOR: !\REF: WARNING		
C2H3OOH<=>CH2CHO+OH	8.400E+014	0.000
43000.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C2H3OOH=>CH2CO+H+OH	1.59E+20	-1.5
42879.46 !\AUTHOR: !\ C ZHOU !REF: ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH CALCULATION		
!ANALOGY TO IC4H7OOH DECOMPOSITION		
C3KET21<=>CH3COCH2O+OH	1.000E+011	0.000
0.0		
PLOG/ 0.0100 1.490E+058 -13.900 54266.9/		
PLOG/ 0.1000 1.800E+054 -12.400 54193.8/		
PLOG/ 1.0000 3.360E+046 -9.810 52468.5/		
PLOG/ 10.0000 2.390E+036 -6.540 49429.0/		
PLOG/ 100.0000 1.280E+027 -3.610 46333.1/		

```
!\SUBSPECIES: \NC3H7O2H
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```
!\REACTIONCLASS: \UNIMOL          \A          \N
\EA
!
```

NC3H7O2H<=>NC3H7O+OH	1.500E+016	0.000
42500.0 !\AUTHOR: !\REF:ESTIMATE		

!

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

NC3H7O2+H2<=>NC3H7O2H+H 3.010E+013 0.000
26030.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986)
NC3H7O2+HO2<=>NC3H7O2H+O2 1.750E+010 0.000
-3275.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
NC3H7O2+CH2O<=>NC3H7O2H+HCO 5.600E+012 0.000
13600.0 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2
NC3H7O2+CH4<=>NC3H7O2H+CH3 1.120E+013 0.000
24640.0 !\AUTHOR: !\REF:ANALOGY TO CH4+HO2
NC3H7O2+CH3OH<=>NC3H7O2H+CH2OH 6.300E+012 0.000
19360.0 !\AUTHOR: !\REF:ANALOGY TO CH3OH+HO2
NC3H7O2+CH3CHO<=>NC3H7O2H+CH3CO 2.800E+012 0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2
NC3H7O2+C2H4<=>NC3H7O2H+C2H3 1.130E+013 0.000
30430.0 !\AUTHOR: !\REF:ANALOGY TO C2H4+HO2
NC3H7O2+C2H6<=>NC3H7O2H+C2H5 1.700E+013 0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
NC3H7O2+C2H3CHO<=>NC3H7O2H+C2H3CO 2.800E+012 0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2
NC3H7O2+C2H5CHO<=>NC3H7O2H+C2H5CO 2.000E+011 0.000
9500.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

!=====
=====
!\ENDSUBSPECIES: \NC3H7O2H
!=====
=====
!

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

NC3H7O2+NC3H7O2=>NC3H7O+NC3H7O+O2 1.400E+016 -1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+CH3CO3=>NC3H7O+CH3CO2+O2 1.400E+016 -1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+C2H5O2=>NC3H7O+C2H5O+O2 1.400E+016 -1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+CH3<=>NC3H7O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+C2H5<=>NC3H7O+C2H5O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+IC3H7<=>NC3H7O+IC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+NC3H7<=>NC3H7O+NC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+C3H5-A<=>NC3H7O+C3H5O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
NC3H7O2+CH3O2=>NC3H7O+CH3O+O2 1.400E+016 -1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE

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

IC3H7O2+IC3H7<=>IC3H7O+IC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC3H7O2+NC3H7<=>IC3H7O+NC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC3H7O2+C3H5-A<=>IC3H7O+C3H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		

!=====
 =====

!\ENDSUBSPECIES: \IC3H7O2H

!=====
 =====

!=====
 =====

!=====
 =====

!=====
 =====

!\SUBSPECIES: C3H6O1-2/C3H6O1-3

!=====
 =====

!=====
 =====

!=====
 =====

!\REACTIONCLASS: \RH_R_ABSTRACTION	\A	\N
------------------------------------	----	----

\EA

!=====
 =====

C3H6O1-2<=>C2H4+CH2O	6.000E+014	0.000
60000.0 !\AUTHOR: !\REF:!\FLOWERS, M. C., J. CHEM. SOC. FAR. TRANS. I 73, 1927 (1977)		
C3H6O1-2+OH=>CH2O+C2H3+H2O	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C3H6O1-2+H=>CH2O+C2H3+H2	2.630E+007	2.000
5000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C3H6O1-2+O=>CH2O+C2H3+OH	8.430E+013	0.000
5200.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C3H6O1-2+HO2=>CH2O+C2H3+H2O2	1.000E+013	0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C3H6O1-2+CH3=>CH2O+C2H3+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		

!=====
 =====

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

!=====
 =====

C3H6O1-3<=>C2H4+CH2O	6.000E+014	0.000
60000.0 !\AUTHOR: !\REF:WESTBROOK AND PITZ ESTIMATE (1983)		
C3H6O1-3+OH=>CH2O+C2H3+H2O	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C3H6O1-3+O=>CH2O+C2H3+OH	8.430E+013	0.000
5200.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C3H6O1-3+H=>CH2O+C2H3+H2	2.630E+007	2.000
5000.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C3H6O1-3+CH3O2=>CH2O+C2H3+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C3H6O1-3+HO2=>CH2O+C2H3+H2O2	1.000E+013	0.000
15000.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C3H6O1-3+CH3=>CH2O+C2H3+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:PITZ ESTIMATE		

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=====
!\\ENDSUBSPECIES: C3H6O1-2/C3H6O1-3
=====
!-----
!\\ENDSUBMECH: C3H8
!-----
!-----
!\\SUBMECH: \\C3H6
!-----
!-----
!-----
!\\REACTIONCLASS: \\UNIMOL                                \\A                                \\N
\\EA
!-----
C2H3+CH3 (+M) <=> C3H6 (+M)                                2.500E+013                                0.000
0.0 !\\AUTHOR: !\\REF:LASKIN ET AL. IJCK 32 589-614 2000
LOW/                                                        4.270E+058                                -11.940
9769.8/
TROE/ 1.750E-001 1.341E+003 6.000E+004 1.014E+004/
CH2 (S)+C2H4<=>CC3H6          1.44E+51          -1.31E+01          1.42E+04
!\\AUTHOR: !\\REF:
PLOG/ 0.01 1.44E+51 -1.31E+01 1.42E+04/
PLOG/ 0.1 3.38E+54 -1.36E+01 1.65E+04/
PLOG/ 1 1.35E+54 -1.30E+01 1.89E+04/
PLOG/ 10 2.73E+47 -1.08E+01 1.42E+04/
PLOG/ 100 2.71E+50 -1.12E+01 1.67E+04/
DUP
CH2 (S)+C2H4<=>CC3H6          6.16E+40          -1.05E+01          5428.1
!\\AUTHOR: !\\REF:
PLOG/ 0.01 6.16E+40 -1.05E+01 5428.1/
PLOG/ 0.1 6.93E+41 -1.03E+01 6188.9/
PLOG/ 1 1.81E+37 -8.55E+00 5521/
PLOG/ 10 4.26E+37 -8.32E+00 4770.2/
PLOG/ 100 4.68E+35 -7.37E+00 4689.1/
DUP
CH2 (S)+C2H4<=>C3H6          4.82E+57          -1.43E+01          1.71E+04
!\\AUTHOR: !\\REF:
PLOG/ 0.01 4.82E+57 -1.43E+01 1.71E+04/
PLOG/ 0.1 3.84E+59 -1.44E+01 1.84E+04/
PLOG/ 1 2.13E+58 -1.35E+01 2.04E+04/
PLOG/ 10 8.48E+52 -1.16E+01 2.07E+04/
PLOG/ 100 6.07E+47 -9.85E+00 2.21E+04/
DUP
CH2 (S)+C2H4<=>C3H6          1.15E+45          -1.11E+01          6145.2 !\\AUTHOR:
!\\REF:
PLOG/ 0.01 1.15E+45 -1.11E+01 6145.2/
PLOG/ 0.1 1.83E+45 -1.07E+01 6638.5/
PLOG/ 1 1.30E+40 -8.77E+00 5863.8/
PLOG/ 10 2.27E+32 -6.14E+00 4317.9/
PLOG/ 100 1.28E+24 -3.49E+00 2529.9/
DUP

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CH2 (S)+C2H4<=>C3H5-A+H 8.20E+19 -2.06E+00 1.15E+03
 !\AUTHOR: !\REF:
 PLOG/ 0.01 8.20E+19 -2.06E+00 1.15E+03/
 PLOG/ 0.1 2.27E+21 -2.44E+00 2.65E+03/
 PLOG/ 1 4.44E+35 -6.55E+00 1.39E+04/
 PLOG/ 10 1.18E+28 -4.09E+00 1.40E+04/
 PLOG/ 100 6.51E+26 -3.58E+00 1.89E+04/
 DUP
 CH2 (S)+C2H4<=>C3H5-A+H 1.08E+07 1.62E+00 -3174.6
 !\AUTHOR: !\REF:
 PLOG/ 0.01 1.08E+07 1.62E+00 -3174.6/
 PLOG/ 0.1 1.37E+05 2.15E+00 -3799.2/
 PLOG/ 1 3.89E+14 -4.20E-01 1237.6/
 PLOG/ 10 2.45E+10 6.70E-01 750.93/
 PLOG/ 100 1.81E+02 2.97E+00 -746.03/
 DUP
 CH2 (S)+C2H4<=>C2H3+CH3 1.77E+19 -1.94E+00 6.79E+03
 !\AUTHOR: !\REF:
 PLOG/ 0.01 1.77E+19 -1.94E+00 6.79E+03/
 PLOG/ 0.1 1.68E+19 -1.80E+00 4.31E+03/
 PLOG/ 1 4.16E+24 -3.19E+00 9.76E+03/
 PLOG/ 10 7.89E+24 -3.07E+00 1.39E+04/
 PLOG/ 100 7.36E+29 -4.28E+00 2.38E+04/
 DUP
 CH2 (S)+C2H4<=>C2H3+CH3 4.30E+12 1.90E-01 -110.41
 !\AUTHOR: !\REF:
 PLOG/ 0.01 4.30E+12 1.90E-01 -110.41/
 PLOG/ 0.1 2.26E+11 5.40E-01 47.81/
 PLOG/ 1 4.92E+09 1.02E+00 599.77/
 PLOG/ 10 1.47E+08 1.33E+00 1228.4/
 PLOG/ 100 8.11E+10 5.50E-01 5506.5/
 DUP
 C2H3+CH3<=>C3H5-A+H 4.12E+29 -4.95E+00 8.00E+03
 !\AUTHOR: !\REF:
 PLOG/ 0.01 4.12E+29 -4.95E+00 8.00E+03/
 PLOG/ 0.1 4.86E+30 -5.03E+00 1.13E+04/
 PLOG/ 1 5.30E+29 -4.57E+00 1.44E+04/
 PLOG/ 10 1.32E+30 -4.54E+00 1.93E+04/
 PLOG/ 100 5.16E+28 -4.03E+00 2.38E+04/
 DUP
 C2H3+CH3<=>C3H5-A+H 5.73E+15 -7.70E-01 1195.9
 !\AUTHOR: !\REF:
 PLOG/ 0.01 5.73E+15 -7.70E-01 1195.9/
 PLOG/ 0.1 2.06E+13 -7.40E-02 1428.7/
 PLOG/ 1 4.48E+10 6.00E-01 1421.6/
 PLOG/ 10 4.10E+06 1.71E+00 1056.9/
 PLOG/ 100 1.37E-01 3.91E+00 -353.55/
 DUP
 C3H6<=>C2H3+CH3 1.88E+78 -1.87E+01 1.30E+05
 !\AUTHOR: !\REF:
 PLOG/ 0.01 1.88E+78 -1.87E+01 1.30E+05/
 PLOG/ 0.1 8.73E+76 -1.79E+01 1.32E+05/
 PLOG/ 1 5.80E+75 -1.72E+01 1.34E+05/
 PLOG/ 10 8.12E+71 -1.58E+01 1.36E+05/
 PLOG/ 100 2.15E+64 -1.34E+01 1.35E+05/
 DUP
 C3H6<=>C2H3+CH3 1.69E+59 -1.36E+01 113290
 !\AUTHOR: !\REF:

PLOG/	0.01	1.69E+59	-1.36E+01	113290/
PLOG/	0.1	2.00E+60	-1.37E+01	114890/
PLOG/	1	6.70E+54	-1.18E+01	113840/
PLOG/	10	1.06E+47	-9.27E+00	111510/
PLOG/	100	7.29E+38	-6.70E+00	108740/
DUP				
C3H6<=>C3H5-A+H		9.16E+74	-1.76E+01	1.20E+05
!\AUTHOR: !\REF:				
PLOG/	0.01	9.16E+74	-1.76E+01	1.20E+05/
PLOG/	0.1	1.73E+70	-1.60E+01	1.20E+05/
PLOG/	1	1.08E+71	-1.59E+01	1.2486E+05/
PLOG/	10	6.40E+65	-1.42E+01	1.25E+05/
PLOG/	100	8.05E+56	-1.15E+01	1.22E+05/
DUP				
C3H6<=>C3H5-A+H		2.98E+54	-1.23E+01	101200
!\AUTHOR: !\REF:				
PLOG/	0.01	2.98E+54	-1.23E+01	101200/
PLOG/	0.1	1.37E+43	-8.87E+00	96365/
PLOG/	1	6.28E+42	-8.51E+00	98004/
PLOG/	10	4.73E+35	-6.26E+00	95644/
PLOG/	100	4.34E+28	-4.06E+00	93114/
DUP				
C3H6<=>CC3H6		1.26E+64	-1.56E+01	9.50E+04
!\AUTHOR: !\REF:				
PLOG/	0.01	1.26E+64	-1.56E+01	9.50E+04/
PLOG/	0.1	3.94E+67	-1.62E+01	1.01E+05/
PLOG/	1	6.14E+68	-1.62E+01	1.06E+05/
PLOG/	10	9.70E+66	-1.53E+01	1.09E+05/
PLOG/	100	1.45E+62	-1.36E+01	1.10E+05/
DUP				
C3H6<=>CC3H6		4.84E+41	-9.62E+00	79528
!\AUTHOR: !\REF:				
PLOG/	0.01	4.84E+41	-9.62E+00	79528/
PLOG/	0.1	8.07E+44	-1.02E+01	82671/
PLOG/	1	1.15E+47	-1.06E+01	85502/
PLOG/	10	1.33E+39	-7.98E+00	83303/
PLOG/	100	4.97E+31	-5.60E+00	80987/
DUP				
CC3H6<=>C3H5-A+H		2.33E+63	-1.46E+01	1.03E+05
!\AUTHOR: !\REF:				
PLOG/	0.01	2.33E+63	-1.46E+01	1.03E+05/
PLOG/	0.1	7.03E+63	-1.44E+01	1.07E+05/
PLOG/	1	5.07E+64	-1.43E+01	1.12E+05/
PLOG/	10	4.92E+61	-1.32E+01	1.15E+05/
PLOG/	100	4.82E+57	-1.17E+01	1.18E+05/
DUP				
CC3H6<=>C3H5-A+H		1.12E+40	-8.37E+00	85836
!\AUTHOR: !\REF:				
PLOG/	0.01	1.12E+40	-8.37E+00	85836/
PLOG/	0.1	1.06E+41	-8.33E+00	88499/
PLOG/	1	8.23E+43	-8.88E+00	92907/
PLOG/	10	1.27E+39	-7.33E+00	93401/
PLOG/	100	1.45E+28	-4.02E+00	90995/
DUP				
CC3H6<=>C2H3+CH3		8.31E+64	-1.51E+01	1.11E+05
!\AUTHOR: !\REF:				
PLOG/	0.01	8.31E+64	-1.51E+01	1.11E+05/
PLOG/	0.1	8.29E+64	-1.47E+01	1.14E+05/

PLOG/	1	1.00E+70	-1.57E+01	1.22E+05/
PLOG/	10	1.66E+67	-1.46E+01	1.24E+05/
PLOG/	100	7.87E+62	-1.31E+01	1.27E+05/
DUP				
CC3H6<=>C2H3+CH3		1.51E+49	-1.10E+01	99748
!\AUTHOR: !\REF:				
PLOG/	0.01	1.51E+49	-1.10E+01	99748/
PLOG/	0.1	1.05E+45	-9.46E+00	99275/
PLOG/	1	3.39E+50	-1.06E+01	104220/
PLOG/	10	1.76E+47	-9.43E+00	104930/
PLOG/	100	1.88E+39	-6.93E+00	103980/
DUP				
C3H5-T+H<=>C3H6		4.96E+60	-1.52E+01	1.80E+04
!\AUTHOR: !\REF:				
PLOG/	0.01	4.96E+60	-1.52E+01	1.80E+04/
PLOG/	0.1	3.20E+62	-1.51E+01	2.01E+04/
PLOG/	1	2.31E+60	-1.40E+01	2.19E+04/
PLOG/	10	3.69E+54	-1.20E+01	2.21E+04/
PLOG/	100	1.15E+50	-1.04E+01	2.33E+04/
DUP				
C3H5-T+H<=>C3H6		1.49E+48	-1.20E+01	7203.3
!\AUTHOR: !\REF:				
PLOG/	0.01	1.49E+48	-1.20E+01	7203.3/
PLOG/	0.1	6.76E+46	-1.11E+01	7629.9/
PLOG/	1	1.09E+40	-8.66E+00	6447.8/
PLOG/	10	2.38E+31	-5.73E+00	4506/
PLOG/	100	5.69E+25	-3.83E+00	3250.4/
DUP				
C3H5-T+H<=>C3H5-A+H		2.11E+17	-1.08E+00	1.29E+03
!\AUTHOR: !\REF:				
PLOG/	0.01	2.11E+17	-1.08E+00	1.29E+03/
PLOG/	0.1	9.05E+29	-4.91E+00	8.54E+03/
PLOG/	1	2.98E+30	-4.79E+00	1.20E+04/
PLOG/	10	8.22E+28	-4.14E+00	1.54E+04/
PLOG/	100	2.28E+29	-4.12E+00	2.09E+04/
DUP				
C3H5-T+H<=>C3H5-A+H		6.41E+03	2.61E+00	-3778.4
!\AUTHOR: !\REF:				
PLOG/	0.01	6.41E+03	2.61E+00	-3778.4/
PLOG/	0.1	5.19E+14	-3.00E-01	1090.4/
PLOG/	1	8.17E+11	4.90E-01	1184.6/
PLOG/	10	2.79E+09	1.09E+00	1187.5/
PLOG/	100	6.75E+03	2.70E+00	373.8/
DUP				
C3H5-T+H<=>C2H3+CH3		3.31E+16	-6.90E-01	5.20E+03
!\AUTHOR: !\REF:				
PLOG/	0.01	3.31E+16	-6.90E-01	5.20E+03/
PLOG/	0.1	9.04E+16	-8.10E-01	4.80E+03/
PLOG/	1	2.01E+24	-2.86E+00	1.09E+04/
PLOG/	10	2.75E+26	-3.31E+00	1.58E+04/
PLOG/	100	3.15E+32	-4.83E+00	2.60E+04/
DUP				
C3H5-T+H<=>C2H3+CH3		8.04E+13	-1.40E-01	1150
!\AUTHOR: !\REF:				
PLOG/	0.01	8.04E+13	-1.40E-01	1150/
PLOG/	0.1	7.17E+10	6.70E-01	673.8/
PLOG/	1	9.97E+08	1.36E+00	1596.4/
PLOG/	10	7.41E+07	1.57E+00	2108.8/

PLOG/	100	2.70E+12	3.20E-01	6791.8/	
DUP					
C3H6<=>C3H5-S+H				7.710E+069	-16.090
140000.0					
!					
<hr/>					
!\REACTIONCLASS:	\RH_R_ABSTRACTION				
!					
<hr/>					
C3H6+H<=>C3H5-A+H2				3.644E+005	2.455
4361.2 !\AUTHOR: !\REF:					
C3H6+O2<=>C3H5-A+HO2				5.960E+019	-1.670
46192.1 !\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE					
C3H6+O<=>C3H5-A+OH				5.240E+011	0.700
5884.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4					
C3H6+OH<=>C3H5-A+H2O				4.460E+006	2.072
1050.8 !\AUTHOR: !\REF: NO REFERENCE					
C3H6+HO2<=>C3H5-A+H2O2				3.070E-002	4.403
13547.2 !\AUTHOR: !\REF:					
C3H6+CH3<=>C3H5-A+CH4				2.210E+000	3.500
5675.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)					
C3H6+CH3O<=>C3H5-A+CH3OH				8.400E+010	0.000
2600.0 !\AUTHOR: !\REF: BILL					
C3H6+CH3O2<=>C3H5-A+CH3O2H				7.680E-002	4.403
13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2					
C3H6+C2H5<=>C3H5-A+C2H6				1.000E+011	0.000
9800.0 !\AUTHOR: !\REF: ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)					
C3H6+C2H5O2<=>C3H5-A+C2H5O2H				7.680E-002	4.403
13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2					
C3H6+CH3CO3<=>C3H5-A+CH3CO3H				7.680E-002	4.403
13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2					
C3H6+NC3H7O2<=>C3H5-A+NC3H7O2H				7.680E-002	4.403
13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2					
C3H6+IC3H7O2<=>C3H5-A+IC3H7O2H				7.680E-002	4.403
13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2					
C3H6+H<=>C3H5-T+H2				1.498E+002	3.381
8909.5 !\AUTHOR: !\REF:					
C3H6+O<=>C3H5-T+OH				6.030E+010	0.700
7632.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4					
C3H6+OH<=>C3H5-T+H2O				1.800E+006	1.979
2235.2 !\AUTHOR: !\REF: ANALOGY WITH C2H4					
C3H6+HO2<=>C3H5-T+H2O2				1.560E+004	2.820
24427.9 !\AUTHOR: !\REF: C3 NUIG CALCULATION J.M					
C3H6+O2<=>C3H5-T+HO2				1.000E+013	0.000
58770.0 !\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE					
C3H6+CH3<=>C3H5-T+CH4				8.400E-001	3.500
11660.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)					
C3H6+H<=>C3H5-S+H2				5.101E+002	3.234
12357.0 !\AUTHOR: !\REF:					
DUP					
C3H6+H<=>C3H5-S+H2				3.969E+002	3.252
12007.0 !\AUTHOR: !\REF:					
DUP					

C3H6+O2<=>C3H5-S+HO2	2.000E+013	0.000
62270.0 !\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE		
C3H6+O<=>C3H5-S+OH	1.200E+011	0.700
8959.1 !\AUTHOR: !\REF: ANALOGY WITH C2H4		
C3H6+OH<=>C3H5-S+H2O	1.860E+005	2.369
2502.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4		
C3H6+HO2<=>C3H5-S+H2O2	9.570E+002	3.059
20798.6 !\AUTHOR: !\REF: C3 NUIG CALCULATION J.M		
C3H6+CH3<=>C3H5-S+CH4	1.348E+000	3.500
12850.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
!		

!\REACTIONCLASS: \R_ADDITION\O

C3H6+O<=>C2H5+HCO	7.450E+006	1.880
183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4		
C3H6+O=>CH2CO+CH3+H	3.050E+006	1.880
183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4		
C3H6+O=>CH3CHCO+H+H	3.050E+006	1.880
183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4		
!		

!\REACTIONCLASS: \R_ADDITION\H

C3H6+H<=>NC3H7	1.000E+000	1.000		
0.0 !\AUTHOR: !\REF: CURRAN EST				
PLOG/	0.0013	7.990E+081	-23.161	22239.0/
PLOG/	0.0400	4.240E+068	-18.427	19665.0/
PLOG/	1.0000	1.040E+049	-11.500	15359.0/
PLOG/	10.0000	6.200E+041	-8.892	14637.0/
PLOG/	100.0000	1E-10	0.0	0.0/
!PLOG/	100.0000	-6.450E+031	-5.851	8177.8/
DUP				
C3H6+H<=>NC3H7	1.000E+000	1.000		
0.0 !\AUTHOR: !\REF: CURRAN EST				
PLOG/	0.0013	1.850E+026	-5.830	3865.8/
PLOG/	0.0400	2.820E+030	-6.490	5470.8/
PLOG/	1.0000	3.780E+028	-5.570	5625.1/
PLOG/	10.0000	1.460E+025	-4.280	5247.8/
PLOG/	100.0000	4.220E+027	-4.390	9345.8/
!PLOG/	100.0000	7.240E+026	-4.210	6825.0/
DUP				
C3H6+H<=>C2H4+CH3	1.000E+000	1.000		
1.0 !\AUTHOR: !\REF: CURRAN EST				
PLOG/	0.0013	1.540E+009	1.350	2542.0/
PLOG/	0.0400	7.880E+010	0.870	3599.6/
PLOG/	1.0000	2.670E+012	0.470	5431.1/
PLOG/	10.0000	9.250E+022	-2.600	12898.0/
PLOG/	100.0000	1.320E+023	-2.420	16500.0/
DUP				
C3H6+H<=>C2H4+CH3	1.000E+000	1.000		
1.0 !\AUTHOR: !\REF: CURRAN EST				
PLOG/	0.0013	1E-10	0.0	0.0/
PLOG/	0.0400	1E-10	0.0	0.0/
PLOG/	1.0000	1E-10	0.0	0.0/
PLOG/	10.0000	1.240E+005	2.520	3679.1/

PLOG/	100.0000	2.510E+003	2.910	3980.9/	
DUP					
C3H6+H<=>IC3H7				1.000E+000	1.000
1.0 !\AUTHOR: !\REF: CURRAN EST					
PLOG/	0.0013	1.350E+044	-10.680	8196.4/	
PLOG/	0.0400	2.110E+057	-14.230	15147.0/	
PLOG/	1.0000	3.260E+061	-14.940	20161.0/	
PLOG/	10.0000	5.300E+056	-13.120	20667.0/	
PLOG/	100.0000	1.110E+050	-10.800	20202.0/	
DUP					
C3H6+H<=>IC3H7				1.000E+000	1.000
1.0 !\AUTHOR: !\REF: CURRAN EST					
PLOG/	0.0013	2.170E+130	-32.580	136140.0/	
PLOG/	0.0400	2.250E+029	-5.840	4241.9/	
PLOG/	1.0000	1.060E+030	-5.630	5613.4/	
PLOG/	10.0000	6.110E+026	-4.440	5182.3/	
PLOG/	100.0000	2.730E+023	-3.260	4597.0/	
DUP					
C2H4+CH3<=>NC3H7				1.000E+000	1.000
1.0 !\AUTHOR: !\REF: CURRAN EST					
PLOG/	0.0013	8.670E+048	-12.540	18206.0/	
PLOG/	0.0400	1.060E+049	-12.040	20001.0/	
PLOG/	1.0000	7.670E+047	-11.170	22366.0/	
PLOG/	10.0000	1.810E+045	-10.030	23769.0/	
PLOG/	100.0000	2.040E+040	-8.250	24214.0/	
DUP					
C2H4+CH3<=>NC3H7				1.000E+000	1.000
1.0 !\AUTHOR: !\REF: CURRAN EST					
PLOG/	0.0013	1.120E+043	-11.300	13080.0/	
PLOG/	0.0400	7.280E+039	-9.880	13164.0/	
PLOG/	1.0000	2.600E+033	-7.460	12416.0/	
PLOG/	10.0000	3.850E+027	-5.380	11455.0/	
PLOG/	100.0000	1.660E+021	-3.170	10241.0/	
DUP					

!

!\REACTIONCLASS: \R_ADDITION\HO2

!

C3H6+HO2<=>C3H6OOH2-1				4.850E-021	2.650
11201.0 !\AUTHOR: !\REF: WARNING					
PLOG/	0.0130	1.310E+013	-1.840	8561.0/	
PLOG/	0.9869	5.930E+017	-2.610	11533.0/	
PLOG/	9.8700	8.340E+024	-4.400	16440.0/	
PLOG/	98.6900	3.750E+023	-3.680	17965.0/	
C3H6+HO2<=>C3H6O1-2+OH				1.130E+019	-1.680
23587.0 !\AUTHOR: !\REF: WARNING					
PLOG/	0.0130	3.730E+003	2.640	11173.0/	
PLOG/	0.9869	1.780E+012	0.110	16137.0/	
PLOG/	9.8700	3.900E+017	-1.400	20077.0/	
PLOG/	98.6900	1.130E+019	-1.680	23587.0/	
C3H6+HO2<=>IC3H7+O2				8.870E+022	-3.090
26586.0 !\AUTHOR: !\REF: WARNING					
PLOG/	0.0130	1.020E+007	1.160	10273.0/	
PLOG/	0.9869	1.310E+020	-2.580	19078.0/	
PLOG/	9.8700	4.140E+028	-4.920	26212.0/	
PLOG/	98.6900	8.870E+022	-3.090	26586.0/	

C3H6OOH2-1<=>C3H6O1-2+OH 6.910E+007 1.370
13373.0 !\AUTHOR: !\REF: WARNING
PLOG/ 0.0130 2.660E+035 -8.360 18056.0/
PLOG/ 0.9869 1.960E+035 -7.660 20595.0/
PLOG/ 9.8700 2.240E+033 -6.750 21619.0/
PLOG/ 98.6900 8.480E+026 -4.580 20278.0/
!

!\REACTIONCLASS: \R_DECOMPOSITION
!

!\REACTIONCLASS: \R_R_ABSTRACTION
!

C3H5-A+H<=>C3H4-A+H2 1.232E+003 3.035
2582.0 !\AUTHOR: !\REF:KLIPPENSTEIN & HARDING 2007
C3H5-A+OH<=>C3H4-A+H2O 6.000E+012 0.000
0.0 !\AUTHOR: !\REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.
C3H5-A+CH3<=>C3H4-A+CH4 3.000E+012 -0.320
-131.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-A+C2H5<=>C3H4-A+C2H6 4.000E+011 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H5-A+C2H3<=>C3H4-A+C2H4 1.000E+012 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H4-A+C3H4-A<=>C3H5-A+C3H3 5.000E+014 0.000
64746.7 !\AUTHOR: !\REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230
(2005)
C3H5-S+H<=>C3H4-A+H2 3.333E+012 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H5-S+CH3<=>C3H4-A+CH4 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H5-S+H<=>C3H4-P+H2 3.340E+012 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-S+CH3<=>C3H4-P+CH4 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000

C3H5-T+H<=>C3H4-P+H2 3.340E+012 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-T+CH3<=>C3H4-P+CH4 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!

!\REACTIONCLASS: \R_R_RECOMB
!

C3H5-A+C3H5-A<=>C3H4-A+C3H6 9.550E+040 -9.300
12470.0 !\AUTHOR: !\REF: FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117,
4762-4776
PLOG/ 1.0000 4.770E+040 -9.300 12470.0/
PLOG/ 4.0000 3.970E+032 -6.800 9180.0/
PLOG/ 10.0000 1.460E+028 -5.500 7410.0/
C3H5-A+C2H5<=>C2H4+C3H6 4.000E+011 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
C3H5-A+HCO<=>C3H6+CO 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000

C3H5-S+HCO<=>C3H6+CO 9.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-T+HCO<=>C3H6+CO 9.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-S+O<=>C2H4+HCO 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-S+OH=>C2H4+HCO+H 5.000E+012 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-S+HO2=>C2H4+HCO+OH 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000

C3H5-T+O<=>CH3+CH2CO 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-T+OH=>CH3+CH2CO+H 5.000E+012 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-T+HO2=>CH3+CH2CO+OH 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000

!

!\REACTIONCLASS: \R+O

!

C3H5-A+O<=>C2H3CHO+H 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.

!

!\REACTIONCLASS: \R+OH

!

C3H5-A+OH=>C2H3CHO+H+H 5.300E+037 -6.710
29306.0 !\AUTHOR: !\REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.
PLOG/ 0.1000 5.300E+037 -6.710 29306.0/
PLOG/ 1.0000 4.200E+032 -5.160 30126.0/
PLOG/ 10.0000 1.600E+020 -1.560 26330.0/

!

!\REACTIONCLASS: \R+O2

!

C3H5-A+O2<=>C3H4-A+HO2 4.990E+015 -1.400
22428.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
PLOG/ 1.0000 4.990E+015 -1.400 22428.0/
PLOG/ 10.0000 2.180E+021 -2.850 30755.0/
C3H5-A+O2<=>CH3CO+CH2O 1.190E+015 -1.010
20128.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
PLOG/ 1.0000 1.190E+015 -1.010 20128.0/
PLOG/ 10.0000 7.140E+015 -1.210 21046.0/
C3H5-A+O2<=>C2H3CHO+OH 1.820E+013 -0.410
22859.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
PLOG/ 1.0000 1.820E+013 -0.410 22859.0/
PLOG/ 10.0000 2.470E+013 -0.450 23017.0/
C3H5-S+O2<=>CH3CHO+HCO 3.100E+031 -5.944
5748.4 !\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN
C3H5-S+O2<=>CH3CHCHO+O 5.380E+018 -2.140
5142.9 !\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN
C3H5-S+O2<=>C2H3CHO+OH 2.700E+019 -2.140
5142.9 !\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN

C3H5-T+O2<=>CH3COCH2+O 9.860E+025 -3.751
11255.4 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-T+O2<=>CH3CO+CH2O 2.550E+020 -2.608
1565.7 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C3H5-T+O2<=>C3H4-A+HO2 3.590E+010 -0.270
-413.6 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!

!\REACTIONCLASS: \R_HO2
!

C3H5-A+HO2<=>C3H5O+OH 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325;SC3346 \COMMENT:
PLOG/ 0.0100 1.020E+013 -0.158 -1417.0/
PLOG/ 0.1000 4.980E+014 -0.642 -349.1/
PLOG/ 1.0000 7.770E+017 -1.520 2379.2/
PLOG/ 10.0000 2.930E+015 -0.684 3615.3/
PLOG/ 100.0000 1.640E+004 2.740 1144.4/
C3H5-A+HO2<=>AC3H5OOH 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325;SC3346 \COMMENT:
PLOG/ 0.0100 1.910E+031 -7.230 1336.2/
PLOG/ 0.1000 6.310E+042 -10.300 5568.9/
PLOG/ 1.0000 1.030E+045 -10.600 7851.5/
PLOG/ 10.0000 2.790E+037 -7.920 6497.9/
PLOG/ 100.0000 1.440E+032 -6.010 6053.6/
C3H5-A+HO2<=>C2H3CHO+H2O 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325;SC3346 \COMMENT:
PLOG/ 0.0100 1.090E+000 3.010 -3421.1/
PLOG/ 0.1000 6.350E+001 2.500 -2341.4/
PLOG/ 1.0000 6.050E+005 1.390 595.1/
PLOG/ 10.0000 3.100E+005 1.590 2677.6/
PLOG/ 100.0000 5.070E-005 4.590 927.5/
AC3H5OOH<=>C2H3CHO+H2O 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325;SC3346 \COMMENT:
PLOG/ 0.0100 1.990E+050 -12.700 53531.9/
PLOG/ 0.1000 4.720E+047 -11.500 54360.9/
PLOG/ 1.0000 1.500E+040 -8.840 53179.2/
PLOG/ 10.0000 2.540E+028 -5.000 49919.4/
PLOG/ 100.0000 1.480E+016 -1.120 45949.3/
AC3H5OOH<=>C3H5O+OH 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325;SC3346 \COMMENT:
PLOG/ 0.0100 1.490E+058 -13.900 54266.9/
PLOG/ 0.1000 1.800E+054 -12.400 54193.8/
PLOG/ 1.0000 3.360E+046 -9.810 52468.5/
PLOG/ 10.0000 2.390E+036 -6.540 49429.0/
PLOG/ 100.0000 1.280E+027 -3.610 46333.1/
C3H5O<=>C2H3+CH2O 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116
(13), PP 3325;SC3346 \COMMENT:
PLOG/ 0.0010 7.260E+006 0.182 17815.5/
PLOG/ 0.0100 6.970E+016 -2.500 20878.7/
PLOG/ 0.1000 6.640E+023 -4.230 23565.0/
PLOG/ 1.0000 1.070E+026 -4.560 24622.9/

PLOG/	10.0000	6.500E+029	-5.370	26645.0/	
PLOG/	100.0000	4.630E+031	-5.590	28915.3/	
PLOG/	1000.0000	8.520E+025	-3.610	27863.4/	
C3H5O<=>CH2CHOCH2				1.000E+011	0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	3.170E+020	-4.150	12121.3/	
PLOG/	0.0100	4.790E+024	-5.030	14606.1/	
PLOG/	0.1000	1.900E+026	-5.160	16124.4/	
PLOG/	1.0000	1.510E+028	-5.400	18165.4/	
PLOG/	10.0000	2.420E+028	-5.170	19691.2/	
PLOG/	100.0000	5.570E+024	-3.860	19395.2/	
PLOG/	1000.0000	1.350E+018	-1.730	17386.5/	
C3H5O<=>CH2CH2CHO				1.000E+011	0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	5.250E-049	15.500	-15639.9/	
PLOG/	0.0100	1.460E-088	27.600	-35995.0/	
PLOG/	0.1000	4.440E-022	8.380	-3819.0/	
PLOG/	1.0000	6.230E+012	-1.440	10829.2/	
PLOG/	10.0000	3.480E+042	-9.910	25297.9/	
PLOG/	100.0000	1.880E+038	-8.160	25974.5/	
PLOG/	1000.0000	1.670E+021	-2.740	20337.7/	
C3H5O<=>C2H3CHO+H				1.000E+011	0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	3.000E+015	-2.310	14667.9/	
PLOG/	0.0100	1.500E+022	-3.960	18283.0/	
PLOG/	0.1000	1.950E+023	-3.990	19143.3/	
PLOG/	1.0000	1.150E+025	-4.240	20311.2/	
PLOG/	10.0000	1.760E+028	-4.890	22765.2/	
PLOG/	100.0000	1.410E+027	-4.280	23770.6/	
PLOG/	1000.0000	2.570E+020	-2.060	22040.1/	
C3H5O<=>C2H4+HCO				1.000E+011	0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	6.620E+016	-2.840	13197.0/	
PLOG/	0.0100	1.260E+020	-3.530	15469.2/	
PLOG/	0.1000	2.130E+021	-3.640	16584.5/	
PLOG/	1.0000	1.070E+024	-4.160	18985.0/	
PLOG/	10.0000	8.420E+025	-4.400	22382.6/	
PLOG/	100.0000	1.860E+021	-2.730	23658.8/	
PLOG/	1000.0000	4.750E+008	1.140	20922.5/	
CH2CHOCH2<=>C2H3+CH2O				1.000E+011	0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	3.300E+009	-0.638	19747.8/	
PLOG/	0.0100	3.360E+021	-3.900	23945.2/	
PLOG/	0.1000	2.910E+029	-5.900	27249.7/	
PLOG/	1.0000	1.830E+034	-6.940	30690.4/	
PLOG/	10.0000	9.720E+033	-6.500	33002.5/	
PLOG/	100.0000	2.680E+027	-4.260	33305.6/	
PLOG/	1000.0000	8.810E+014	-0.326	31553.1/	
CH2CHOCH2<=>CH2CH2CHO				1.000E+011	0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	8.010E-092	27.800	-37321.2/	
PLOG/	0.0100	7.780E-011	3.700	-2766.9/	

PLOG/	0.1000	5.110E+015	-2.760	15937.6/	
PLOG/	1.0000	4.480E+025	-5.200	21532.2/	
PLOG/	10.0000	3.970E+034	-7.410	28116.9/	
PLOG/	100.0000	5.620E+022	-3.560	25806.7/	
PLOG/	1000.0000	2.510E+020	-2.630	29288.4/	
CH2CHOCH2<=>C2H3CHO+H					1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	4.930E+024	-5.050	20108.4/	
PLOG/	0.0100	2.140E+028	-5.800	22219.4/	
PLOG/	0.1000	1.930E+032	-6.640	25108.2/	
PLOG/	1.0000	8.600E+034	-7.110	28209.1/	
PLOG/	10.0000	2.170E+034	-6.640	30647.6/	
PLOG/	100.0000	4.170E+028	-4.710	31231.9/	
PLOG/	1000.0000	3.980E+018	-1.620	30129.8/	
CH2CHOCH2<=>C2H4+HCO					1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	8.230E+026	-5.840	19356.9/	
PLOG/	0.0100	1.320E+029	-6.210	21293.6/	
PLOG/	0.1000	3.470E+032	-6.960	24197.3/	
PLOG/	1.0000	1.440E+036	-7.760	28007.8/	
PLOG/	10.0000	9.720E+037	-8.020	32394.6/	
PLOG/	100.0000	2.430E+031	-5.810	34295.8/	
PLOG/	1000.0000	3.730E+014	-0.726	32008.3/	
CH2CH2CHO<=>C2H3+CH2O					1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	6.890E-069	21.500	2638.0/	
PLOG/	0.0100	5.340E-033	11.100	16749.1/	
PLOG/	0.1000	6.110E+026	-6.010	44116.7/	
PLOG/	1.0000	8.040E+035	-8.310	46919.7/	
PLOG/	10.0000	5.520E+040	-9.190	50508.7/	
PLOG/	100.0000	5.850E+035	-7.180	52038.4/	
PLOG/	1000.0000	1.930E+019	-1.940	48440.0/	
CH2CH2CHO<=>C2H3CHO+H					1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	1.610E+010	-1.240	32371.3/	
PLOG/	0.0100	5.840E+015	-2.610	32878.4/	
PLOG/	0.1000	3.640E+023	-4.600	34275.3/	
PLOG/	1.0000	7.580E+031	-6.630	37895.4/	
PLOG/	10.0000	2.860E+032	-6.300	39990.7/	
PLOG/	100.0000	1.570E+023	-3.140	38011.7/	
PLOG/	1000.0000	4.520E+012	0.214	34570.5/	
CH2CH2CHO<=>C2H4+HCO					1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					
PLOG/	0.0010	2.900E+032	-7.240	25687.5/	
PLOG/	0.0100	5.300E+033	-7.280	27100.6/	
PLOG/	0.1000	2.000E+035	-7.410	29027.3/	
PLOG/	1.0000	1.010E+034	-6.700	30018.1/	
PLOG/	10.0000	9.760E+027	-4.630	28923.9/	
PLOG/	100.0000	2.110E+019	-1.850	26239.8/	
PLOG/	1000.0000	1.590E+013	0.063	24086.3/	
C2H3+CH2O<=>C2H3CHO+H					1.000E+011 0.000
0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116					
(13), PP 3325;SC3346 \COMMENT:					

PLOG/	0.0010	2.600E+004	2.260	1510.3/
PLOG/	0.0100	5.130E+004	2.170	1675.5/
PLOG/	0.1000	3.990E+005	1.910	2218.3/
PLOG/	1.0000	1.750E+007	1.450	3428.0/
PLOG/	10.0000	1.350E+009	0.933	5173.0/
PLOG/	100.0000	2.240E+011	0.357	8001.3/
PLOG/	1000.0000	6.010E+005	2.090	7895.6/

C2H3+CH2O<=>C2H4+HCO 1.000E+011 0.000

0.0 !\AUTHOR: !\REF:FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116

(13), PP 3325;§C3346 \COMMENT:

PLOG/	0.0010	1.110E+007	1.090	1807.2/
PLOG/	0.0100	2.470E+007	0.993	1994.9/
PLOG/	0.1000	2.470E+008	0.704	2596.2/
PLOG/	1.0000	1.420E+010	0.209	3934.2/
PLOG/	10.0000	3.450E+013	-0.726	6944.3/
PLOG/	100.0000	3.310E+014	-0.866	10965.7/
PLOG/	1000.0000	1.650E+001	3.170	9399.8/

!

!\REACTIONCLASS: \R+CH3O2

!

C3H5-A+CH3O2<=>C3H5O+CH3O 1.000E+011 0.000

0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2

PLOG/	0.0100	3.330E+012	-0.158	-1417.0/
PLOG/	0.1000	1.660E+014	-0.642	-349.1/
PLOG/	1.0000	2.595E+017	-1.520	2379.2/
PLOG/	10.0000	9.780E+014	-0.684	3615.3/
PLOG/	100.0000	5.470E+003	2.740	1144.4/

C3H5-A+CH3O2<=>AC4H7OOH 1.000E+011 0.000

0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2

PLOG/	0.0100	1.910E+031	-7.230	1336.2/
PLOG/	0.1000	6.310E+042	-10.300	5568.9/
PLOG/	1.0000	1.030E+045	-10.600	7851.5/
PLOG/	10.0000	2.790E+037	-7.920	6497.9/
PLOG/	100.0000	3.400E+029	-5.280	4539.8/

AC4H7OOH<=>C3H5O+CH3O 1.000E+011 0.000

0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2

PLOG/	0.0100	1.490E+058	-13.900	54266.9/
PLOG/	0.1000	1.800E+054	-12.400	54193.8/
PLOG/	1.0000	3.360E+046	-9.810	52468.5/
PLOG/	10.0000	2.390E+036	-6.540	49429.0/
PLOG/	100.0000	2.560E+027	-3.610	46333.1/

!

!\REACTIONCLASS: \RADICAL_ADDITION\OH

!

C3H6+OH<=>C3H5OH+H 2.290E+013 0.070

10580.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040;§C11053

PLOG/	0.0013	2.670E+013	0.050	10611.0/
PLOG/	0.0100	2.750E+013	0.050	10623.0/
PLOG/	0.0130	2.870E+013	0.040	10634.0/
PLOG/	0.0250	1.590E+014	-0.160	11125.0/
PLOG/	0.1000	3.100E+014	-0.220	11407.0/
PLOG/	0.1315	3.780E+014	-0.240	11458.0/
PLOG/	1.0000	9.150E+007	1.420	10087.0/

PLOG/	10.0000	3.660E+005	2.140	10410.0/	
PLOG/	100.0000	8.190E+002	2.840	10481.0/	
C3H6+OH<=>C2H3OH+CH3					1.290E+006 1.650
1233.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,					
11040;\\$C11053					
PLOG/	0.0013	1.290E+006	1.650	1233.0/	
PLOG/	0.0100	1.820E+004	2.100	1162.0/	
PLOG/	0.0130	2.040E+003	2.480	1128.0/	
PLOG/	0.0250	2.880E+002	2.800	1152.0/	
PLOG/	0.1000	1.400E+001	3.210	1208.0/	
PLOG/	0.1315	7.710E+000	3.290	1216.0/	
PLOG/	1.0000	1.130E+004	2.500	3238.0/	
PLOG/	10.0000	2.410E+019	-1.740	13107.0/	
PLOG/	100.0000	3.300E-001	3.700	3665.0/	
C3H6+OH<=>IC3H5OH+H					2.870E+000 2.920
625.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,					
11040;\\$C11053					
PLOG/	0.0013	2.870E+000	2.920	625.0/	
PLOG/	0.0100	4.840E-001	2.980	704.0/	
PLOG/	0.0130	3.130E-001	3.040	721.0/	
PLOG/	0.0250	9.330E-003	3.620	677.0/	
PLOG/	0.1000	4.640E-005	4.480	687.0/	
PLOG/	0.1315	2.710E-005	4.560	707.0/	
PLOG/	1.0000	7.650E-007	5.050	874.0/	
PLOG/	10.0000	2.640E+015	-0.800	12728.0/	
PLOG/	100.0000	4.870E-004	4.320	4020.0/	
C3H6+OH<=>SC3H5OH+H					2.870E+000 2.920
625.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,					
11040;\\$C11053					
PLOG/	0.0013	3.470E+006	1.530	4288.0/	
PLOG/	0.0100	1.080E+007	1.340	4576.0/	
PLOG/	0.0130	9.760E+006	1.330	4589.0/	
PLOG/	0.0250	5.140E+006	1.360	4594.0/	
PLOG/	0.1000	3.130E+005	1.690	4603.0/	
PLOG/	0.1315	1.390E+005	1.800	4603.0/	
PLOG/	1.0000	1.030E+002	2.830	4530.0/	
PLOG/	10.0000	3.400E-002	3.890	4390.0/	
PLOG/	100.0000	4.460E-006	5.030	4132.0/	
C3H6+OH<=>CH3CHO+CH3					6.930E+005 1.490
-536.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,					
11040;\\$C11053					
PLOG/	0.0013	6.930E+005	1.490	-536.0/	
PLOG/	0.0100	5.940E+003	2.010	-560.0/	
PLOG/	0.0130	1.100E+003	2.220	-680.0/	
PLOG/	0.0250	1.070E+002	2.500	-759.0/	
PLOG/	0.1000	7.830E-001	3.100	-919.0/	
PLOG/	0.1315	3.070E-001	3.220	-946.0/	
PLOG/	1.0000	3.160E-004	4.050	-1144.0/	
PLOG/	10.0000	7.590E-006	4.490	-680.0/	
PLOG/	100.0000	5.450E-005	4.220	1141.0/	
C3H6+OH<=>C3H6OH1-2					5.100E+054 -20.700
32402.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,					
11040;\\$C11053					
PLOG/	0.0013	2.300E+078	-20.700	32402.0/	
PLOG/	0.0100	2.740E+077	-20.000	33874.0/	
PLOG/	0.0130	1.070E+076	-19.580	32874.0/	
PLOG/	0.0250	3.680E+073	-18.790	31361.0/	
PLOG/	0.1000	1.040E+068	-17.010	27909.0/	

PLOG/ 0.1315 7.230E+066 -16.640 27162.0/
PLOG/ 1.0000 1.950E+059 -14.170 23079.0/
PLOG/ 10.0000 7.580E+053 -12.230 22976.0/
PLOG/ 100.0000 1.430E+048 -10.230 23772.0/

DUP

C3H6+OH<=>C3H6OH1-2 1.420E+036 -15.840
11594.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,
11040;§C11053

PLOG/ 0.0013 6.410E+059 -15.840 11594.0/
PLOG/ 0.0100 7.280E+059 -15.510 12898.0/
PLOG/ 0.0130 2.790E+059 -15.340 12913.0/
PLOG/ 0.0250 2.650E+058 -14.930 12936.0/
PLOG/ 0.1000 1.350E+056 -14.040 12945.0/
PLOG/ 0.1315 3.980E+055 -13.850 12887.0/
PLOG/ 1.0000 1.550E+050 -12.040 11493.0/
PLOG/ 10.0000 6.410E+041 -9.350 8921.0/
PLOG/ 100.0000 2.300E+032 -6.310 6088.0/

DUP

C3H6+OH<=>C3H6OH2-1 5.100E+054 -20.700
32402.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,
11040;§C11053

PLOG/ 0.0013 2.140E+059 -15.840 11594.0/
PLOG/ 0.0100 2.430E+059 -15.510 12898.0/
PLOG/ 0.0130 9.300E+058 -15.340 12913.0/
PLOG/ 0.0250 8.830E+057 -14.930 12936.0/
PLOG/ 0.1000 4.500E+055 -14.040 12945.0/
PLOG/ 0.1315 1.330E+055 -13.850 12887.0/
PLOG/ 1.0000 5.180E+049 -12.040 11493.0/
PLOG/ 10.0000 2.140E+041 -9.350 8921.0/
PLOG/ 100.0000 7.650E+031 -6.310 6088.0/

DUP

C3H6+OH<=>C3H6OH2-1 1.420E+036 -15.840
11594.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11,
11040;§C11053

PLOG/ 0.0013 7.680E+077 -20.700 32402.0/
PLOG/ 0.0100 9.130E+076 -20.000 33874.0/
PLOG/ 0.0130 3.550E+075 -19.580 32874.0/
PLOG/ 0.0250 1.230E+073 -18.790 31361.0/
PLOG/ 0.1000 3.450E+067 -17.010 27909.0/
PLOG/ 0.1315 2.410E+066 -16.640 27162.0/
PLOG/ 1.0000 6.500E+058 -14.170 23079.0/
PLOG/ 10.0000 2.530E+053 -12.230 22976.0/
PLOG/ 100.0000 4.780E+047 -10.230 23772.0/

DUP

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!\SUBSPECIES: \C3H5OH

!=====

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!

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!

CH2CCH2OH+H<=>C3H5OH 1.000E+014 0.000

0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE


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!
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!\REACTIONCLASS: \RH_R_ABSTRACTION           \A           \N
\EA
!
-----
C3H5OH+H<=>CH2CCH2OH+H2                    3.900E+005      2.500
5821.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
C3H5OH+O2<=>CH2CCH2OH+HO2                  4.000E+013      0.000
60690.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
C3H5OH+OH<=>CH2CCH2OH+H2O                  5.060E+012      0.000
5960.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
C3H5OH+CH3<=>CH2CCH2OH+CH4                 2.400E+011      0.000
8030.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
CH2CCH2OH+H2O2<=>C3H5OH+HO2                3.010E+009      0.000
2583.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
!
-----
!\REACTIONCLASS: \R_DECOMPOSITION           \A           \N
\EA
!
-----
CH2CCH2OH<=>C2H2+CH2OH                      2.163E+040     -8.310
45110.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
CH2CCH2OH<=>CH2O+C2H3                       9.240E+010      0.870
30460.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP
CH2CCH2OH<=>C2H3CHO+H                       1.110E+011      0.480
36770.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP
CH2CCH2OH<=>HCO+C2H4                         9.240E+010      0.870
30460.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP
!
-----
!\REACTIONCLASS: \R_O2_PRODUCTS             \A           \N
\EA
!
-----
CH2CCH2OH+O2=>CH2OH+CO+CH2O                4.335E+012      0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
C3H5O+O2<=>C2H3CHO+HO2                      1.000E+012      0.000
6000.0 !\AUTHOR: !\REF:ACETALDEHYDE ANALOG
!=====
=====
!\ENDSUBSPECIES: \C3H5OH
!=====
=====
!=====
=====
!\SUBSPECIES: \C3H6OH2-1/C3H6OH2-1
!=====
=====
!
-----
!\REACTIONCLASS: \RADICAL_DECOMPOSITION     \A           \N
\EA
!
-----
CH3COCH3+H<=>C3H6OH2-1                      8.000E+012      0.000
9500.0 !\AUTHOR: !\REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13

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IC3H5OH+H<=>C3H6OH2-1 6.250E+011 0.510
4020.0 !\AUTHOR: !\REF:BASED ON IC4H8+H<=>IC4H9
C2H5CHO+H<=>C3H6OH1-2 8.000E+012 0.000
9500.0 !\AUTHOR: !\REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13
C3H5-T+OH<=>IC3H5OH 5.000E+013 0.000
0.0 !\AUTHOR: !\REF:REVERSE BY ANALOGY HCO+OH -->PRODUCTS
!

!\REACTIONCLASS: \R_O2_ALKENE_HO2 \A \N
\EA
!

C3H6OH2-1+O2<=>CH3COCH3+HO2 1.500E+012 0.000
5000.0 !\AUTHOR: !\REF:!\MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS.
CHEM. 1990, 94, 3016
C3H6OH1-2+O2<=>C2H5CHO+HO2 1.500E+012 0.000
5000.0 !\AUTHOR: !\REF:!\MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS.
CHEM. 1990, 94, 3016
!

!\REACTIONCLASS: \R+O2
!

C3H6OH1-2+O2<=>HOC3H6O2 1.200E+011 0.000
-1100.0 !\AUTHOR: !\ WILK, CERNANSKY, PITZ, AND WESTBROOK, C&F 1988.
C3H6OH2-1+O2<=>HOC3H6O2 1.200E+011 0.000
-1100.0 !\AUTHOR: !\ WILK, CERNANSKY, PITZ, AND WESTBROOK, C&F 1988.
HOC3H6O2=>CH3CHO+CH2O+OH 1.250E+010 0.000
18900.0 !\AUTHOR: !\

!\SUBSPECIES: \SC3H5OH

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

SC3H5OH<=>C2H5CHO 8.590E+011 0.318
55900.0 !\AUTHOR: !\REF:SARATHY ET AL. CNF2012
!

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

SC3H5OH+O2=>C2H3CHO+H+HO2 3.000E+013 0.000
39100.0 !\AUTHOR: !\REF:BILL SEPT 2013 AND SAUDI ARAMCO MECH 1.3 (NO
REFERENCE)
SC3H5OH+OH=>C2H3CHO+H+H2O 3.100E+006 2.000
-298.0 !\AUTHOR: !\REF: TSANG 1991
SC3H5OH+H=>C2H3CHO+H+H2 1.730E+005 2.500
2492.0 !\AUTHOR: !\REF: TSANG 1991
SC3H5OH+O=>C2H3CHO+H+OH 1.750E+012 0.700
5884.0 !\AUTHOR: !\REF: TSANG 1991

SC3H5OH+HO2=>C2H3CHO+H+H2O2	9.600E+003	2.600
13900.0 !\AUTHOR: !\REF: TSANG 1991		
SC3H5OH+CH3=>C2H3CHO+H+CH4	2.210E+000	3.500
5675.0 !\AUTHOR: !\REF: TSANG 1991		
SC3H5OH+CH3O2=>C2H3CHO+H+CH3O2H	9.600E+003	2.600
13900.0 !\AUTHOR: !\REF: USE HO2 ABSTRACTION RATE CONSTANT		
SC3H5OH+CH3O=>C2H3CHO+H+CH3OH	8.300E+010	0.000
2600.0 !\AUTHOR: !\REF: LITERATURE SOURCE UNKNOWN		
SC3H5OH+HO2<=>C2H5CHO+HO2	1.490E+005	1.670
6810.0 !\AUTHOR: !\REF: DASILVA, BOZZELLI, CHEM. PHYS. LETT. 483 (2009) 25;§C29.		
SC3H5OH+HOCHO<=>C2H5CHO+HOCHO	2.810E-002	3.286
-4509.0 !\AUTHOR: !\REF: DASILVA, ANGEW. CHEM. 122 (2010) 7685;§C7687		

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

!\REACTIONCLASS: \AROMATIC_GROWTH	\A	\N
\EA		

C3H5-A+C2H2<=>CVCCVCCJ	1.000E+012	0.000
6883.4 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C3H5-A+C2H3=>C5H6+H+H	1.600E+035	-14.000
61137.7 !\AUTHOR: !\REF:CURRAN ESTIMATE		

!-----
 !\ENDSUBMECH: C3H6
 !-----
 !-----
 !\SUBMECH: \C3H4-A\C3H4-P
 !-----
 !

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

C2H+CH3<=>C3H4-P	8.000E+013	0.000
0.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
C3H4-A<=>C3H4-P	4.786E+048	-10.000
88685.0 !\AUTHOR: !\REF:		
PLOG/ 1.0000 7.762E+039 -7.800 78446.0/		
PLOG/ 10.0000 4.786E+048 -10.000 88685.0/		
CC3H4<=>C3H4-P	1.660E+037	-7.240
48013.0 !\AUTHOR: !\REF:		
PLOG/ 0.0395 2.512E+050 -11.820 50914.0/		
PLOG/ 1.0000 1.230E+037 -7.510 45551.0/		
PLOG/ 10.0000 1.660E+037 -7.240 48013.0/		
CC3H4<=>C3H4-A	5.012E+035	-6.870
51298.0 !\AUTHOR: !\REF:		
PLOG/ 0.0395 9.772E+043 -9.970 56007.0/		

PLOG/	1.0000	2.512E+026	-4.560	43922.0/	
PLOG/	10.0000	5.012E+035	-6.870	51298.0/	
C3H4-P<=>C3H3+H				6.480E+030	-4.655
93925.2 !\AUTHOR: !\REF:					
PLOG/	1.0000	6.480E+030	-4.655	93925.2/	
PLOG/	10.0000	1.210E+025	-2.787	92376.1/	
C3H4-A<=>C3H3+H				1.320E+031	-4.749
92079.5 !\AUTHOR: !\REF:					
PLOG/	1.0000	1.320E+031	-4.749	92079.5/	
PLOG/	10.0000	3.650E+025	-2.950	90624.9/	
C3H3+H<=>CC3H4				3.236E+018	-2.050
2053.0 !\AUTHOR: !\REF:					
PLOG/	0.0395	8.913E+112	-28.260	83611.0/	
PLOG/	1.0000	1.072E+021	-2.950	2687.0/	
PLOG/	10.0000	3.236E+018	-2.050	2053.0/	

!

!\REACTIONCLASS: \R_CAT_ISO	\A	\N
\EA		

!

C3H4-P+C3H3<=>C3H4-A+C3H3	6.140E+006	1.740
10450.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		

!

!\REACTIONCLASS: \RH_R_ABSTRACTION	A	\N
\EA		

!

C3H4-P+O2<=>C3H3+HO2	3.000E+013	0.000
42630.0 !\AUTHOR: !\REF:		
C3H4-P+O<=>C3H3+OH	7.650E+008	1.500
8600.0 !\AUTHOR: !\REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST		
C3H4-P+H<=>C3H3+H2	3.572E+004	2.825
4821.0 !\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S		
C3H4-P+OH<=>C3H3+H2O	4.940E+006	2.027
1059.6 !\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S		
C3H4-P+HO2<=>C3H3+H2O2	9.550E-002	4.170
9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).		
C3H4-P+CH3<=>C3H3+CH4	1.800E+012	0.000
7700.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H4-P+CH3O2<=>C3H3+CH3O2H	9.550E-002	4.170
9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).		
C3H4-P+C2H<=>C2H2+C3H3	1.000E+013	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H4-P+C2H3<=>C3H3+C2H4	1.000E+012	0.000
7700.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).		
C3H4-P+C3H5-A<=>C3H3+C3H6	3.000E+012	0.000
7700.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).		
C3H4-A+H<=>C3H3+H2	6.625E+003	3.095
5522.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP		
C3H4-A+O2<=>C3H3+HO2	4.000E+013	0.000
41320.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP		
C3H4-A+OH<=>C3H3+H2O	1.482E+005	2.492
1807.2 !\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S		
C3H4-A+CH3<=>C3H3+CH4	1.300E+012	0.000
7700.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		

C3H4-A+HO2<=>C3H3+H2O2 3.580E-002 4.170
 9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 C3H4-A+CH3O2<=>C3H3+CH3O2H 7.161E-002 4.170
 9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 C3H4-A+C3H5-A<=>C3H3+C3H6 2.000E+011 0.000
 7700.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 !

!\REACTIONCLASS: \R_ADDITION\H \A \N
 \EA
 !

C3H4-A+H<=>C3H4-P+H 2.440E+010 1.040
 2159.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438

PLOG/ 0.0010 8.490E+010 0.890 2503.0/
 PLOG/ 0.0390 1.480E+013 0.260 4103.0/
 PLOG/ 1.0000 2.480E+015 -0.330 6436.0/
 PLOG/ 10.0000 2.350E+025 -3.230 13165.0/
 PLOG/ 100.0000 1.020E+024 -2.670 15552.0/

DUP

C3H4-A+H<=>C3H4-P+H 2.440E+010 1.040
 2159.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438

PLOG/ 0.0010 1E-10 0.0 0.0/
 PLOG/ 0.0390 1E-10 0.0 0.0/
 PLOG/ 1.0000 1E-10 0.0 0.0/
 PLOG/ 10.0000 1.790E+007 1.980 4521.0/
 PLOG/ 100.0000 4.630E+004 2.620 4466.0/

DUP

C3H4-A+H<=>C3H5-A 2.210E+061 -15.250
 20076.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438

PLOG/ 0.0010 2.210E+061 -15.250 20076.0/
 PLOG/ 0.0390 1.240E+052 -12.020 17839.0/
 PLOG/ 1.0000 4.670E+051 -11.450 21340.0/
 PLOG/ 10.0000 3.750E+048 -10.270 22511.0/
 PLOG/ 100.0000 4.230E+043 -8.610 22522.0/

DUP

C3H4-A+H<=>C3H5-A 2.210E+061 -15.250
 20076.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438

PLOG/ 0.0010 2.800E+038 -8.670 8035.0/
 PLOG/ 0.0390 9.330E+036 -8.190 7462.0/
 PLOG/ 1.0000 3.320E+030 -5.780 6913.0/
 PLOG/ 10.0000 2.290E+026 -4.320 6163.0/
 PLOG/ 100.0000 4.380E+021 -2.710 5187.0/

DUP

C3H4-A+H<=>C3H5-S 1.100E+030 -6.520
 15200.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-
 589

PLOG/ 0.1000 1.100E+030 -6.520 15200.0/
 PLOG/ 1.0000 5.400E+029 -6.090 16300.0/
 PLOG/ 10.0000 2.600E+031 -6.230 18700.0/
 PLOG/ 100.0000 3.200E+031 -5.880 21500.0/

C3H4-A+H<=>C3H5-T 6.440E+102 -27.510
 51768.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438

PLOG/	0.0010	6.440E+102	-27.510	51768.0/
PLOG/	0.0390	1.550E+053	-13.100	14472.0/
PLOG/	1.0000	1.900E+053	-12.590	16726.0/
PLOG/	10.0000	7.950E+051	-11.820	18286.0/
PLOG/	100.0000	4.210E+052	-11.640	22262.0/
DUP				
C3H4-A+H<=>C3H5-T				6.440E+102 -27.510
51768.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;\\$C9438				
PLOG/	0.0010	1.100E+054	-14.290	10809.0/
PLOG/	0.0390	9.880E+044	-11.210	8212.0/
PLOG/	1.0000	2.810E+040	-9.420	7850.0/
PLOG/	10.0000	2.600E+035	-7.570	7147.0/
PLOG/	100.0000	9.880E+029	-5.530	6581.0/
DUP				
C3H4-A+H<=>CH3+C2H2				3.740E+001 3.350
57.8 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;\\$C9438				
PLOG/	0.0010	1.230E+008	1.530	4737.0/
PLOG/	0.0390	2.720E+009	1.200	6834.0/
PLOG/	1.0000	1.260E+020	-1.830	15003.0/
PLOG/	10.0000	1.680E+016	-0.600	14754.0/
PLOG/	100.0000	1.370E+017	-0.790	17603.0/
DUP				
C3H4-A+H<=>CH3+C2H2				3.740E+001 3.350
57.8 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;\\$C9438				
PLOG/	0.0010	1E-10	0.0	0.0/
PLOG/	0.0390	1E-10	0.0	0.0/
PLOG/	1.0000	1.230E+004	2.680	6335.0/
PLOG/	10.0000	3.310E+008	1.140	8886.0/
PLOG/	100.0000	1.280E+006	1.710	9774.0/
DUP				
C3H4-P+H<=>C3H5-T				8.850E+051 -13.040
12325.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;\\$C9438				
PLOG/	0.0010	8.850E+051	-13.040	12325.0/
PLOG/	0.0390	3.170E+052	-12.690	14226.0/
PLOG/	1.0000	2.870E+053	-12.510	16853.0/
PLOG/	10.0000	9.510E+051	-11.740	18331.0/
PLOG/	100.0000	4.510E+052	-11.580	22207.0/
DUP				
C3H4-P+H<=>C3H5-S				8.850E+051 -13.040
12325.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;\\$C9438				
PLOG/	0.0010	1.970E+046	-11.910	7456.0/
PLOG/	0.0390	2.590E+045	-11.230	8046.0/
PLOG/	1.0000	6.930E+039	-9.110	7458.0/
PLOG/	10.0000	6.800E+034	-7.290	6722.0/
PLOG/	100.0000	5.650E+029	-5.390	6150.0/
DUP				
C3H4-P+H<=>C3H5-S				3.380E+049 -12.750
14072.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;\\$C9438				
PLOG/	0.0010	1E-10	0.0	0.0/
PLOG/	0.0390	3.380E+049	-12.750	14072.0/
PLOG/	1.0000	1.370E+051	-12.550	15428.0/
PLOG/	10.0000	3.880E+050	-11.900	16915.0/

PLOG/ 100.0000 2.170E+049 -11.100 18746.0/
 DUP
 C3H4-P+H<=>C3H5-S 3.380E+049 -12.750
 14072.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438
 PLOG/ 0.0010 1.490E+038 -10.110 7458.0/
 PLOG/ 0.0390 2.980E+043 -11.430 8736.0/
 PLOG/ 1.0000 5.750E+039 -9.510 8772.0/
 PLOG/ 10.0000 4.330E+040 -9.600 9401.0/
 PLOG/ 100.0000 3.440E+034 -7.360 8558.0/
 DUP
 C3H4-P+H<=>CH3+C2H2 2.120E+010 1.060
 3945.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112,
 9429;\\$C9438
 PLOG/ 0.0010 2.440E+010 1.040 3980.0/
 PLOG/ 0.0390 3.890E+010 0.989 4114.0/
 PLOG/ 1.0000 3.460E+012 0.442 5463.0/
 PLOG/ 10.0000 1.720E+014 -0.010 7134.0/
 PLOG/ 100.0000 1.900E+015 -0.290 8306.0/
 C3H4-P+H<=>C3H5-A 1.100E+060 -14.560
 28100.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-
 589
 PLOG/ 0.1000 1.100E+060 -14.560 28100.0/
 PLOG/ 1.0000 4.910E+060 -14.370 31644.0/
 PLOG/ 2.0000 3.040E+060 -14.190 32642.0/
 PLOG/ 5.0000 9.020E+059 -13.890 33953.0/
 PLOG/ 10.0000 2.200E+059 -13.610 34900.0/
 PLOG/ 100.0000 1.600E+055 -12.070 37500.0/
 C3H5-A<=>C3H5-T 3.900E+059 -15.420
 75400.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-
 589
 PLOG/ 0.1000 3.900E+059 -15.420 75400.0/
 PLOG/ 1.0000 7.060E+056 -14.080 75868.0/
 PLOG/ 2.0000 4.800E+055 -13.590 75949.0/
 PLOG/ 5.0000 4.860E+053 -12.810 75883.0/
 PLOG/ 10.0000 6.400E+051 -12.120 75700.0/
 PLOG/ 100.0000 2.800E+043 -9.270 74000.0/
 C3H5-A<=>C3H5-S 1.300E+055 -14.530
 73800.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-
 589
 PLOG/ 0.1000 1.300E+055 -14.530 73800.0/
 PLOG/ 1.0000 5.000E+051 -13.020 73300.0/
 PLOG/ 10.0000 9.700E+048 -11.730 73700.0/
 PLOG/ 100.0000 4.860E+044 -9.840 73400.0/
 C2H2+CH3<=>C3H5-T 6.800E+020 -4.160
 18000.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-
 589
 PLOG/ 0.1000 6.800E+020 -4.160 18000.0/
 PLOG/ 1.0000 4.990E+022 -4.390 18850.0/
 PLOG/ 2.0000 6.000E+023 -4.600 19571.0/
 PLOG/ 5.0000 7.310E+025 -5.060 21150.0/
 PLOG/ 10.0000 9.300E+027 -5.550 22900.0/
 PLOG/ 100.0000 3.800E+036 -7.580 31300.0/
 C3H5-T<=>C3H5-S 1.600E+044 -12.160
 52200.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-
 589
 PLOG/ 0.1000 1.600E+044 -12.160 52200.0/
 PLOG/ 1.0000 1.500E+048 -12.710 53900.0/

PLOG/	10.0000	5.100E+052	-13.370	57200.0/
PLOG/	100.0000	5.800E+051	-12.430	59200.0/
C2H2+CH3<=>C3H5-A				8.200E+053 -13.320
33200.0 !\AUTHOR:	!\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589			
PLOG/	0.1000	8.200E+053	-13.320	33200.0/
PLOG/	1.0000	2.680E+053	-12.820	35730.0/
PLOG/	2.0000	3.640E+052	-12.460	36127.0/
PLOG/	5.0000	1.040E+051	-11.890	36476.0/
PLOG/	10.0000	4.400E+049	-11.400	36700.0/
PLOG/	100.0000	3.800E+044	-9.630	37600.0/
CH3+C2H2<=>C3H5-S				1.780E+042 -10.400
13647.0 !\AUTHOR:	!\REF:MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;§C9438			
PLOG/	0.0010	1.780E+042	-10.400	13647.0/
PLOG/	0.0390	1.520E+044	-10.730	15256.0/
PLOG/	1.0000	1.190E+044	-10.190	18728.0/
PLOG/	10.0000	6.020E+043	-9.740	20561.0/
PLOG/	100.0000	1.420E+042	-8.910	22235.0/
DUP				
CH3+C2H2<=>C3H5-S				1.780E+042 -10.400
13647.0 !\AUTHOR:	!\REF:MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429;§C9438			
PLOG/	0.0010	1E-10	0.0	0.0/
PLOG/	0.0390	1E-10	0.0	0.0/
PLOG/	1.0000	8.490E+035	-8.430	12356.0/
PLOG/	10.0000	3.040E+032	-7.010	12357.0/
PLOG/	100.0000	1.690E+027	-5.070	11690.0/
DUP				

!

!\REACTIONCLASS: \R_ADDITION\O	\A	\N
\EA		

!

C3H4-P+O<=>HCCO+CH3	7.300E+012	0.000
2250.0 !\AUTHOR:	!\REF:LASKIN ET AL. IJCK 32 589-614 2000	
C3H4-P+O<=>C2H4+CO	1.000E+013	0.000
2250.0 !\AUTHOR:	!\REF:LASKIN ET AL. IJCK 32 589-614 2000	
C3H4-P+O<=>C2H3+HCO	3.200E+012	0.000
2010.0 !\AUTHOR:	!\REF:DAGAUT, P. ET AL., CST 71, 111(1990).	
C3H4-A+O<=>C2H4+CO	2.000E+007	1.800
1000.0 !\AUTHOR:	!\REF:LASKIN ET AL. IJCK 32 589-614 2000	
C3H4-A+O<=>C2H2+CH2O	3.000E-003	4.610
-4243.0 !\AUTHOR:	!\REF:DAGAUT, P. ET AL., CST 71, 111(1990).	

!

!\REACTIONCLASS: \R_ADDITION\OH	\A	\N
\EA		

!

C3H4-A+OH<=>CH2CCH2OH	1.110E+012	0.000
-304.0 !\AUTHOR:	!\REF: ESTIMATE ATKINSON 1984 C3 NUIG S.M.B	
C3H4-A+OH<=>SC3H4OH	2.220E+012	0.000
-304.0 !\AUTHOR:	!\REF: ESTIMATE ATKINSON 1984 C3 NUIG S.M.B	
SC3H4OH<=>CH2CO+CH3	9.240E+010	0.870
30460.0 !\AUTHOR:	!\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP	

C3H4-P+OH<=>PC3H4OH-2 3.930E+011 0.000
 0.0 !\AUTHOR: !\REF: ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984
 C3H4-P+OH<=>SC3H4OH 2.360E+012 0.000
 0.0 !\AUTHOR: !\REF: ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984
 PC3H4OH-2<=>CH3CHCHO 3.560E+010 0.880
 23238.0 !\AUTHOR: !\REF: MATHEU ET AL. IJCK, 2003, 35, 95--119
 CH3CHCHO<=>C2H3CHO+H 1.0 1.0 1.0!IC3H7<=>C3H6+H 1.0 1.0 1.0
 PLOG / 1.000E-002 1.740E+050 -11.73 52870. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 11%
 PLOG / 1.000E-001 1.130E+047 -10.57 50479. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 10%
 PLOG / 1.000E+000 2.940E+043 -9.29 48810. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 8%
 PLOG / 2.500E+000 1.160E+042 -8.78 48382. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 7%
 PLOG / 5.000E+000 9.480E+040 -8.40 48095. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 6%
 PLOG / 1.000E+001 7.190E+039 -8.01 47818. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 5%
 PLOG / 2.500E+001 2.130E+038 -7.49 47438. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 5%
 PLOG / 5.000E+001 1.420E+037 -7.09 47128. / !FIT FROM: 700-2250 K
 ERROR IN FIT: 4%
 CH3CHCHO<=>CH3CHCO+H 8.328E+012 -0.020
 32410.0 !\AUTHOR: !\REF: PELUCCHI ECM 2013
 !\MISC
 CH3CHCHO+H2<=>C2H5CHO+H 2.160E+005 2.380
 18990.0 !\AUTHOR: !\REF:
 !

!\REACTIONCLASS: \R_ADDITION\HO2 \A \N
 \EA
 !

C3H4-P+HO2=>C2H4+CO+OH 3.000E+012 0.000
 19000.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 C3H4-A+HO2=>C2H4+CO+OH 1.000E+011 0.000
 14000.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 C3H4-A+HO2=>CH2CO+CH2+OH 4.000E+012 0.000
 19000.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
 !

!\REACTIONCLASS: \R_ADDITION\CH2 \A \N
 \EA
 !

C3H4-A+C2H<=>C2H2+C3H3 1.000E+013 0.000
 0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 !=====

!\SUBSPECIES: \C3H3
 !=====

!

!\REACTIONCLASS: \R_R_PRODUCTS \A \N
 \EA

!

C3H3+O<=>CH2O+C2H	2.000E+013	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H3+HO2=>OH+CO+C2H3	8.000E+011	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H3+HCO<=>C3H4-A+CO	2.500E+013	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H3+HCO<=>C3H4-P+CO	2.500E+013	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
C2H5+C2H<=>C3H3+CH3	1.810E+013	0.000
0.0 !\AUTHOR: !\REF:Tsang, W.; Hampson, R.F., J. Phys. Chem. Ref. Data 15, 1087 (1986)		
C3H3+O2<=>CH2CO+HCO	1.700E+005	1.700
1500.0 !\AUTHOR: !\REF:		
C3H3+CH<=>C4H3-N+H	7.0E13	0.0
0.0 !\AUTHOR: !\REF: JAM		

!

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

!

C3H3+HO2<=>C3H3O+OH	1.000E+011	0.000
0.0 !\AUTHOR: !\REF: ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS. CHEM. A, 2012, 116 (13), PP 3325;SC3346		
PLOG/ 0.0100	1.020E+013	-0.158 -1417.0/
PLOG/ 0.1000	4.980E+014	-0.642 -349.1/
PLOG/ 1.0000	7.770E+017	-1.520 2379.2/
PLOG/ 10.0000	2.930E+015	-0.684 3615.3/
PLOG/ 100.0000	1.640E+004	2.740 1144.4/
C3H3+HO2<=>C3H3O2H	1.000E+011	0.000
0.0 !\AUTHOR: !\REF: ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS. CHEM. A, 2012, 116 (13), PP 3325;SC3346		
PLOG/ 0.0100	1.910E+031	-7.230 1336.2/
PLOG/ 0.1000	6.310E+042	-10.300 5568.9/
PLOG/ 1.0000	1.030E+045	-10.600 7851.5/
PLOG/ 10.0000	2.790E+037	-7.920 6497.9/
PLOG/ 100.0000	4.730E+025	-4.130 2923.8/
C3H3+HO2<=>C2HCHO+H2O	1.000E+011	0.000
0.0 !\AUTHOR: !\REF: ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS. CHEM. A, 2012, 116 (13), PP 3325;SC3346		
PLOG/ 0.0100	1.090E+000	3.010 -3421.1/
PLOG/ 0.1000	6.350E+001	2.500 -2341.4/
PLOG/ 1.0000	6.050E+005	1.390 595.1/
PLOG/ 10.0000	3.100E+005	1.590 2677.6/
PLOG/ 100.0000	5.070E-005	4.590 927.5/
C3H3O2H<=>C2HCHO+H2O	1.000E+011	0.000
0.0 !\AUTHOR: !\REF: ANALOGY WITH C3H5-A+HO2 !\KINETICS FROM FRANKLIN C GOLDSMITH !\J. PHYS. CHEM. A, 2012, 116 (13), PP 3325;SC3346		
PLOG/ 0.0100	1.990E+050	-12.700 53531.9/
PLOG/ 0.1000	4.720E+047	-11.500 54360.9/
PLOG/ 1.0000	1.500E+040	-8.840 53179.2/
PLOG/ 10.0000	2.540E+028	-5.000 49919.4/
PLOG/ 100.0000	1.480E+016	-1.120 45949.3/
C2H+CH2O<=>C3H3O	1.000E+011	0.000
0.0		
PLOG/ 0.0010	5.925E-004	2.609 -4297.3/

PLOG/	0.0100	5.688E+006	-0.073	-1234.1/		
PLOG/	0.1000	5.390E+013	-1.803	1452.2/		
PLOG/	1.0000	8.733E+015	-2.074	2510.1/		
PLOG/	10.0000	5.305E+019	-2.943	4532.2/		
PLOG/	100.0000	3.779E+021	-3.163	6802.5/		
!\C2HCHO						
C2HCHO<=>C2H2+CO				2.510E+014		0.000
68000.0 !\AUTHOR: !\REF:						
C2H+HCO<=>C2HCHO				1.000E+013		0.000
0.0 !\AUTHOR: !\REF:						
!						

!\REACTIONCLASS: \R_R_RECOMB\H				\A		\N
\EA						
!						

C3H3+H<=>C3H2+H2				2.140E+005		2.520
7453.0 !\AUTHOR: !\REF:						
C3H3+H<=>C3H2(S)+H2				3.311E+013		0.195
17579.0 !\AUTHOR: !\REF:						
PLOG/	0.0395	2.951E+009	1.280	13474.0/		
PLOG/	1.0000	1.097E+010	1.130	13929.0/		
PLOG/	10.0000	3.311E+013	0.195	17579.0/		
C3H3+H<=>H2CCC(S)+H2				1.000E+018		-1.230
15111.0 !\AUTHOR: !\REF:						
PLOG/	0.0395	2.692E+009	1.050	5371.0/		
PLOG/	1.0000	2.884E+013	-0.030	9448.0/		
PLOG/	10.0000	1.000E+018	-1.230	15111.0/		
C3H3+H<=>C3H2C+H2				7.244E+009		0.606
18356.0 !\AUTHOR: !\REF:						
PLOG/	0.0395	1.072E+007	1.370	15557.0/		
PLOG/	1.0000	1.349E+007	1.340	15560.0/		
PLOG/	10.0000	7.244E+009	0.606	18356.0/		
C3H2C+O2<=>C2H2+CO2				1.000E+013		0.000
0.0 !\AUTHOR: !\REF:						
!						

!\REACTIONCLASS: \R_R_RECOMB\OH				\A		\N
\EA						
!						

C3H3+OH<=>C3H2+H2O				2.000E+013		0.000
8000.0 !\AUTHOR: !\REF:						
C3H3+OH<=>CH2O+C2H2				2.000E+012		0.000
0.0 !\AUTHOR: !\REF:						
C3H3+OH<=>C2H3+HCO				1.000E+013		0.000
0.0 !\AUTHOR: !\REF:						
C3H3+OH<=>C2H4+CO				1.000E+013		0.000
0.0 !\AUTHOR: !\REF:						
C3H3+OH<=>C3H2(S)+H2O				1.000E+012		0.000
0.0 !\AUTHOR: !\REF:						
C3H3+OH<=>H2CCC(S)+H2O				1.000E+012		0.000
0.0 !\AUTHOR: !\REF:						

!=====
=====

!\SUBSPECIES: \C3H2						
!===== =====						

C3H2(S)+M<=>C3H2+M 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:
C3H2(S)+H<=>H2CCC(S)+H 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:
H2CCC(S)+O2<=>CO2+C2H2 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:

!=====
=====

!\ENDSUBSPECIES: \C3H2

!=====
=====

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!

!\REACTIONCLASS: \AROMATIC_GROWTH \A \N
\EA

!

C3H3+C3H3<=>C6H5+H 1.0467E+54 -11.88 28757.
!\AUTHOR: !\REF: FROM MILLER, BUT SLIGHTLY DIFFERENT THAN IN PUBLISHED
PAPER

PLOG /0.03947 1.0467E+54 -11.88 28757./
PLOG /1. 1.6975E+48 -9.977 36755./
PLOG /10. 3.6712E+26 -3.879 28963./

C3H3+C3H3<=>C6H6 1.8189E+74 -18.14 31896.

!\AUTHOR: !\REF: FROM SCOTT SKEEN 2011 WHO GOT IT FROM MILLER: (SLIGHTLY
DIFFERENT THAN IN MILLER AND KLIPPENSTEIN 2003 PUBLICATION)

PLOG /0.03947 1.64E66 -15.902 27529./
PLOG /1. 3.1609E+55 -12.55 22264./
PLOG /10. 3.8888E+50 -11.01 20320./

C3H3+C3H3<=>FULVENE 6.3069E+76 -19.07 31542.

!\AUTHOR: !\REF: FROM SCOTT SKEEN 2011 WHO GOT IT FROM MILLER: (SLIGHTLY
DIFFERENT THAN IN MILLER AND KLIPPENSTEIN 2003 PUBLICATION)

PLOG /0.03947 7.25E65 -16.015 25035./
PLOG /1. 1.3798E+66 -15.66 28260./
PLOG /10. 1.2584E+56 -12.61 23515./

C3H3+C3H5-A=>FULVENE+H+H 3.26E29 -5.397 3390.

!\AUTHOR: !\ JAM, YG, ET AL 2007

C3H3+C3H4-A<=>C6H6+H 1.400E+012 0.000

9990.4 !\AUTHOR: !\REF:CURRAN ESTIMATE

!-----

!\ENDSUBMECH: C3H4-A/C3H4-P

!-----

!=====
=====

!\SUBSPECIES: \CH3CHCO

!=====
=====

=====

!

!\REACTIONCLASS: \RH_R_LUMPED \A \N
\EA

!

CH3CHCO+OH<=>C2H5+CO2 1.730E+012 0.000
-1010.0 !\AUTHOR: !\REF:ESTIMATE

CH3CHCO+OH<=>SC2H4OH+CO 2.000E+012 0.000
 -1010.0 !\AUTHOR: !\REF:ESTIMATE
 CH3CHCO+H<=>C2H5+CO 4.400E+012 0.000
 1459.0 !\AUTHOR: !\REF:ESTIMATE
 CH3CHCO+O<=>CH3CHO+CO 3.200E+012 0.000
 -437.0 !\AUTHOR: !\REF:ESTIMATE

!=====
 =====
 !\SUBSPECIES: \CH3CHCO
 !=====
 =====

!-----

 !\SUBMECH: \CH3COCH3
 !-----

 !

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

CH3COCH3<=>CH3CO+CH3 2.050E+058 -12.796
 100030.1 !\AUTHOR: !\REF: SAXENA ET AL. PROCEEDINGS. 32 123-130 (2009)
 PLOG/ 0.0100 2.050E+058 -12.796 100030.1/
 PLOG/ 0.1000 3.300E+051 -10.574 98221.2/
 PLOG/ 1.0000 1.310E+042 -7.657 94660.6/
 PLOG/ 10.0000 2.160E+033 -4.989 90916.5/
 PLOG/ 100.0000 9.400E+028 -3.669 89022.8/
 CH3COCH2+H<=>CH3COCH3 1.000E+013 0.000
 0.0 !\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
 !

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

CH3COCH3+OH<=>CH3COCH2+H2O 1.250E+005 2.483
 445.0 !\AUTHOR:
 CH3COCH3+H<=>CH3COCH2+H2 9.800E+005 2.430
 5160.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
 CH3COCH3+O<=>CH3COCH2+OH 5.130E+011 0.211
 4890.0 !\AUTHOR: !\REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17
 -2Q98
 CH3COCH3+CH3<=>CH3COCH2+CH4 3.960E+011 0.000
 9784.0 !\AUTHOR: !\REF:S. Pichon, Combustion and Flame (2009) 156(2)
 494;§C504.
 CH3COCH3+CH3O<=>CH3COCH2+CH3OH 4.340E+011 0.000
 6460.0 !\AUTHOR:
 CH3COCH3+O2<=>CH3COCH2+HO2 6.030E+013 0.000
 48500.0 !\AUTHOR: !\REF:A-FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM
 DHRXN
 CH3COCH3+HO2<=>CH3COCH2+H2O2 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF:ANALOGY TO ETHANE
 CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF:ANALOGY TO ETHANE

CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21 1.000E+011 0.000
5000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
!

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

CH3COCH2+HO2<=>CH3COCH2O+OH 2.410E+013 0.000
0.0 !\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
CH3COCH2+CH3O2<=>CH3COCH2O+CH3O 1.205E+013 0.000
0.0 !\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
CH3COCH2O<=>CH3CO+CH2O 5.872E+20 -2.4218
10535.8 !\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., REVERSED REACTION.
!

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

CH3COCH2+O2<=>CH3COCH2O2 1.200E+011 0.000
-1100.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
CH2CO+CH3<=>CH3COCH2 1.760E+004 2.480
6130.0 !\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
CH2O+CH3COCH2O2<=>HCO+C3KET21 1.288E+011 0.000
9000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
HO2+CH3COCH2O2<=>C3KET21+O2 1.000E+012 0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
!

!\ENDSUBMECH: \CH3COCH3
!-----
!-----
!-----
!-----
!\SUBMECH: \C2H3CHO
!-----
!-----
!

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

C2H3+HCO<=>C2H3CHO 1.810E+013 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE
!

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

C2H3CHO+H<=>C2H3CO+H2 1.340E+013 0.000
3300.0 !\AUTHOR: !\REF:BASED ON CH3CHO+H
C2H3CHO+O<=>C2H3CO+OH 5.940E+012 0.000
1868.0 !\AUTHOR: !\REF:BASED ON CH3CHO+H

C2H3CHO+OH<=>C2H3CO+H2O	9.240E+006	1.500
-962.0 !\AUTHOR: !\REF:TAYLOR ET AL. 1996		
C2H3CHO+O2<=>C2H3CO+HO2	1.005E+013	0.000
40700.0 !\AUTHOR: !\REF:TAYLOR ET AL. 1996		
C2H3CHO+HO2<=>C2H3CO+H2O2	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2		
C2H3CHO+CH3<=>C2H3CO+CH4	2.608E+006	1.780
5911.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2		
C2H3CHO+C2H3<=>C2H3CO+C2H4	1.740E+012	0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE.		
C2H3CHO+CH3O<=>C2H3CO+CH3OH	1.000E+012	0.000
3300.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+CH3O		
C2H3CHO+CH3O2<=>C2H3CO+CH3O2H	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2		

!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION	\A	\N
\EA		

!

C2H3+CO<=>C2H3CO	1.510E+011	0.000
4810.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		

!

!\ENDSUBMECH: CH3COCH3

!

!\SUBMECH: \C2H5CHO

!

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

!

C2H5+HCO<=>C2H5CHO	1.810E+013	0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		

!

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

!

C2H5CHO+H<=>C2H5CO+H2	4.000E+013	0.000
4200.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+H		
C2H5CHO+O<=>C2H5CO+OH	5.000E+012	0.000
1790.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+O		
C2H5CHO+OH<=>C2H5CO+H2O	2.690E+010	0.760
-340.0 !\AUTHOR:		
C2H5CHO+CH3<=>C2H5CO+CH4	2.608E+006	1.780
5911.0 !\AUTHOR: !\REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17-2Q98		
C2H5CHO+HO2<=>C2H5CO+H2O2	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+HO2		

C2H5CHO+CH3O<=>C2H5CO+CH3OH	1.000E+012	0.000
3300.0 !\AUTHOR: !\REF: ANALOGY WITH CH3CHO+CH3O		
C2H5CHO+CH3O2<=>C2H5CO+CH3O2H	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+HO2		
C2H5CHO+C2H5<=>C2H5CO+C2H6	1.000E+012	0.000
8000.0 !\AUTHOR: !\REF:ACETALDEHYDE ANALOG		
C2H5CHO+C2H5O<=>C2H5CO+C2H5OH	6.026E+011	0.000
3300.0 !\AUTHOR: !\REF:ACETALDEHYDE ANALOG		
C2H5CHO+C2H5O2<=>C2H5CO+C2H5O2H	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2		
C2H5CHO+O2<=>C2H5CO+HO2	1.005E+013	0.000
40700.0 !\AUTHOR:		
C2H5CHO+CH3CO3<=>C2H5CO+CH3CO3H	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2		
C2H5CHO+C2H3<=>C2H5CO+C2H4	1.700E+012	0.000
8440.0 !\AUTHOR: !\REF: ANALOGY WITH ACETALDEHYDE		
C2H5CHO+NC3H7<=>C2H5CO+C3H8	1.700E+012	0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE		
C2H5CHO+IC3H7<=>C2H5CO+C3H8	1.700E+012	0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE		
C2H5CHO+C3H5-A<=>C2H5CO+C3H6	1.700E+012	0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE		

!

!\REACTIONCLASS: \RADICAL_ALPHA_SCISSION	\A	\N
\EA		

!

C2H5+CO<=>C2H5CO	1.510E+011	0.000
4810.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,		
15:1087 (1986)		

!-----

!\ENDSUBMECH: C2H5CHO

!-----

!\END_KINETICS_MODULE: \C3

!+++++

!+++++

!\KINETICS_MODULE: \C4

!\MODSUBMECHS:

!+++++

!-----

!\SUBMECH: \C4H10

!-----

!

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

!

C4H10(+M)<=>C2H5+C2H5(+M) 1.355E+037 -6.036
92929.0 !\AUTHOR: !\REF:BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A
2004, 108:4247-4253
LOW/ 4.720E+018 0.000
49578.0/
TROE/ 7.998E-002 1.000E-020 3.243E+004 4.858E+003/
C4H10(+M)<=>NC3H7+CH3(+M) 6.600E+052 -10.626
100330.0 !\AUTHOR: !\REF:BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A
2004, 108:4247-4253
LOW/ 5.340E+017 0.000
42959.0/
TROE/ 9.502E-002 1.000E-020 5.348E+003 4.326E+003/
C4H10<=>PC4H9+H 4.80E+40 -7.06 115302 !\AUTHOR:
!\REF:ESTIMATE FROM RECOMBINATION (1E14 0 0)
PLOG/0.01 4.45E+90 -21.91 140564/ !\
PLOG/0.1 4.63E+76 -17.64 134669/ !\
PLOG/1 4.94E+58 -12.32 125435/ !\
PLOG/10 4.80E+40 -7.06 115302/ !\
PLOG/100 1.49E+27 -3.15 107323/ !\
C4H10<=>SC4H9+H 8.52E+38 -6.58 110556 !\AUTHOR:
!\REF:ESTIMATE FROM RECOMBINATION (1E14 0 0)
PLOG/0.01 3.10E+88 -21.24 136355/ !\
PLOG/0.1 4.34E+73 -16.76 129590/ !\
PLOG/1 7.39E+55 -11.52 120199/ !\
PLOG/10 8.52E+38 -6.58 110556/ !\
PLOG/100 5.40E+26 -3.05 103313/ !\
!

!\REACTIONCLASS: \RH_H_ABSTRACTION \A \N
\EA
!

C4H10+H<=>PC4H9+H2 3.490E+005 2.690
6450.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
C4H10+O2<=>PC4H9+HO2 6.000E+013 0.000
52340.0 !\AUTHOR: !\REF: ANALOGY WITH C4H10+O2<=>PC4H9+HO2
C4H10+O<=>PC4H9+OH 1.130E+014 0.000
7850.0 !\AUTHOR: !\REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705
(1983)
C4H10+OH<=>PC4H9+H2O 1.054E+010 0.970
1586.0 !\AUTHOR: !\REF: Droege, A. T. and Tully, F. P.: Hydrogen-atom
abstraction from alkanes by OH. 3. Propane, J. Phys. Chem., 90,
1949;§C1955
C4H10+HO2<=>PC4H9+H2O2 4.080E+001 3.590
17160.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
(2008) 112(30): 7047-7054.
C4H10+CH3<=>PC4H9+CH4 9.040E-001 3.650
7154.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
C4H10+CH3O<=>PC4H9+CH3OH 3.000E+011 0.000
7000.0 !\AUTHOR: !\REF:DRYER ESTIMATE
C4H10+CH3O2<=>PC4H9+CH3O2H 1.386E+000 3.970
18280.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
(2008) 112(30): 7047-7054.,
C4H10+O2CHO<=>PC4H9+HO2CHO 1.680E+013 0.000
20440.0 !\AUTHOR: !\REF:ANALOGY WITH RH+RO2 -->R+RO2H

C4H10+C2H5<=>PC4H9+C2H6	1.580E+011	0.000
12300.0 !\AUTHOR: !\REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
C4H10+C2H3<=>PC4H9+C2H4	1.000E+012	0.000
18000.0 !\AUTHOR: !\REF:SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17, 174 (1978)		
C4H10+C2H5O<=>PC4H9+C2H5OH	3.000E+011	0.000
7000.0 !\AUTHOR: !\REF:ANOLOGY TO CH3O		
C4H10+C2H5O2<=>PC4H9+C2H5O2H	4.080E+001	3.590
17160.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.,		
C4H10+CH3CO3<=>PC4H9+CH3CO3H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+C3H5-A<=>PC4H9+C3H6	7.940E+011	0.000
20500.0 !\AUTHOR: !\REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
C4H10+NC3H7O2<=>PC4H9+NC3H7O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+IC3H7O2<=>PC4H9+IC3H7O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+PC4H9<=>SC4H9+C4H10	1.000E+011	0.000
10400.0 !\AUTHOR: !\REF: WESTBROOK AND PITZ ESTIMATE (1983)		
C4H10+PC4H9O2<=>PC4H9+PC4H9O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+SC4H9O2<=>PC4H9+SC4H9O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+IC4H9O2<=>PC4H9+IC4H9O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+TC4H9O2<=>PC4H9+TC4H9O2H	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+H<=>SC4H9+H2	2.600E+006	2.400
4471.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
C4H10+O2<=>SC4H9+HO2	4.000E+013	0.000
49800.0 !\AUTHOR: !\REF: Ingham,T.; Walker,R.W.; Woolford,R.E., Symp. Int. Combust. Proc. 25, 767-774 (1994)		
C4H10+O<=>SC4H9+OH	5.620E+013	0.000
5200.0 !\AUTHOR: !\REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705 (1983)		
C4H10+OH<=>SC4H9+H2O	9.340E+007	1.610
-35.0 !\AUTHOR: !\REF: Droege, A. T. and Tully, F. P.: Hydrogen-atom abstraction from alkanes by OH. 3. Propane, J. Phys. Chem., 90, 1949;§C1955		
C4H10+HO2<=>SC4H9+H2O2	1.264E+002	3.370
13720.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C4H10+CH3<=>SC4H9+CH4	3.020E+000	3.460
5481.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
C4H10+CH3O<=>SC4H9+CH3OH	6.000E+011	0.000
7000.0 !\AUTHOR: !\REF:DRYER ESTIMATE		
C4H10+CH3O2<=>SC4H9+CH3O2H	2.037E+001	3.580
14810.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.,		
C4H10+O2CHO<=>SC4H9+HO2CHO	1.120E+013	0.000
17690.0 !\AUTHOR: !\REF:ANALOGY WITH RH+RO2 -->R+RO2H		
C4H10+C2H5<=>SC4H9+C2H6	1.000E+011	0.000
10400.0 !\AUTHOR: !\REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		

C4H10+C2H3<=>SC4H9+C2H4	8.000E+011	0.000
16800.0 !\AUTHOR: !\REF:SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17, 174 (1978)		
C4H10+C2H5O<=>SC4H9+C2H5OH	6.000E+011	0.000
7000.0 !\AUTHOR: !\REF:ANOLOGY TO CH3O		
C4H10+C2H5O2<=>SC4H9+C2H5O2H	1.264E+002	3.370
13720.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C4H10+CH3CO3<=>SC4H9+CH3CO3H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:!\WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE AUGUST 1988		
C4H10+C3H5-A<=>SC4H9+C3H6	3.160E+011	0.000
16400.0 !\AUTHOR: !\REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
C4H10+NC3H7O2<=>SC4H9+NC3H7O2H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+IC3H7O2<=>SC4H9+IC3H7O2H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+PC4H9O2<=>SC4H9+PC4H9O2H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+SC4H9O2<=>SC4H9+SC4H9O2H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+IC4H9O2<=>SC4H9+IC4H9O2H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
C4H10+TC4H9O2<=>SC4H9+TC4H9O2H	1.120E+013	0.000
17700.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		

!\REACTIONCLASS: \RADICAL_UNIMOL	\A	\N
\EA		

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

PC4H9+HO2<=>PC4H9O+OH	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
CH3O2+PC4H9<=>CH3O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9+HO2<=>SC4H9O+OH	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9+CH3O2<=>CH3O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		

!\REACTIONCLASS: \R_BETA_SCISSION	\A	\N
\EA		

C2H5+CH3CHO<=>SC4H9O	3.330E+010	0.000
6397.0 !\AUTHOR: !\REF:Henry J. Curran International Journal of Chemical Kinetics (2006) 38: 250;SC275.		

!\REACTIONCLASS: \R+O2	\A	\N
PC4H9+O2<=>C4H8-1+HO2	8.370E-001	3.590
11960.0 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N, IC3H7+O2)		
PC4H9+O2<=>PC4H9O2	6.865E+016	-1.627
198.7 !\AUTHOR: !\REF:Miyoshi		
SC4H9+O2<=>C4H8-1+HO2	5.350E-001	3.710
9322.0 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N, IC3H7+O2)		
SC4H9+O2<=>C4H8-2+HO2	1.070E+000	3.710
9322.0 !\AUTHOR: !\REF:IN ARAMCO (BASED ON KLIPPENSTEIN ET AL. N, IC3H7+O2)		
SC4H9+O2<=>SC4H9O2	3.487E+014	-0.816
-536.5 !\AUTHOR: !\REF:Miyoshi		
!=====		
!\SUBSPECIES: \PC4H9O2		
!=====		
!\REACTIONCLASS: \RO2+RH_RO2H_R		
!\EA		
!		
PC4H9O2+H2<=>PC4H9O2H+H	3.010E+013	0.000
26030.0 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
PC4H9O2+HO2<=>PC4H9O2H+O2	1.750E+010	0.000
-3275.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)		
PC4H9O2+H2O2<=>PC4H9O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:ANALOGY TO H2O2+CH3O2<=>HO2+CH3O2H		
PC4H9O2+CH4<=>PC4H9O2H+CH3	1.120E+013	0.000
24640.0 !\AUTHOR: !\REF:ANALOGY TO CH4+HO2		
PC4H9O2+CH3OH<=>PC4H9O2H+CH2OH	6.300E+012	0.000
19360.0 !\AUTHOR: !\REF:ANALOGY TO CH3OH+HO2		
PC4H9O2+CH2O<=>PC4H9O2H+HCO	5.600E+012	0.000
13600.0 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2		
PC4H9O2+C2H6<=>PC4H9O2H+C2H5	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
PC4H9O2+CH3CHO<=>PC4H9O2H+CH3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
PC4H9O2+C2H4<=>PC4H9O2H+C2H3	1.130E+013	0.000
30430.0 !\AUTHOR: !\REF:ANALOGY TO C2H4+HO2		
PC4H9O2+C3H6<=>PC4H9O2H+C3H5-A	5.350E-002	4.207
13288.1 !\AUTHOR: !\REF:ANALOGY TO C3H6+HO2		
PC4H9O2+C2H5CHO<=>PC4H9O2H+C2H5CO	2.000E+011	0.000
9500.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
PC4H9O2+C2H3CHO<=>PC4H9O2H+C2H3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
PC4H9O2+C3H8<=>PC4H9O2H+NC3H7	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
PC4H9O2+C3H8<=>PC4H9O2H+IC3H7	2.000E+012	0.000
17000.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		

!\REACTIONCLASS: \RO2+R_PRODUCTS		
\EA	\A	\N
PC4H9O2+CH3<=>PC4H9O+CH3O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+C2H5<=>PC4H9O+C2H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+IC3H7<=>PC4H9O+IC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+NC3H7<=>PC4H9O+NC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+C3H5-A<=>PC4H9O+C3H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+PC4H9<=>PC4H9O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+SC4H9<=>PC4H9O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
PC4H9O2+C4H71-3<=>PC4H9O+C4H71-O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
!\REACTIONCLASS: \KHP_DECOMP		
\EA	\A	\N
PC4H9O2H<=>PC4H9O+OH	1.500E+016	0.000
42500.0 !\AUTHOR: !\REF:ESTIMATE		
!\REACTIONCLASS: \RO2+RO2_PRODUCTS		
\EA	\A	\N
PC4H9O2+CH3O2=>PC4H9O+CH3O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
PC4H9O2+CH3CO3=>PC4H9O+CH3CO2+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
PC4H9O2+C2H5O2=>PC4H9O+C2H5O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
PC4H9O2+NC3H7O2=>PC4H9O+NC3H7O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
PC4H9O2+IC3H7O2=>PC4H9O+IC3H7O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
PC4H9O2+PC4H9O2=>PC4H9O+PC4H9O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
PC4H9O2+SC4H9O2=>PC4H9O+SC4H9O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
!\REACTIONCLASS: \RO2_QOOH		
\EA	\A	\N
PC4H9O2<=>C4H8OOH1-2	4.009E+008	1.100
30100.0 !\AUTHOR: !\REF:Sharma		

PC4H9O2<=>C4H8OOH1-3	1.360E+007	1.300
18200.0 !\AUTHOR: !\REF:Sharma		
PC4H9O2<=>C4H8OOH1-4	1.233E+006	1.500
20000.0 !\AUTHOR: !\REF:Sharma		

!

!\REACTIONCLASS: \RO2_ALKENE_HO2	\A	\N
\EA		

!

PC4H9O2<=>C4H8-1+HO2	1.258E+008	1.380
28900.0 !\AUTHOR: !\REF:Villano		

!=====
=====

!\SUBSPECIES: \SC4H9O2

!=====
=====

IC3H7O2+PC4H9<=>IC3H7O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
NC3H7O2+PC4H9<=>NC3H7O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+PC4H9<=>SC4H9O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC3H7O2+SC4H9<=>IC3H7O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
NC3H7O2+SC4H9<=>NC3H7O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		

!

!\REACTIONCLASS: \RO2+RH_RO2H_R	\A	\N
\EA		

!

SC4H9O2+H2<=>SC4H9O2H+H	3.010E+013	0.000
26030.0 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
SC4H9O2+HO2<=>SC4H9O2H+O2	1.750E+010	0.000
-3275.0 !\AUTHOR:		
SC4H9O2+CH2O<=>SC4H9O2H+HCO	5.600E+012	0.000
13600.0 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2		
SC4H9O2+CH3CHO<=>SC4H9O2H+CH3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2		
SC4H9O2+C2H6<=>SC4H9O2H+C2H5	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
SC4H9O2+C2H5CHO<=>SC4H9O2H+C2H5CO	2.000E+011	0.000
9500.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
SC4H9O2+C3H6<=>SC4H9O2H+C3H5-A	5.350E-002	4.207
13288.1 !\AUTHOR: !\REF:ANALOGY TO C3H6+HO2		
SC4H9O2+C2H4<=>SC4H9O2H+C2H3	1.130E+013	0.000
30430.0 !\AUTHOR: !\REF:ANALOGY TO C2H4+HO2		
SC4H9O2+CH3OH<=>SC4H9O2H+CH2OH	6.300E+012	0.000
19360.0 !\AUTHOR: !\REF:ANALOGY TO CH3OH+HO2		
SC4H9O2+C2H3CHO<=>SC4H9O2H+C2H3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
SC4H9O2+CH4<=>SC4H9O2H+CH3	1.120E+013	0.000
24640.0 !\AUTHOR: !\REF:ANALOGY TO CH4+HO2		
SC4H9O2+H2O2<=>SC4H9O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:ANALOGY TO H2O2+CH3O2<=>HO2+CH3O2H		

SC4H9O2+C3H8<=>SC4H9O2H+NC3H7	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
SC4H9O2+C3H8<=>SC4H9O2H+IC3H7	2.000E+012	0.000
17000.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		

!

!\REACTIONCLASS: \RO2+RO2_PRODUCTS	\A	\N
\EA		

!

SC4H9O2+CH3O2=>SC4H9O+CH3O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+SC4H9O2=>SC4H9O+SC4H9O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:ESTIMATE		

!

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

!

SC4H9O2+CH3<=>SC4H9O+CH3O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+C2H5<=>SC4H9O+C2H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+IC3H7<=>SC4H9O+IC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+NC3H7<=>SC4H9O+NC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+SC4H9<=>SC4H9O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+C3H5-A<=>SC4H9O+C3H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
SC4H9O2+C4H71-3<=>SC4H9O+C4H71-O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		

!

!\REACTIONCLASS: \KHP_DECOMP	\A	\N
\EA		

!

SC4H9O+OH<=>SC4H9O2H	1.000E+015	-0.800
0.0 !\AUTHOR: !\REF:PITZ ESTIMATE		

!

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

!

SC4H9O2<=>C4H8OOH2-1	1.458E+009	1.100
33500.0 !\AUTHOR: !\REF:Sharma		
SC4H9O2<=>C4H8OOH2-3	1.716E+009	0.900
29500.0 !\AUTHOR: !\REF:Sharma		
SC4H9O2<=>C4H8OOH2-4	1.439E+007	1.400
20800.0 !\AUTHOR: !\REF:Sharma		

```
!\REACTIONCLASS: \RO2+ALKENE_HO2      \A      \N
\EA
!
```

SC4H9O2<=>C4H8-1+HO2	5.130E+009	1.000
30400.0 !\AUTHOR: !\REF:Villano		

```
!\REACTIONCLASS: \QOOH_ALKENE_HO2      \A      \N
\EA
!
```

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

C4H8OOH1-2<=>C4H8O1-2+OH	1.710E+009	1.060
10900.0 !\AUTHOR: !\REF:Villano (From Kuiwen's Mech)		
C4H8OOH1-3<=>C4H8O1-3+OH	2.590E+009	0.690
16000.0 !\AUTHOR: !\REF:Villano (From Kuiwen's Mech)		
C4H8OOH1-4<=>C4H8O1-4+OH	1.720E+008	0.760
11100.0 !\AUTHOR: !\REF:Villano (From Kuiwen's Mech)		
C4H8OOH2-4<=>C4H8O1-3+OH	2.440E+009	0.780
18000.0 !\AUTHOR: !\REF:Villano (From Kuiwen's Mech)		

```
!\SUBSPECIES: \C4_CYC_ETH
```

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

C4H8O1-2+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-2+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-2+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-2+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-2+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-2+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		

C4H8O1-3+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-3+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-3+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-3+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-4+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-4+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-4+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-4+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O2-3+H=>CH2O+C3H5-A+H2	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O2-3+OH=>CH2O+C3H5-A+H2O	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O2-3+O=>CH2O+C3H5-A+OH	5.000E+012	0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O2-3+HO2=>CH2O+C3H5-A+H2O2	1.000E+013	0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O2-3+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
C4H8O2-3+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CH2CHO+C2H4<=>C4H7O12-4	1.000E+11	0.0000
7800.0		
C2H4+CH2CHO<=>C4H7O13-4	1.000E+11	0.0000
7800.0		
CH3+C2H3CHO<=>C4H7O23-1	1.000E+11	0.0000
7800.0		
!=====		
=====		
!\ENDSUBSPECIES: \C4_CYC_ETH		
!=====		
=====		
!		
<hr/>		
!\REACTIONCLASS: \QOOH_DECOMP	\A	\N
\EA		
!		
<hr/>		
C4H8OOH1-3=>OH+CH2O+C3H6	1.230E+009	1.300
24900.0 !\AUTHOR: !\REF:Villano (From Kuiwen's Mech)		
C4H8OOH2-4=>OH+CH3CHO+C2H4	3.080E+008	1.500
23500.0 !\AUTHOR: !\REF:Villano (From Kuiwen's Mech)		

!\REACTIONCLASS: \QOOH+O2_PRODUCTS		
\EA	\A	\N
C4H8OOH1-2+O2<=>C4H8OOH1-2O2	1.744E+014	-0.816
-536.5 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-3+O2<=>C4H8OOH1-3O2	1.744E+014	-0.816
-536.5 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-4+O2<=>C4H8OOH1-4O2	3.433E+016	-1.627
198.7 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-1+O2<=>C4H8OOH2-1O2	3.433E+016	-1.627
198.7 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-3+O2<=>C4H8OOH2-3O2	1.744E+014	-0.816
-536.5 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-4+O2<=>C4H8OOH2-4O2	3.433E+016	-1.627
198.7 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
!\REACTIONCLASS: \O2QOOH_ALKENEKHP_HO2		
\EA	\A	\N
C4H8OOH1-2O2<=>C4H72-1OOH+HO2	2.540E+010	0.804
30098.5 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-3O2<=>C4H71-4OOH+HO2	5.130E+009	1.000
30400.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-3O2<=>C4H72-1OOH+HO2	2.540E+010	0.804
30098.5 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-4O2<=>C4H71-4OOH+HO2	1.440E+007	1.380
28900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-3O2<=>C4H71-3OOH+HO2	5.130E+009	1.000
30400.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-4O2<=>C4H71-3OOH+HO2	1.440E+007	1.380
28900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
!\REACTIONCLASS: \O2QOOH_POOH		
\EA	\A	\N
C4H8OOH1-2O2<=>C4H71-3,4OOH	1.440E+007	1.400
20800.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-2O2<=>C4H72-3,4OOH	1.720E+009	0.900
29500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-2O2<=>NC4KET12+OH	2.440E+007	1.600
27900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-3O2<=>C4H71-2,4OOH	1.460E+009	1.100
33500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-3O2<=>C4H72-1,3OOH	1.720E+009	0.900
29500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-3O2<=>NC4KET13+OH	1.090E+004	2.400
19900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH1-4O2<=>C4H72-1,4OOH	1.360E+007	1.300
18200.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
DUP		

C4H8OOH1-4O2<=>C4H72-1,4OOH	4.010E+008	1.100
30100.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A DUP		
C4H8OOH1-4O2<=>NC4KET14+OH	4.800E+003	1.700
16600.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-1O2<=>C4H72-3,4OOH	1.720E+009	0.900
29500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-1O2<=>C4H71-3,4OOH	1.230E+006	1.500
20000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-1O2<=>NC4KET21+OH	2.760E+008	1.200
25700.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-3O2<=>C4H71-2,3OOH	1.460E+009	1.100
33500.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A DUP		
C4H8OOH2-3O2<=>C4H71-2,3OOH	1.440E+007	1.400
20800.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A DUP		
C4H8OOH2-3O2<=>NC4KET23+OH	1.750E+006	1.700
26000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-4O2<=>C4H71-2,4OOH	1.230E+006	1.500
20000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-4O2<=>C4H72-1,3OOH	4.010E+008	1.100
30100.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H8OOH2-4O2<=>NC4KET24+OH	5.790E+001	2.900
17000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A !		

!\REACTIONCLASS: \POOH_PRODUCTS1	\A	\N
\EA		
!		

C4H71-3,4OOH<=>C4H7O1-3OOH-4+OH	2.440E+009	0.780
18000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H71-3,4OOH<=>C4H7O1-4OOH-2+OH	1.720E+009	0.760
11100.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H72-3,4OOH<=>C4H7O2-3OOH-1+OH	6.990E+009	0.815
9788.3 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H72-3,4OOH<=>C4H7O1-3OOH-2+OH	2.590E+009	0.690
16000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H71-2,4OOH<=>C4H7O1-2OOH-4+OH	2.350E+010	0.680
10800.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H71-2,4OOH<=>C4H7O1-4OOH-2+OH	1.720E+009	0.760
11100.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H72-1,3OOH<=>C4H7O1-2OOH-3+OH	1.710E+009	1.060
10900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H72-1,3OOH<=>C4H7O2-3OOH-1+OH	6.990E+009	0.815
9788.3 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H72-1,4OOH<=>C4H7O1-2OOH-4+OH	1.710E+009	1.060
10900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H72-1,4OOH<=>C4H7O1-3OOH-4+OH	2.590E+009	0.690
16000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H71-2,3OOH<=>C4H7O1-2OOH-3+OH	2.350E+010	0.680
10800.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H71-2,3OOH<=>C4H7O1-3OOH-2+OH	2.440E+009	0.780
18000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		
C4H71-3,4OOH=>C2H4+OH+HO2CH2CHO	1.230E+009	1.300
24900.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2 080415A		

!-----

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

!

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

IC4H10 (+M) <=> CH3+IC3H7 (+M) 2.520E+031 -4.102
91495.0 !\AUTHOR: !\REF:OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004,
108:4247-4253
LOW/ 2.410E+019 0.000
52576.0/
TROE/ 3.662E-001 8.153E+002 6.079E+001 1.000E+020/
IC4H10 <=> TC4H9+H 2.510E+098 -23.810
145300.0 !\AUTHOR: !\REF:OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004,
108:4247-4253.
IC4H10 <=> IC4H9+H 9.850E+095 -23.110
147600.0 !\AUTHOR: !\REF:OEHLSCHLAEGGER ET AL. J. PHYS. CHEM. A 2004,
108:4247-4253.
!

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

IC4H10+CH3 <=> IC4H9+CH4 1.360E+000 3.650
7154.0 !\AUTHOR: !\REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)
IC4H10+H <=> IC4H9+H2 1.810E+006 2.540
6756.0 !\AUTHOR: !\REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)
IC4H10+OH <=> IC4H9+H2O 6.654E+004 2.665
-168.9 !\AUTHOR: !\REF:JOE MICHAELS SYMP. PAPER 2008.
IC4H10+C2H5 <=> IC4H9+C2H6 1.510E+012 0.000
10400.0 !\AUTHOR: !\REF:ALLARA AND SHAW ANALOG
IC4H10+HO2 <=> IC4H9+H2O2 6.120E+001 3.590
17160.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
(2008) 112(30): 7047-7054.
IC4H10+O <=> IC4H9+OH 4.046E+007 2.034
5136.0 !\AUTHOR: !\REF:NIST STANDARD REFERENCE DATABASE 17 -2Q98
IC4H10+CH3O <=> IC4H9+CH3OH 4.800E+011 0.000
7000.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+CH3O
IC4H10+O2 <=> IC4H9+HO2 9.000E+013 0.000
52290.0 !\AUTHOR: !\REF: ANALOGY WITH C4H10+O2 <=> PC4H9+HO2
IC4H10+CH3O2 <=> IC4H9+CH3O2H 2.079E+000 3.970
18280.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
(2008) 112(30): 7047-7054.
IC4H10+C2H5O2 <=> IC4H9+C2H5O2H 2.550E+013 0.000
20460.0 !\AUTHOR: !\REF:SCOTT AND WALKER C&F 129(4) 365--377 2002 (*1.5)
IC4H10+CH3CO3 <=> IC4H9+CH3CO3H 2.550E+013 0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2
IC4H10+NC3H7O2 <=> IC4H9+NC3H7O2H 2.550E+013 0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2
IC4H10+IC3H7O2 <=> IC4H9+IC3H7O2H 2.550E+013 0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2

IC4H10+IC4H9O2<=>IC4H9+IC4H9O2H	2.550E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
IC4H10+TC4H9O2<=>IC4H9+TC4H9O2H	2.550E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
IC4H10+O2CHO<=>IC4H9+HO2CHO	2.520E+013	0.000
20440.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
IC4H10+SC4H9O2<=>IC4H9+SC4H9O2H	2.250E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
IC4H10+SC4H9O2<=>TC4H9+SC4H9O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+PC4H9O2<=>IC4H9+PC4H9O2H	2.250E+013	0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO C2H6+HO2		
IC4H10+H<=>TC4H9+H2	6.020E+005	2.400
2583.0 !\AUTHOR: !\REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)		
IC4H10+CH3<=>TC4H9+CH4	9.040E-001	3.460
4598.0 !\AUTHOR: !\REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)		
IC4H10+OH<=>TC4H9+H2O	2.925E+004	2.531
-1659.0 !\AUTHOR: !\REF:JOE MICHAELS SYMP. PAPER 2008.		
IC4H10+C2H5<=>TC4H9+C2H6	1.000E+011	0.000
7900.0 !\AUTHOR: !\REF:FROM ISOBUTYL RATE		
IC4H10+HO2<=>TC4H9+H2O2	4.332E+002	3.010
12090.0 !\AUTHOR: !\REF: X0.666		
IC4H10+O<=>TC4H9+OH	1.968E+005	2.402
1150.0 !\AUTHOR: !\REF:NIST STANDARD REFERENCE DATABASE 17 -2Q98		
IC4H10+CH3O<=>TC4H9+CH3OH	1.900E+010	0.000
2800.0 !\AUTHOR: !\REF:TAMURA ESTIMATE		
IC4H10+O2<=>TC4H9+HO2	1.000E+013	0.000
48200.0 !\AUTHOR: !\REF: Ingham, T.; Walker, R.W.; Woolford, R.E., Symp. Int. Combust. Proc. 25, 767-774 (1994)		
IC4H10+O2CHO<=>TC4H9+HO2CHO	2.800E+012	0.000
16010.0 !\AUTHOR: !\REF:ANALOGY WITH RH+RO2 -->R+RO2H		
IC4H10+PC4H9O2<=>TC4H9+PC4H9O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+CH3O2<=>TC4H9+CH3O2H	1.366E+002	3.120
13190.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
IC4H10+C2H5O2<=>TC4H9+C2H5O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+CH3CO3<=>TC4H9+CH3CO3H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+NC3H7O2<=>TC4H9+NC3H7O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+IC3H7O2<=>TC4H9+IC3H7O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+IC4H9O2<=>TC4H9+IC4H9O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+TC4H9O2<=>TC4H9+TC4H9O2H	2.800E+012	0.000
16000.0 !\AUTHOR: !\REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+IC4H9<=>TC4H9+IC4H10	2.500E+010	0.000
7900.0 !\AUTHOR: !\REF:WESTBROOK AND PITZ ESTIMATE (1983)		

!

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

IC4H9<=>TC4H9 3.560E+010 0.880
34600.0 !\AUTHOR: !\REF:D.M. Matheu, W.H. Green, J.M. Grenda, Int. J.
Chem. Kin. 2003 Volume 35, Issue 3, 2003, Pages: 95;SC119
!

!\REACTIONCLASS: \R_BETA_SCISSION \A \N
\EA
!

IC4H9<=>C3H6+CH3 1.0 1.0 1.0
!\AUTHOR: !\ FROM K. ZHANG ESTIMATED
PLOG / 1.000E-001 3.150E+041 -9.50 33486. / !FIT FROM: 500-2000 K
ERROR IN FIT: 34%
PLOG / 1.000E+000 6.750E+044 -10.07 37209. / !FIT FROM: 500-2000 K
ERROR IN FIT: 29%
PLOG / 1.000E+001 7.790E+044 -9.70 39751. / !FIT FROM: 500-2000 K
ERROR IN FIT: 19%
PLOG / 1.000E+002 3.610E+039 -7.78 39583. / !FIT FROM: 500-2000 K
ERROR IN FIT: 10%
!

!\REACTIONCLASS: \R_RO2 \A \N
\EA
!

TC4H9+HO2<=>TC4H9O+OH 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
TC4H9+CH3O2<=>TC4H9O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
TC4H9+NC3H7O2<=>TC4H9O+NC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
TC4H9+SC4H9O2<=>TC4H9O+SC4H9O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
TC4H9+PC4H9O2<=>TC4H9O+PC4H9O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
TC4H9+IC3H7O2<=>TC4H9O+IC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
IC4H9+HO2<=>IC4H9O+OH 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
IC4H9+CH3O2<=>IC4H9O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
IC4H9+NC3H7O2<=>IC4H9O+NC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
IC4H9+SC4H9O2<=>IC4H9O+SC4H9O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
IC4H9+PC4H9O2<=>IC4H9O+PC4H9O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE
IC4H9+IC3H7O2<=>IC4H9O+IC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE

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!\SUBSPECIES: \TC4H9O

!=====
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!

!\REACTIONCLASS: \R_BETA_SCISSION \A \N
\EA
!

CH3COCH3+CH3<=>TC4H9O 1.500E+011 0.000
11900.0 !\AUTHOR: !\REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006
!

!\REACTIONCLASS: \R_O2 \A \N
\EA
!

TC4H9O+O2<=>IC4H8O+HO2 8.100E+011 0.000
4700.0 !\AUTHOR: !\REF:PITZ ESTIMATE

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!

!\ENDSUBSPECIES: \TC4H9O

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!

!\SUBSPECIES: \IC4H9O

!=====
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!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

IC4H9O+H<=>IC3H7CHO+H2 1.990E+013 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX TSANG/ HAMPSON 86
IC4H9O+O2<=>IC3H7CHO+HO2 1.930E+011 0.000
1660.0 !\AUTHOR: !\REF:!\ZABARNICK, S. AND HEICKLEN, J., IJCK, 17, 503
(1985).
IC4H9O+O<=>IC3H7CHO+OH 6.000E+012 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX TSANG/ HAMPSON 86
IC4H9O+OH<=>IC3H7CHO+H2O 1.810E+013 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX TSANG/ HAMPSON 86
IC4H9O+HO2<=>IC3H7CHO+H2O2 1.000E+012 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX TSANG/ HAMPSON 86
IC4H9O+CH3<=>IC3H7CHO+CH4 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX TSANG/ HAMPSON 86
!

!\REACTIONCLASS: \R_BETA_SCISSION \A \N
\EA
!

IC3H7CHO+H<=>IC4H9O 1.000E+012 0.000
5860.0 !\AUTHOR: !\REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006
CH2O+IC3H7<=>IC4H9O 5.000E+010 0.000
2330.0 !\AUTHOR: !\REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006

IC3H7CHO+OH<=>TC3H6CHO+H2O	1.684E+012	0.000
-781.0 !\AUTHOR: !\REF:SEMMES ET AL. INTL. J. CHEM. KINET. 1985, 17, 303.		
IC4H8O+OH<=>IC3H6CHO+H2O	7.520E+004	2.490
-1474.1 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		
IC4H8O+H<=>IC3H6CHO+H2	8.790E+004	2.680
2910.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		
IC4H8O+HO2<=>IC3H6CHO+H2O2	2.450E-005	5.260
7475.1 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		
IC4H8O+CH3O2<=>IC3H6CHO+CH3O2H	1.225E-005	5.260
7475.1 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		
IC4H8O+CH3<=>IC3H6CHO+CH4	1.993E+001	3.370
7634.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		
IC4H8O+O<=>IC3H6CHO+OH	1.450E+005	2.470
876.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		
IC4H8O+O2<=>IC3H6CHO+HO2	1.500E+013	0.000
50150.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+R=SC2H4OH+RH		

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!\SUBSPECIES: \TC3H6CHO

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!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA

!

IC3H5CHO+H<=>TC3H6CHO	1.300E+013	0.000
1200.0 !\AUTHOR: !\REF:H.J. Curran, International Journal of Chemical Kinetics (2006) 38: 250;§C275.		
IC3H6CO+H<=>TC3H6CHO	1.300E+013	0.000
4800.0 !\AUTHOR: !\REF:H.J. Curran, International Journal of Chemical Kinetics (2006) 38: 250;§C275.		
IC3H6CO+OH<=>IC3H7+CO2	1.730E+012	0.000
-1010.0 !\AUTHOR: !\REF:ANALOGY TO 1C4H8+OH		
IC3H6CO+OH<=>C3H6OH2-1+CO	2.000E+012	0.000
-1010.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		

!

!\REACTIONCLASS: \R_RH_ABSTRACTION \A \N
\EA

!

TC3H6CHO+HO2<=>IC3H7CHO+O2	3.675E+012	0.000
1310.0 !\AUTHOR: !\REF:!\LOHDI, Z.H.; WALKER, R.W.; J. CHEM. SOC. FARAD. 1991 87, 2361 (C3H5-A+HO2) (X 0.5)		
TC3H6CHO+CH3<=>IC3H5CHO+CH4	3.010E+012	-0.320
-131.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
TC3H6CHO+CH2O<=>IC3H7CHO+HCO	2.520E+008	1.900
18190.0 !\AUTHOR: !\REF:ANALOGY WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES		
TC3H6CHO+IC4H8<=>IC3H7CHO+IC4H7	4.700E+002	3.300
19840.0 !\AUTHOR: !\REF:ANALOGY WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES		

!

!\REACTIONCLASS: \R_O2_RO2 \A \N
\EA

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TC3H6CHO+O2<=>TC3H6O2CHO	1.990E+017	-2.100
0.0 !\AUTHOR: !\REF:ANALOGY TO NEOPENTYL, Xi, Z.; Han, W-J.; Bayes, K.D., J. Phys. Chem. 92, 3450 (1988)		
TC3H6O2CHO<=>IC3H5O2HCHO	6.000E+011	0.000
29880.0 !\AUTHOR: !\REF:ANALOGY TO NEOPENTYL, Xi, Z.; Han, W-J.; Bayes, K.D., J. Phys. Chem. 92, 3450 (1988)		
TC3H6O2CHO<=>TC3H6O2HCO	1.000E+011	0.000
25750.0 !\AUTHOR: !\REF:ANALOGY TO NEOPENTYL, Xi, Z.; Han, W-J.; Bayes, K.D., J. Phys. Chem. 92, 3450 (1988)		
IC3H5CHO+HO2<=>IC3H5O2HCHO	2.230E+011	0.000
10600.0 !\AUTHOR: !\REF:SLAGLE ET AL. J. PHYS. CHEM. 1991, 95		

! _____

!\REACTIONCLASS: \R_HO2_PRODUCTS \A \N
 \EA
 ! _____

TC3H6OCHO+OH<=>TC3H6CHO+HO2	2.018E+017	-1.200
21010.0 !\AUTHOR: !\REF:ANALOGY WITH C3H5-A+CH3 -->1-C4H8 TSANG 91 (PROPENE).		
TC3H6OCHO<=>CH3COCH3+HCO	3.980E+013	0.000
9700.0 !\AUTHOR: !\REF:CURRAN AND GAFFURI, 1995.		

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!\REACTIONCLASS: \R_OH_TERMINATION \A \N
 \EA
 ! _____

TC3H6CHO+OH<=>IC3H6OHCHO	5.000E+013	0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C3H6OH2-1+HCO<=>IC3H6OHCHO	1.810E+013	0.000
0.0 !\AUTHOR: !\REF:!\TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		

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 !\SUBSPECIES: \IC3H5CHO
 ! =====
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 ! _____

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

IC3H5CHO+H<=>IC3H5CO+H2	714740.3558	2.35674
1577.16272 !\AUTHOR: !\REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
IC3H5CHO+O2<=>IC3H5CO+HO2	2.000E+013	0.000
40700.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
IC3H5CHO+O<=>IC3H5CO+OH	7.180E+012	0.000
1389.0 !\AUTHOR: !\REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
IC3H5CHO+OH<=>IC3H5CO+H2O	61329.9	2.65 -
4586.4 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.		
IC3H5CHO+HO2<=>IC3H5CO+H2O2	1.1773E-4	4.91966
3684.27444 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.		

IC3H5CHO+CH3<=>IC3H5CO+CH4	1.24879	3.63386
4328.93484 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-12104.		
IC3H5CHO+H<=>IC3H4CHO-A+H2	3.64E+05	2.455
4361.2 !\AUTHOR: !\REF: ANALOGY TO ALLYL RADICAL IN C3H6		
IC3H5CHO+O2<=>IC3H4CHO-A+HO2	5.96E+19	-1.67
46192.1 !\AUTHOR: !\REF: ANALOGY TO ALLYL RADICAL IN C3H6		
IC3H5CHO+OH<=>IC3H4CHO-A+H2O	4.46E+06	2.072
1050.8 !\AUTHOR: !\REF: ANALOGY TO ALLYL RADICAL IN C3H6		
IC3H5CHO+O<=>IC3H4CHO-A+OH	5.24E+11	0.7
5884 !\AUTHOR: !\REF: ANALOGY TO ALLYL RADICAL IN C3H6		
IC3H5CHO+HO2<=>IC3H4CHO-A+H2O2	3.07E-02	4.403
13547.2 !\AUTHOR: !\REF: ANALOGY TO ALLYL RADICAL IN C3H6		
IC3H5CHO+CH3<=>IC3H4CHO-A+CH4	2.21E+00	3.5
5675 !\AUTHOR: !\REF: ANALOGY TO ALLYL RADICAL IN C3H6		

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!\REACTIONCLASS: \RADICAL_DECOMPOSITION      \A      \N
\EA
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!

IC3H5CO<=>C3H5-T+CO	1.278E+020	-1.890
34460.0 !\AUTHOR: !\REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
C3H4-A+HCO<=>IC3H4CHO-A	40209.73013	2.51815
8847.53569 !\AUTHOR: !\REF: ANALOGY TO C3H4-A+CH3--->IC4H7 ZHOU		
CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY		

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!\REACTIONCLASS: \RADICAL_DECOMPOSITION      \A      \N
\EA
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!

IC3H7+CO<=>IC3H7CO	1.500E+011	0.000
4810.0 !\AUTHOR: !\REF:NAROZNIK, M; NIEDZIELSKI, J. J. PHOTOCHEM. 1986, 32, 281		
C2H3CHO+CH3<=>IC3H6CHO	1.000E+011	0.000
7800.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		

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!\ENDSUBSPECIES: \IC3H5CHO
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!\ENDSUBSPECIES: \TC3H6CHO
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!\SUBSPECIES: \SC4H7OH-I
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!\REACTIONCLASS: \R_CAT_ISO      \A      \N
\EA
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SC4H7OH-I+HO2<=>IC3H7CHO+HO2 1.490E+05 1.67 6.810E+03 !\AUTHOR: !\
KETO-ENOL ISOMERIZATIONS
SC4H7OH-I+HOCHO<=>IC3H7CHO+HOCHO 2.81E-02 3.286 -4509 !\AUTHOR: !\
KETO-ENOL ISOMERIZATIONS

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

SC4H7OH-I+H<=>IC4H6OH+H2 7.29E+05 2.455 4361.2
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION
SC4H7OH-I+O<=>IC4H6OH+OH 1.05E+12 0.700 5884.0
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION
SC4H7OH-I+OH<=>IC4H6OH+H2O 43950.16898 2.67841 -827.103
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION
SC4H7OH-I+HO2<=>IC4H6OH+H2O2 2.92E-01 4.12 12802.0
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION
SC4H7OH-I+CH3<=>IC4H6OH+CH4 4.420E+000 3.500 5675.0
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION
SC4H7OH-I+CH3O<=>IC4H6OH+CH3OH 1.68E+11 0.000 2600.0
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION
SC4H7OH-I+CH3O2<=>IC4H6OH+CH3O2H 1.928E+004 2.600 13910.0
!\AUTHOR: !\REF: ANALOGY TO IC4H8 IN ALLYL RADICAL FORMATION

!\REACTIONCLASS: \R_R_PRODUCTS \A \N \EA

IC4H6OH+H=>CH3+C3H4-A+OH 40209.73013 2.51815 8847.53569
!\AUTHOR: !\ BUTENOL RADICAL DECOMPOSITION

!\ENDSUBSPECIES: \SC4H7OH-I

!\ENDSUBSPECIES: \IC3H7CHO\IC4H8O

!\REACTIONCLASS: \R_O2_ALKENE_HO2 \A \N
\EA

TC4H9+O2<=>IC4H8+HO2 8.370E-001 3.590
11960.0 !\AUTHOR: !\REF: IN ARAMCO (BASED ON KLIPPENSTEIN ET AL.
N, IC3H7+O2)
IC4H9+O2<=>IC4H8+HO2 1.070E+000 3.710
9322.0 !\AUTHOR: !\REF: IN ARAMCO (BASED ON KLIPPENSTEIN ET AL.
N, IC3H7+O2)

!\REACTIONCLASS: \R_O2_RO2 \A \N
\EA

! _____
 IC4H9+O2<=>IC4H9O2 6.6946E+13 -0.3 -
 187.2 !\AUTHOR: !\REF: F. GOLDSMITH JPCA, 2012
 TC4H9+O2<=>TC4H9O2 6.6946E+13 -0.3 -
 187.2 !\AUTHOR: !\REF: F. GOLDSMITH JPCA, 2012
 ! _____

!\REACTIONCLASS: \RO2_ALKENE_HO2 \A \N
 \EA
 ! _____

IC4H9O2<=>IC4H8+HO2 1.94E+08 1.27
 29600.0 !\AUTHOR: !\ ALL USE DEAN'S DATA FIRST TWO 2011, SECOND TWO 2013
 ! _____

!\REACTIONCLASS: \RO2_QOOH \A \N
 \EA
 ! _____

IC4H9O2<=>IC4H8O2H-I 9.82E+07 1.3
 21500 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701
 IC4H9O2<=>IC4H8O2H-T 2.31E+09 0.8
 27100 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701
 TC4H9O2<=>TC4H8O2H-I 4.521E+009 1.2
 33500.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701
 ! _____

!\REACTIONCLASS: \QOOH_DECOMP \A \N
 \EA
 ! _____

IC4H8O2H-I<=>CC4H8O+OH 4.470E+011 0.000
 21900.0 !\AUTHOR: !\REF:GREEN 2003
 IC4H8O2H-I=>OH+CH2O+C3H6 8.451E+015 -0.680
 29170.0 !\AUTHOR: !\REF:GREEN 2003
 ! _____

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 !\SUBSPECIES: \CC4H8O
 ! _____
 =====

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

CC4H8O+OH=>CH2O+C3H5-A+H2O 5.000E+012 0.000
 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CC4H8O+H=>CH2O+C3H5-A+H2 3.510E+007 2.000
 5000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CC4H8O+O=>CH2O+C3H5-A+OH 1.124E+014 0.000
 5200.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CC4H8O+HO2=>CH2O+C3H5-A+H2O2 1.000E+013 0.000
 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

CC4H8O+CH3O2=>CH2O+C3H5-A+CH3O2H	1.000E+013	0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CC4H8O+CH3=>CH2O+C3H5-A+CH4	2.000E+011	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
!=====		
=====		
!\ENDSUBSPECIES: \CC4H8O		
!=====		
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!		
<hr/>		
!\REACTIONCLASS: \QOOH_O2	\A	\N
\EA		
!		
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IC4H8O2H-I+O2<=>IC4H8OOH-IO2	9.35316E+11	0.1 -
1010.88 !\AUTHOR: !\REF:GOLDSMITH, JPCA, 2012		
IC4H8O2H-T+O2<=>IC4H8OOH-TO2	5.04482E+12	-0.1 -
655.2 !\AUTHOR: !\REF:GOLDSMITH, JPCA, 2012		
TC4H8O2H-I+O2<=>TC4H8OOH-IO2	22844293817	0.5 -
786.24 !\AUTHOR: !\REF:GOLDSMITH, JPCA, 2012		
!		
<hr/>		
!\REACTIONCLASS: \O2QOOH_PRODUCTS	\A	\N
\EA		
!		
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IC4H8OOH-IO2<=>IC4KETII+OH	5.000E+010	0.000
21400.0 !\AUTHOR: !\REF: GREEN 2003		
IC4H8OOH-TO2<=>IC4KETIT+OH	4.000E+011	0.000
31500.0 !\AUTHOR: !\REF: GREEN 2003		
IC4H8OOH-TO2<=>TIC4H7Q2-I	6.000E+011	0.000
34500.0 !\AUTHOR: !\REF: GREEN 2003		
IC4H8OOH-IO2<=>IIC4H7Q2-I	3.750E+010	0.000
24400.0 !\AUTHOR: !\REF: GREEN 2003		
IC4H8OOH-IO2<=>IIC4H7Q2-T	1.000E+011	0.000
29200.0 !\AUTHOR: !\REF: GREEN 2003		
TC4H8OOH-IO2<=>TIC4H7Q2-I	9.820E+007	1.300
21500.0 !\AUTHOR: !\REF: GREEN 2003		
IC4H8O2H-T<=>IC4H8O+OH	1.55E+012	0.000
13400.0 !\AUTHOR: !\REF: GREEN 2003		
!		
<hr/>		
!\REACTIONCLASS: \POOH_DECOMP	\A	\N
\EA		
!		
<hr/>		
AC3H5OOH+CH2O2H<=>IIC4H7Q2-I	8.500E+010	0.000
10600.0 !\AUTHOR: !\REF: CURRAN ESTIMATED		
IC4H7OOH+HO2<=>IIC4H7Q2-T	1.000E+011	0.000
7800.0 !\AUTHOR: !\REF: CURRAN ESTIMATED		
TIC4H7Q2-I<=>IC4H7OOH+HO2	1.600E+012	0.230
15200.0 !\AUTHOR: !\REF: GREEN 2003		
!=====		
=====		
!\SUBSPECIES: \IC4KETII\IC4KETIT		
!=====		
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!

!\REACTIONCLASS: \RO2_R \A \N
\EA
!

IC4H9O2+CH3<=>IC4H9O+CH3O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+C2H5<=>IC4H9O+C2H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+IC3H7<=>IC4H9O+IC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+NC3H7<=>IC4H9O+NC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+PC4H9<=>IC4H9O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+SC4H9<=>IC4H9O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+IC4H9<=>IC4H9O+IC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+TC4H9<=>IC4H9O+TC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+C3H5-A<=>IC4H9O+C3H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+C4H71-3<=>IC4H9O+C4H71-O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
IC4H9O2+IC4H7<=>IC4H9O+IC4H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+CH3<=>TC4H9O+CH3O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+C2H5<=>TC4H9O+C2H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+IC3H7<=>TC4H9O+IC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+NC3H7<=>TC4H9O+NC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+PC4H9<=>TC4H9O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+SC4H9<=>TC4H9O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+IC4H9<=>TC4H9O+IC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+TC4H9<=>TC4H9O+TC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+C3H5-A<=>TC4H9O+C3H5O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		
TC4H9O2+C4H71-3<=>TC4H9O+C4H71-O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:		

!=====
=====
!\SUBSPECIES: \IC4H9O2H
!=====
=====
!

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

! _____
 IC4H9O2H<=>IC4H9O+OH 1.500E+016 0.000
 42500.0 !\AUTHOR: !\REF:ESTIMATE
 ! _____

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

IC4H9O2+HO2<=>IC4H9O2H+O2 1.750E+010 0.000
 -3275.0 !\AUTHOR:
 IC4H9O2+H2O2<=>IC4H9O2H+HO2 2.400E+012 0.000
 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+H2<=>IC4H9O2H+H 3.010E+013 0.000
 26030.0 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF.
 DATA, VOL 15, 1986
 IC4H9O2+CH4<=>IC4H9O2H+CH3 1.130E+013 0.000
 20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+CH3OH<=>IC4H9O2H+CH2OH 6.300E+012 0.000
 19360.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+CH2O<=>IC4H9O2H+HCO 1.300E+011 0.000
 9000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+C2H6<=>IC4H9O2H+C2H5 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+C2H4<=>IC4H9O2H+C2H3 8.590E+000 3.754
 27132.0 !\AUTHOR: !\REF:PITZ ESTIMATE: ANALOGY WITH C2H4+CH3O2
 IC4H9O2+C2H5OH<=>IC4H9O2H+PC2H4OH 6.300E+012 0.000
 19360.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+C2H5OH<=>IC4H9O2H+SC2H4OH 4.200E+012 0.000
 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+CH3CHO<=>IC4H9O2H+CH3CO 2.800E+012 0.000
 13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2
 IC4H9O2+C3H8<=>IC4H9O2H+IC3H7 2.000E+012 0.000
 17000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+C3H8<=>IC4H9O2H+NC3H7 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 IC4H9O2+C2H3CHO<=>IC4H9O2H+C2H3CO 2.800E+012 0.000
 13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2
 IC4H9O2+C2H5CHO<=>IC4H9O2H+C2H5CO 2.800E+012 0.000
 13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2
 IC4H9O2+C3H6<=>IC4H9O2H+C3H5-A 5.350E-002 4.207
 13288.1 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2

!=====
 !\SUBSPECIES: \TC4H9O2H
 !=====
 ! _____

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

TC4H9O2H<=>TC4H9O+OH 5.950E+015 0.000
 42540.0 !\AUTHOR: !\REF:ESTIMATE
 ! _____

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

TC4H9O2+CH4<=>TC4H9O2H+CH3	1.130E+013	0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+C2H6<=>TC4H9O2H+C2H5	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+C3H8<=>TC4H9O2H+IC3H7	2.000E+012	0.000
17000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+C3H8<=>TC4H9O2H+NC3H7	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+CH3OH<=>TC4H9O2H+CH2OH	6.300E+012	0.000
19360.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+C2H5OH<=>TC4H9O2H+PC2H4OH	6.300E+012	0.000
19360.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+C2H5OH<=>TC4H9O2H+SC2H4OH	4.200E+012	0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+CH3CHO<=>TC4H9O2H+CH3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
TC4H9O2+C2H3CHO<=>TC4H9O2H+C2H3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
TC4H9O2+C2H5CHO<=>TC4H9O2H+C2H5CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
TC4H9O2+HO2<=>TC4H9O2H+O2	1.750E+010	0.000
-3275.0 !\AUTHOR:		
TC4H9O2+H2O2<=>TC4H9O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+CH2O<=>TC4H9O2H+HCO	1.300E+011	0.000
9000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
TC4H9O2+C2H4<=>TC4H9O2H+C2H3	8.590E+000	3.754
27132.0 !\AUTHOR: !\REF:PITZ ESTIMATE		
TC4H9O2+H2<=>TC4H9O2H+H	3.010E+013	0.000
26030.0 !\AUTHOR: !\REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
TC4H9O2+C3H6<=>TC4H9O2H+C3H5-A	5.350E-002	4.207
13288.1 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2		

!\ENDSUBMECH: \IC4H10

!\SUBMECH: \IC4H8

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

IC4H8<=>IC4H7-I1+H	7.710E+069	-16.090
140000.0 ! 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 1.42E+93 -22.79 133825.
! 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/	0.100	1.26E+94	-22.99	134024./
PLOG/	1.0000	6.76E+93	-22.51	137933./
PLOG/	3.5000	3.14E+90	-21.37	137866./
PLOG/	10.0000	9.20E+85	-19.94	136498./
PLOG/	35.0000	6.05E+78	-17.76	133437./
PLOG/	100.0000	4.87E+71	-15.65	129919./

IC4H8<=>IC4H7+H 4.66E+92 -22.45 129059.
! 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/	0.100	7.51E+95	-23.38	129214./
PLOG/	1.0000	3.59E+88	-20.99	127813./
PLOG/	3.5000	2.96E+82	-19.12	125456./
PLOG/	10.0000	2.13E+76	-17.27	122629./
PLOG/	35.0000	1.13E+68	-14.82	118416./
PLOG/	100.0000	4.73E+60	-12.66	114404./

!

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

!

IC4H8+OH<=>IC4H7+H2O 43950.16898 2.67841 -
827.103
IC4H8+OH<=>IC4H7-I1+H2O 10930.0948 2.81477
1114.19989 !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 3.12E+13 0.00E+00
37450 !AUTHOR: !REF: YASUNAGA, PROC. COMBUST INST., 2009, 32, 453-460.
INCREASED BY 40% AT 800-1000 K.
IC4H8+O2<=>IC4H7-I1+HO2 2.000E+013 0.000
62270.0 !AUTHOR: !REF: C-J CHEN AND J. W. BOZZELLI J. PHYS. CHEM. A,
2000, 104, 9715-9732.
IC4H8+H<=>IC4H7+H2 7.29E+05 2.455
4361.2 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013,
117, 2718-2727
IC4H8+H<=>IC4H7-I1+H2 8.621E+02 3.25
12166.98 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013,
117, 2718-2727
IC4H8+O<=>IC4H7+OH 1.05E+12 0.700
5884.0 !AUTHOR: !REF: ANALOGY WITH C2H4
IC4H8+O<=>IC4H7-I1+OH 1.200E+011 0.700
8959.1 !AUTHOR: !REF: ANALOGY WITH C2H4
IC4H8+HO2<=>IC4H7+H2O2 2.92E-01 4.12
12802.0 !AUTHOR: !REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
IC4H8+HO2<=>IC4H7-I1+H2O2 97038.94079 2.54892
24733.17153 !AUTHOR: !REF: C3 NUIG CALCULATION J.MENDES
IC4H8+CH3<=>IC4H7+CH4 3.2E+12 0.000
10000.0 !AUTHOR: !REF: YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.
IC4H8+CH3<=>IC4H7-I1+CH4 2.0E+12 0.000
15000.0 !AUTHOR: !REF: YASUNAGA, K. PROC. COMBUT. INST. 2009, 32, 453.
IC4H8+CH3O<=>IC4H7+CH3OH 1.68E+11 0.000
2600.0 !AUTHOR: !REF: ANALOGY TO C3H6+CH3O

IC4H8+C3H5-A<=>IC4H7+C3H6	7.940E+011	0.000
20500.0 ! AUTHOR: !REF:WESTBROOK AND PITZ ESTIMATE 1983		
IC4H8+C3H5-S<=>IC4H7+C3H6	7.940E+011	0.000
20500.0 ! AUTHOR: !REF:WESTBROOK AND PITZ ESTIMATE 1983		
IC4H8+C3H5-T<=>IC4H7+C3H6	7.940E+011	0.000
20500.0 ! AUTHOR: !REF:WESTBROOK AND PITZ ESTIMATE 1983		
IC4H8+CH3O2<=>IC4H7+CH3O2H	1.54E-01	4.403
13547.2 !AUTHOR: !REF:ANALOGY TO C3H6+CH3O2		
IC4H8+CH3CO3<=>IC4H7+CH3CO3H	1.54E-01	4.403
13547.2 !AUTHOR: !REF:ANALOGY TO C3H6+CH3O2		
IC4H8+O2CHO<=>IC4H7+HO2CHO	1.928E+004	2.600
13910.0 !AUTHOR: !REF:ANALOGY WITH RH+RO2 --> R+RO2H		
IC4H9O2+IC4H8<=>IC4H9O2H+IC4H7	1.400E+012	0.000
14900.0 !AUTHOR: !REF:WESTBROOK ESTIMATE		
TC4H9O2+IC4H8<=>TC4H9O2H+IC4H7	1.400E+012	0.000
14900.0 !AUTHOR: !REF:WESTBROOK ESTIMATE		
PC4H9O2+IC4H8<=>PC4H9O2H+IC4H7	1.400E+012	0.000
14900.0 !AUTHOR: !REF:WESTBROOK ESTIMATE		
SC4H9O2+IC4H8<=>SC4H9O2H+IC4H7	1.400E+012	0.000
14900.0 !AUTHOR: !REF:WESTBROOK ESTIMATE		
IC3H7O2+IC4H8<=>IC3H7O2H+IC4H7	1.400E+012	0.000
14900.0 !AUTHOR: !REF:WESTBROOK ESTIMATE		
NC3H7O2+IC4H8<=>NC3H7O2H+IC4H7	1.400E+012	0.000
14900.0 !AUTHOR: !REF:WESTBROOK ESTIMATE		
IC4H7O+IC4H8<=>IC4H7OH+IC4H7	2.700E+011	0.000
4000.0 !AUTHOR: !REF:PITZ ESTIMATE		
IC4H8+CH2CCH2OH<=>IC4H7+C3H5OH	7.940E+011	0.000
20500.0 !AUTHOR: !REF:CURRAN ESTIMATE		

!

!\REACTIONCLASS: \RA_DECOMPOSITION \A \N
 \EA

!

IC4H7<=>IC4H7-I1	1.300E+055	-14.530
73800.0 !\AUTHOR: !\REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589		
PLOG/ 0.1000	1.300E+055	-14.530
PLOG/ 1.0000	5.000E+051	-13.020
PLOG/ 10.0000	9.700E+048	-11.730
PLOG/ 100.0000	4.860E+044	-9.840

C3H4-A+CH3<=>IC4H7	40209.7	2.5	8847.5
!\AUTHOR: !\REF: C ZHOU CALCULATED AT QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY			

!

!\REACTIONCLASS: \RA_HO2_PRODUCTS \A \N
 \EA

!

IC4H7+HO2<=>IC4H7O+OH	1.000E+011	0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346		
PLOG/ 0.0100	1.020E+013	-0.158
PLOG/ 0.1000	4.980E+014	-0.642
PLOG/ 1.0000	7.770E+017	-1.520
PLOG/ 10.0000	2.930E+015	-0.684
PLOG/ 100.0000	1.640E+004	2.740

IC4H7+HO2<=>IC4H7OOH 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0100 1.910E+031 -7.230 1336.2/
 PLOG/ 0.1000 6.310E+042 -10.300 5568.9/
 PLOG/ 1.0000 1.030E+045 -10.600 7851.5/
 PLOG/ 10.0000 2.790E+037 -7.920 6497.9/
 PLOG/ 100.0000 1.440E+032 -6.010 6053.6/

IC4H7+HO2<=>IC3H5CHO+H2O 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0100 1.090E+000 3.010 -3421.1/
 PLOG/ 0.1000 6.350E+001 2.500 -2341.4/
 PLOG/ 1.0000 6.050E+005 1.390 595.1/
 PLOG/ 10.0000 3.100E+005 1.590 2677.6/
 PLOG/ 100.0000 5.070E-005 4.590 927.5/

IC4H7OOH<=>IC3H5CHO+H2O 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0100 1.990E+050 -12.700 53531.9/
 PLOG/ 0.1000 4.720E+047 -11.500 54360.9/
 PLOG/ 1.0000 1.500E+040 -8.840 53179.2/
 PLOG/ 10.0000 2.540E+028 -5.000 49919.4/
 PLOG/ 100.0000 1.480E+016 -1.120 45949.3/

IC4H7OOH<=>IC4H7O+OH 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0100 1.490E+058 -13.900 54266.9/
 PLOG/ 0.1000 1.800E+054 -12.400 54193.8/
 PLOG/ 1.0000 3.360E+046 -9.810 52468.5/
 PLOG/ 10.0000 2.390E+036 -6.540 49429.0/
 PLOG/ 100.0000 1.280E+027 -3.610 46333.1/

IC4H7O<=>C3H5-T+CH2O 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0010 7.260E+006 0.182 17815.5/
 PLOG/ 0.0100 6.970E+016 -2.500 20878.7/
 PLOG/ 0.1000 6.640E+023 -4.230 23565.0/
 PLOG/ 1.0000 1.070E+026 -4.560 24622.9/
 PLOG/ 10.0000 6.500E+029 -5.370 26645.0/
 PLOG/ 100.0000 4.630E+031 -5.590 28915.3/
 PLOG/ 1000.0000 8.520E+025 -3.610 27863.4/

IC4H7O<=>IC3H5OCH2 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0010 3.170E+020 -4.150 12121.3/
 PLOG/ 0.0100 4.790E+024 -5.030 14606.1/
 PLOG/ 0.1000 1.900E+026 -5.160 16124.4/
 PLOG/ 1.0000 1.510E+028 -5.400 18165.4/
 PLOG/ 10.0000 2.420E+028 -5.170 19691.2/
 PLOG/ 100.0000 5.570E+024 -3.860 19395.2/
 PLOG/ 1000.0000 1.350E+018 -1.730 17386.5/

IC4H7O<=>IC3H6CHO 1.000E+011 0.000
 0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG/ 0.0010 5.250E-049 15.500 -15639.9/
 PLOG/ 0.0100 1.460E-088 27.600 -35995.0/
 PLOG/ 0.1000 4.440E-022 8.380 -3819.0/

PLOG/	1.0000	6.230E+012	-1.440	10829.2/	
PLOG/	10.0000	3.480E+042	-9.910	25297.9/	
PLOG/	100.0000	1.880E+038	-8.160	25974.5/	
PLOG/	1000.0000	1.670E+021	-2.740	20337.7/	
IC4H7O<=>IC3H5CHO+H					1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
PLOG/	0.0010	3.000E+015	-2.310	14667.9/	
PLOG/	0.0100	1.500E+022	-3.960	18283.0/	
PLOG/	0.1000	1.950E+023	-3.990	19143.3/	
PLOG/	1.0000	1.150E+025	-4.240	20311.2/	
PLOG/	10.0000	1.760E+028	-4.890	22765.2/	
PLOG/	100.0000	1.410E+027	-4.280	23770.6/	
PLOG/	1000.0000	2.570E+020	-2.060	22040.1/	
IC4H7O<=>C3H6+HCO					1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
PLOG/	0.0010	6.620E+016	-2.840	13197.0/	
PLOG/	0.0100	1.260E+020	-3.530	15469.2/	
PLOG/	0.1000	2.130E+021	-3.640	16584.5/	
PLOG/	1.0000	1.070E+024	-4.160	18985.0/	
PLOG/	10.0000	8.420E+025	-4.400	22382.6/	
PLOG/	100.0000	1.860E+021	-2.730	23658.8/	
PLOG/	1000.0000	4.750E+008	1.140	20922.5/	
IC3H5OCH2<=>C3H5-T+CH2O					1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
PLOG/	0.0010	3.300E+009	-0.638	19747.8/	
PLOG/	0.0100	3.360E+021	-3.900	23945.2/	
PLOG/	0.1000	2.910E+029	-5.900	27249.7/	
PLOG/	1.0000	1.830E+034	-6.940	30690.4/	
PLOG/	10.0000	9.720E+033	-6.500	33002.5/	
PLOG/	100.0000	2.680E+027	-4.260	33305.6/	
PLOG/	1000.0000	8.810E+014	-0.326	31553.1/	
IC3H5OCH2<=>IC3H6CHO					1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
PLOG/	0.0010	8.010E-092	27.800	-37321.2/	
PLOG/	0.0100	7.780E-011	3.700	-2766.9/	
PLOG/	0.1000	5.110E+015	-2.760	15937.6/	
PLOG/	1.0000	4.480E+025	-5.200	21532.2/	
PLOG/	10.0000	3.970E+034	-7.410	28116.9/	
PLOG/	100.0000	5.620E+022	-3.560	25806.7/	
PLOG/	1000.0000	2.510E+020	-2.630	29288.4/	
IC3H5OCH2<=>IC3H5CHO+H					1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
PLOG/	0.0010	4.930E+024	-5.050	20108.4/	
PLOG/	0.0100	2.140E+028	-5.800	22219.4/	
PLOG/	0.1000	1.930E+032	-6.640	25108.2/	
PLOG/	1.0000	8.600E+034	-7.110	28209.1/	
PLOG/	10.0000	2.170E+034	-6.640	30647.6/	
PLOG/	100.0000	4.170E+028	-4.710	31231.9/	
PLOG/	1000.0000	3.980E+018	-1.620	30129.8/	
IC3H5OCH2<=>C3H6+HCO					1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346					
PLOG/	0.0010	8.230E+026	-5.840	19356.9/	

PLOG/	0.0100	1.320E+029	-6.210	21293.6/
PLOG/	0.1000	3.470E+032	-6.960	24197.3/
PLOG/	1.0000	1.440E+036	-7.760	28007.8/
PLOG/	10.0000	9.720E+037	-8.020	32394.6/
PLOG/	100.0000	2.430E+031	-5.810	34295.8/
PLOG/	1000.0000	3.730E+014	-0.726	32008.3/
IC3H6CHO<=>C3H5-T+CH2O				1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346				
PLOG/	0.0010	6.890E-069	21.500	2638.0/
PLOG/	0.0100	5.340E-033	11.100	16749.1/
PLOG/	0.1000	6.110E+026	-6.010	44116.7/
PLOG/	1.0000	8.040E+035	-8.310	46919.7/
PLOG/	10.0000	5.520E+040	-9.190	50508.7/
PLOG/	100.0000	5.850E+035	-7.180	52038.4/
PLOG/	1000.0000	1.930E+019	-1.940	48440.0/
IC3H6CHO<=>IC3H5CHO+H				1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346				
PLOG/	0.0010	1.610E+010	-1.240	32371.3/
PLOG/	0.0100	5.840E+015	-2.610	32878.4/
PLOG/	0.1000	3.640E+023	-4.600	34275.3/
PLOG/	1.0000	7.580E+031	-6.630	37895.4/
PLOG/	10.0000	2.860E+032	-6.300	39990.7/
PLOG/	100.0000	1.570E+023	-3.140	38011.7/
PLOG/	1000.0000	4.520E+012	0.214	34570.5/
IC3H6CHO<=>C3H6+HCO				1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346				
PLOG/	0.0010	2.900E+032	-7.240	25687.5/
PLOG/	0.0100	5.300E+033	-7.280	27100.6/
PLOG/	0.1000	2.000E+035	-7.410	29027.3/
PLOG/	1.0000	1.010E+034	-6.700	30018.1/
PLOG/	10.0000	9.760E+027	-4.630	28923.9/
PLOG/	100.0000	2.110E+019	-1.850	26239.8/
PLOG/	1000.0000	1.590E+013	0.063	24086.3/
C3H5-T+CH2O<=>IC3H5CHO+H				1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346				
PLOG/	0.0010	2.600E+004	2.260	1510.3/
PLOG/	0.0100	5.130E+004	2.170	1675.5/
PLOG/	0.1000	3.990E+005	1.910	2218.3/
PLOG/	1.0000	1.750E+007	1.450	3428.0/
PLOG/	10.0000	1.350E+009	0.933	5173.0/
PLOG/	100.0000	2.240E+011	0.357	8001.3/
PLOG/	1000.0000	6.010E+005	2.090	7895.6/
C3H5-T+CH2O<=>C3H6+HCO				1.000E+011 0.000
0.0 !AUTHOR: !REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346				
PLOG/	0.0010	1.110E+007	1.090	1807.2/
PLOG/	0.0100	2.470E+007	0.993	1994.9/
PLOG/	0.1000	2.470E+008	0.704	2596.2/
PLOG/	1.0000	1.420E+010	0.209	3934.2/
PLOG/	10.0000	3.450E+013	-0.726	6944.3/
PLOG/	100.0000	3.310E+014	-0.866	10965.7/
PLOG/	1000.0000	1.650E+001	3.170	9399.8/

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!\REACTIONCLASS: \R_CH3O2_PRODUCTS           \A           \N
\EA
!
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IC4H7+CH3O2<=>IC4H7O+CH3O           1.000E+011      0.000
0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2
PLOG/      0.0100      3.330E+012      -0.158      -1417.0/
PLOG/      0.1000      1.660E+014      -0.642      -349.1/
PLOG/      1.0000      2.595E+017      -1.520      2379.2/
PLOG/     10.0000      9.780E+014      -0.684      3615.3/
PLOG/    100.0000      5.470E+003       2.740      1144.4/
IC4H7+CH3O2<=>IC4H7OOCH3           1.000E+011      0.000
0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2
PLOG/      0.0100      1.910E+031      -7.230      1336.2/
PLOG/      0.1000      6.310E+042     -10.300      5568.9/
PLOG/      1.0000      1.030E+045     -10.600      7851.5/
PLOG/     10.0000      2.790E+037      -7.920      6497.9/
PLOG/    100.0000      3.400E+029      -5.280      4539.8/
IC4H7OOCH3<=>IC4H7O+CH3O           1.000E+011      0.000
0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2
PLOG/      0.0100      1.490E+058     -13.900     54266.9/
PLOG/      0.1000      1.800E+054     -12.400     54193.8/
PLOG/      1.0000      3.360E+046      -9.810     52468.5/
PLOG/     10.0000      2.390E+036      -6.540     49429.0/
PLOG/    100.0000      2.560E+027      -3.610     46333.1/

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!\REACTIONCLASS: \R_IC4H7O2_PRODUCCTS       \A           \N
\EA
!
-----
IC4H7O2+IC4H7<=>IC4H7O+IC4H7O           1.000E+011
0.000      0.0 !\AUTHOR: !\ ANALOGY TO IC4H7+HO2 DIVIDED 4
PLOG/      0.0100      2.55E+12       -0.158     -1417.0/
PLOG/      0.1000      1.25E+14       -0.642     -349.1/
PLOG/      1.0000      1.94E+17       -1.520     2379.2/
PLOG/     10.0000      7.33E+14       -0.684     3615.3/
PLOG/    100.0000      4.10E+03       2.740     1144.4/
IC4H7O2+IC4H7<=>IC4H7OOIC4H7         1.000E+011
0.000      0.0 !\AUTHOR: !\ ANALOGY TO IC4H7+HO2 DIVIDED 4
PLOG/      0.0100      4.78E+30       -7.230     1336.2/
PLOG/      0.1000      1.58E+42      -10.300     5568.9/
PLOG/      1.0000      2.58E+44      -10.600     7851.5/
PLOG/     10.0000      6.98E+36       -7.920     6497.9/
PLOG/    100.0000      3.60E+31       -6.010     6053.6/
IC4H7OOIC4H7<=>IC4H7O+IC4H7O         1.000E+011
0.000      0.0 !\AUTHOR: !\ ANALOGY TO IC4H7+HO2 DIVIDED 4
PLOG/      0.0100      3.73E+57      -13.900     54266.9/
PLOG/      0.1000      4.50E+53      -12.400     54193.8/
PLOG/      1.0000      8.40E+45       -9.810     52468.5/
PLOG/     10.0000      5.98E+35       -6.540     49429.0/
PLOG/    100.0000      3.20E+26       -3.610     46333.1/

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!\REACTIONCLASS: \R_RO2                   \A           \N
\EA

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!

IC4H7+NC3H7O2<=>IC4H7O+NC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC4H7+PC4H9O2<=>IC4H7O+PC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC4H7+SC4H9O2<=>IC4H7O+SC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC4H7+IC3H7O2<=>IC4H7O+IC3H7O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		
IC4H7+TC4H9O2<=>IC4H7O+TC4H9O	7.000E+012	0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE		

!

!\REACTIONCLASS: \RA_RA_RECOMBINATION \A
 \N \EA
 !

IC4H7+IC4H7<=>C3H4-A+AC5H10		9.550E+040
-9.300 12470.0 !\AUTHOR: \REF: FRIDLAND ET AL. J. PHYS. CHEM. A,		
2013, 117, 4750-4761		
PLOG/ 1.0000 4.10E+40 -9.300 12470.0/		
PLOG/ 4.0000 3.41E+32 -6.800 9180.0/		
PLOG/ 10.0000 1.26E+28 -5.500 7410.0/		
IC4H7+IC4H7<=>H15DE25DM	1.000E+011	0.000
0.0 !AUTHOR: ! ANALOGY FROM PROPENE, DEVIDED BY 2.3		
PLOG/ 0.039 3.27E+64 -15.935 20230/		
PLOG/ 0.078 7.50E+59 -14.49 18600/		
PLOG/ 0.156 1.14E+55 -12.995 16700/		
H15DE25DM+H<=>H15DE25DM-S+H2		1.42E+06
2.315165407 2075.955844 !\AUTHOR: !\REF:		
H15DE25DM+O2<=>H15DE25DM-S+HO2		4.000E+014
0.000 38890.0 !\AUTHOR: !\REF:		
H15DE25DM+O<=>H15DE25DM-S+OH		1.59243E+11
0.7 1.30E+01 !\AUTHOR: !\REF:		
H15DE25DM+OH<=>H15DE25DM-S+H2O		8.95E+04
2.636965672 -6.0 !\AUTHOR: !\REF:		
H15DE25DM+HO2<=>H15DE25DM-S+H2O2		1.00E+00
3.887366896 9386.357213 !\AUTHOR: !\REF:		
H15DE25DM+CH3<=>H15DE25DM-S+CH4		1.00E+00
3.649020008 3374.05195 !\AUTHOR: !\REF:		
H15DE25DM+H<=>H15DE25DM-A+H2		7.29E+05
2.455 4361.2 !\AUTHOR: !\REF:		
H15DE25DM+O2<=>H15DE25DM-A+HO2		1.86E+9
1.301 40939 !\AUTHOR: !\REF:		
H15DE25DM+O<=>H15DE25DM-A+OH		1.05E+12
0.700 5884.0 !\AUTHOR: !\REF:		
H15DE25DM+OH<=>H15DE25DM-A+H2O		2.53E+05
2.46 729.44 !\AUTHOR: !\REF:		
H15DE25DM+HO2<=>H15DE25DM-A+H2O2		2.92E-01
4.12 12802.0 !\AUTHOR: !\REF:		
H15DE25DM+CH3<=>H15DE25DM-A+CH4		4.420E+000
3.500 5675.0 !\AUTHOR: !\REF:		
C3H5-T+B13DE2M<=>H15DE25DM-S	7.07E+03	2.48
6130 !\AUTHOR: !\REF:C ZHOU ESTIMATEDG		
C3H4-A+AC5H9-D<=>H15DE25DM-A	2.84E+04	2.5
8847.5 !\AUTHOR: !\REF: C ZHOU CALCULATED AT		

QCISD(T)/CBS//M062X/6-311++G(D,P) LEVEL OF THEORY

H15DE25DM-S+HO2<=>H15DE25DM-SO+OH -1000.0	!	\AUTHOR: !\REF:	7.000E+012	0.000
IC3H5CHO+IC4H7<=>H15DE25DM-SO 6329.74	!	\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275	2.5E+010	0.00
C3H5-T+IC4H7CHO<=>H15DE25DM-SO 15526.42	!	\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4) (2006) 250-275	2.5E+010	0.00
IC4H7CHO+OH=>CH2CHO+C3H4-A+H2O 2.46 729.44	!	\AUTHOR: !\REF:	5.064E+07	
H15DE25DM-A+HO2<=>H15DE25DM-AO+OH -1000.0	!	\AUTHOR: !\REF: THE SAME AS ALLYL+HO2	7.000E+012	0.000
H15DE2M-T+CH2O<=>H15DE25DM-AO 4786.58	!	\AUTHOR: !\REF: ESTIMATE BASED ON CURRAN IJCK 2006, 38, 250	2.5E+010	0.00
IC4H7+C3H4-A<=>H15DE2M-T 6130.0	!	\AUTHOR: !\REF: ESTIMATE BASED ON CURRAN IJCK 2006, 38, 250	8.8E+03	2.48
!				

!\REACTIONCLASS: \RS_R_PRODUCTS	\A	\N
\EA		
!		

IC4H7-I1+H<=>C3H4-A+CH4 0.0	!	\AUTHOR: !\REF: DAGAUT, P. ET AL., CST 71, 111 (1990).	3.333E+012	0.000
IC4H7-I1+H<=>C3H4-P+CH4 0.0	!	\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000	3.340E+012	0.000
IC4H7-I1+O<=>C3H6+HCO 0.0	!	\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000	6.000E+013	0.000
IC4H7-I1+OH=>C3H6+HCO+H 0.0	!	\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000	5.000E+012	0.000
IC4H7-I1+HO2=>C3H6+HCO+OH 0.0	!	\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000	2.000E+013	0.000
IC4H7-I1+HCO<=>IC4H8+CO 0.0	!	\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000	9.000E+013	0.000
IC4H7-I1+CH3<=>C3H4-P+C2H6 0.0	!	\AUTHOR: !\REF: LASKIN ET AL. IJCK 32 589-614 2000	1.000E+011	0.000
!				

!\REACTIONCLASS: \RS_O2_PRODUCTS	\A	\N
\EA		
!		

IC4H7-I1+O2<=>CH3COCH3+HCO 5748.4	!	\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN	3.100E+031	-5.944
IC4H7-I1+O2<=>TC3H6CHO+O 5142.9	!	\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN	5.380E+018	-2.140
IC4H7-I1+O2<=>IC3H5CHO+OH 5142.9	!	\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN	2.700E+019	-2.140
!				

!\REACTIONCLASS: \RA_O2	\A	\N
\EA		
!		

IC4H7+O2<=>IC4H7O2 1.09E+010 0.56725
2290 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
IC4H7+O<=>IC3H5CHO+H 6.030E+013 0.000
0.0!\AUTHOR: !\REF: CURRAN ESTIMATE
!

!\REACTIONCLASS: \RAO2_ISOMERISATION \A \N
\EA
!

IC4H7O2<=>IC4H6OOH-I 1.41E+005 1.83586
19820 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
IC4H7O2<=>CCYCCOOC-T1 1.19E+008 0.80412
28020 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
IC4H7O2<=>C2CYCOOC-I1 1.07E+008 0.89161
29720 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
!

!\REACTIONCLASS: \RAO2_DECOMPOSITION \A \N
\EA
!

IC4H7O2<=>IC4H7O+O 1.82E+014 0.0
60620 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
IC4H7O2<=>IC3H5CHO+OH 1.52E+009 1.02524
39460 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
!

!\REACTIONCLASS: \RAO2_ISOMERISATION_PRODUCTS_DECOMP \A \N
\EA
!

IC4H6OOH-I<=>CVCYCCOC+OH 6.82E+012 -0.34545
42140 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
IC4H6OOH-I<=>C3H4-A+CH2O2H 1.18E+012 0.91203
51390 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
IC4H6OOH-I<=>IC3H5CHO+OH 2.42E+009 0.87390
54090 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
CCYCCOOC-T1<=>CCYCC2OCO 4.56E+011 0.92729
17470 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
CCYCCOOC-T1<=>CCYCCOOC-I2 3.56E+013 0.0
38820 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.
CCYCCOOC-I2<=>CHOIC3H6O 3.19E+014 0.0
3000 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
A., 2000, 104, 9715-9732.

C2CYCOOC-I1<=>IC3H5OOCH2 4.41E+013 -0.22618
 18500 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
 A., 2000, 104, 9715-9732.
 IC3H5OOCH2<=>CH3COCH2+CH2O 1.41E+010 0.0
 1000 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
 A., 2000, 104, 9715-9732.
 CHOIC3H6O<=>CH3CHCHO+CH2O 4.30E+012 0.0
 9780 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
 A., 2000, 104, 9715-9732.
 CCYC2OCO<=>CCYCCO-T1+CH2O 1.74E+013 0.0
 18150 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
 A., 2000, 104, 9715-9732.
 C2CYCOOC-I1<=>CCYC2OCO 1.21E+013 0.10180
 20320 !\AUTHOR: !\REF: CHIUNG-JU CHEN AND J. W. BOZZELLI, J. PHYS. CHEM.
 A., 2000, 104, 9715-9732.

!

!\REACTIONCLASS: \RAO2_RAO2 \A \N
 \EA

!

IC4H7O2+IC4H7O2=>IC4H7O+IC4H7O+O2 1.40E+16 -1.61
 1860.0 !\AUTHOR: !\REF: ALKANES ESTIMATED
 ! IC4H8+HO2<=>IC4H7+H2O2 DIVIDED BY 2
 IC4H7O2+IC4H8<=>IC4H7+IC4H7OOH 1.46E-01 4.12
 12802.0

!

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
 \EA

!

IC4H8+H<=>IC4H9 1.000E+000 1.000
 0.0 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117,
 2718-2727
 PLOG/ 0.0013 7.990E+081 -23.161 22239.0/
 PLOG/ 0.0400 4.240E+068 -18.427 19665.0/
 PLOG/ 1.0000 1.040E+049 -11.500 15359.0/
 PLOG/ 10.0000 6.200E+041 -8.892 14637.0/
 !PLOG/ 100.0000 -6.450E+031 -5.851 8177.8/

DUP

IC4H8+H<=>IC4H9 1.000E+000 1.000
 0.0 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117,
 2718-2727
 PLOG/ 0.0013 1.850E+026 -5.830 3865.8/
 PLOG/ 0.0400 2.820E+030 -6.490 5470.8/
 PLOG/ 1.0000 3.780E+028 -5.570 5625.1/
 PLOG/ 10.0000 1.460E+025 -4.280 5247.8/
 PLOG/ 100.0000 4.220E+027 -4.390 9345.8/ !REF: REFIT TO

ONE PARAMETER TO AVOID PROBLEMS WITH NEGATIVE K

DUP

IC4H8+H<=>TC4H9 1.000E+000 1.000
 1.0 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117,
 2718-2727
 PLOG/ 0.0013 1.350E+044 -10.680 8196.4/
 PLOG/ 0.0400 2.110E+057 -14.230 15147.0/
 PLOG/ 1.0000 3.260E+061 -14.940 20161.0/
 PLOG/ 10.0000 5.300E+056 -13.120 20667.0/

PLOG/ 100.0000 1.110E+050 -10.800 20202.0/
 DUP
 IC4H8+H<=>TC4H9 1.000E+000 1.000
 1.0 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117,
 2718-2727
 PLOG/ 0.0013 2.170E+130 -32.580 136140.0/
 PLOG/ 0.0400 2.250E+029 -5.840 4241.9/
 PLOG/ 1.0000 1.060E+030 -5.630 5613.4/
 PLOG/ 10.0000 6.110E+026 -4.440 5182.3/
 PLOG/ 100.0000 2.730E+023 -3.260 4597.0/

DUP
 !DIVIDED BY 3 TO HAVE BETTER PREDICTION OF PROPENE IN FR
 IC4H8+H<=>C3H6+CH3 1.000E+000 1.000
 1.0 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117,
 2718-2727
 PLOG/ 0.0013 5.13E+08 1.350 2542.0/
 PLOG/ 0.0400 2.63E+10 0.870 3599.6/
 PLOG/ 1.0000 8.90E+11 0.470 5431.1/
 PLOG/ 10.0000 3.08E+22 -2.600 12898.0/
 PLOG/ 100.0000 4.40E+22 -2.420 16500.0/

DUP
 IC4H8+H<=>C3H6+CH3 1.000E+000 1.000
 1.0 !AUTHOR: !REF: MILLER AND KLIPPENSTEIN |J. PHYS. CHEM. A 2013, 117,
 2718-2727
 PLOG/ 0.0013 7.70E+02 1.350 2542.0/
 PLOG/ 0.0400 3.94E+04 0.870 3599.6/
 PLOG/ 1.0000 1.34E+06 0.470 5431.1/
 PLOG/ 10.0000 4.13E+04 2.520 3679.1/
 PLOG/ 100.0000 8.37E+02 2.910 3980.9/

DUP

!

!\REACTIONCLASS: \RADICAL_ADDITION\HO2 \A \N
 \EA

!

IC4H8+HO2<=>TC4H9O2 1.04E-01 3.45
 4338.0 !\AUTHOR: !\REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
 IC4H8+HO2<=>IC4H8O2H-T 1.64E4 2.43
 8300 !\AUTHOR: !\ REF: VILLANO, S, M.; CARSTENSEN, H-H.; DEAN, A. M. J.
 PHYS. CHEM. A., 2013, 117, 6458.
 IC4H8+HO2<=>TC4H8O2H-I 1.000E+011 0.000
 0.0 !\AUTHOR: !\REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
 PLOG/ 0.013 6.67E+14 -2.14 14188/
 PLOG/ 0.9869 6.25E+06 0.64 9073 /
 PLOG/ 9.869 7.96E+06 0.82 8771 /
 PLOG/ 98.69 2.05E+13 -0.82 12919/
 IC4H8+HO2<=>IC4H8O+OH 1.000E+011 0.000
 0.0 !\AUTHOR: !\REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
 PLOG/ 0.013 1.18E+04 2.29 11321/
 PLOG/ 0.9869 5.30E+04 2.10 11797/
 PLOG/ 9.869 1.47E+09 0.83 14808/
 PLOG/ 98.69 1.96E+17 -1.45 21195/
 TC4H8O2H-I<=>IC4H8O+OH 1.000E+011 0.000
 0.0 !\AUTHOR: !\REF: ZADOR (J. PHYS. CHEM. A., 2011,115,10218)
 PLOG/ 0.013 5.23E+17 -2.97 8215/
 PLOG/ 0.9869 4.39E+22 -3.90 11424/
 PLOG/ 9.869 4.00E+25 -4.50 13952/

PLOG/ 98.69 1.21E+27 -4.66 16324/
!

!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N
\EA
!

IC4H8+O<=>IC3H7+HCO 7.450E+006 1.880
183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4
IC4H8+O=>CH2CO+CH3+CH3 3.050E+006 1.880
183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4
IC4H8+O=>IC3H6CO+H+H 3.050E+006 1.880
183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4
!

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA
!

IC4H8+OH<=>IC4H7OH+H 2.290E+013 0.070
10580.0 !AUTHOR: ! ANALOGY TO C3H6+OH
PLOG/ 0.0013 2.670E+013 0.050 10611.0/
PLOG/ 0.0100 2.750E+013 0.050 10623.0/
PLOG/ 0.0130 2.870E+013 0.040 10634.0/
PLOG/ 0.0250 1.590E+014 -0.160 11125.0/
PLOG/ 0.1000 3.100E+014 -0.220 11407.0/
PLOG/ 0.1315 3.780E+014 -0.240 11458.0/
PLOG/ 1.0000 9.150E+007 1.420 10087.0/
PLOG/ 10.0000 3.660E+005 2.140 10410.0/
PLOG/ 100.0000 8.190E+002 2.840 10481.0/
IC4H8+OH<=>SC3H5OH+CH3 1.290E+006 1.650
1233.0 !AUTHOR: ! ANALOGY TO C3H6+OH
PLOG/ 0.0013 5.16E+05 1.650 1233.0/
PLOG/ 0.0100 7.28E+03 2.100 1162.0/
PLOG/ 0.0130 8.16E+02 2.480 1128.0/
PLOG/ 0.0250 1.15E+02 2.800 1152.0/
PLOG/ 0.1000 5.60E+00 3.210 1208.0/
PLOG/ 0.1315 3.08E+00 3.290 1216.0/
PLOG/ 1.0000 4.52E+03 2.500 3238.0/
PLOG/ 10.0000 9.64E+18 -1.740 13107.0/
PLOG/ 100.0000 1.32E-01 3.700 3665.0/
IC4H8+OH<=>IC3H5OH+CH3 1.290E+006 1.650
1233.0 !AUTHOR: ! ANALOGY TO C3H6+OH
PLOG/ 0.0013 2.06E+06 1.650 1233.0/
PLOG/ 0.0100 2.91E+04 2.100 1162.0/
PLOG/ 0.0130 3.26E+03 2.480 1128.0/
PLOG/ 0.0250 4.61E+02 2.800 1152.0/
PLOG/ 0.1000 2.24E+01 3.210 1208.0/
PLOG/ 0.1315 1.23E+01 3.290 1216.0/
PLOG/ 1.0000 1.81E+04 2.500 3238.0/
PLOG/ 10.0000 3.86E+19 -1.740 13107.0/
PLOG/ 100.0000 5.28E-01 3.700 3665.0/
IC4H8+OH<=>SC4H7OH-I+H 2.870E+000 2.920
625.0 !AUTHOR: ! ANALOGY TO C3H6+OH
PLOG/ 0.0013 2.870E+000 2.920 625.0/
PLOG/ 0.0100 4.840E-001 2.980 704.0/
PLOG/ 0.0130 3.130E-001 3.040 721.0/
PLOG/ 0.0250 9.330E-003 3.620 677.0/

PLOG/	0.1000	4.640E-005	4.480	687.0/	
PLOG/	0.1315	2.710E-005	4.560	707.0/	
PLOG/	1.0000	7.650E-007	5.050	874.0/	
PLOG/	10.0000	2.640E+015	-0.800	12728.0/	
PLOG/	100.0000	4.870E-004	4.320	4020.0/	
IC4H8+OH<=>CH3COCH3+CH3				6.930E+005	1.490
-536.0 !AUTHOR: ! ANALOGY TO C3H6+OH					
PLOG/	0.0013	6.930E+005	1.490	-536.0/	
PLOG/	0.0100	5.940E+003	2.010	-560.0/	
PLOG/	0.0130	1.100E+003	2.220	-680.0/	
PLOG/	0.0250	1.070E+002	2.500	-759.0/	
PLOG/	0.1000	7.830E-001	3.100	-919.0/	
PLOG/	0.1315	3.070E-001	3.220	-946.0/	
PLOG/	1.0000	3.160E-004	4.050	-1144.0/	
PLOG/	10.0000	7.590E-006	4.490	-680.0/	
PLOG/	100.0000	5.450E-005	4.220	1141.0/	
IC4H8+OH<=>IC4H8OH-IT				5.100E+054	-20.700
32402.0 !AUTHOR: ! ANALOGY TO C3H6+OH					
PLOG/	0.0013	2.300E+078	-20.700	32402.0/	
PLOG/	0.0100	2.740E+077	-20.000	33874.0/	
PLOG/	0.0130	1.070E+076	-19.580	32874.0/	
PLOG/	0.0250	3.680E+073	-18.790	31361.0/	
PLOG/	0.1000	1.040E+068	-17.010	27909.0/	
PLOG/	0.1315	7.230E+066	-16.640	27162.0/	
PLOG/	1.0000	1.950E+059	-14.170	23079.0/	
PLOG/	10.0000	7.580E+053	-12.230	22976.0/	
PLOG/	100.0000	1.430E+048	-10.230	23772.0/	
DUP					
IC4H8+OH<=>IC4H8OH-IT				1.420E+036	-15.840
11594.0 !AUTHOR: ! ANALOGY TO C3H6+OH					
PLOG/	0.0013	6.410E+059	-15.840	11594.0/	
PLOG/	0.0100	7.280E+059	-15.510	12898.0/	
PLOG/	0.0130	2.790E+059	-15.340	12913.0/	
PLOG/	0.0250	2.650E+058	-14.930	12936.0/	
PLOG/	0.1000	1.350E+056	-14.040	12945.0/	
PLOG/	0.1315	3.980E+055	-13.850	12887.0/	
PLOG/	1.0000	1.550E+050	-12.040	11493.0/	
PLOG/	10.0000	6.410E+041	-9.350	8921.0/	
PLOG/	100.0000	2.300E+032	-6.310	6088.0/	
DUP					
IC4H8+OH<=>IC4H8OH-TI				5.100E+054	-20.700
32402.0 !AUTHOR: ! ANALOGY TO C3H6+OH					
PLOG/	0.0013	2.140E+059	-15.840	11594.0/	
PLOG/	0.0100	2.430E+059	-15.510	12898.0/	
PLOG/	0.0130	9.300E+058	-15.340	12913.0/	
PLOG/	0.0250	8.830E+057	-14.930	12936.0/	
PLOG/	0.1000	4.500E+055	-14.040	12945.0/	
PLOG/	0.1315	1.330E+055	-13.850	12887.0/	
PLOG/	1.0000	5.180E+049	-12.040	11493.0/	
PLOG/	10.0000	2.140E+041	-9.350	8921.0/	
PLOG/	100.0000	7.650E+031	-6.310	6088.0/	
DUP					
IC4H8+OH<=>IC4H8OH-TI				1.420E+036	-15.840
11594.0 !AUTHOR: ! ANALOGY TO C3H6+OH					
PLOG/	0.0013	7.680E+077	-20.700	32402.0/	
PLOG/	0.0100	9.130E+076	-20.000	33874.0/	
PLOG/	0.0130	3.550E+075	-19.580	32874.0/	
PLOG/	0.0250	1.230E+073	-18.790	31361.0/	

PLOG/	0.1000	3.450E+067	-17.010	27909.0/
PLOG/	0.1315	2.410E+066	-16.640	27162.0/
PLOG/	1.0000	6.500E+058	-14.170	23079.0/
PLOG/	10.0000	2.530E+053	-12.230	22976.0/
PLOG/	100.0000	4.780E+047	-10.230	23772.0/

DUP

!

!\REACTIONCLASS: \ROH_O2	\A	\N	\EA
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IC4H8OH-IT+O2<=>TQJC4H8OH 1.420E+036 -15.840 11594.0

!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.05E+114	-33.81	24741/
PLOG/	0.01	2.13E+114	-33.44	26448/
PLOG/	0.1	1.62E+110	-31.75	26612/
PLOG/	1	6.00E+101	-28.79	25197/
PLOG/	10	5.36E+89	-24.76	22402/
PLOG/	40	1.55E+81	-21.95	20197/
PLOG/	100	1.51E+75	-20	18578/
PLOG/	200	3.16E+70	-18.48	17287/

IC4H8OH-IT+O2<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0

!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.21E+26	-5.09	5755/
PLOG/	0.01	1.41E+31	-6.55	8781/
PLOG/	0.1	5.08E+34	-7.53	11702/
PLOG/	1	1.67E+34	-7.27	13418/
PLOG/	10	2.82E+28	-5.41	13318/
PLOG/	40	2.50E+22	-3.52	12314/
PLOG/	100	2.82E+17	-1.99	11286/
PLOG/	200	1.93E+13	-0.71	10340/

DUP

IC4H8OH-IT+O2<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0 !AUTHOR:

! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	2.45E+21	-4.19	6837/
PLOG/	0.01	1.40E+30	-6.75	11554/
PLOG/	0.1	9.11E+39	-9.56	17834/
PLOG/	1	5.16E+42	-10.17	22412/
PLOG/	10	6.07E+32	-6.94	22738/
PLOG/	40	3.88E+20	-3.14	20677/
PLOG/	100	3.32E+10	-0.03	18552/
PLOG/	200	1.22E+02	2.57	16623/

DUP

IC4H8OH-IT+O2<=>SC4H7OH-I+HO2 1.420E+036 -15.840 11594.0

!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.26E+25	-4.69	5755/
PLOG/	0.01	1.44E+30	-6.15	8785/
PLOG/	0.1	4.78E+33	-7.11	11695/
PLOG/	1	1.40E+33	-6.84	13395/
PLOG/	10	2.12E+27	-4.96	13277/
PLOG/	40	1.78E+21	-3.07	12265/
PLOG/	100	1.97E+16	-1.53	11234/
PLOG/	200	1.32E+12	-0.25	10285/

DUP

IC4H8OH-IT+O2<=>SC4H7OH-I+HO2 1.420E+036 -15.840 11594.0

!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	3.22E+23	-4.69	5341/
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PLOG/	0.01	4.80E+28	-6.18	8461/
PLOG/	0.1	1.71E+32	-7.16	11410/
PLOG/	1	1.53E+32	-7.02	13378/
PLOG/	10	5.55E+29	-6.14	15100/
PLOG/	40	1.72E+26	-4.97	15849/
PLOG/	100	4.46E+21	-3.51	15644/
PLOG/	200	5.06E+16	-1.96	14979/
DUP				
IC4H8OH-IT+O2<=>TQC4H8OI 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	6.36E+104	-33.74	22390/
PLOG/	0.01	7.96E+103	-33.01	22966/
PLOG/	0.1	6.99E+96	-30.48	20584/
PLOG/	1	1.04E+88	-27.47	16629/
PLOG/	10	3.13E+96	-29.62	20346/
PLOG/	40	2.79E+105	-32.04	24971/
PLOG/	100	4.64E+109	-33.12	27657/
PLOG/	200	2.06E+111	-33.48	29197/
IC4H8OH-IT+O2=>CH3COCH3+CH2O+OH 1.420E+036 -15.840 11594.0				
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	3.03E+37	-8.35	6940/
PLOG/	0.01	1.07E+42	-9.64	9965/
PLOG/	0.1	9.22E+43	-10.12	12427/
PLOG/	1	1.14E+42	-9.42	13806/
PLOG/	10	1.80E+38	-8.13	15131/
PLOG/	40	1.61E+34	-6.8	15691/
PLOG/	100	7.00E+29	-5.41	15552/
PLOG/	200	3.74E+25	-4.06	15118/
IC4H8OH-IT+O2<=>QC4H7OHP 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	1.18E+118	-37.6	26229 /
PLOG/	0.01	1.91E+131	-40.73	34079/
PLOG/	0.1	5.81E+138	-42.17	40750/
PLOG/	1	5.05E+134	-40.19	43580/
PLOG/	10	2.07E+117	-34.26	41516/
PLOG/	40	1.71E+101	-29.04	38094/
PLOG/	100	1.25E+89	-25.15	35203/
PLOG/	200	2.98E+79	-22.09	32802/
IC4H8OH-IT+O2<=>CCY(CCO)COH+OH 1.420E+036 -15.840 11594.0				
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	2.11E+18	-2.87	6870/
PLOG/	0.01	3.02E+27	-5.54	11842/
PLOG/	0.1	1.36E+37	-8.29	18165/
PLOG/	1	1.21E+39	-8.66	22517/
PLOG/	10	1.53E+28	-5.13	22530/
PLOG/	40	2.72E+15	-1.16	20283/
PLOG/	100	1.06E+05	2.06	18044/
PLOG/	200	2.30E-04	4.73	16037/
IC4H8OH-IT+O2<=>TQC4H7OHI 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	1.76E+53	-19.87	9019/
PLOG/	0.01	4.68E+67	-23.92	11892/
PLOG/	0.1	2.07E+91	-30.58	17347/
PLOG/	1	2.84E+100	-32.4	20041/
PLOG/	10	1.16E+115	-35.81	27656/
PLOG/	40	4.87E+123	-37.83	33314/
PLOG/	100	7.95E+124	-37.82	35683/
PLOG/	200	4.58E+122	-36.86	36374/

IC4H8OH-IT+O2<=>C2CY(COC)OH+OH 1.420E+036 -15.840 11594.0
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/ 0.001 1.42E+32 -6.95 6210/
PLOG/ 0.01 5.19E+36 -8.24 9233/
PLOG/ 0.1 5.77E+38 -8.76 11715/
PLOG/ 1 2.86E+36 -7.95 12823/
PLOG/ 10 1.37E+32 -6.51 13646/
PLOG/ 40 2.15E+29 -5.56 14541/
PLOG/ 100 1.20E+26 -4.51 14778/
PLOG/ 200 3.31E+22 -3.37 14606/

TQJC4H8OH<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0 !AUTHOR: !
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/ 0.001 9.73E+65 -18.5 42975/
PLOG/ 0.01 1.04E+64 -17.25 44419/
PLOG/ 0.1 7.90E+59 -15.59 44504/
PLOG/ 1 9.35E+53 -13.49 43566/
PLOG/ 10 4.13E+44 -10.39 41279/
PLOG/ 40 6.57E+38 -8.49 39745/
PLOG/ 100 8.32E+34 -7.23 38675/
PLOG/ 200 9.46E+31 -6.28 37849/

DUP

TQJC4H8OH<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0 !AUTHOR: !
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/ 0.001 5.27E+64 -18 42872/
PLOG/ 0.01 4.82E+62 -16.74 44284/
PLOG/ 0.1 3.42E+58 -15.07 44348/
PLOG/ 1 4.05E+52 -12.97 43402/
PLOG/ 10 1.93E+43 -9.88 41120/
PLOG/ 40 3.28E+37 -7.99 39593/
PLOG/ 100 4.35E+33 -6.74 38527/
PLOG/ 200 5.13E+30 -5.79 37706/

DUP

TQJC4H8OH<=>TQC4H8OI 1.420E+036 -15.840 11594.0 !AUTHOR: ! REF:
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/ 0.001 3.78E+50 -12.91 31539/
PLOG/ 0.01 1.42E+45 -10.94 30864/
PLOG/ 0.1 1.50E+40 -9.21 29932/
PLOG/ 1 3.12E+35 -7.64 28864/
PLOG/ 10 2.73E+29 -5.67 27243/
PLOG/ 40 8.88E+25 -4.54 26272/
PLOG/ 100 4.60E+23 -3.8 25622/
PLOG/ 200 9.08E+21 -3.25 25131/

TQJC4H8OH<=>QC4H7OHP 1.420E+036 -15.840 11594.0 !AUTHOR: ! REF:
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/ 0.001 9.16E+62 -18.02 45297/
PLOG/ 0.01 2.56E+62 -17.1 47393/
PLOG/ 0.1 1.25E+59 -15.61 47984/
PLOG/ 1 1.97E+53 -13.49 47281/
PLOG/ 10 1.91E+43 -10.15 44926/
PLOG/ 40 7.68E+36 -8.05 43267/
PLOG/ 100 3.49E+32 -6.64 42089/
PLOG/ 200 1.77E+29 -5.57 41173/

TQJC4H8OH<=>TQC4H7OHI 1.420E+036 -15.840 11594.0 !AUTHOR: ! REF:
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/ 0.001 9.57E+58 -15.99 38293/
PLOG/ 0.01 7.27E+54 -14.25 38593/
PLOG/ 0.1 8.30E+49 -12.44 38031/
PLOG/ 1 1.90E+44 -10.51 36905/

PLOG/	10	2.18E+36	-7.9	34865/
PLOG/	40	4.10E+31	-6.36	33581/
PLOG/	100	3.00E+28	-5.35	32704/
PLOG/	200	1.34E+26	-4.59	32035/
TQC4H8OI=>CH3COCH3+CH2O+OH 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	8.09E+38	-9.91	19096/
PLOG/	0.01	9.09E+39	-9.93	19135/
PLOG/	0.1	1.89E+41	-10.02	19407/
PLOG/	1	7.47E+23	-4.1	14658/
PLOG/	10	2.95E+33	-6.75	18685/
PLOG/	40	4.24E+36	-7.56	20307/
PLOG/	100	7.83E+36	-7.54	20747/
PLOG/	200	7.63E+35	-7.17	20641/
QC4H7OHP<=>IC4H7OH+HO2 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	3.29E+57	-15.64	28576/
PLOG/	0.01	9.65E+58	-15.75	29927/
PLOG/	0.1	2.19E+50	-12.66	28547/
PLOG/	1	1.67E+49	-12.05	29204/
PLOG/	10	7.08E+40	-9.26	27188/
PLOG/	40	1.32E+30	-5.82	24071/
PLOG/	100	1.15E+30	-5.8	24053/
PLOG/	200	1.12E+30	-5.8	24050/
QC4H7OHP<=>CCY(CCO)COH+OH 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	1.11E+51	-12.97	28497/
PLOG/	0.01	5.58E+51	-12.87	29529/
PLOG/	0.1	3.03E+44	-10.28	28326/
PLOG/	1	1.42E+44	-9.98	28986/
PLOG/	10	9.69E+37	-7.93	27491/
PLOG/	40	5.90E+29	-5.3	25095/
PLOG/	100	5.27E+29	-5.29	25081/
PLOG/	200	5.15E+29	-5.28	25078/
TQC4H7OHI<=>C2CY(COC)OH+OH 1.420E+036 -15.840 11594.0 !AUTHOR: !				
! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	1.10E+31	-7.21	14640/
PLOG/	0.01	1.37E+32	-7.24	14716/
PLOG/	0.1	3.34E+33	-7.35	15127/
PLOG/	1	1.86E+23	-3.68	12864/
PLOG/	10	9.88E+31	-6.23	16040/
PLOG/	40	1.25E+34	-6.78	17056/
PLOG/	100	7.73E+33	-6.67	17176/
PLOG/	200	2.13E+33	-6.45	17170/
TQC4H7OHI<=>SC4H7OH-I+HO2 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	6.01E+27	-7.27	14658/
PLOG/	0.01	7.78E+28	-7.3	14733/
PLOG/	0.1	3.27E+30	-7.48	15191/
PLOG/	1	2.81E+17	-2.82	12336/
PLOG/	10	1.92E+26	-5.22	16146/
PLOG/	40	7.61E+27	-5.49	17483/
PLOG/	100	1.91E+26	-4.86	17429/
PLOG/	200	2.94E+24	-4.18	17285/
IC4H8OH-TI+O2<=>IQJC4H8OH 1.420E+036 -15.840 11594.0 !AUTHOR: !				
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.				
PLOG/	0.001	3.34E+111	-32.67	25143/
PLOG/	0.01	4.84E+107	-31.05	25460/

PLOG/	0.1	2.41E+100	-28.42	24474/
PLOG/	1	4.55E+89	-24.78	22176/
PLOG/	10	1.14E+76	-20.31	18721/
PLOG/	40	9.25E+66	-17.35	16238/
PLOG/	100	6.20E+60	-15.36	14499/
PLOG/	200	1.30E+56	-13.86	13159/

IC4H8OH-TI+O2<=>IC3H6OHCHO+OH 1.420E+036 -15.840 11594.0
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.59E+15	-1.63	8947/
PLOG/	0.01	5.07E+20	-3.24	11938/
PLOG/	0.1	5.00E+25	-4.66	15251/
PLOG/	1	3.18E+26	-4.79	17388/
PLOG/	10	6.00E+20	-2.95	17297/
PLOG/	40	1.70E+14	-0.91	16099/
PLOG/	100	7.91E+08	0.73	14913/
PLOG/	200	3.03E+04	2.08	13854/

IC4H8OH-TI+O2<=>IQC4H8OT 1.420E+036 -15.840 11594.0 !AUTHOR: !
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.12E+102	-32.4	23496/
PLOG/	0.01	4.23E+95	-30.04	22067/
PLOG/	0.1	3.45E+83	-26.08	17114/
PLOG/	1	8.16E+82	-25.61	16198/
PLOG/	10	1.04E+97	-29.54	22648/
PLOG/	40	7.25E+103	-31.42	26487/
PLOG/	100	2.48E+106	-32.06	28397/
PLOG/	200	1.39E+107	-32.2	29446/

IC4H8OH-TI+O2=>CH3COCH3+CH2O+OH 1.420E+036 -15.840 11594.0
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	4.39E+48	-11.88	11603/
PLOG/	0.01	9.82E+50	-12.49	14143/
PLOG/	0.1	3.43E+49	-11.94	15561/
PLOG/	1	2.43E+45	-10.56	16415/
PLOG/	10	4.98E+39	-8.68	17473/
PLOG/	40	7.99E+33	-6.83	17502/
PLOG/	100	1.02E+29	-5.28	17165/
PLOG/	200	7.18E+24	-3.99	16747/

IC4H8OH-TI+O2<=>CH3+C3KET21 1.420E+036 -15.840 11594.0 !AUTHOR:
! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	2.91E+40	-9.23	10830/
PLOG/	0.01	9.66E+43	-10.2	13698/
PLOG/	0.1	1.34E+44	-10.13	15661/
PLOG/	1	2.57E+41	-9.18	17047/
PLOG/	10	1.82E+36	-7.46	18330/
PLOG/	40	8.82E+29	-5.44	18205/
PLOG/	100	1.74E+24	-3.65	17600/
PLOG/	200	2.16E+19	-2.12	16925/

IC4H8OH-TI+O2<=>IQC4H7OHT 1.420E+036 -15.840 11594.0 !AUTHOR: !
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.03E+115	-35.13	25407/
PLOG/	0.01	1.10E+129	-38.89	32891/
PLOG/	0.1	5.15E+135	-40.38	38573/
PLOG/	1	7.27E+129	-38.13	39933/
PLOG/	10	4.50E+112	-32.49	37045/

PLOG/	40	7.72E+97	-27.79	33612/
PLOG/	100	5.17E+86	-24.26	30799/
PLOG/	200	4.70E+77	-21.41	28440/

IC4H8OH-TI+O2=>IC3H5OH+CH2O+OH 1.420E+036 -15.840 11594.0
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	5.10E+24	-4.31	13009/
PLOG/	0.01	6.91E+33	-6.97	17935/
PLOG/	0.1	1.74E+41	-9.03	23613/
PLOG/	1	2.26E+36	-7.32	25633/
PLOG/	10	3.15E+17	-1.4	22782/
PLOG/	40	9.35E+00	3.71	19114/
PLOG/	100	5.59E-12	7.46	16156/
PLOG/	200	1.27E-21	10.41	13733/

IC4H8OH-TI+O2<=>CCY(CCOC)OH+OH 1.420E+036 -15.840 11594.0
!AUTHOR: ! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	3.06E+33	-7.24	11476/
PLOG/	0.01	6.56E+42	-9.92	17197/
PLOG/	0.1	8.24E+46	-10.95	22090/
PLOG/	1	4.48E+38	-8.22	23019/
PLOG/	10	1.01E+18	-1.77	19496/
PLOG/	40	1.16E+01	3.44	15637/
PLOG/	100	4.85E-12	7.23	12599/
PLOG/	200	8.64E-22	10.21	10126/

! IQJC4H8OH<=>IC3H6OHCHO+OH 1.420E+036 -15.840 11594.0 !AUTHOR: !
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	3.58E+71	-20.62	52656/
PLOG/	0.01	9.67E+71	-20.08	54935/
PLOG/	0.1	3.39E+67	-18.18	55330/
PLOG/	1	7.26E+58	-15.09	54016/
PLOG/	10	4.57E+46	-11.01	51172/
PLOG/	40	4.31E+38	-8.38	49054/
PLOG/	100	2.12E+33	-6.66	47587/
PLOG/	200	2.72E+29	-5.41	46486/

! IQJC4H8OH<=>IQC4H8OT 1.420E+036 -15.840 11594.0 !AUTHOR: ! REF:
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.04E+45	-11.2	31755/
PLOG/	0.01	2.90E+40	-9.62	30945/
PLOG/	0.1	4.85E+35	-8.01	29850/
PLOG/	1	2.62E+30	-6.28	28498/
PLOG/	10	3.37E+24	-4.37	26873/
PLOG/	40	9.75E+20	-3.23	25861/
PLOG/	100	5.61E+18	-2.52	25208/
PLOG/	200	1.44E+17	-2.01	24740/

IQJC4H8OH<=>IQC4H7OHT 1.420E+036 -15.840 11594.0 !AUTHOR: ! REF:
H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

PLOG/	0.001	1.36E+50	-12.93	36743/
PLOG/	0.01	3.36E+45	-11.27	36143/
PLOG/	0.1	1.13E+40	-9.41	34990/
PLOG/	1	5.93E+33	-7.33	33438/
PLOG/	10	4.24E+26	-5	31502/
PLOG/	40	1.97E+22	-3.61	30275/
PLOG/	100	3.43E+19	-2.72	29477/
PLOG/	200	3.69E+17	-2.09	28900/

IQC4H7OHT=>IC3H5OH+CH2O+OH 1.420E+036 -15.840 11594.0 !AUTHOR:
! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PLOG/ 0.001 4.25E+16 -3.66 19364/
PLOG/ 0.01 2.98E+33 -8.01 27106/
PLOG/ 0.1 3.46E+38 -8.83 31412/
PLOG/ 1 7.07E+28 -5.46 29633/
PLOG/ 10 2.01E+13 -0.43 25278/
PLOG/ 40 1.43E+13 -0.38 25238/
PLOG/ 100 1.38E+13 -0.38 25234/
PLOG/ 200 1.37E+13 -0.37 25233/

IQC4H7OHT<=>CCY(CCOC)OH+OH 1.420E+036 -15.840 11594.0 !AUTHOR:
! REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PLOG/ 0.001 1.12E+25 -5.59 19349/
PLOG/ 0.01 7.20E+32 -7.6 23093/
PLOG/ 0.1 2.22E+34 -7.65 25130/
PLOG/ 1 2.40E+27 -5.28 23663/
PLOG/ 10 2.24E+17 -2.04 20810/
PLOG/ 40 1.82E+17 -2.01 20786/
PLOG/ 100 1.78E+17 -2.01 20783/
PLOG/ 200 1.77E+17 -2.01 20782/

IQC4H7OHT<=>IC4H7OOH+OH 1.420E+036 -15.840 11594.0 !AUTHOR: !
REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
PLOG/ 0.001 6.07E+13 -4.21 22478/
PLOG/ 0.01 9.74E+39 -10.89 33616/
PLOG/ 0.1 2.18E+49 -12.65 40359/
PLOG/ 1 3.32E+37 -8.42 38539/
PLOG/ 10 2.34E+16 -1.56 32712/
PLOG/ 40 1.44E+16 -1.49 32656/
PLOG/ 100 1.38E+16 -1.48 32651/
PLOG/ 200 1.37E+16 -1.48 32649/

IQC4H8OT=>CH3COCH3+CH2O+OH 3.64E+09 1.3 23700.0 !\AUTHOR: !REF:
VILLANO, L. HUYNH, H-H CARTENSEN, A M. DEAN., J. PHYS. CHEM A, 2012, 116,
5068.

IQC4H8OT<=>CH3+C3KET21 4.95E+10 0.83 27900 !\AUTHOR:
!REF: VILLANO, L. HUYNH, H-H CARTENSEN, A M. DEAN., J. PHYS. CHEM A,
2012, 116, 5068.

IQC4H7OHT<=>CH2COHCH2OOH+CH3 4.95E+10 0.83 27900 !\AUTHOR:
!REF: VILLANO, L. HUYNH, H-H CARTENSEN, A M. DEAN., J. PHYS. CHEM A,
2012, 116, 5068.

!

!\REACTIONCLASS: \O2ROH_O2_PRODUCTS \A \N
\EA
!

TQC4H7OHIO2<=>TQC4H7OHIQ-I 2.56E+12 -0.13 34360
!\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION.

TQC4H7OHIQ-I=>HO2CHO+CH3COCH3+OH 5.819E+05 2.40 22790
!\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION.

TQC4H7OHIQ-I<=>IC4KETIT+HO2 1.829E+10 0.790 15100
!\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION.

$\text{IC4KETIT} \Rightarrow \text{CH3COCH3} + \text{HCO} + \text{OH}$ 9.500E+015 0.000 42540.0
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{IC4KETIT} + \text{OH} \Leftrightarrow \text{TC3H6O2HCO} + \text{H2O}$ 61329.94775 2.65419 -
 4586.39996 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION
 FROM F. GOLDSMITH CALCULATION.

$\text{IC4KETIT} + \text{HO2} \Leftrightarrow \text{TC3H6O2HCO} + \text{H2O2}$ 1.1773E-4 4.91966
 3684.27444 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION
 FROM F. GOLDSMITH CALCULATION.

$\text{TC3H6O2HCO} \Rightarrow \text{CH3COCH3} + \text{CO} + \text{OH}$ 1.278E+020 -1.890 34460.0
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{TQC4H7OHIO2} \Leftrightarrow \text{TQC4H7OHIQ} - \text{P}$ 5.69E+08 7.80E-01 21850
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{TQC4H7OHIQ} - \text{P} \Leftrightarrow \text{IC3H5COHQ} + \text{HO2}$ 1.83E+10 7.90E-01 15100
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{TQC4H7OHIQ} - \text{P} \Leftrightarrow \text{CH2CQCOHQ} + \text{CH3}$ 5.38E+11 0.070 24800
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{TQC4H7OHIQ} - \text{P} \Rightarrow \text{IC3H5Q} + \text{HOCHO} + \text{OH}$ 5.38E+11 0.070 24800
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{TQC4H7OHIQ} - \text{P} \Leftrightarrow \text{COHQCYC} (\text{COC}) + \text{OH}$ 2.28E+08 1.29E+00 9890
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{TQC4H7OHIQ} - \text{P} \Leftrightarrow \text{QCYC} (\text{CCOC}) \text{OH} + \text{OH}$ 4.58E+15 -1.08E+00 18440
 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
 CALCULATION.

$\text{IC3H5COHQ} \Rightarrow \text{HOCHO} + \text{C3H5} - \text{T} + \text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM
 F. GOLDSMITH CALCULATION.

$\text{CH2CQCOHQ} \Rightarrow \text{HOCHO} + \text{CH2CO} + 2\text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM
 F. GOLDSMITH CALCULATION.

$\text{CH2CQCOHQ} \Rightarrow \text{HCO} + \text{CH2CO} + 3\text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM
 F. GOLDSMITH CALCULATION.

$\text{IC3H5Q} \Rightarrow \text{CH2CO} + \text{CH3} + \text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM
 F. GOLDSMITH CALCULATION.

$\text{COHQCYC} (\text{COC}) \Rightarrow \text{HOCHO} + \text{CH2O} + \text{C2H3} + \text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM
 F. GOLDSMITH CALCULATION.

$\text{QCYC} (\text{CCOC}) \text{OH} \Rightarrow \text{HOCHO} + \text{CH2CO} + \text{CH3} + \text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !\REF: C ZHOU ESTIMATED SECOND-O2 ADDITION FROM
 F. GOLDSMITH CALCULATION.

$\text{TQC4H7OHIO2} \Leftrightarrow \text{TQC4H7OHTO2}$ 2.956E+09 0.04 16350
 !\AUTHOR: !REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010,
 114, 5689-5701

$\text{TQC4H7OHTO2} \Leftrightarrow \text{HOCOCQ} (\text{CH3})_2 + \text{OH}$ 1.75E+8 1.7 26000
 !\AUTHOR: !REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010,
 114, 5689-5701

$\text{HOCOCQ} (\text{CH3})_2 \Rightarrow \text{CO} + \text{CH3COCH3} + 2\text{OH}$ 1.59E+20 -1.5
 42879.46 !\AUTHOR: !REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701

IQC4H7OHTO2<=>IQC4H7OHTQ-P 2.063E+07 1.0 21070
 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010,
 114, 5689-5701
 IQC4H7OHTQ-P=>OH+CH2O+CH2COHCH2OOH 1.20E+10 0.35 15700
 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010,
 114, 5689-5701
 CH2COHCH2OOH=>OH+CH2O+CH2CO+H 1.59E+20 -1.5
 42879.46 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701
 IQC4H7OHTQ-P<=>OH+IC4H6Q2-II 1.0E+11 0.0 0.0
 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010,
 114, 5689-5701
 PLOG/ 0.01 2.53E+040 -9.91 32631.4/
 PLOG/ 0.1 2.54E+037 -8.72 32909.5/
 PLOG/ 1 1.12E+031 -6.53 31806.6/
 PLOG/ 10 1.98E+021 -3.34 29137.8/
 PLOG/ 100 1.95E+010 0.154 25612/
 IC4H6Q2-II=>OH+CH2O+HO2+C3H4-A 1.59E+20 -1.5
 42879.46 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701
 IQC4H7OHTO2<=>IQC4H8OTQ-I 4.13E+07 1.0 21070
 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010,
 114, 5689-5701
 IQC4H8OTQ-I=>OH+CH2O+C3KET21 1.20E+10 0.35
 15700 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS.
 CHEM. A 2010, 114, 5689-5701
 IQC4H8OTQ-I<=>CH3+CO(CH2OOH)2 2.740E+13 0.24 29830
 CO(CH2OOH)2=>2OH+2CH2O+CO 1.59E+20 -1.5
 42879.46 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM.
 A 2010, 114, 5689-5701
 IQC4H7OHTO2<=>CHOC(CH3)OHCH2Q+OH 1.20E+10 0.35 15700
 CHOC(CH3)OHCH2Q=>OH+CH2O+H+CH3COCHO 1.59E+20 -1.5
 42879.46 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM.
 A 2010, 114, 5689-5701
 CH3COCHO+OH=>2CO+CH3+H2O 61329.94775 2.65419 -
 4586.39996 !\AUTHOR: !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J.
 PHYS. CHEM. A 2010, 114, 5689-5701
 TQC4H7OHI+O2<=>TQC4H7OHIO2 3.49E+14 -0.816 -536.49
 !\AUTHOR: ! REF: MIYOSHI A., IJCK, 2012, 44, 59-74
 IQC4H7OHT+O2<=>IQC4H7OHTO2 6.87E+16 -1.627 198.7
 !\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 2.26E3 2.73
 -4688 !\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010,
 12, 7221-7233
 C2CY(COC)OH+HO2=>IC3H6CO+OH+H2O2 8.6 3.46
 9732.326 !\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014,
 118, 1300-1308
 CCY(CCO)COH+OH=>IC3H5CHO+OH+H2O 5.66E2 2.93 -
 4039.4 !\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP,
 2010, 12, 7221-7233
 CCY(CCO)COH+HO2=>IC3H5CHO+OH+H2O2 1.81E-1 3.98
 9056.7 !\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014,
 118, 1300-1308

CCY(CCO)COH+OH=>PC3H4OH-2+CH2O+H2O 1.26E3 2.97 -
 2660.6 !\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP,
 2010, 12, 7221-7233
 CCY(CCO)COH+HO2=>PC3H4OH-2+CH2O+H2O2 1.4E-5 5.26
 8267.9 !\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014,
 118, 1300-1308
 CCY(CCOC)OH+OH=>CH2O+SC3H4OH+H2O 5.66E2 2.93 -
 4039.4 !\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP,
 2010, 12, 7221-7233
 CCY(CCOC)OH+HO2=>CH2O+SC3H4OH+H2O2 1.81E-1 3.98
 9056.7 !\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014,
 118, 1300-1308

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 =====

!\ENDSUBSPECIES: \C2CY(COC)OH\CCY(CCO)COH\CCY(CCO)COH\CCY(CCOC)OH

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 =====

!\SUBSPECIES: \IC4H7OH

!=====
 =====

!_____

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!_____

IC4H7+OH<=>IC4H7OH 3.000E+013 0.000

0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

IC4H7O+H<=>IC4H7OH 4.000E+013 0.000

0.0 !\AUTHOR: !\REF:ANALOGY WITH C3H5-A+X -->PRODUCTS. LITERATURE VALUES

IC4H6OH+H<=>IC4H7OH 1.000E+014 0.000

0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

CH2CCH2OH+CH3<=>IC4H7OH 3.000E+013 0.000

0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!_____

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!_____

!\IC4H6OH

IC4H7OH+O2<=>IC4H6OH+HO2 6.000E+013 0.000

3990.0 !\AUTHOR: !\REF: Ingham,T.; Walker,R.W.; Woolford,R.E., Symp.
 Int. Combust. Proc. 25, 767-774 (1994)

IC4H7OH+OH<=>IC4H6OH+H2O 1.26E+03 2.97

-2660.593 !\AUTHOR: !\ REF: C ZHOU, ET AL. COMBUST & FLAME, 2011, 158,
 726.

IC4H7OH+HO2<=>IC4H6OH+H2O2 1.45E-05 5.26

8267.907 !\AUTHOR: !\ REF: C ZHOU, ET AL. IJCK, 2012, 44, 155.

IC4H6OH+H2<=>IC4H7OH+H 2.160E+004 2.380

18990.0 !\AUTHOR: !\REF:ANALOGY C3H5-A+X -->PRODUCTS

IC4H6OH+CH2O<=>IC4H7OH+HCO 6.300E+008 1.900

18190.0 !\AUTHOR: !\REF:RATE CONSTANT ANALOGY TO C3H5-A+CH2O (X 5)

IC4H6OH+IC4H8<=>IC4H7OH+IC4H7 4.700E+002 3.300

19840.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!\IC4H7O

IC4H7O+H2<=>IC4H7OH+H 9.050E+006 2.000
17830.0 !\AUTHOR: !\REF:(TSANG/ HAMPSON 86) X 5
IC4H7OH+HCO<=>IC4H7O+CH2O 3.020E+011 0.000
18160.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA
!

C3H4-A+CH2OH<=>IC4H6OH 1.000E+011 0.000
9200.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
IC4H7O<=>IC4H6OH 1.391E+011 0.000
15600.0 !\AUTHOR: !\REF:EA<=>8.6+7 (RING STRAIN+EABS OF PRIMARY H BY RO)
!

!\REACTIONCLASS: \R_HO2 \A \N
\EA
!

IC4H6OH+HO2=>CH2CCH2OH+CH2O+OH 1.446E+013 0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
!

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
\EA
!

IC4H7OH+H<=>IC4H8OH 1.000E+013 0.000
1200.0 !\AUTHOR: !\REF:ANALOGY WITH IC4H9 -->IC4H8+H
!

!\REACTIONCLASS: \R_R_ABSORPTION \A \N
\EA
!

IC4H7O+O2<=>IC3H5CHO+HO2 3.000E+010 0.000
1649.0 !\AUTHOR: !\REF:FROM BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 21,
411--429, 1992
IC4H7O+HO2<=>IC3H5CHO+H2O2 3.000E+011 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX
IC4H7O+CH3<=>IC3H5CHO+CH4 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX
IC4H7O+O<=>IC3H5CHO+OH 6.000E+012 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX
IC4H7O+OH<=>IC3H5CHO+H2O 1.810E+013 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX
IC4H7O+H<=>IC3H5CHO+H2 1.990E+013 0.000
0.0 !\AUTHOR: !\REF:ANALOGY CH3O+X -->CH2O+HX
!

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!\ENDSUBSPECIES: \IC4H7OH
!=====

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!\SUBSPECIES: \IC3H6OHCHO

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!=====
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IC3H6OHCHO+OH=>TC3H6OH+CO+H2O          61329.9      2.65      -
4586.4 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014,
118, 12089-12104.
IC3H6OHCHO+H=>TC3H6OH+CO+H2            8.66E5        2.3      1426
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104.
IC3H6OHCHO+HO2=>TC3H6OH+CO+H2O2        1.01E-4       5.0      3429
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104.
IC3H6OHCHO+CH3=>TC3H6OH+CO+CH4          3.94          3.6      4223
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104.
!=====
=====
!\ENDSUBSPECIES: \IC3H6OHCHO
!=====
=====
!\SUBSPECIES: \TC3H6OH
!=====
=====
TC3H6OH<=>CH3COCH3+H                    8.981E11      0.271
3.299E+04 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA,
2014, 118, 12089-12104.
TC3H6OH<=>IC3H5OH+H                      4.211E10      1.005
4.090E+04 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA,
2014, 118, 12089-12104.
TC3H6OH+O2<=>CH3COCH3+HO2               2.230E13      0.000
0.000E+00 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA,
2014, 118, 12089-12104.
!=====
=====
!\ENDSUBSPECIES: \TC3H6OH
!=====
=====
!-----
-----
!\ENDSUBMECH: \IC4H8
!-----
-----
!\SUBMECH: \C4H8-1\C4H8-2
!-----
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!
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!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
-----
C3H5-A+CH3(+M)<=>C4H8-1(+M)              1.00E+14      -0.32      -262.3
!\AUTHOR: !\REF: Yijun Zhang et al. Combustion and Flame 159 (2012)
905?;iC917
LOW / 3.91E+60 -12.81      6250.0      /

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TROE / 0.104 1606.0 60000.0 6118.4 /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C2H5+C2H3(+M)<=>C4H8-1(+M) 1.50E+13 0.00 0.0
!\AUTHOR: !\REF: Yijun Zhang et al. Combustion and Flame 159 (2012)
905?;iC917
LOW / 1.55E+56 -11.79 8984.5 /
TROE / 0.198 2277.9 60000.0 5723.2 /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C4H71-4+H(+M)<=>C4H8-1(+M) 3.60E+13 0.00
0.0 !\AUTHOR: !\REF: Yijun Zhang et al. Combustion and Flame 159 (2012)
905?;iC917
LOW / 3.01E+48 -9.32 5833.6 /
TROE / 0.498 1314.0 1314.0 50000.0 /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/
C4H71-3+H<=>C4H8-1 5.00E+13 0.0
5000.0 !\AUTHOR: !\REF: EST
C3H5-S+CH3(+M)<=>C4H8-2(+M) 5.00E+13 0.0
0.00 !\AUTHOR: !\REF C2H3+CH3(+M)=C3H6(+M)
LOW /8.54E+58 -11.940 9769.80 /
TROE /0.175 1340.6 60000.0 10139.8 /
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/C2H2/3.00/ C2H4/3.00/
C4H8-2<=>C3H5-A+CH3 0.75E+66 -15.6
97300 !\AUTHOR: !\REF: ASSUME BY THIS WORK
C4H8-2<=>H+C4H71-3 4.60E+84 -20.03
132787 !\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 7.769E+005 2.200
-437.18 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A
2011, 115, 2549?;iC2556
C4H8-1+OH<=>C4H71-4+H2O 8.60E+006 2.030
2623.10 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A
2011, 115, 2549?;iC2556
C4H8-1+OH<=>C4H71-2+H2O 3.000E+006 1.970
2847.66 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A
2011, 115, 2549?;iC2556
C4H8-1+OH<=>C4H71-1+H2O 6.930E+006 1.920
4962.04 !\AUTHOR: !\REF:Subith S. Vasu ET AL. J. Phys. Chem. A
2011, 115, 2549?;iC2556
C4H8-2+OH<=>C4H71-3+H2O 4.460E+006 2.072
1050.8 !\AUTHOR: !\REF:ANALOGY WITH C3H6+OH<=>C3H5-A+H2O *2/2
C4H8-2+OH<=>C4H72-2+H2O 6.000E+006 1.970
2845.9 !\AUTHOR: !\REF: ANALOGY WITH C4H8-1 *2

!***** ABSTRACTION BY

HO2*****!

C4H8-1+HO2<=>C4H71-3+H2O 7.82E-01 3.97
11702 !\AUTHOR: !\REF:Judith Zador,Stephen J. Klippenstein,and
James A. Miller J. Phys. Chem. A 2011, 115, 10218?;iC10225
C4H8-2+HO2<=>C4H71-3+H2O 6.90E-01 4.00
12103 !\AUTHOR: !\REF:Judith Zador,Stephen J. Klippenstein,and
James A. Miller J. Phys. Chem. A 2011, 115, 10218?;iC10225

C4H8-1+HO2<=>C4H71-4+H2O2			4.080E+001	3.590
17160.0	!\AUTHOR: !\REF:ANALOGY WITH C4H10+HO2<=>PC4H9+H2O2			
C4H8-1+HO2<=>C4H71-1+H2O2			9.570E+002	3.059
20798.6	!\AUTHOR: !\REF:ANALOGY WITH C3H6+HO2			
C4H8-1+HO2<=>C4H71-2+H2O2			1.560E+004	2.820
24427.9	!\AUTHOR: !\REF:ANALOGY WITH C3H6+HO2			
C4H8-2+HO2<=>C4H72-2+H2O2			3.120E+004	2.820
24427.9	!\AUTHOR: !\REF:ANALOGY WITH C3H6+HO2 *2			
C4H8-1+H<=>C4H71-4+H2	3.84E+004	2.87	6.611E+03	
!\AUTHOR: !\REF: TST/RRHO+HRS				
C4H8-1+H<=>C4H71-3+H2	2.42E+003	3.05	1.995E+03	
!\AUTHOR: !\REF: TST/RRHO+HRS				
C4H8-1+H<=>C4H71-2+H2	2.37E+004	2.85	8.917E+03	
!\AUTHOR: !\REF: TST/RRHO+HRS				
C4H8-1+H<=>C4H71-1+H2	2.63E+004	2.83	1.205E+04	
!\AUTHOR: !\REF: TST/RRHO+HRS				
DUP				
C4H8-1+H<=>C4H71-1+H2	2.23E+004	2.85	1.171E+04	
!\AUTHOR: !\REF: TST/RRHO+HRS				
DUP				
C4H8-2+H<=>C4H71-3+H2	5.62E+002	3.50	1.627E+03	!\AUTHOR:
!\REF: TST/RRHO+HRS !*2 Ea-1				
C4H8-2+H<=>C4H72-2+H2	8.47E+004	2.76	9.304E+03	!\AUTHOR:
!\REF: TST/RRHO+HRS				
C4H8-1+O<=>C4H71-3+OH			1.750E+011	0.700
5884.0	!\AUTHOR: !\REF: IN ARAMCO			
C4H8-2+O<=>C4H71-3+OH			2.190E+011	0.810
7550.0	!\AUTHOR: !\REF: IN ARAMCO			
C4H8-1+O<=>C4H71-1+OH			1.200E+011	0.700
8959.1	!\AUTHOR: !\REF: ANALOGY WITH C2H4+O			
C4H8-1+O<=>C4H71-2+OH			6.030E+010	0.700
7632.0	!\AUTHOR: !\REF: ANALOGY WITH C2H4+O			
C4H8-2+O<=>C4H72-2+OH			1.206E+011	0.700
7632.0	!\AUTHOR: !\REF: ANALOGY WITH C2H4+O !*2			
C4H8-1+O<=>C4H71-4+OH			1.130E+014	0.000
7850.0	!\AUTHOR: !\REF: ANALOGY WITH C4H10+O<=>PC4H9+OH			
C4H8-1+O2<=>C4H71-3+HO2			1.000E+014	0.000
37190.0	!\AUTHOR: !\REF: IN ARAMCO !*5			
C4H8-2+O2<=>C4H71-3+HO2			2.000E+014	0.000
39390.0	!\AUTHOR: !\REF: IN ARAMCO !*5			
C4H8-1+O2<=>C4H71-1+HO2			2.000E+013	0.000
62270.0	!\AUTHOR: !\REF: ANALOGY WITH C3H6+O2			
C4H8-1+O2<=>C4H71-2+HO2			1.000E+013	0.000
58770.0	!\AUTHOR: !\REF: ANALOGY WITH C3H6+O2			
C4H8-2+O2<=>C4H72-2+HO2			2.000E+013	0.000
58770.0	!\AUTHOR: !\REF: ANALOGY WITH C3H6+O2 !*2			
C4H8-1+O2<=>C4H71-4+HO2			6.000E+013	0.000
52340.0	!\AUTHOR: !\REF: ANALOGY WITH C4H10+O2<=>PC4H9+HO2			
C4H8-1+CH3<=>C4H71-3+CH4			2.210E+000	3.500
5675.0	!\AUTHOR: !\REF: IN ARAMCO (TSANG '91)			
C4H8-1+CH3<=>C4H71-4+CH4			4.520E-001	3.650
7154.0	!\AUTHOR: !\REF: IN ARAMCO (TSANG '91)			
C4H8-2+CH3<=>C4H71-3+CH4			7.140E+000	3.570
7642.0	!\AUTHOR: !\REF: IN ARAMCO (TSANG '91)			
C4H8-1+CH3<=>C4H71-1+CH4			1.348E+000	3.500
12850.0	!\AUTHOR: !\REF: ANALOGY WITH C3H6+CH3			
C4H8-1+CH3<=>C4H71-2+CH4			8.400E-001	3.500
11660.0	!\AUTHOR: !\REF: ANALOGY WITH C3H6+CH3			

C4H8-2+CH3<=>C4H72-2+CH4	1.680E+000	3.500
11660.0	!\AUTHOR: !\REF:ANALOGY WITH C3H6+CH3 !*2	
C4H8-1+CH3O2<=>C4H71-3+CH3O2H	2.700E+004	0.700
5884.0	!\AUTHOR: !\REF:IN ARAMCO (TSANG '91)	
C4H8-1+CH3O2<=>C4H71-4+CH3O2H	2.380E+003	2.550
16490.0	!\AUTHOR: !\REF:IN ARAMCO (TSANG '91)	
C4H8-1+CH3O<=>C4H71-3+CH3OH	4.000E+001	2.900
8609.0	!\AUTHOR: !\REF:IN ARAMCO (TSANG '91)	
C4H8-1+CH3O<=>C4H71-4+CH3OH	2.170E+011	0.000
6458.0	!\AUTHOR: !\REF:IN ARAMCO (TSANG '91)	
C4H8-2+CH3O<=>C4H71-3+CH3OH	1.800E+001	2.950
11990.0	!\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)	
C4H8-1+CH3CO3<=>C4H71-3+CH3CO3H	1.000E+011	0.000
8000.0	!\AUTHOR: !\REF:IN ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))	
C4H8-1+C3H5-A<=>C4H71-3+C3H6	7.900E+010	0.000
12400.0	!\AUTHOR: !\REF:IN ARAMCO (DECHAUX, J.C., OXID. COMM. 2, 95 (1981))	
C4H8-1+C2H5O2<=>C4H71-3+C2H5O2H	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).)	
C4H8-1+NC3H7O2<=>C4H71-3+NC3H7O2H	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).)	
C4H8-1+IC3H7O2<=>C4H71-3+IC3H7O2H	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).)	
C4H8-1+PC4H9O2<=>C4H71-3+PC4H9O2H	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).)	
C4H8-1+SC4H9O2<=>C4H71-3+SC4H9O2H	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).)	
C4H8-2+NC3H7O2<=>C4H71-3+NC3H7O2H	3.200E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (!TWICE RATE OF C3H6+HO2)	
C4H8-2+IC3H7O2<=>C4H71-3+IC3H7O2H	3.200E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (!TWICE RATE OF C3H6+HO2)	
C4H8-2+PC4H9O2<=>C4H71-3+PC4H9O2H	3.200E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (!TWICE RATE OF C3H6+HO2)	
C4H8-2+SC4H9O2<=>C4H71-3+SC4H9O2H	3.200E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (!TWICE RATE OF C3H6+HO2)	
C4H71-3+C2H5<=>C4H8-1+C2H4	2.590E+012	0.000
-131.0	!\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)	
C4H71-3+CH3O<=>C4H8-1+CH2O	2.410E+013	0.000
0.0	!\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)	
IC4H9O2+C4H8-1<=>IC4H9O2H+C4H71-3	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (WESTBROOK ESTIMATE)	
TC4H9O2+C4H8-1<=>TC4H9O2H+C4H71-3	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (WESTBROOK ESTIMATE)	
IC4H9O2+C4H8-2<=>IC4H9O2H+C4H71-3	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (WESTBROOK ESTIMATE)	
TC4H9O2+C4H8-2<=>TC4H9O2H+C4H71-3	1.400E+012	0.000
14900.0	!\AUTHOR: !\REF:IN ARAMCO (WESTBROOK ESTIMATE)	

!\REACTIONCLASS: \R_DECOMPOSITION
\EA

\A \N

C4H71-1<=>C4H6-1+H	8.95E+08	1.14
35636.4576 !\AUTHOR: !\REF:		
C4H71-1<=>C2H5+C2H2	2.85E+12	0.68
33178.2912 !\AUTHOR: !\REF:		
C4H71-2<=>C4H6-1+H	9.79E+08	1.2
38080.7136 !\AUTHOR: !\REF:		
C4H71-2<=>C4H612+H	1.99E+08	1.56
37683.2736 !\AUTHOR: !\REF:		
C4H71-2<=>C3H4-A+CH3	1.23E+10	1.19
32915.9808 !\AUTHOR: !\REF:		
C4H71-3<=>C4H612+H	3.95E+11	0.93
61611.1488 !\AUTHOR: !\REF:		
C4H71-3<=>C4H6+H	8.53E+07	1.95
47490.1056 !\AUTHOR: !\REF:		
C4H71-4<=>C2H4+C2H3	2.84E+10	0.99
38998.8 !\AUTHOR: !\REF:		
C4H71-4<=>C4H6+H	1.32E+05	2.28
33245.856 !\AUTHOR: !\REF:		
C4H72-2<=>C4H6-2+H	7.87E+09	1.16
36173.0016 !\AUTHOR: !\REF:		
C4H72-2<=>C4H612+H	9.54E+07	1.81
38992.8384 !\AUTHOR: !\REF:		
C4H72-2<=>C3H4-P+CH3	6.30E+11	0.93
34754.1408 !\AUTHOR: !\REF:		
C4H71-3<=>C4H71-4	5.62E-12	7.19
36200.8224 !\AUTHOR: !\REF:		
C4H71-3<=>C4H72-2	6.76E-23	10.21
41574.2112 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \RA_HO2_PRODUCTS \A \N
 \EA
 !

C4H71-3+HO2<=>C4H71-3OOH 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG / 1.000E-002 2.050E+001 1.24 -22589. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 11%
 PLOG / 1.000E-001 3.690E+006 0.08 -18331. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 12%
 PLOG / 1.000E+000 2.020E+013 -1.45 -11709. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 11%
 PLOG / 2.000E+000 1.490E+015 -1.87 -9604. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 10%
 PLOG / 5.000E+000 1.850E+017 -2.31 -6991. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 9%
 PLOG / 1.000E+001 2.880E+018 -2.55 -5260. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 8%
 PLOG / 3.000E+001 3.450E+019 -2.71 -3140. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 7%
 PLOG / 5.000E+001 5.330E+019 -2.70 -2438. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 C4H71-3+HO2<=>C4H71-O+OH 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346

PLOG / 1.000E-002 6.90E+20 -2.68 229. / !FIT FROM: 800-2000 K ERROR
IN FIT: 0%
PLOG / 1.000E-001 4.50E+22 -3.18 1760. / !FIT FROM: 800-2000 K ERROR
IN FIT: 1%
PLOG / 1.000E+000 8.61E+27 -4.63 6415. / !FIT FROM: 800-2000 K ERROR
IN FIT: 2%
PLOG / 2.000E+000 1.92E+30 -5.28 8578. / !FIT FROM: 800-2000 K ERROR
IN FIT: 2%
PLOG / 5.000E+000 5.46E+33 -6.22 11879. / !FIT FROM: 800-2000 K ERROR
IN FIT: 3%
PLOG / 1.000E+001 2.98E+36 -6.97 14600. / !FIT FROM: 800-2000 K ERROR
IN FIT: 2%
PLOG / 3.000E+001 5.58E+40 -8.14 19040. / !FIT FROM: 800-2000 K ERROR
IN FIT: 2%
PLOG / 5.000E+001 4.44E+42 -8.67 21071. / !FIT FROM: 800-2000 K ERROR
IN FIT: 1%

C4H71-3+HO2<=>C2H3COCH3+H2O 1.0 1.0 1.0

!\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
2012, 116 (13), PP 3325-3346

PLOG / 1.000E-002 5.160E+014 -1.74 1910. / !FIT FROM: 800-2000 K
ERROR IN FIT: 0%
PLOG / 1.000E-001 1.620E+016 -2.16 3167. / !FIT FROM: 800-2000 K
ERROR IN FIT: 0%
PLOG / 1.000E+000 9.730E+020 -3.47 7339. / !FIT FROM: 800-2000 K
ERROR IN FIT: 1%
PLOG / 2.000E+000 1.700E+023 -4.09 9378. / !FIT FROM: 800-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 4.330E+026 -5.02 12574. / !FIT FROM: 800-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 2.590E+029 -5.78 15275. / !FIT FROM: 800-2000 K
ERROR IN FIT: 2%
PLOG / 3.000E+001 7.850E+033 -7.01 19801. / !FIT FROM: 800-2000 K
ERROR IN FIT: 1%
PLOG / 5.000E+001 8.840E+035 -7.58 21918. / !FIT FROM: 800-2000 K
ERROR IN FIT: 1%

C4H71-3OOH<=>C4H71-O+OH 1.0 1.0 1.0

!\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
2012, 116 (13), PP 3325-3346

PLOG / 1.000E-002 4.410E+035 -7.37 39745. / !FIT FROM: 800-2000 K
ERROR IN FIT: 9%
PLOG / 1.000E-001 6.640E+037 -7.60 44224. / !FIT FROM: 800-2000 K
ERROR IN FIT: 8%
PLOG / 1.000E+000 7.090E+037 -7.24 47692. / !FIT FROM: 800-2000 K
ERROR IN FIT: 5%
PLOG / 2.000E+000 1.920E+037 -6.97 48350. / !FIT FROM: 800-2000 K
ERROR IN FIT: 4%
PLOG / 5.000E+000 1.200E+036 -6.51 48849. / !FIT FROM: 800-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E+001 7.170E+034 -6.08 48933. / !FIT FROM: 800-2000 K
ERROR IN FIT: 2%
PLOG / 3.000E+001 3.690E+032 -5.32 48614. / !FIT FROM: 800-2000 K
ERROR IN FIT: 1%
PLOG / 5.000E+001 3.040E+031 -4.97 48341. / !FIT FROM: 800-2000 K
ERROR IN FIT: 1%

C4H71-3OOH<=>C2H3COCH3+H2O 1.0 1.0 1.0

!\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
2012, 116 (13), PP 3325-3346

PLOG / 1.000E-002 3.580E+023 -4.64 38121. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 9%
 PLOG / 1.000E-001 2.850E+027 -5.36 43407. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 8%
 PLOG / 1.000E+000 2.630E+029 -5.53 48042. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 PLOG / 2.000E+000 2.830E+029 -5.43 49101. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 5%
 PLOG / 5.000E+000 1.040E+029 -5.18 50137. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 4%
 PLOG / 1.000E+001 2.120E+028 -4.89 50610. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 3%
 PLOG / 3.000E+001 5.390E+026 -4.33 50818. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 5.000E+001 7.760E+025 -4.04 50737. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 C4H71-O<=>C2H3+CH3CHO 8.520E+025 -3.610
 27863.4 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H71-O<=>AC3H5OCH2 1.350E+018 -1.730
 17386.5 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H71-O<=>CH2CH2COCH3 1.670E+021 -2.740
 20337.7 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H71-O<=>C2H3COCH3+H 2.570E+020 -2.060
 22040.1 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H71-O<=>C2H4+CH3CO 4.750E+008 1.140
 20922.5 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 AC3H5OCH2<=>C3H5-A+CH2O 8.810E+014 -0.326
 31553.1 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 AC3H5OCH2<=>CH2CH2COCH3 2.510E+020 -2.630
 29288.4 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 AC3H5OCH2<=>C2H3COCH3+H 3.980E+018 -1.620
 30129.8 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 AC3H5OCH2<=>C3H6+HCO 3.730E+014 -0.726
 32008.3 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 CH2CH2COCH3<=>C2H3+CH3CHO 1.930E+019 -1.940
 48440.0 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 CH2CH2COCH3<=>C2H3COCH3+H 4.520E+012 0.214
 34570.5 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 CH2CH2COCH3<=>C2H4+CH3CO 1.590E+013 0.063
 24086.3 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C2H3+CH3CHO<=>C2H4+CH3CO 1.650E+001 3.170
 9399.8 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H71-3+HO2<=>C4H72-1OOH 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346

PLOG / 1.000E-002 1.000E+007 -0.33 -17896. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 11%
 PLOG / 1.000E-001 1.150E+011 -1.16 -14831. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 12%
 PLOG / 1.000E+000 2.950E+016 -2.33 -9451. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 11%
 PLOG / 2.000E+000 7.680E+017 -2.62 -7705. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 11%
 PLOG / 5.000E+000 2.210E+019 -2.89 -5556. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 10%
 PLOG / 1.000E+001 1.140E+020 -2.99 -4159. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 9%
 PLOG / 3.000E+001 2.800E+020 -2.96 -2503. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 7%
 PLOG / 5.000E+001 2.400E+020 -2.88 -1971. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 C4H71-3+HO2<=>C4H7O2-1+OH 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG / 1.000E-002 6.81E+20 -2.68 217. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 0%
 PLOG / 1.000E-001 2.25E+22 -3.10 1516. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 1.000E+000 2.75E+27 -4.49 6067. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 2.000E+000 6.27E+29 -5.14 8273. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 5.000E+000 1.96E+33 -6.09 11661. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 1.000E+001 1.16E+36 -6.85 14456. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 3.000E+001 2.51E+40 -8.04 19009. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 5.000E+001 2.18E+42 -8.58 21090. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 C4H71-3+HO2<=>SC3H5CHO+H2O 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG / 1.000E-002 1.620E+014 -1.60 1519. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 1.000E-001 3.190E+015 -1.96 2620. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+000 1.690E+020 -3.26 6800. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 2.000E+000 3.390E+022 -3.89 8918. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 5.000E+000 1.090E+026 -4.85 12249. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+001 7.810E+028 -5.63 15058. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 3.000E+001 3.140E+033 -6.89 19743. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 5.000E+001 4.070E+035 -7.48 21927. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 2%
 C4H72-1OOH<=>C4H7O2-1+OH 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346

PLOG / 1.000E-002 5.070E+035 -7.39 39733. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 9%
 PLOG / 1.000E-001 7.690E+037 -7.63 43994. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 8%
 PLOG / 1.000E+000 2.760E+037 -7.14 47024. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 PLOG / 2.000E+000 4.320E+036 -6.81 47507. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 5%
 PLOG / 5.000E+000 1.210E+035 -6.24 47760. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 4%
 PLOG / 1.000E+001 3.920E+033 -5.74 47658. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 3%
 PLOG / 3.000E+001 8.620E+030 -4.88 47084. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 PLOG / 5.000E+001 5.290E+029 -4.50 46721. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 C4H72-10OH<=>SC3H5CHO+H2O 1.0 1.0 1.0
 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A,
 2012, 116 (13), PP 3325-3346
 PLOG / 1.000E-002 1.150E+024 -4.78 38584. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 9%
 PLOG / 1.000E-001 9.650E+027 -5.51 43561. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 8%
 PLOG / 1.000E+000 2.330E+029 -5.53 47626. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 PLOG / 2.000E+000 1.290E+029 -5.35 48469. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 PLOG / 5.000E+000 1.810E+028 -4.98 49208. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 4%
 PLOG / 1.000E+001 1.760E+027 -4.61 49458. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 3%
 PLOG / 3.000E+001 1.590E+025 -3.91 49357. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 2%
 PLOG / 5.000E+001 1.580E+024 -3.58 49164. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 1%
 C4H7O2-1<=>C3H5-S+CH2O 8.520E+025 -3.610
 27863.4 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H7O2-1<=>SC3H5OCH2-1 1.350E+018 -1.730
 17386.5 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H7O2-1<=>C3H6CHO-2 1.670E+021 -2.740
 20337.7 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H7O2-1<=>SC3H5CHO+H 2.570E+020 -2.060
 22040.1 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C4H7O2-1<=>C3H6+HCO 4.750E+008 1.140
 20922.5 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 SC3H5OCH2-1<=>C3H5-S+CH2O 8.810E+014 -0.326
 31553.1 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 SC3H5OCH2-1<=>C3H6CHO-2 2.510E+020 -2.630
 29288.4 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346

SC3H5OCH2-1<=>SC3H5CHO+H 3.980E+018 -1.620
 30129.8 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 SC3H5OCH2-1<=>C3H6+HCO 3.730E+014 -0.726
 32008.3 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C3H6CHO-2<=>C3H5-S+CH2O 1.930E+019 -1.940
 48440.0 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C3H6CHO-2<=>SC3H5CHO+H 4.520E+012 0.214
 34570.5 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C3H6CHO-2<=>C3H6+HCO 1.590E+013 0.063
 24086.3 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346
 C3H5-S+CH2O<=>C3H6+HCO 1.650E+001 3.170
 9399.8 !\AUTHOR: !\REF: KINETICS FROM FRANKLIN C GOLDSMITH J.
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346

!

!\REACTIONCLASS: \RA_RO2_PRODUCTS \A \N

\EA

!

C4H71-3+CH3O2<=>C4H71-3OOCH3 1.0 1.0 1.0
 !\AUTHOR: !\REF: ANALOGY WITH C4H71-3+HO2 /2
 PLOG / 1.000E-002 1.03E+01 1.24 -22589. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 11%
 PLOG / 1.000E-001 1.85E+06 0.08 -18331. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 12%
 PLOG / 1.000E+000 1.01E+13 -1.45 -11709. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 11%
 PLOG / 2.000E+000 7.45E+14 -1.87 -9604. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 10%
 PLOG / 5.000E+000 9.25E+16 -2.31 -6991. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 9%
 PLOG / 1.000E+001 1.44E+18 -2.55 -5260. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 8%
 PLOG / 3.000E+001 1.73E+19 -2.71 -3140. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 7%
 PLOG / 5.000E+001 2.67E+19 -2.70 -2438. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 6%
 C4H71-3+CH3O2<=>C4H71-O+CH3O 1.0 1.0 1.0
 !\AUTHOR: !\REF: ANALOGY WITH C4H71-3+HO2 /2
 PLOG / 1.000E-002 3.45E+20 -2.68 229. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 0%
 PLOG / 1.000E-001 2.25E+22 -3.18 1760. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 1.000E+000 4.31E+27 -4.63 6415. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 2.000E+000 9.60E+29 -5.28 8578. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 5.000E+000 2.73E+33 -6.22 11879. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 3%
 PLOG / 1.000E+001 1.49E+36 -6.97 14600. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 3.000E+001 2.79E+40 -8.14 19040. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%

PLOG / 5.000E+001 2.22E+42 -8.67 21071. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 C4H71-3OCH3<=>C4H71-O+CH3O 1.0 1.0 1.0
 !\AUTHOR: !\REF: ANALOGY WITH C4H71-3+HO2 /2
 PLOG / 1.000E-002 2.21E+35 -7.37 39745. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 9%
 PLOG / 1.000E-001 3.32E+37 -7.60 44224. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 8%
 PLOG / 1.000E+000 3.55E+37 -7.24 47692. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 5%
 PLOG / 2.000E+000 9.60E+36 -6.97 48350. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 4%
 PLOG / 5.000E+000 6.00E+35 -6.51 48849. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 3%
 PLOG / 1.000E+001 3.59E+34 -6.08 48933. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 3.000E+001 1.85E+32 -5.32 48614. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 5.000E+001 1.52E+31 -4.97 48341. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 C4H71-3+CH3O2<=>C4H72-1OCH3 1.0 1.0 1.0
 !\AUTHOR: !\REF: ANALOGY WITH C4H71-3+HO2 /2
 PLOG / 1.000E-002 5.00E+06 -0.33 -17896. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 11%
 PLOG / 1.000E-001 5.75E+10 -1.16 -14831. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 12%
 PLOG / 1.000E+000 1.48E+16 -2.33 -9451. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 11%
 PLOG / 2.000E+000 3.84E+17 -2.62 -7705. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 11%
 PLOG / 5.000E+000 1.11E+19 -2.89 -5556. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 10%
 PLOG / 1.000E+001 5.70E+19 -2.99 -4159. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 9%
 PLOG / 3.000E+001 1.40E+20 -2.96 -2503. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 7%
 PLOG / 5.000E+001 1.20E+20 -2.88 -1971. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 6%
 C4H71-3+CH3O2<=>C4H7O2-1+CH3O 1.0 1.0 1.0
 !\AUTHOR: !\REF: ANALOGY WITH C4H71-3+HO2 /2
 PLOG / 1.000E-002 3.41E+20 -2.68 217. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 0%
 PLOG / 1.000E-001 1.13E+22 -3.10 1516. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 1.000E+000 1.38E+27 -4.49 6067. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 2.000E+000 3.14E+29 -5.14 8273. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 5.000E+000 9.80E+32 -6.09 11661. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 1.000E+001 5.80E+35 -6.85 14456. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 PLOG / 3.000E+001 1.26E+40 -8.04 19009. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 5.000E+001 1.09E+42 -8.58 21090. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 2%
 C4H72-1OCH3<=>C4H7O2-1+CH3O 1.0 1.0 1.0
 !\AUTHOR: !\REF: ANALOGY WITH C4H71-3+HO2 /2

PLOG / 1.000E-002 2.54E+35 -7.39 39733. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 9%
 PLOG / 1.000E-001 3.85E+37 -7.63 43994. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 8%
 PLOG / 1.000E+000 1.38E+37 -7.14 47024. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 6%
 PLOG / 2.000E+000 2.16E+36 -6.81 47507. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 5%
 PLOG / 5.000E+000 6.05E+34 -6.24 47760. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 4%
 PLOG / 1.000E+001 1.96E+33 -5.74 47658. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 3%
 PLOG / 3.000E+001 4.31E+30 -4.88 47084. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 PLOG / 5.000E+001 2.65E+29 -4.50 46721. / !FIT FROM: 800-2000 K ERROR
 IN FIT: 1%
 C4H71-3+C2H5O2<=>C4H71-O+C2H5O 3.800E+012 0.000
 -1200.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH3
 IC3H7O2+C4H71-3<=>IC3H7O+C4H71-O 3.800E+012 0.000
 -1200.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH3
 NC3H7O2+C4H71-3<=>NC3H7O+C4H71-O 3.800E+012 0.000
 -1200.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH3
 C4H71-O<=>C2H3CHO+CH3 7.940E+014 0.000
 19000.0 !\AUTHOR: !\REF:ANALOGY TO BATT'S RATE FOR S-
 BUTOXY DECOMPOSITION
 C4H71-3+O<=>C2H3CHO+CH3 6.030E+013 0.000
 0.0 !\AUTHOR: !\REF:IN ARAMCO (ESTIMATE)
 !

!\REACTIONCLASS: \RA_R_ABSTRACTION \A \N
 \EA
 !

C4H71-3+O2<=>C4H6+HO2 1.07 3.710
 9322.0 !\AUTHOR: !\REF: J. D. DESAIN, S. J. KLIPPENSTEIN, J. A.
 MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427
 H+C4H71-3<=>C4H6+H2 3.160E+013 0.000
 0.0 !\AUTHOR: !\REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF.
 DATA 9, 523 (1980)
 C2H5+C4H71-3<=>C4H6+C2H6 3.980E+012 0.000
 0.0 !\AUTHOR: !\REF:EDELSON AND ALLARA, 1980
 C2H3+C4H71-3<=>C2H4+C4H6 3.980E+012 0.000
 0.0 !\AUTHOR: !\REF:EDELSON AND ALLARA, 1980
 C3H5-A+C4H71-3<=>C3H6+C4H6 6.310E+012 0.000
 0.0 !\AUTHOR: !\REF:EDELSON AND ALLARA, 1980
 !

!\REACTIONCLASS: \RA_RA_RECOMBINATION \A
 \N \EA
 !

C4H71-3+C4H71-3<=>C8H141-5,3-4 4.11E+16 -
 1.260 1560.62 !\AUTHOR: !\REF: FRIDLAND ET AL. J. PHYS.
 CHEM. A, 2013, 117, 4762-4776
 C4H71-3+C4H71-3<=>C8H141-5,3 4.11E+16 -
 1.260 1560.62 !\AUTHOR: !\REF: FRIDLAND ET AL. J. PHYS.
 CHEM. A, 2013, 117, 4762-4776

C4H71-3+C4H71-3<=>C8H142-6	4.11E+16	-
1.260 1560.62 !\AUTHOR: !\REF: FRIDLAND ET AL. J. PHYS. CHEM. A, 2013, 117, 4762-4776		
C8H141-5,3-4+OH<=>C8H131-5,3-4,TA+H2O	2.5E+6	
2.0 -2629.06 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+OH<=>C8H131-5,3,TA+H2O	1.3E+6	
2.0 -2629.06 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+OH<=>C8H131-5,3,SA+H2O	3.2E+6	
2.0 -1434.03 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+OH<=>C8H131-5,3,PA+H2O	3.0E+6	
2.0 -239.01 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+OH<=>C8H132-6,SA+H2O	6.3E+6	
2.0 -1434.03 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+OH<=>C8H132-6,PA+H2O	6.0E+6	
2.0 -239.01 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3-4+HO2<=>C8H131-5,3-4,TA+H2O2	3.2E+4	
2.6 10755.26 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+HO2<=>C8H131-5,3,TA+H2O2	1.6E+4	
2.6 10755.26 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+HO2<=>C8H131-5,3,SA+H2O2	6.3E+3	
2.6 12428.30 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+HO2<=>C8H131-5,3,PA+H2O2	9.5E+3	
2.6 13862.33 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+HO2<=>C8H132-6,SA+H2O2	1.3E+4	
2.6 12428.30 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+HO2<=>C8H132-6,PA+H2O2	1.9E+4	
2.6 13862.33 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3-4+H<=>C8H131-5,3-4,TA+H2	5.0E+4	
2.5 -2868.07 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+H<=>C8H131-5,3,TA+H2	2.5E+4	
2.5 -2868.07 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+H<=>C8H131-5,3,SA+H2	5.0E+4	
2.5 -1673.04 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+H<=>C8H131-5,3,PA+H2	1.9E+5	
2.5 2390.06 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+H<=>C8H132-6,SA+H2	1.0E+5	
2.5 -1673.04 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+H<=>C8H132-6,PA+H2	3.8E+5	
2.5 2390.06 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3-4+O<=>C8H131-5,3-4,TA+OH	6.3E+10	
0.7 1195.03 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+O<=>C8H131-5,3,TA+OH	3.2E+10	
0.7 1195.03 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+O<=>C8H131-5,3,SA+OH	8.0E+10	
0.7 3107.07 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+O<=>C8H131-5,3,PA+OH	6.3E+10	
0.7 5975.14 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+O<=>C8H132-6,SA+OH	1.6E+11	
0.7 3107.07 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H142-6+O<=>C8H132-6,PA+OH	1.3E+11	
0.7 5975.14 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3-4+CH3<=>C8H131-5,3-4,TA+CH4	1.6E+12	
0.0 5258.13 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+CH3<=>C8H131-5,3,TA+CH4	7.9E+11	
0.0 5258.13 !\AUTHOR: !\REF: HENRY'S SLIDES		
C8H141-5,3+CH3<=>C8H131-5,3,SA+CH4	1.6E+12	
0.0 6931.17 !\AUTHOR: !\REF: HENRY'S SLIDES		

C8H141-5,3+CH3<=>C8H131-5,3,PA+CH4 1.5E-1
3.5 5736.14 !\AUTHOR: !\REF: HENRY'S SLIDES
C8H142-6+CH3<=>C8H132-6,SA+CH4 3.2E+12
0.0 6931.17 !\AUTHOR: !\REF: HENRY'S SLIDES
C8H142-6+CH3<=>C8H132-6,PA+CH4 3.0E-1
3.5 5736.14 !\AUTHOR: !\REF: HENRY'S SLIDES
C8H141-5,3-4+O2<=>C8H131-5,3-4,TA+HO2 1.60E+13
0.0 35420 !\AUTHOR: !\REF: C4H8-1, C4H8-2 AND LLNL ANALOGY
C8H141-5,3+O2<=>C8H131-5,3,TA+HO2 8.00E+12
0.0 35420 !\AUTHOR: !\REF: C4H8-1, C4H8-2 AND LLNL ANALOGY
C8H141-5,3+O2<=>C8H131-5,3,SA+HO2 2.000E+013
0.0 37190.0 !\AUTHOR: !\REF: C4H8-1, C4H8-2 AND LLNL ANALOGY
C8H141-5,3+O2<=>C8H131-5,3,PA+HO2 2.000E+013
0.0 39390.0 !\AUTHOR: !\REF: C4H8-1, C4H8-2 AND LLNL ANALOGY
C8H142-6+O2<=>C8H132-6,SA+HO2 4.000E+013
0.0 37190.0 !\AUTHOR: !\REF: C4H8-1, C4H8-2 AND LLNL ANALOGY
C8H142-6+O2<=>C8H132-6,PA+HO2 4.000E+013
0.0 39390.0 !\AUTHOR: !\REF: C4H8-1, C4H8-2 AND LLNL ANALOGY
C6H101-3,3+C2H3<=>C8H131-5,3-4,TA 4.40E+04
2.48 6130 !\AUTHOR: !\REF: H. J. CURRAN INC. INT J CHEM KINET
38: 250?;iC275, 2006
B13DE2M+C3H5-S<=>C8H131-5,3,TA 4.40E+04
2.48 6130 !\AUTHOR: !\REF: H. J. CURRAN INC. INT J CHEM KINET
38: 250?;iC275, 2006
C6H10D24+C2H3<=>C8H131-5,3,SA 8.80E+03
2.48 6130 !\AUTHOR: !\REF: H. J. CURRAN INC. INT J CHEM KINET
38: 250?;iC275, 2006
C4H6+C4H71-3<=>C8H131-5,3,PA 1.30E+03
2.48 8520 !\AUTHOR: !\REF: H. J. CURRAN INC. INT J CHEM KINET
38: 250?;iC275, 2006
C5H81-3+C3H5-S<=>C8H132-6,SA 8.80E+03
2.48 6130 !\AUTHOR: !\REF: H. J. CURRAN INC. INT J CHEM KINET
38: 250?;iC275, 2006
C4H6+C4H71-3<=>C8H132-6,PA 1.30E+03
2.48 8520 !\AUTHOR: !\REF: H. J. CURRAN INC. INT J CHEM KINET
38: 250?;iC275, 2006
C6H101-3,3<=>C2H3+C4H72-2 2.500E+15 0.0000
99500.0 !\AUTHOR: !\REF: ANALOGY TO KUIWEN'S MECH
C6H10D24<=>C3H5-S+C3H5-S 2.500E+15 0.0000
99500.0 !\AUTHOR: !\REF: ANALOGY TO KUIWEN'S MECH
C8H131-5,3-4,TA+HO2<=>C8H131-5,3-4,TAO+OH 1.64e+004 2.74
1144.38 !\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 1.64e+004 2.74
1144.38 !\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 1.64e+004 2.74
1144.38 !\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 1.64e+004 2.74
1144.38 !\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 1.64e+004 2.74
1144.38 !\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 1.64e+004 2.74
1144.38 !\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	2.5E+10	0.0
10090 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
C4H71-3+C2H3COCH3<=>C8H131-5,3,TAO	2.5E+10	0.0
10090 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
C4H71-3+SC3H5CHO<=>C8H131-5,3,SAO	3.33E+10	0.0
6397 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
C7H111-5,3,6P+CH2O<=>C8H131-5,3,PAO	1.00E+11	0.0
3496 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
C4H71-3+SC3H5CHO<=>C8H132-6,SAO	3.33E+10	0.0
6397 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
C7H111-5,1P+CH2O<=>C8H132-6,PAO	1.00E+11	0.0
3496 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
CC5H9-A+C2H2<=>C7H111-5,3,6P	1.32E+04	2.48
6130 !\AUTHOR: !\REF: H.J. CURRAN, INT. J. CHEM. KIN. 38 (4)		
(2006) 250-275.		
C5H92-5+C2H2<=>C7H111-5,1P	1.32E+04	2.48
6130 !\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	1.0E+011	0.0
0.0 !\AUTHOR: !\REF: !JET SURF 2.0		
C4H71-4+O2<=>C4H71-4O2	6.865E+016	-
1.627 198.7		
C4H71-4+HO2<=>C4H7O1-4+OH	7.000E+012	
0.000 -1000.0		
CH3O2+C4H71-4<=>CH3O+C4H7O1-4	7.000E+012	
0.000 -1000.0		
C4H71-4O2+H2<=>C4H71-4OOH+H	3.010E+013	
0.000 26030.0		
C4H71-4O2+HO2<=>C4H71-4OOH+O2	1.750E+010	
0.000 -3275.0		
C4H71-4O2+H2O2<=>C4H71-4OOH+HO2	2.400E+012	
0.000 10000.0		
C4H71-4O2+CH4<=>C4H71-4OOH+CH3	1.120E+013	
0.000 24640.0		
C4H71-4O2+CH3OH<=>C4H71-4OOH+CH2OH	6.300E+012	
0.000 19360.0		
C4H71-4O2+CH2O<=>C4H71-4OOH+HCO	5.600E+012	
0.000 13600.0		
C4H71-4O2+C2H6<=>C4H71-4OOH+C2H5	1.700E+013	
0.000 20460.0		
C4H71-4O2+CH3CHO<=>C4H71-4OOH+CH3CO	2.800E+012	
0.000 13600.0		
C4H71-4O2+C2H4<=>C4H71-4OOH+C2H3	1.130E+013	
0.000 30430.0		
C4H71-4O2+C3H6<=>C4H71-4OOH+C3H5-A	5.350E-002	
4.207 13288.1		

C4H71-4O2+C2H5CHO<=>C4H71-4OOH+C2H5CO	2.000E+011	
0.000 9500.0		
C4H71-4O2+C2H3CHO<=>C4H71-4OOH+C2H3CO	2.800E+012	
0.000 13600.0		
C4H71-4O2+C3H8<=>C4H71-4OOH+NC3H7	1.700E+013	
0.000 20460.0		
C4H71-4O2+C3H8<=>C4H71-4OOH+IC3H7	2.000E+012	
0.000 17000.0		
C4H71-4O2+CH3<=>C4H7O1-4+CH3O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+C2H5<=>C4H7O1-4+C2H5O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+IC3H7<=>C4H7O1-4+IC3H7O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+NC3H7<=>C4H7O1-4+NC3H7O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+C3H5-A<=>C4H7O1-4+C3H5O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+PC4H9<=>C4H7O1-4+PC4H9O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+SC4H9<=>C4H7O1-4+SC4H9O	7.000E+012	
0.000 -1000.0		
C4H71-4O2+C4H71-3<=>C4H7O1-4+C4H71-O	7.000E+012	
0.000 -1000.0		
C4H71-4OOH<=>C4H7O1-4+OH	1.500E+016	
0.000 42500.0		
C4H71-4O2+CH3O2=>C4H7O1-4+CH3O+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2+CH3CO3=>C4H7O1-4+CH3CO2+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2+C2H5O2=>C4H7O1-4+C2H5O+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2+NC3H7O2=>C4H7O1-4+NC3H7O+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2+IC3H7O2=>C4H7O1-4+IC3H7O+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2+C4H71-4O2=>C4H7O1-4+C4H7O1-4+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2+SC4H9O2=>C4H7O1-4+SC4H9O+O2	1.400E+016	-
1.610 1860.0		
C4H71-4O2<=>C4H61-3OOH4	4.009E+008	1.100
30100.0		
C4H61-3OOH4<=>C2H3CHOCH2+OH	1.710E+009	1.060
10900.0		
C4H61-3OOH4<=>C4H6O25+OH	1.720E+008	0.760
11100.0		
C2H3CHOCH2+H=>C2H3+CH2CO+H2	5.000E+012	0.000
0.0		
C2H3CHOCH2+O=>C2H3+CH2CO+OH	5.000E+012	0.000
0.0		
C2H3CHOCH2+OH=>C2H3+CH2CO+H2O	5.000E+012	0.000
0.0		
C2H3CHOCH2+HO2=>C2H3+CH2CO+H2O2	1.000E+013	0.000
15000.0		
C2H3CHOCH2+CH3=>C2H3+CH2CO+CH4	2.000E+011	0.000
10000.0		
C2H3CHOCH2+CH3O2=>C2H3+CH2CO+CH3O2H	1.000E+013	0.000
19000.0		

C4H6O25+H<=>CH2CHCHCHO+H2	5.000E+012	0.000
0.0		
C4H6O25+O<=>CH2CHCHCHO+OH	5.000E+012	0.000
0.0		
C4H6O25+OH<=>CH2CHCHCHO+H2O	5.000E+012	0.000
0.0		
C4H6O25+HO2<=>CH2CHCHCHO+H2O2	1.000E+013	0.000
15000.0		
C4H6O25+CH3<=>CH2CHCHCHO+CH4	2.000E+011	0.000
10000.0		
C4H6O25+CH3O2<=>CH2CHCHCHO+CH3O2H	1.000E+013	0.000
19000.0		
C4H61-3OOH4+HO2<=>C4H6O1-3OOH4+OH		4.10E+03
2.740 1144.4 !\AUTHOR: !\REF:ANALOGY TO C4H71-3+HO2		
ADDITION, FOLLOWED BY WDM		
C4H61-3OOH4+HO2<=>C4H6O2-1OOH4+OH		4.10E+03
2.740 1144.4 !\AUTHOR: !\REF:ANALOGY TO C4H71-3+HO2		
ADDITION, FOLLOWED BY WDM		
C4H6O1-3OOH4<=>C2H3CHO+CH2O+OH		6.70E+39
-8.38 22782 !\AUTHOR: !\REF:ANALOGY TO C4H71-3+HO2		
ADDITION, FOLLOWED BY WDM		
C4H6O1-3OOH4<=>C2H3+HO2CH2CHO		2.67E+34
-6.63 22672 !\AUTHOR: !\REF:ANALOGY TO C4H71-3+HO2		
ADDITION, FOLLOWED BY WDM		

!

!\REACTIONCLASS: \RSP_O2	\A	\N
\EA		

!

C4H71-1+O2<=>C4H71-1O2		4.07E+27
-4.67 5222.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH		
C2H3+O2 J. PHYS. CHEM. A		
C4H71-1O2<=>C3H6CHO-3+O		1.22E+29
-4.71 42340.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH		
C2H3+O2 J. PHYS. CHEM. A		
C4H71-1O2<=>C2H5CHCO+OH		1.55E+24
-3.87 49850.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH		
C2H3+O2 J. PHYS. CHEM. A		

!

!\REACTIONCLASS: \RSV_O2	\A	\N
\EA		

!

C4H71-2+O2<=>C4H71-2O2		4.07E+27
-4.67 5222.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH		
C2H3+O2 J. PHYS. CHEM. A		
C4H71-2O2<=>C2H5COCH2+O		1.22E+29
-4.71 42340.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH		
C2H3+O2 J. PHYS. CHEM. A		
C4H72-2+O2<=>C4H72-2O2		4.07E+27
-4.67 5222.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH C2H3+O2 J.		
PHYS. CHEM. A		
C4H72-2O2<=>CH3CHCOCH3+O		1.22E+29
-4.71 42340.0 !\AUTHOR: !\REF:C. FRANKLIN GOLDSMITH C2H3+O2 J.		
PHYS. CHEM. A		

!

!\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:
PLOG / 1.0000000E-003 2.5500000E+006 1.9300000E+000 5.5640000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E-002 5.5600000E+006 1.8300000E+000 5.8020000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E-001 1.2100000E+009 1.1800000E+000 7.4720000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 1%
PLOG / 1.0000000E+000 9.4700000E+016 -1.0300000E+000 1.3413000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 6%
PLOG / 1.0000000E+001 4.5000000E+028 -4.2400000E+000 2.3618000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 7%
PLOG / 1.0000000E+002 7.0200000E+032 -5.2200000E+000 3.1754000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 18%
DUP
C4H8-1+H<=>C2H4+C2H5 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 3.4500000E+007 1.8100000E+000 2.2630000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 0%
PLOG / 1.0000000E-002 8.0600000E+007 1.7100000E+000 2.5220000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 0%
PLOG / 1.0000000E-001 1.1800000E+010 1.1000000E+000 4.0770000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E+000 6.0200000E+015 -4.9000000E-001 8.4520000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 5%
PLOG / 1.0000000E+001 7.5800000E+021 -2.1400000E+000 1.4245000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 6%
PLOG / 1.0000000E+002 2.2900000E+021 -1.8700000E+000 1.7243000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 15%
DUP
C4H8-1+H<=>C3H6+CH3 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 7.8300000E+009 1.1700000E+000 1.4420000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 0%
PLOG / 1.0000000E-002 3.3900000E+010 1.0000000E+000 1.8950000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 1%
PLOG / 1.0000000E-001 3.7000000E+013 1.4000000E-001 4.1270000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 3%
PLOG / 1.0000000E+000 4.5700000E+019 -1.5400000E+000 9.0610000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 5%
PLOG / 1.0000000E+001 8.5700000E+023 -2.6600000E+000 1.4140000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 7%
PLOG / 1.0000000E+002 1.3200000E+020 -1.4600000E+000 1.5383000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 20%
DUP
C4H8-1+H<=>C3H6+CH3 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 1.8000000E+006 1.7600000E+000 5.9000000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%

PLOG / 1.0000000E-002 3.4600000E+006 1.6800000E+000 6.1000000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E-001 4.0200000E+008 1.1000000E+000 7.5740000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 1%
PLOG / 1.0000000E+000 1.2100000E+016 -9.9000000E-001 1.3175000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 5%
PLOG / 1.0000000E+001 7.1400000E+027 -4.2300000E+000 2.3319000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 7%
PLOG / 1.0000000E+002 1.0000000E+033 -5.4900000E+000 3.1922000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 18%

DUP

C4H8-1+H<=>PC4H9

1.0000000E+000

1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:

PLOG / 1.0000000E-003 1.3500000E+015 -2.8100000E+000 1.5700000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 20%
PLOG / 1.0000000E-002 5.2000000E+016 -2.9700000E+000 1.9920000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 21%
PLOG / 1.0000000E-001 1.9100000E+021 -3.9700000E+000 4.6360000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 24%
PLOG / 1.0000000E+000 1.9000000E+031 -6.4600000E+000 1.1968000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 28%
PLOG / 1.0000000E+001 2.1000000E+040 -8.6000000E+000 2.1058000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 21%
PLOG / 1.0000000E+002 1.4400000E+037 -7.2100000E+000 2.4896000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 15%

DUP

C4H8-1+H<=>PC4H9

1.0000000E+000

1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:

PLOG / 1.0000000E-003 4.3300000E+020 -4.1600000E+000 -2.6300000E+002 /
! FIT FROM 500-2000 K ERROR IN FIT 25%
PLOG / 1.0000000E-002 1.7800000E+022 -4.3300000E+000 1.8600000E+002 /
! FIT FROM 500-2000 K ERROR IN FIT 26%
PLOG / 1.0000000E-001 1.9800000E+026 -5.1800000E+000 2.5180000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 28%
PLOG / 1.0000000E+000 3.7800000E+032 -6.6300000E+000 7.2650000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 28%
PLOG / 1.0000000E+001 8.7900000E+034 -6.9100000E+000 1.0952000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 18%
PLOG / 1.0000000E+002 7.8000000E+028 -4.7900000E+000 1.0355000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 9%

DUP

C4H8-1+H<=>SC4H9

1.0000000E+000

1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:

PLOG / 1.0000000E-003 4.0700000E+022 -4.5100000E+000 -7.7100000E+002 /
! FIT FROM 500-2000 K ERROR IN FIT 24%
PLOG / 1.0000000E-002 3.9000000E+024 -4.7800000E+000 -3.4000000E+001 /
! FIT FROM 500-2000 K ERROR IN FIT 25%
PLOG / 1.0000000E-001 2.0300000E+029 -5.8100000E+000 2.9700000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 26%
PLOG / 1.0000000E+000 3.5300000E+034 -6.9500000E+000 7.5250000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 22%
PLOG / 1.0000000E+001 1.1900000E+034 -6.4200000E+000 9.8100000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 12%
PLOG / 1.0000000E+002 1.3700000E+026 -3.7900000E+000 8.0120000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 6%

DUP

C4H8-1+H<=>SC4H9

1.0000000E+000

1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:

PLOG / 1.0000000E-003 3.5200000E+012 -2.1500000E+000 1.4660000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 23%
PLOG / 1.0000000E-002 1.0200000E+014 -2.2800000E+000 1.7990000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 23%
PLOG / 1.0000000E-001 1.1600000E+018 -3.1300000E+000 4.0490000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 26%
PLOG / 1.0000000E+000 5.2200000E+027 -5.5300000E+000 1.0963000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 31%
PLOG / 1.0000000E+001 4.3300000E+037 -7.9200000E+000 2.0354000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 24%
PLOG / 1.0000000E+002 2.2200000E+036 -7.0600000E+000 2.5203000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 15%

DUP

C4H8-2+H<=>C2H4+C2H5 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 8.9600000E+006 1.8600000E+000 6.2090000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 3%
PLOG / 1.0000000E-002 1.9200000E+007 1.7700000E+000 6.4430000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 3%
PLOG / 1.0000000E-001 3.9700000E+009 1.1100000E+000 8.0970000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 1%
PLOG / 1.0000000E+000 3.0100000E+017 -1.0900000E+000 1.4023000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 5%
PLOG / 1.0000000E+001 1.8800000E+029 -4.3300000E+000 2.4297000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 6%
PLOG / 1.0000000E+002 5.1500000E+033 -5.3900000E+000 3.2601000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 19%

C4H8-2+H<=>C3H6+CH3 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 6.3900000E+009 1.2900000E+000 1.8340000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 0%
PLOG / 1.0000000E-002 2.6000000E+010 1.1200000E+000 2.2670000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 1%
PLOG / 1.0000000E-001 2.4800000E+013 2.9000000E-001 4.4560000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 3%
PLOG / 1.0000000E+000 2.9100000E+019 -1.3900000E+000 9.3650000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 5%
PLOG / 1.0000000E+001 6.1300000E+023 -2.5300000E+000 1.4463000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 7%
PLOG / 1.0000000E+002 1.2300000E+020 -1.3500000E+000 1.5762000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 19%

C4H8-2+H<=>PC4H9 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 3.9000000E+014 -2.5500000E+000 1.7290000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 22%
PLOG / 1.0000000E-002 1.4100000E+016 -2.7100000E+000 2.1330000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 22%
PLOG / 1.0000000E-001 4.3100000E+020 -3.6900000E+000 4.7190000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 25%
PLOG / 1.0000000E+000 4.0300000E+030 -6.1700000E+000 1.2020000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 29%
PLOG / 1.0000000E+001 5.1900000E+039 -8.3300000E+000 2.1137000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 22%
PLOG / 1.0000000E+002 5.1700000E+036 -6.9800000E+000 2.5063000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 15%

C4H8-2+H<=>SC4H9 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:

```

PLOG / 1.0000000E-003 8.3400000E+021 -4.2100000E+000 -6.0200000E+002 /
! FIT FROM 500-2000 K ERROR IN FIT 25%
PLOG / 1.0000000E-002 6.7900000E+023 -4.4600000E+000 8.2000000E+001 /
! FIT FROM 500-2000 K ERROR IN FIT 26%
PLOG / 1.0000000E-001 2.8500000E+028 -5.4700000E+000 3.0030000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 28%
PLOG / 1.0000000E+000 5.4500000E+033 -6.6100000E+000 7.5590000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 24%
PLOG / 1.0000000E+001 2.3300000E+033 -6.1100000E+000 9.8930000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 14%
PLOG / 1.0000000E+002 3.2700000E+025 -3.5100000E+000 8.1450000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 7%
C4H8-1+H<=>C4H8-2+H 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 2.9800000E+007 1.8600000E+000 3.5750000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E-002 6.1100000E+007 1.7700000E+000 3.7940000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E-001 4.7800000E+009 1.2400000E+000 5.1520000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 0%
PLOG / 1.0000000E+000 1.0200000E+015 -2.5000000E-001 9.2330000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 3%
PLOG / 1.0000000E+001 6.5100000E+020 -1.8200000E+000 1.4806000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 5%
PLOG / 1.0000000E+002 4.4400000E+019 -1.3700000E+000 1.7409000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 16%
DUP
C4H8-1+H<=>C4H8-2+H 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 1.5500000E+004 2.3200000E+000 7.0490000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 4%
PLOG / 1.0000000E-002 2.3600000E+004 2.2700000E+000 7.1770000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 4%
PLOG / 1.0000000E-001 6.6000000E+005 1.8600000E+000 8.2010000E+003 /
! FIT FROM 500-2000 K ERROR IN FIT 2%
PLOG / 1.0000000E+000 1.1500000E+012 1.1000000E-001 1.2789000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 3%
PLOG / 1.0000000E+001 8.8000000E+023 -3.1700000E+000 2.2546000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 6%
PLOG / 1.0000000E+002 3.7200000E+031 -5.1600000E+000 3.2234000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 15%
DUP
SC4H9<=>PC4H9 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
PLOG / 1.0000000E-003 9.6000000E+037 -1.1040000E+001 3.8840000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 43%
PLOG / 1.0000000E-002 6.0500000E+040 -1.1260000E+001 3.9461000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 44%
PLOG / 1.0000000E-001 1.6400000E+047 -1.2490000E+001 4.3112000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 46%
PLOG / 1.0000000E+000 6.5300000E+055 -1.4270000E+001 5.0351000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 40%
PLOG / 1.0000000E+001 2.1300000E+056 -1.3710000E+001 5.4866000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 23%
PLOG / 1.0000000E+002 6.0200000E+045 -1.0070000E+001 5.3399000E+004 /
! FIT FROM 500-2000 K ERROR IN FIT 10%
PC4H9<=>C2H4+C2H5 1.0000000E+000
1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:

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PLOG / 1.0000000E-003 3.4400000E+034 -8.1000000E+000 2.8397000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 35%
 PLOG / 1.0000000E-002 1.1100000E+039 -9.0500000E+000 3.1891000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 34%
 PLOG / 1.0000000E-001 7.7400000E+042 -9.7800000E+000 3.5771000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 29%
 PLOG / 1.0000000E+000 7.4700000E+043 -9.6700000E+000 3.8722000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 20%
 PLOG / 1.0000000E+001 2.0600000E+039 -7.9700000E+000 3.8955000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 10%
 PLOG / 1.0000000E+002 1.4800000E+029 -4.7100000E+000 3.5950000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 6%
 PC4H9<=>C3H6+CH3 1.0000000E+000
 1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
 PLOG / 1.0000000E-003 3.7100000E+025 -5.8100000E+000 3.4965000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 24%
 PLOG / 1.0000000E-002 1.8500000E+027 -6.0100000E+000 3.5481000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 25%
 PLOG / 1.0000000E-001 2.4600000E+032 -7.1600000E+000 3.8637000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 28%
 PLOG / 1.0000000E+000 2.0500000E+042 -9.6100000E+000 4.6415000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 29%
 PLOG / 1.0000000E+001 4.9800000E+048 -1.0970000E+001 5.4456000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 19%
 PLOG / 1.0000000E+002 2.2300000E+042 -8.6800000E+000 5.6601000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 14%
 SC4H9<=>C2H4+C2H5 1.0000000E+000
 1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
 PLOG / 1.0000000E-003 8.3000000E+025 -5.7500000E+000 3.9343000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 24%
 PLOG / 1.0000000E-002 4.1200000E+027 -5.9400000E+000 3.9859000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 25%
 PLOG / 1.0000000E-001 5.5700000E+032 -7.1000000E+000 4.3029000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 28%
 PLOG / 1.0000000E+000 4.5400000E+042 -9.5400000E+000 5.0839000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 29%
 PLOG / 1.0000000E+001 1.0600000E+049 -1.0900000E+001 5.8899000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 18%
 PLOG / 1.0000000E+002 9.9400000E+042 -8.7000000E+000 6.1203000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 15%
 SC4H9<=>C3H6+CH3 1.0000000E+000
 1.0000000E+000 1.0000000E+000 !\AUTHOR: !\REF:
 PLOG / 1.0000000E-003 2.8900000E+040 -9.7600000E+000 3.3601000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 32%
 PLOG / 1.0000000E-002 1.8000000E+044 -1.0500000E+001 3.7007000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 30%
 PLOG / 1.0000000E-001 2.5100000E+046 -1.0730000E+001 4.0237000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 23%
 PLOG / 1.0000000E+000 4.7400000E+044 -9.8500000E+000 4.1841000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 15%
 PLOG / 1.0000000E+001 3.7900000E+037 -7.4400000E+000 4.0604000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 8%
 PLOG / 1.0000000E+002 4.7900000E+026 -4.0100000E+000 3.6898000E+004 /
 ! FIT FROM 500-2000 K ERROR IN FIT 6%
 !

!\REACTIONCLASS: \R_ADDITION\OH

\A

\N

\EA

!

C4H71-1OH+H<=>PC4H8OH-1 4267949684205.41
0.492750689836384 4444.57662660868 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

NC3H7CHO+H<=>PC4H8OH-1 9.8E+10
1.19205556991972 8785.56579045593 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C2H3OH+C2H5<=>PC4H8OH-1 3.0E+06
1.8344227669761 7337.92313843988 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C4H8-1+OH<=>PC4H8OH-2 2.1E+06
1.80584359238537 -3292.33399356593 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C4H71-1OH+H<=>PC4H8OH-2 1.6E+10
1.11403297478319 4389.23773365885 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C4H72-1OH+H<=>PC4H8OH-2 2.7E+11 -
0.134331624130482 1584.65884107689 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C3H6+CH2OH<=>PC4H8OH-3 7.0E+03
2.42680725691275 7063.5142949433 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C4H71-4OH+H<=>PC4H8OH-3 1.5E+11
0.88281161510281 2750.62938509725 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

SC4H8OH-1<=>PC4H8OH-3 2.9E+08
1.37714323923115 37865.9705441062 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C3H6+CH2OH<=>PC4H8OH-4 7.0E+03
2.42680725691275 7063.5142949433 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C4H71-4OH+H<=>PC4H8OH-4 1.5E+11
0.88281161510281 2750.62938509725 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

SC4H8OH-1<=>PC4H8OH-4 2.9E+08
1.37714323923115 37865.9705441062 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

NC3H7CHO+H<=>PC4H9O 4.7E+09
1.43469379654107 4357.89006047953 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

NC3H7+CH2O<=>PC4H9O 5.0E+03
2.42516348673951 3238.89516310988 !\AUTHOR: !\REF:J. ZA??
DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
519?;iC526

C4H71-2OH+H<=>SC4H8OH-2 1.4E+08
 1.51550214630697 218.841417907051 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C2H5COCH3+H<=>SC4H8OH-2 7.0E+07
 1.80134205573461 13223.1219632522 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C4H8-1+OH<=>SC4H8OH-1 7E+05
 1.80188194674497 -3290.24380570477 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C2H3OH+C2H5<=>SC4H8OH-1 6.4E+06
 1.67089578770901 10270.2427563368 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C4H8-2+OH<=>SC4H8OH-3 1.4E+06
 1.80188194674497 -3290.24380570477 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 SC3H5OH+CH3<=>SC4H8OH-3 6.4E+06
 1.67089578770901 10270.2427563368 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C2H5COCH3+H<=>SC4H9O 2.7E+07
 1.75632567406421 6206.15193211754 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C2H5CHO+CH3<=>SC4H9O 1.2E+04
 2.28382558987551 7978.10227873491 !\AUTHOR: !\REF:J. ZA??
 DOR, J.A. MILLER / PROCEEDINGS OF THE COMBUSTION INSTITUTE 34 (2013)
 519?;iC526
 C4H71-4OH+OH<=>C4H64,2-1OH+H2O 2.020E+006
 2.200 -437.2 !\AUTHOR: !\REF:ANALOGY WITH C4H8-1+OH
 C4H71-4OH+HO2<=>C4H64,2-1OH+H2O 3.91E-01
 3.97 11702 !\AUTHOR: !\REF:ANALOGY WITH C4H8-1+OH
 !

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

PC4H8OH-2+O2<=>PC4H8OH-2O2 3.60E+12 0.0
 0.0 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A.,
 2007, 111, 4974.
 PC4H8OH-2O2<=>SQC4H8OP 2.91E+12 -0.226
 22300 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A.,
 2007, 111, 4974.
 PC4H8OH-2O2<=>C4H72-1OH+HO2 3.64E+14 -0.711
 32710 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A.,
 2007, 111, 4974.
 PC4H8OH-2O2<=>C4H71-1OH+HO2 2.44E+13 -0.253
 32590 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A.,
 2007, 111, 4974.
 SQC4H8OP=>C2H5CHO+CH2O+OH 5.36E+12 -0.080
 10790 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A.,
 2007, 111, 4974.

PC4H8OH-2O2<=>NC4KET21OH+OH	1.49E+09	0.109	
41390	!\AUTHOR: !\REF: !DIFFERENT FROM IC4H8 SYSTEM		
(ANALOGY WITH SC4H8OH-1 SYSTEM)			
C4H72-1OH+OH<=>C4H64,2-1OH+H2O	2.02E+06		
2.200 -436.92	!\AUTHOR: !\REF: !ANALOGY WITH C4H8-2+OH		
(CONSIDER THE NUMBER OF H ATOM AND OH GROUP AFFACT *2)			
C4H72-1OH+OH<=>C4H63,1-1OH+H2O	2.69E+06		
2.200 -436.92	!\AUTHOR: !\REF: !ANALOGY WITH C4H8-2+OH		
(CONSIDER THE NUMBER OF H ATOM AND OH GROUP AFFACT *2)			
C4H72-1OH+HO2<=>C4H64,2-1OH+H2O2	1.725E-01		
4.00 12103	!\AUTHOR: !\REF: !ANALOGY WITH C4H8-2+OH		
(CONSIDER THE NUMBER OF H ATOM AND OH GROUP AFFACT *2)			
C4H72-1OH+HO2<=>C4H63,1-1OH+H2O2	2.30E-01		
4.00 12103	!\AUTHOR: !\REF: !ANALOGY WITH C4H8-2+OH		
(CONSIDER THE NUMBER OF H ATOM AND OH GROUP AFFACT *2)			
C4H71-1OH+OH<=>C4H63,1-1OH+H2O	2.020E+006		
2.200 -437.2	!\AUTHOR: !\REF: !ANALOGY WITH C4H8-1+OH		
C4H71-1OH+HO2<=>C4H63,1-1OH+H2O2	3.91E-01		
3.97 11702	!\AUTHOR: !\REF: !ANALOGY WITH C4H8-1+OH		
C4H64,2-1OH<=>C4H6+OH	7.035E+16		-
1.012 3.607E+04	!\AUTHOR: !\REF:S.M. SARATHY ET AL. /		
COMBUSTION AND FLAME 159 (2012) 2028?;iC2055			
C4H63,1-1OH<=>C4H5OH-13+H	7.722E+12		
0.488 4.394E+04	!\AUTHOR: !\REF:S.M. SARATHY ET AL. /		
COMBUSTION AND FLAME 159 (2012) 2028?;iC2055			
C4H5OH-13<=>C4H5-N+OH	5.610E+21		-
1.612 1.060E+05	!\AUTHOR: !\REF:S.M. SARATHY ET AL. /		
COMBUSTION AND FLAME 159 (2012) 2028?;iC2055			
C4H5OH-13<=>C2H3+CH2CHO	2.816E+24		-
2.381 9.013E+04	!\AUTHOR: !\REF:S.M. SARATHY ET AL. /		
COMBUSTION AND FLAME 159 (2012) 2028?;iC2055			
NC4KET21OH+OH<=>C2H4COCH2OH+H2O	8.450E+011	0.000	
-228.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+HO2<=>C2H4COCH2OH+H2O2	2.000E+011	0.000	
8698.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+O<=>C2H4COCH2OH+OH	3.070E+013	0.000	
3400.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+H<=>C2H4COCH2OH+H2	4.460E+006	2.000	
3200.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+O2<=>C2H4COCH2OH+HO2	1.550E+013	0.000	
41970.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+CH3<=>C2H4COCH2OH+CH4	1.740E+000	3.460	
3680.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+CH3O<=>C2H4COCH2OH+CH3OH	1.450E+011	0.000	
2771.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+CH3O2<=>C2H4COCH2OH+CH3O2H	2.000E+012	0.000	
15250.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+C2H3<=>C2H4COCH2OH+C2H4	3.000E+011	0.000	
3400.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
NC4KET21OH+C2H5<=>C2H4COCH2OH+C2H6	3.000E+010	0.000	
8600.0	!\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS		
C2H4COCH2OH<=>CH3CHCO+CH2OH	9.440E+029	-4.93	
38330	!\AUTHOR: !\REF:ANALOGY WITH SC4H9<=>C3H6+CH3		
PC4H8OH-2O2<=>SQC4H7OHP-4	1.439E+007	1.400	
20800.0	!\AUTHOR: !\REF:SHARMA		
SQC4H7OHP-4<=>CY(CCCO)COH+OH	2.440E+009		
0.780 18000.0	!\AUTHOR: !\REF:VILLANO (FROM KUIWEN'S MECH)		

SQC4H7OHP-4=>OH+HOCH2CHO+C2H4 3.080E+008
 1.500 23500.0 !\AUTHOR: !\REF:VILLANO (FROM KUIWEN'S MECH)
 CY(CCCO) COH+H=>C2H4+HOCH2CO+H2 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+O=>C2H4+HOCH2CO+OH 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+OH=>C2H4+HOCH2CO+H2O 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+HO2=>C2H4+HOCH2CO+H2O2 1.000E+013
 0.000 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+CH3=>C2H4+HOCH2CO+CH4 2.000E+011
 0.000 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+CH3O2=>C2H4+HOCH2CO+CH3O2H 1.000E+013
 0.000 19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+H=>CH2O+CH2CCH2OH+H2 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+O=>CH2O+CH2CCH2OH+OH 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+OH=>CH2O+CH2CCH2OH+H2O 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+HO2=>CH2O+CH2CCH2OH+H2O2 1.000E+013
 0.000 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+CH3=>CH2O+CH2CCH2OH+CH4 2.000E+011
 0.000 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 CY(CCCO) COH+CH3O2=>CH2O+CH2CCH2OH+CH3O2H 1.000E+013
 0.000 19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
 HOCH2CO<=>CH2OH+CO 1.070E+012
 0.630 16900.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CO<=>CH3+CO
 SQC4H7OHP-4+O2<=>SQC4H7OHP-4O2 3.433E+016 -
 1.627 198.7 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO
 R+O2
 SQC4H7OHP-4O2<=>C4H6OHOH1-4-3+HO2 1.440E+007
 1.380 28900.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO
 R+O2
 SQC4H7OHP-4O2<=>NC4KET24OH-1+OH 5.790E+001
 2.900 17000.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO
 R+O2
 C4H6OHOH1-4-3=>C2H3CHO+CH2OH+OH 1.050E+016
 0.000 41600.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO
 R+O2
 C4H6OHOH1-4-3=>HOCH2CHO+C2H3+OH 1.050E+016
 0.000 41600.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO
 R+O2
 NC4KET24OH-1=>CH2O+HOCH2COCH2+OH 1.500E+016
 0.000 43000.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO
 R+O2
 HOCH2CHO+O2<=>HOCH2CO+HO2 3.010E+013
 0.000 39150.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
 ABSTRACTION REACTIONS
 HOCH2CHO+O<=>HOCH2CO+OH 5.940E+012
 0.000 1868.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
 ABSTRACTION REACTIONS
 HOCH2CHO+H<=>HOCH2CO+H2 1.310E+005
 2.580 1220.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
 ABSTRACTION REACTIONS
 HOCH2CHO+OH<=>HOCH2CO+H2O 3.370E+012
 0.000 -619.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
 ABSTRACTION REACTIONS

HOCH2CHO+HO2<=>HOCH2CO+H2O2 3.010E+012
0.000 11920.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
ABSTRACTION REACTIONS
HOCH2CHO+CH3<=>HOCH2CO+CH4 7.080E-004
4.580 1966.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
ABSTRACTION REACTIONS
HOCH2CHO+CH3O2<=>HOCH2CO+CH3O2H 3.010E+012
0.000 11920.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
ABSTRACTION REACTIONS
HOCH2CHO+CH3CO3<=>HOCH2CO+CH3CO3H 3.010E+012
0.000 11920.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO
ABSTRACTION REACTIONS
!

!\REACTIONCLASS: \SC4H8OH-1_O2_PRODUCTS \A
\N \EA
!

SC4H8OH-1+O2<=>SC4H8OH-1O2 3.60E+12 0.0
0.0 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM.
A., 2007, 111, 4974.
SC4H8OH-1O2<=>PQC4H8OS 9.30E+10 -0.036
22890 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM.
A., 2007, 111, 4974.
SC4H8OH-1O2<=>NC4KET12OH+OH 1.49E+09 0.109
41390 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM.
A., 2007, 111, 4974.
PQC4H8OS=>C2H5CHO+CH2O+OH 6.70E+39 -8.38
22782 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM.
A., 2007, 111, 4974.
PQC4H8OS=>C2H5+HO2CH2CHO 2.67E+34 -6.63
22672 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM.
A., 2007, 111, 4974.
SC4H8OH-1O2<=>C4H71-2OH+HO2 2.44E+13 -0.253
32590 !\AUTHOR: !\REF:DIFFERENT FROM IC4H8 SYSTEM
(ANALOGY WITH PC4H8OH-2 SYSTEM)
SC4H8OH-1O2<=>PQC4H7OHS-3 1.360E+007
1.300 18200.0 !\AUTHOR: !\REF:SHARMA
PQC4H7OHS-3<=>CCY(COCC)OH+OH 2.590E+009
0.690 16000.0 !\AUTHOR: !\REF:VILLANO (FROM KUIWEN'S
MECH)
PQC4H7OHS-3=>OH+CH2O+SC3H5OH 1.230E+009
1.300 24900.0 !\AUTHOR: !\REF:VILLANO (FROM KUIWEN'S
MECH)
C4H71-2OH+OH<=>C4H63,1-2OH+H2O 2.020E+006
2.200 -437.2 !\AUTHOR: !\REF:ANALOGY WITH C4H8-1+OH
C4H71-2OH+HO2<=>C4H63,1-2OH+H2O2 3.91E-01
3.97 11702 !\AUTHOR: !\REF:ANALOGY WITH C4H8-1+OH
C4H63,1-2OH<=>C4H612+OH 7.035E+16
-1.012 3.607E+04 !\AUTHOR: !\REF:S.M. SARATHY ET AL. /
COMBUSTION AND FLAME 159 (2012) 2028?;iC2055
NC4KET12OH+H<=>C2H5CHOHCO+H2 1.000E+005
2.580 1220.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.
NC4KET12OH+OH<=>C2H5CHOHCO+H2O 1.700E+012
0.000 -619.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+O} \rightleftharpoons \text{C2H5CHOHCO+OH}$ 5.940E+012
 0.000 1868.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+HO2} \rightleftharpoons \text{C2H5CHOHCO+H2O2}$ 0.950E+004
 2.70 11520.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL. COMBUSTION
 AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+CH3} \rightleftharpoons \text{C2H5CHOHCO+CH4}$ 1.420E-003
 4.580 1966.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+C2H5} \rightleftharpoons \text{C2H5CHOHCO+C2H6}$ 7.360E+004
 2.000 5917.09 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+CH3O} \rightleftharpoons \text{C2H5CHOHCO+CH3OH}$ 1.000E+012
 0.000 3300.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+CH3O2} \rightleftharpoons \text{C2H5CHOHCO+CH3O2H}$ 3.010E+012
 0.000 11920.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+O2} \rightleftharpoons \text{C2H5CHOHCO+HO2}$ 9.030E+013
 0.000 43320.0 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+C2H3} \rightleftharpoons \text{C2H5CHOHCO+C2H4}$ 3.256E+005
 2.000 3965.69 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{NC4KET12OH+C2H5O} \rightleftharpoons \text{C2H5CHOHCO+C2H5OH}$ 6.030E+011
 0.000 3300.00 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{C2H5CHOHCO} \rightleftharpoons \text{C3H6OH1-1+CO}$ 5.78E+014
 0.00 16843.51 !\AUTHOR: !\REF:M. PELUCCHI ET AL.
 COMBUSTION AND FLAME (2015) 162(2) 265?;iC286.

$\text{C3H6OH1-1} \rightleftharpoons \text{C2H5CHO+H}$ 8.981E11
 0.271 3.299E+04 !\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H.
 J. CURRAN. JPCA, 2014, 118, 12089-12104.

$\text{C2H3OH+CH3} \rightleftharpoons \text{C3H6OH1-1}$ 2.040E+040 -
 8.250 24214.0 !\AUTHOR: !\REF:ANALOGY WITH

$\text{C2H4+CH3} \rightleftharpoons \text{NC3H7}$
 DUP

$\text{C2H3OH+CH3} \rightleftharpoons \text{C3H6OH1-1}$ 1.660E+021 -
 3.170 10241.0 !\AUTHOR: !\REF:ANALOGY WITH

$\text{C2H4+CH3} \rightleftharpoons \text{NC3H7}$
 DUP

$\text{CCY(COCC)OH+H} \Rightarrow \text{OH+C2H3COCH3+H2}$ 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+O} \Rightarrow \text{OH+C2H3COCH3+OH}$ 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+OH} \Rightarrow \text{OH+C2H3COCH3+H2O}$ 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+HO2} \Rightarrow \text{OH+C2H3COCH3+H2O2}$ 1.000E+013
 0.000 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+CH3} \Rightarrow \text{OH+C2H3COCH3+CH4}$ 2.000E+011
 0.000 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+CH3O2} \Rightarrow \text{OH+C2H3COCH3+CH3O2H}$ 1.000E+013
 0.000 19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+H} \Rightarrow \text{OH+SC3H5CHO+H2}$ 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

$\text{CCY(COCC)OH+O} \Rightarrow \text{OH+SC3H5CHO+OH}$ 5.000E+012
 0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE

CCY (COCC) OH+OH=>OH+SC3H5CHO+H2O	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+HO2=>OH+SC3H5CHO+H2O2	1.000E+013	
0.000 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+CH3=>OH+SC3H5CHO+CH4	2.000E+011	
0.000 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+CH3O2=>OH+SC3H5CHO+CH3O2H	1.000E+013	
0.000 19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+H=>C2H3OH+CH3CO+H2	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+O=>C2H3OH+CH3CO+OH	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+OH=>C2H3OH+CH3CO+H2O	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+HO2=>C2H3OH+CH3CO+H2O2	1.000E+013	
0.000 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+CH3=>C2H3OH+CH3CO+CH4	2.000E+011	
0.000 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+CH3O2=>C2H3OH+CH3CO+CH3O2H	1.000E+013	
0.000 19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+H=>HCO+SC3H5OH+H2	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+O=>HCO+SC3H5OH+OH	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+OH=>HCO+SC3H5OH+H2O	5.000E+012	
0.000 0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+HO2=>HCO+SC3H5OH+H2O2	1.000E+013	
0.000 15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+CH3=>HCO+SC3H5OH+CH4	2.000E+011	
0.000 10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
CCY (COCC) OH+CH3O2=>HCO+SC3H5OH+CH3O2H	1.000E+013	
0.000 19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
PQC4H7OHS-3+O2<=>PQC4H7OHS-3O2	1.744E+014	-0.816
-536.5 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2		
PQC4H7OHS-3O2<=>NC4KET13OH-2+OH	1.090E+004	2.400
19900.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2		
NC4KET13OH-2=>CH3CHO+HOCHCHO+OH	1.050E+016	0.000
43000.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2		
PQC4H7OHS-3O2<=>C4H7O2-1,3OOH	2.91E+12	-
0.226 22300 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS.		
CHEM. A., 2007, 111, 4974.		
PQC4H7OHS-3O2<=>C4H6OHOOH1-3-4+HO2	3.64E+14	-
0.711 32710 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS.		
CHEM. A., 2007, 111, 4974.		
PQC4H7OHS-3O2<=>C4H6OHOOH2-2-1+HO2	2.44E+13	-
0.253 32590 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS.		
CHEM. A., 2007, 111, 4974.		
C4H7O2-1,3OOH=>C3KET12+CH2O+OH	5.36E+12	-
0.080 10790 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS.		
CHEM. A., 2007, 111, 4974.		
C4H7O2-1,3OOH=>HO2CH2CHO+CH3CHO+OH	6.70E+39	-
8.38 22782 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS.		
CHEM. A., 2007, 111, 4974.		
PQC4H7OHS-3O2<=>NC4KET24OH-3+OH	1.49E+09	
0.109 41390 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS.		
CHEM. A., 2007, 111, 4974.		
HOCHCHO+O<=>CHOCHO+OH	1.460E-003	4.730
1727.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5OH+OH<=>C2H5O+H2O		

HOCHCHO+OH<=>CHOCHO+H2O	5.810E-003	4.280
-3560.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5OH+OH<=>C2H5O+H2O		
HOCHCHO+H<=>CHOCHO+H2	9.450E+002	3.140
8701.1 !\AUTHOR: !\REF:ANALOGY WITH C2H5OH+OH<=>C2H5O+H2O		
HOCHCHO+HO2<=>CHOCHO+H2O2	6.470E-007	5.300
10533.1 !\AUTHOR: !\REF:ANALOGY WITH C2H5OH+OH<=>C2H5O+H2O		
HOCHCHO+CH3<=>CHOCHO+CH4	2.035E+000	3.570
7721.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5OH+OH<=>C2H5O+H2O		
HOCHCHO+CH3O2<=>CHOCHO+CH3O2H	3.236E-007	5.300
10533.1 !\AUTHOR: !\REF:ANALOGY WITH C2H5OH+OH<=>C2H5O+H2O		
C4H6OHOH1-3-4=>CH2O+PC3H4OH-3+OH	1.500E+016	
0.000 42000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2		
C4H6OHOH2-2-1=>CH2O+PC3H4OH-1+OH	1.500E+016	
0.000 42000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2		
NC4KET24OH-3=>CH2O+CH3COCHOH+OH	1.500E+016	
0.000 43000.0 !\AUTHOR: !\REF:Miyoshi A/2 compared to R+O2		
PC3H4OH-3<=>C2H3CHO+H	5.690E+052	-
13.380 45049.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
PC3H4OH-3<=>C3H5O	5.480E+045	-
11.630 44328.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
PC3H4OH-3<=>CH2CCH2OH	2.650E+036	-
8.860 51019.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
PC3H4OH-3+O2<=>C2H3CHO+HO2	5.260E+017	-
1.638 869.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
PC3H4OH-1<=>CH3CHCO+H	5.690E+052	-
13.380 45049.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
PC3H4OH-1<=>PC3H4OH-2	2.650E+036	-
8.860 51019.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
PC3H4OH-1+O2<=>CH3CHCO+HO2	5.260E+017	-
1.638 869.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
CH3COCHOH<=>CH3COCHO+H	5.690E+052	-
13.380 45049.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
CH3COCHOH<=>CH3COCH2O	5.480E+045	-
11.630 44328.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
CH3COCHOH+O2<=>CH3COCHO+HO2	5.260E+017	-
1.638 869.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		

!\REACTIONCLASS: \SC4H8OH-3_O2_PRODUCTS \A

\N \EA

!

SC4H8OH-3+O2<=>SC4H8OH-3O2	3.60E+12	0.0
0.0 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.		
SC4H8OH-3O2<=>SQC4H8OS	2.91E+12	-0.226
22300 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.		
SC4H8OH-3O2<=>C4H71-3OH+HO2	3.64E+14	-0.711
32710 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.		
SC4H8OH-3O2<=>C4H72-2OH+HO2	2.44E+13	-0.253
32590 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.		
SQC4H8OS=>CH3CHO+CH3CHO+OH	2.68E+13	-0.080
10790 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.		

SC4H8OH-3O2<=>NC4KET23OH+OH 1.49E+09 0.109
 41390 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007,
 111, 4974.
 SC4H8OH-3O2<=>SQC4H7OHS-4 1.439E+007
 1.400 20800.0 !\AUTHOR: !\REF:SHARMA
 SQC4H7OHS-4<=>CCY(COCC)OH+OH 2.440E+009
 0.780 18000.0 !\AUTHOR: !\REF:VILLANO (FROM KUIWEN'S MECH)
 SQC4H7OHS-4=>OH+CH3CHO+C2H3OH 3.080E+008
 1.500 23500.0 !\AUTHOR: !\REF:VILLANO (FROM KUIWEN'S MECH)
 C4H71-3OH+OH<=>C4H63,1-3OH+H2O 2.020E+006
 2.200 -437.2 !\AUTHOR: \REF:ANALOGY WITH C4H8-1+OH
 C4H71-3OH+HO2<=>C4H63,1-3OH+H2O2 3.91E-01
 3.97 11702 !\AUTHOR: \REF:ANALOGY WITH C4H8-1+OH
 C4H72-2OH+OH<=>C4H63,1-3OH+H2O 2.020E+006
 2.200 -437.2 !\AUTHOR: \REF:ANALOGY WITH C4H8-1+OH
 C4H72-2OH+HO2<=>C4H63,1-3OH+H2O2 3.91E-01
 3.97 11702 !\AUTHOR: \REF:ANALOGY WITH C4H8-1+OH
 C4H63,1-3OH<=>C4H6+OH 7.035E+16 -
 1.012 3.607E+04 !\AUTHOR: !\REF:S.M. SARATHY ET AL. /
 COMBUSTION AND FLAME 159 (2012) 2028?;iC2055
 NC4KET23OH+OH<=>CH3COCOCH3+H2O 8.450E+011 0.000
 -228.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+HO2<=>CH3COCOCH3+H2O2 2.000E+011 0.000
 8698.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+O<=>CH3COCOCH3+OH 3.070E+013 0.000
 3400.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+H<=>CH3COCOCH3+H2 4.460E+006 2.000
 3200.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+O2<=>CH3COCOCH3+HO2 1.550E+013 0.000
 41970.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+CH3<=>CH3COCOCH3+CH4 1.740E+000 3.460
 3680.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+CH3O<=>CH3COCOCH3+CH3OH 1.450E+011 0.000
 2771.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+CH3O2<=>CH3COCOCH3+CH3O2H 2.000E+012 0.000
 15250.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+C2H3<=>CH3COCOCH3+C2H4 3.000E+011 0.000
 3400.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 NC4KET23OH+C2H5<=>CH3COCOCH3+C2H6 3.000E+010 0.000
 8600.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 CH3COHCO+CH3<=>CH3COCOCH3 1.230E+011 0.000
 7800.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 CH3COHCO+OH<=>SC2H4OH+CO2 1.730E+012 0.000
 -1010.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 CH3COHCO+H<=>SC2H4OH+CO 4.400E+012 0.000
 1459.0 !\AUTHOR: !\REF:ANALOGY WITH C2H5COCH3 REACTIONS
 SQC4H7OHS-4+O2<=>SQC4H7OHS-4O2 3.433E+016 -1.627
 198.7 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2
 SQC4H7OHS-4O2<=>NC4KET24OH-3+OH 5.790E+001
 2.900 17000.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2
 SQC4H7OHS-4O2<=>C4H7O2-1,3OOH 9.30E+10 -0.036
 22890 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007,
 111, 4974.
 SQC4H7OHS-4O2<=>C4H6OHOH1-2-3+HO2 2.44E+13 -
 0.253 32590 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM.
 A., 2007, 111, 4974.

SQC4H7OHS-4O2<=>NC4KET13OH-2+OH	1.49E+09	
0.109 41390 !\AUTHOR: !\REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.		
C4H6OHOH1-2-3=>CH2COHCHO+CH3+OH	1.050E+016	
0.000 41600.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2		
C4H6OHOH1-2-3=>CH3CHO+SC2H2OH+OH	1.050E+016	
0.000 41600.0 !\AUTHOR: !\REF:MIYOSHI A/2 COMPARED TO R+O2		
SC2H2OH+HCO<=>CH2COHCHO	1.810E+013	
0.000 0.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+H<=>CH2COHCO+H2	1.340E+013	
0.000 3300.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+O<=>CH2COHCO+OH	5.940E+012	
0.000 1868.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+OH<=>CH2COHCO+H2O	9.240E+006	
1.500 -962.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+O2<=>CH2COHCO+HO2	1.005E+013	
0.000 40700.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+HO2<=>CH2COHCO+H2O2	3.010E+012	
0.000 11920.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+CH3<=>CH2COHCO+CH4	2.608E+006	
1.780 5911.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+C2H3<=>CH2COHCO+C2H4	1.740E+012	
0.000 8440.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+CH3O<=>CH2COHCO+CH3OH	1.000E+012	
0.000 3300.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
CH2COHCHO+CH3O2<=>CH2COHCO+CH3O2H	3.010E+012	
0.000 11920.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
SC2H2OH+CO<=>CH2COHCO	1.510E+011	
0.000 4810.0 !\AUTHOR: !\REF:ANALOGY WITH C2H3CHO REACTIONS		
SC2H2OH<=>CH2CO+H	5.690E+052 -13.380	
45049.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
SC2H2OH<=>HCCOH+H	5.400E+046 -11.630	
44323.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
SC2H2OH<=>C2H2OH	2.650E+036 -8.860	
51019.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
SC2H2OH+O2<=>CH2CO+HO2	5.260E+017 -1.638	
869.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		
SC2H2OH+O2<=>HCCOH+HO2	5.512E+003 2.495	
-414.0 !\AUTHOR: !\REF:ANALOGY WITH SC2H4OH REACTIONS		

!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N
 \EA
 !

C4H8-1+O<=>NC3H7+HCO	7.450E+006	1.880
183.0 !\AUTHOR: !\REF:ANALOGY WITH C3H6+O		
C4H8-1+O=>CH2CO+C2H5+H	3.050E+006	1.880
183.0 !\AUTHOR: !\REF:ANALOGY WITH C3H6+O		
C4H8-1+O=>C2H5CHCO+H+H	3.050E+006	1.880
183.0 !\AUTHOR: !\REF:ANALOGY WITH C3H6+O		
C4H8-2+O<=>CH3+C2H5CO	7.450E+006	1.880
183.0 !\AUTHOR: !\REF:ANALOGY WITH C3H6+O		
C4H8-2+O=>CH2CO+C2H5+H	3.050E+006	1.880
183.0 !\AUTHOR: !\REF:ANALOGY WITH C3H6+O		
C4H8-2+O=>C2H5CHCO+H+H	3.050E+006	1.880
183.0 !\AUTHOR: !\REF:ANALOGY WITH C3H6+O		

C4H8-2+HO2<=>C4H8O2-3+OH 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:JUDIT ZADOR,STEPHEN J. KLIPPENSTEIN,AND
JAMES A. MILLER J. PHYS. CHEM. A 2011, 115, 10218?;iC10225
PLOG/ 0.0133 7.65E+05 1.92622 10745/
PLOG/ 1.0000 1.79E+08 1.25089 12370/
PLOG/ 10.0000 1.75E+15 -0.74 17220/
PLOG/ 100.0000 8.37E+20 -2.28314 22838/

C4H8OOH2-3<=>C4H8O2-3+OH 1.05E+10 0.68
11964 !\AUTHOR: !\REF:JUDIT ZADOR,STEPHEN J.
KLIPPENSTEIN,AND JAMES A. MILLER J. PHYS. CHEM. A 2011, 115,
10218?;iC10225
PLOG/ 0.0133 3.02E+19 -3.51 9746/
PLOG/ 1.0000 6.37E+24 -4.55 13480/
PLOG/ 10.0000 1.39E+28 -5.25 16470/
PLOG/ 100.0000 1.54E+27 -4.69 17832/

!

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

!

C4H8-1+CH3O2<=>C4H8O1-2+CH3O 1.000E+012 0.000
14340.0 !\AUTHOR: !\REF:IN ARAMCO (ALLARA, D. L. AND EDELSON,
D., INT. J. CHEM. KINET. 7, 479 (1975).

C4H8-2+CH3O2<=>C4H8O2-3+CH3O 5.620E+011 0.000
12310.0 !\AUTHOR: !\REF:IN ARAMCO (SEATTLE, AUGUST, 1988)

!

!\ENDSUBMECH: \C4H8-1\C4H8-2

!

!\SUBMECH: \C4H6

!

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

!

C4H6<=>C4H5-I+H 5.700E+036 -6.270
112353.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H6<=>C4H5-N+H 5.300E+044 -8.620
123608.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H6<=>C4H4+H2 2.500E+015 0.000
94700.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
H2CC+C2H4<=>C4H6 1.000E+012 0.000
0.0 !\AUTHOR: !\REF:

!

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

!

C4H6+H<=>C4H5-N+H2 1.330E+006 2.530
12240.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000

C4H5-N+HO2<=>C4H6+O2	6.000E+011	0.000
0.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+O<=>C4H5-N+OH	7.500E+006	1.900
3740.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+OH<=>C4H5-N+H2O	6.200E+006	2.000
3430.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H5-N+H2O2<=>C4H6+HO2	1.210E+010	0.000
-596.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+CH3<=>C4H5-N+CH4	2.000E+014	0.000
22800.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+C2H3<=>C4H5-N+C2H4	5.000E+013	0.000
22800.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+C3H3<=>C4H5-N+C3H4-A	1.000E+013	0.000
22500.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+C3H5-A<=>C4H5-N+C3H6	1.000E+013	0.000
22500.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+H<=>C4H5-I+H2	6.650E+005	2.530
9240.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H5-I+HO2<=>C4H6+O2	6.000E+011	0.000
0.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+O<=>C4H5-I+OH	7.500E+006	1.900
3740.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+OH<=>C4H5-I+H2O	3.100E+006	2.000
430.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H5-I+H2O2<=>C4H6+HO2	1.210E+010	0.000
-596.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+CH3<=>C4H5-I+CH4	1.000E+014	0.000
19800.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+C2H3<=>C4H5-I+C2H4	2.500E+013	0.000
19800.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+C3H3<=>C4H5-I+C3H4-A	5.000E+012	0.000
19500.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+C3H5-A<=>C4H5-I+C3H6	5.000E+012	0.000
19500.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		

!\REACTIONCLASS: \R_ADDITION\H \A \N
 \EA
 !

C4H6+H<=>C2H4+C2H3	1.460E+030	-4.340
21647.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
PLOG/ 1.0000 1.460E+030 -4.340 21647.0/		
PLOG/ 10.0000 5.450E+030 -4.510 21877.0/		
C4H6+H<=>C3H4-P+CH3	2.000E+012	0.000
7000.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		
C4H6+H<=>C3H4-A+CH3	2.000E+012	0.000
7000.0 !\AUTHOR: !\REF: WARNING SOURCE UNCLEAR		

!\REACTIONCLASS: \R_ADDITION\O \A \N
 \EA
 !

C4H6+O<=>C2H2+C2H4O1-2	1.000E+008	1.450
-860.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.		

C4H6+O<=>SC3H5CO+H 5.000E+007 1.450
-860.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

C4H6+O<=>CH2CHCHCHO+H 4.500E+008 1.450
-860.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

!

!\REACTIONCLASS: \R_ADDITION\OH \A \N
\EA
!

C4H6+OH<=>C2H3CHO+CH3 1.370e+12 0.00 -1040.0
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
C4H6+OH<=>C3H5-A+CH2O 1.370e+12 0.00 -1040.0
!\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

!\REACTIONCLASS: \R_ADDITION\HO2 \A \N
\EA
!

C4H6+HO2<=>C4H6O25+OH 1.200E+012 0.000
14000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
C4H6+HO2<=>C2H3CHOCH2+OH 4.800E+012 0.000
14000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

!=====
=====
!\SUBSPECIES: \C2H3CHOCH2\C4H6O25\C4H6O23
!=====
=====
!

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

C4H6O25<=>C4H4O+H2 5.300E+012 0.000
48500.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
C2H3CHOCH2<=>C4H6O23 2.000E+014 0.000
50600.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
C4H6O23<=>SC3H5CHO 1.950E+013 0.000
49400.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
C4H6O23<=>C2H4+CH2CO 5.750E+015 0.000
69300.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
C4H6O23<=>C2H2+C2H4O1-2 1.000E+016 0.000
75800.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

!=====
=====
!\ENDSUBSPECIES: \C2H3CHOCH2\C4H6O25\C4H6O23

PLOG/ 0.1200 1.500E+052 -11.970 16056.0/
 PLOG/ 1.0000 1.500E+042 -8.840 12483.0/
 C2H3+C2H3<=>C4H5-I+H 1.500E+030 -4.950
 12958.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 PLOG/ 0.0263 1.500E+030 -4.950 12958.0/
 PLOG/ 0.1200 7.200E+028 -4.490 14273.0/
 PLOG/ 1.0000 1.200E+022 -2.440 13654.0/
 C2H3+C2H3<=>C4H5-N+H 1.100E+024 -3.280
 12395.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 PLOG/ 0.0263 1.100E+024 -3.280 12395.0/
 PLOG/ 0.1200 4.600E+024 -3.380 14650.0/
 PLOG/ 1.0000 2.400E+020 -2.040 15361.0/
 C4H5-N<=>C4H5-I 2.400E+060 -16.080
 47500.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 PLOG/ 0.0132 2.400E+060 -16.080 47500.0/
 PLOG/ 0.0263 1.300E+062 -16.380 49600.0/
 PLOG/ 0.1200 4.900E+066 -17.260 55400.0/
 PLOG/ 1.0000 1.500E+067 -16.890 59100.0/
 PLOG/ 10.0000 2.000E+060 -14.460 58600.0/
 C4H4+H<=>C4H5-N 1.200E+051 -12.570
 12300.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 PLOG/ 0.0132 1.200E+051 -12.570 12300.0/
 PLOG/ 0.0263 4.200E+050 -12.340 12500.0/
 PLOG/ 0.1200 1.100E+050 -11.940 13400.0/
 PLOG/ 1.0000 1.300E+051 -11.920 16500.0/
 PLOG/ 10.0000 6.200E+045 -10.080 15800.0/
 C4H4+H<=>C4H5-I 6.100E+053 -13.190
 14200.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 PLOG/ 0.0132 6.100E+053 -13.190 14200.0/
 PLOG/ 0.0263 9.600E+052 -12.850 14300.0/
 PLOG/ 0.1200 2.100E+052 -12.440 15500.0/
 PLOG/ 1.0000 4.900E+051 -11.920 17700.0/
 PLOG/ 10.0000 1.500E+048 -10.580 18800.0/
 !

!\REACTIONCLASS: \R_R_PRODUCTS \A \N
 \EA
 !

C4H5-N+H<=>C4H5-I+H 3.100E+026 -3.350
 17423.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 C4H5-N+H<=>C4H4+H2 1.500E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-N+OH<=>C4H4+H2O 2.000E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-N+HCO<=>C4H6+CO 5.000E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.

C4H5-N+HO2=>C2H3+CH2CO+OH 6.600E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-N+O2<=>CH2CHCHCHO+O 3.000E+011 0.290
 11.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-N+O2<=>HCO+C2H3CHO 9.200E+016 -1.390
 1010.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-N+O2=>H+CO+C2H3CHO 5.19E+15 -1.26 3312.62
 !<BASED ON C2H3+O2 FROM KLIPPENSTEIN>
 !\C2
 C4H5-I+H<=>C4H4+H2 3.000E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-I+H<=>C3H3+CH3 2.000E+013 0.000
 2000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-I+OH<=>C4H4+H2O 4.000E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-I+HCO<=>C4H6+CO 5.000E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-I+HO2=>C2H3+CH2CO+OH 6.600E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-I+O2<=>CH2CO+CH2CHO 2.160E+010 0.000
 2500.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-2<=>C4H5-I 1.500E+067 -16.890
 59100.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 C4H5-2+H<=>C4H5-I+H 3.100E+026 -3.350
 17423.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 C4H5-2+HO2=>OH+C2H2+CH3CO 8.000E+011 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-2+O2<=>CH3CO+CH2CO 2.160E+010 0.000
 2500.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H5-2+OH<=>CH2OH+C3H3 3.0E12 0.0 0.0
 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H5-2+O<=>CH2O+C3H3 3.0E13 0.0 0.0
 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 !

!\REACTIONCLASS: \AROMATIC_GROWTH \A \N
 \EA
 !

C4H6+C2H3=>C6H6+H2+H 5.620E+011 0.000
 3240.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H5-I+C2H2<=>FULVENE+H 9.738E+26 -3.76
 21329.0 !\AUTHOR: !\ 10ATM/SENOSIAIN&MILLER, J.PHYS.CHEM.A, 2007, PP.
 3740-3747

C4H5-N+C2H2<=>FULVENE+H 1.740E+19 -1.86
 12384.0 !\AUTHOR: !\ 10ATM/SENOSIAIN&MILLER, J.PHYS.CHEM.A, 2007, PP.
 3740-3747
 C4H5-N+C2H2<=>C6H6+H 1.600E+016 -1.330
 5400.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H5-N+C2H3<=>C6H6+H2 1.840E-013 7.070
 -3611.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H5-2+C2H<=>C3H3+C3H3 4.0E+12 0.0
 0.0 !\AUTHOR: !\ JAM6
 C4H5-2+C2H2<=>C6H6+H 5.000E+014 0.000
 25000.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H5-2+C2H4<=>C5H6+CH3 5.000E+014 0.000
 25000.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000

!-----

!\ENDSUBMECH: \C4H6

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!-----

!-----

!\SUBMECH: \C4H612

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!-----

!-----

!-----

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!\REACTIONCLASS: \UNIMOL \A \N

\EA

!-----

C4H612<=>C4H5-I+H 4.200E+015 0.000
 92600.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 C4H612<=>C4H6 3.000E+013 0.000
 65000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 C3H3+CH3 (+M)<=>C4H612 (+M) 1.500E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 LOW/ 2.600E+057 -11.940
 9770.0/
 TROE/ 1.750E-001 1.341E+003 6.000E+004 9.770E+003/
 H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
 0.70/

!-----

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!-----

C4H612+H<=>C4H5-I+H2 1.700E+005 2.500
 2490.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.
 C4H612+CH3<=>C4H5-I+CH4 7.000E+013 0.000
 18500.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
 ET AL.
 C4H612+O<=>C4H5-I+OH 1.800E+011 0.700
 5880.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
 AL.

C4H612+OH<=>C4H5-I+H2O 3.100E+006 2.000
-298.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.
!

!\REACTIONCLASS: \H_CAT_ISO \A \N
\EA
!

C4H612+H<=>C4H6+H 2.000E+013 0.000
4000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.
!

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
\EA
!

C4H612+H<=>C3H4-A+CH3 2.000E+013 0.000
2000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H612+H<=>C3H4-P+CH3 2.000E+013 0.000
2000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.
!

!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N
\EA
!

C4H612+O<=>CH2CO+C2H4 1.200E+008 1.650
327.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

!-----
!-----
!\ENDSUBMECH: \C4H612
!-----
!-----

!\SUBMECH: \C4H6-2
!-----
!-----

C4H6-2<=>C4H6 3.000E+013 0.000
65000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.

C4H6-2<=>C4H612 3.000E+013 0.000
67000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.

C4H6-2+H<=>C4H612+H 2.000E+013 0.000
4000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H6-2+H<=>C4H5-2+H2 3.400E+005 2.500
2490.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H6-2+H<=>CH3+C3H4-P 2.600E+005 2.500
1000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H6-2<=>H+C4H5-2 5.000E+015 0.000
87300.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.

C4H6-2+CH3<=>C4H5-2+CH4 1.400E+014 0.000
18500.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.

!-----

!\ENDSUBMECH: \C4H6-2

!-----

!\SUBMECH: \C4H4

!-----

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

C4H3-I+H<=>C4H4 3.400E+043 -9.010
12120.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.

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

C4H4+H<=>C4H3-N+H2 6.650E+005 2.530
12240.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.

C4H4+OH<=>C4H3-N+H2O 3.100E+007 2.000
3430.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H4+H<=>C4H3-I+H2 3.330E+005 2.530
9240.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H4+OH<=>C4H3-I+H2O 1.550E+007 2.000
430.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

C4H4+CH3<=>C4H3-I+CH4 0.500E+14 0.0 19800.0

!\<HALF THE RATES OF ABSTRACTION FROM 1,3-BUTADIENE>

C4H4+CH3<=>C4H3-N+CH4 1.000E+14 0.0 22800.0

!\<HALF THE RATES OF ABSTRACTION FROM 1,3-BUTADIENE>

!-----

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
\EA

C3H3+CH2<=>C4H4+H 5.000E+013 0.000
0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.

!-----

!\REACTIONCLASS: \RADICAL_ADDITION\O \A \N
\EA
!

C4H4+O<=>C3H3+HCO 6.000E+008 1.450
-860.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
!

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA
!

C4H4+OH<=>CH2O+C3H3 5.0E12 0.0 0.0 !\AUTHOR: !\ JAM
!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA
!

C2H2+C2H(+M)<=>C4H3-N(+M) 8.300E+010 0.899
-363.0
LOW/ 1.240E+031 -4.718
1871.0/

TROE/ 1.000E+000 1.000E+002 5.613E+003 1.339E+004/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/
2.50/ C2H4/ 2.50/

C2H2+C2H(+M)<=>C4H3-I(+M) 8.300E+010 0.899
-363.0
LOW/ 1.240E+031 -4.718
1871.0/

TROE/ 1.000E+000 1.000E+002 5.613E+003 1.339E+004/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/
2.50/ C2H4/ 2.50/

C4H2+H<=>C4H3-N 1.100E+042 -8.720
15300.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H2+H<=>C4H3-I 1.100E+030 -4.920
10800.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

C4H3-N<=>C4H3-I 4.100E+043 -9.490
53000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
!

!\REACTIONCLASS: \R_R_PRODUCTS \A \N
\EA
!

C4H3-N+H<=>C4H3-I+H 2.500E+020 -1.670
10800.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

C4H3-N+H<=>C2H2+H2CC 6.300E+025 -3.340
10014.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

C4H3-N+H<=>C4H4 2.000E+047 -10.260
13070.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

C4H3-N+H<=>C4H2+H2 3.000E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-N+OH<=>C4H2+H2O 2.000E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-N+C2H3<=>C3H3+C3H3 4.0E+12 0.0
 0.0 !\AUTHOR: !\ JAM6
 C3H3+CH<=>C4H3-I+H 5.000E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-I+H<=>C2H2+H2CC 2.800E+023 -2.550
 10780.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-I+H<=>C4H2+H2 6.000E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-I+OH<=>C4H2+H2O 4.000E+012 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-I+O2<=>HCCO+CH2CO 7.860E+016 -1.800
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 C4H3-I+CH2<=>C3H4-A+C2H 2.000E+013 0.000
 0.0 !\AUTHOR: !\REF: ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)
 !

!\REACTIONCLASS: \AROMATIC_GROWTH \A \N
 \EA
 !

C4H4+C2H<=>L-C6H4+H 1.200E+013 0.000
 0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H3-N+C2H2<=>L-C6H4+H 2.500E+014 -0.560
 10600.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H3-N+C2H2<=>C-C6H4+H 6.900E+046 -10.010
 30100.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H3-N+C2H2<=>C6H5 9.600E+070 -17.770
 31300.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
 C4H3-I+CH3<=>C5H6 1.000E+012 0.000
 0.0 !\AUTHOR: !\REF: ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)
 !

!\REACTIONCLASS: \MISCELLANEOUS \A \N
 \EA
 !

C3H3+HCCO<=>C4H4+CO 2.500E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 !-----

 !\ENDSUBMECH: \C4H4
 !-----

!-----

!\SUBMECH: \C4H2
!-----

!

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

H2CC+C2H2 (+M) <=> C4H4 (+M) 3.500E+005 2.055
-2400.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
LOW/ 1.400E+060 -12.599
7417.0/
TROE/ 9.800E-001 5.600E+001 5.800E+002 4.164E+003/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/
3.00/ C2H4/ 3.00/
!

!\REACTIONCLASS: \RADICAL_ADDITION\OH \A \N
\EA
!

C2H2+C2H <=> C4H2+H 9.600E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H2+OH <=> H2C4O+H 6.600E+012 0.000
-410.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H2+OH <=> CO+C3H3 2.58E+19 -2.44
3034. !\AUTHOR: !\ PROC COMB INST 31 185-193 (2007)
H2C4O+H <=> C2H2+HCCO 5.000E+013 0.000
3000.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
H2C4O+OH <=> CH2CO+HCCO 1.000E+007 2.000
2000.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!

!\REACTIONCLASS: \AROMATIC_GROWTH \A \N
\EA
!

C4H2+C2H <=> C6H2+H 9.600E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
C4H2+C2H <=> C6H3 4.500E+037 -7.680
7100.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!-----

!\ENDSUBMECH: \C4H2
!-----

!\SUBMECH: \NC3H7CHO
!-----

!

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

!

!

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

NC3H7CHO+O2<=>NC3H7CO+HO2	3.010E+013	
0.000 39150.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+O<=>NC3H7CO+OH	5.940E+012	
0.000 1868.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+H<=>NC3H7CO+H2	1.310E+005	
2.580 1220.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+OH<=>NC3H7CO+H2O	3.370E+012	
0.000 -619.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+HO2<=>NC3H7CO+H2O2	3.010E+012	
0.000 11920.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+CH3<=>NC3H7CO+CH4	7.080E-004	
4.580 1966.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H	3.010E+012	
0.000 11920.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC3H7CHO+OH<=>C3H6CHO-3+H2O	5.520E+002	3.120
-1176.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+HO2<=>C3H6CHO-3+H2O2	3.440E+012	0.050
17880.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+CH3O2<=>C3H6CHO-3+CH3O2H	3.440E+012	0.050
17880.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+OH<=>C3H6CHO-2+H2O	4.680E+007	1.610
-35.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+HO2<=>C3H6CHO-2+H2O2	9.640E+003	2.600
13910.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+CH3O2<=>C3H6CHO-2+CH3O2H	9.640E+003	2.600
13910.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+OH<=>C3H6CHO-1+H2O	5.280E+009	0.970
1586.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+HO2<=>C3H6CHO-1+H2O2	2.379E+004	2.550
16490.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
NC3H7CHO+CH3O2<=>C3H6CHO-1+CH3O2H	2.379E+004	2.550
16490.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		

!\REACTIONCLASS: \RADICAL_DECOMP \A \N
\EA
!

NC3H7CO<=>NC3H7+CO	1.000E+011	0.000
9600.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H5CHCO+H<=>C3H6CHO-3	5.000E+012	0.000
1200.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H3CHO+CH3<=>C3H6CHO-3	1.230E+011	0.000
7800.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C3H6CHO-1<=>C2H4+CH2CHO	7.400E+011	0.000
21970.0 !\AUTHOR: !\REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95.		

!=====
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!\SUBSPECIES: \C2H5CHCO

!=====
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!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA
!

C2H5CHCO+OH<=>NC3H7+CO2 3.730E+012 0.000
-1010.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
C2H5CHCO+H<=>NC3H7+CO 4.400E+012 0.000
1459.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
C2H5CHCO+O<=>C3H6+CO2 3.200E+012 0.000
-437.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

!=====
=====
!\ENDSUBSPECIES: \C2H5CHCO
!=====
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!

!\SUBSPECIES: \SC3H5CHO
!=====
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!

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

SC3H5CHO<=>C3H6+CO 3.900E+014 0.000
69000.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN
ET AL.
SC3H5CO+H<=>SC3H5CHO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET
AL.
CH2CHCHCHO+H<=>SC3H5CHO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF: PITZ ESTIMATE

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

SC3H5CHO+OH<=>SC3H5CO+H2O 3.370E+12 0.000
-619.0 !\AUTHOR: !\REF:BILL ADDED
SC3H5CHO+HO2<=>SC3H5CO+H2O2 1.000E+012 0.000
11920.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H5CHO+X -->IC3H5CO+HX
SC3H5CHO+CH3<=>SC3H5CO+CH4 3.980E+012 0.000
8700.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H5CHO+X -->IC3H5CO+HX
SC3H5CHO+O<=>SC3H5CO+OH 7.180E+012 0.000
1389.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H5CHO+X -->IC3H5CO+HX
SC3H5CHO+O2<=>SC3H5CO+HO2 4.000E+013 0.000
37600.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H5CHO+X -->IC3H5CO+HX
SC3H5CHO+H<=>SC3H5CO+H2 2.600E+012 0.000
2600.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H5CHO+X -->IC3H5CO+HX

$SC3H5CHO + C2H3 \rightleftharpoons SC3H5CO + C2H4$ 1.110E+000 3.500
 4682.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 $SC3H5CHO + H \rightleftharpoons CH2CHCHCHO + H2$ 1.700E+005 2.500
 2490.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 $SC3H5CHO + O \rightleftharpoons CH2CHCHCHO + OH$ 5.240E+11 0.700
 5884.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 $SC3H5CHO + OH \rightleftharpoons CH2CHCHCHO + H2O$ 4.460E+6 2.072
 1051.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 $SC3H5CHO + CH3 \rightleftharpoons CH2CHCHCHO + CH4$ 2.100E+000 3.500
 5675.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 $SC3H5CHO + C2H3 \rightleftharpoons CH2CHCHCHO + C2H4$ 2.210E+000 3.500
 4682.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

!

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N
 \EA

!

$SC3H5CHO + H \rightleftharpoons CH3 + C2H3CHO$ 4.000E+021 -2.390
 11180.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.
 $SC3H5CHO + H \rightleftharpoons C3H6 + HCO$ 4.000E+021 -2.390
 11180.0 !\AUTHOR: !\REF: WARNING PRIMARY SOURCE UNCLEAR PROBABLY LASKIN ET AL.

!

!\REACTIONCLASS: \R_DECOMPOSITION \A \N
 \EA

!

$C3H5-S + CO \rightleftharpoons SC3H5CO$ 5.000E+012 0.000
 8000.0 !\AUTHOR: !\REF: PITZ ESTIMATE
 $CH2CHCHCHO \rightleftharpoons C3H5-A + CO$ 6.100E+005 0.920
 -1120.0 !\AUTHOR: !\REF: ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
 $CH2CHCHCHO + O2 \rightleftharpoons C2H3CHO + HOCO$ 1.200E+036 -7.250
 33600.0 !\AUTHOR: !\REF: ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

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!\ENDSUBSPECIES: \SC3H5CHO

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!=====

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!\SUBSPECIES: \C2H3COCH3

!=====

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!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
 \EA

!

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C2H3COCH3+OH<=>CH3CHO+CH3CO	1.000E+011	0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H3COCH3+OH=>CH2CO+C2H3+H2O	5.100E+011	0.000
1192.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H3COCH3+HO2=>CH2CHO+CH3CO+OH	6.030E+009	0.000
7949.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H3COCH3+HO2=>CH2CO+C2H3+H2O2	8.500E+012	0.000
20460.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H3COCH3+CH3O2=>CH2CHO+CH3CO+CH3O	3.970E+011	0.000
17050.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		
C2H3COCH3+CH3O2=>CH2CO+C2H3+CH3O2H	3.010E+012	0.000
17580.0 !\AUTHOR: !\REF:CURRAN ESTIMATE		

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!\ENDSUBSPECIES: \C2H3COCH3

!=====
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!\ENDSUBMECH: \NC3H7CHO

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!\SUBMECH: \C2H5COCH3

!-----

!-----

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!-----

!-----

!\REACTIONCLASS: \RADICAL_ADDITION\H \A \N

\EA

!-----

C2H5COCH3+OH<=>CH2CH2COCH3+H2O	7.550E+009	0.970
1586.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+HO2<=>CH2CH2COCH3+H2O2	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995		
C2H5COCH3+O<=>CH2CH2COCH3+OH	2.250E+013	0.000
7700.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+H<=>CH2CH2COCH3+H2	9.160E+006	2.000
7700.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+O2<=>CH2CH2COCH3+HO2	2.050E+013	0.000
51310.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+CH3<=>CH2CH2COCH3+CH4	3.190E+001	3.170
7172.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3OH	2.170E+011	0.000
6460.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995		
C2H5COCH3+CH3O2<=>CH2CH2COCH3+CH3O2H	3.010E+012	0.000
19380.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995		

C2H5COCH3+C2H3<=>CH2CH2COCH3+C2H4	5.000E+011	0.000
10400.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+C2H5<=>CH2CH2COCH3+C2H6	5.000E+010	0.000
13400.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+OH<=>CH3CHCOCH3+H2O	8.450E+011	0.000
-228.0 !\AUTHOR: !\REF:ANALOGY TO C2H5COC2H5+OH<=>PRODUCTS; CURRAN 1995		
C2H5COCH3+HO2<=>CH3CHCOCH3+H2O2	2.000E+011	0.000
8698.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+O<=>CH3CHCOCH3+OH	3.070E+013	0.000
3400.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+H<=>CH3CHCOCH3+H2	4.460E+006	2.000
3200.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+O2<=>CH3CHCOCH3+HO2	1.550E+013	0.000
41970.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3<=>CH3CHCOCH3+CH4	1.740E+000	3.460
3680.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3OH	1.450E+011	0.000
2771.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O2<=>CH3CHCOCH3+CH3O2H	2.000E+012	0.000
15250.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+C2H3<=>CH3CHCOCH3+C2H4	3.000E+011	0.000
3400.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+C2H5<=>CH3CHCOCH3+C2H6	3.000E+010	0.000
8600.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+OH<=>C2H5COCH2+H2O	5.100E+011	0.000
1192.0 !\AUTHOR: !\REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+HO2<=>C2H5COCH2+H2O2	2.380E+004	2.550
14690.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+O<=>C2H5COCH2+OH	5.000E+012	0.000
5962.0 !\AUTHOR: !\REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+H<=>C2H5COCH2+H2	9.300E+012	0.000
6357.0 !\AUTHOR: !\REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+O2<=>C2H5COCH2+HO2	2.050E+013	0.000
49150.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3<=>C2H5COCH2+CH4	1.620E+011	0.000
9630.0 !\AUTHOR: !\REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+CH3O<=>C2H5COCH2+CH3OH	2.170E+011	0.000
4660.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+CH3O2<=>C2H5COCH2+CH3O2H	3.010E+012	0.000
17580.0 !\AUTHOR: !\REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		

C2H5COCH3+C2H3<=>C2H5COCH2+C2H4 6.150E+010 0.000
4278.0 !\AUTHOR: !\REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN
1995
C2H5COCH3+C2H5<=>C2H5COCH2+C2H6 5.000E+010 0.000
11600.0 !\AUTHOR: !\REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3)
KCAL/ MOL (C<=>O); CURRAN 1995
!

!\REACTIONCLASS: \R_DECOMP \A \N
\EA
!

C2H3COCH3+H<=>CH3CHCOCH3 5.000E+012 0.000
1200.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H6CHO+X -->PRODUCTS
CH3CHCO+CH3<=>CH3CHCOCH3 1.230E+011 0.000
7800.0 !\AUTHOR: !\REF:ANALOGY WITH IC3H6CHO+X -->PRODUCTS
C2H5COCH2<=>CH2CO+C2H5 1.000E+014 0.000
35000.0 !\AUTHOR: !\REF: WKM 19/ 04/ 2010
!

!\REACTIONCLASS: \R_O2 \A \N
\EA
!

CH3CHCOCH3+O2<=>CH3CHOOCH3 1.000E+011 0.000
0.0 !\AUTHOR: !\REF: CURRAN AND GAFFURI, 1995
CH3CHOOCH3<=>CH2CHOOHCOCH3 8.900E+012 0.000
29700.0 !\AUTHOR: !\REF: CURRAN AND GAFFURI, 1995
C2H3COCH3+HO2<=>CH2CHOOHCOCH3 7.000E+010 0.000
7800.0 !\AUTHOR: !\REF: CURRAN AND GAFFURI, 1995
!

!\ENDSUBMECH: \C2H5COCH3
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!\END_KINETICS_MODULE: \C4

!++++
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!++++
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!\KINETICS_MODULE: \C5

!\MODSUBMECHS:

!++++
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!

!\SUBMECH: \NC5H12
!-----

!

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

NC5H12<=>NC3H7+C2H5 5.203E+024 -2.071 88080.0
!\AUTHOR: !\REF: A. W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014),
101-110
PLOG / 1.000E-002 1.180E+096 -23.17 126046. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E-001 1.855E+089 -20.90 125630. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+000 3.550E+076 -17.02 120458. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+000 3.475E+071 -15.54 117854. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 2.160E+064 -13.43 113815. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E+001 4.550E+058 -11.79 110456. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 2.000E+001 1.020E+053 -10.15 106996. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 5.000E+001 9.000E+045 -8.13 102538. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
NC5H12<=>PC4H9+CH3 1.451E+022 -1.522 89100.0
!\AUTHOR: !\REF: A. W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014),
101-110
PLOG / 1.000E-002 7.090E+092 -22.46 126235. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E-001 4.830E+086 -20.36 126331. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+000 3.240E+074 -16.63 121640. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+000 4.030E+069 -15.18 119142. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 3.000E+062 -13.09 115199. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 6.470E+056 -11.44 111875. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 2.000E+001 1.360E+051 -9.80 108418. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 5.000E+001 9.740E+043 -7.75 103923. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
NC5H12<=>C5H11-1+H 4.205E+017 -0.390 101180.0
!\AUTHOR: !\REF: A. W. JASPER, J. A. MILLER, COMBUST. FLAME, 161 (2014),
101-110
PLOG / 1.000E-002 1.990E+074 -17.75 124798. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG / 1.000E-001 5.720E+076 -18.01 131106. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG / 1.000E+000 4.420E+072 -16.46 132942. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+000 4.560E+069 -15.52 132148. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 2.640E+064 -13.92 130026. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 3.800E+059 -12.48 127648. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

NC5H12+OH<=>C5H11-1+H2O	2.732E+07	1.813
868.4 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060		
NC5H12+HO2<=>C5H11-1+H2O2	4.080E+001	3.590
17160.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M. SIMMIE, J. PHYS. CHEM. A, 112, 2008, 7047-7054		
NC5H12+CH3<=>C5H11-1+CH4	9.040E-001	3.650
7154.0 !\AUTHOR: !\REF: W. TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951		
NC5H12+CH3O<=>C5H11-1+CH3OH	3.000E+011	0.000
7000.0 !\AUTHOR: !\REF:		
NC5H12+CH3O2<=>C5H11-1+CH3O2H	1.386E+000	3.970
18280.0 !\AUTHOR: !\REF:		
NC5H12+C2H5<=>C5H11-1+C2H6	1.000E+011	0.000
13400.0 !\AUTHOR: !\REF:		
NC5H12+C2H3<=>C5H11-1+C2H4	1.000E+012	0.000
18000.0 !\AUTHOR: !\REF: K. M. SUNDARAM, G. F. FROMENT, IND. ENG. CHEM. FUNDAM., 17, 1978, 174-182		
NC5H12+O2CHO<=>C5H11-1+HO2CHO	1.386E+000	3.970
18280.0 !\AUTHOR: !\REF:		
NC5H12+O2<=>C5H11-2+HO2	2.800E+013	0.000
50160.0 !\AUTHOR: !\REF:		
NC5H12+O2<=>C5H11-3+HO2	1.400E+013	0.000
50160.0 !\AUTHOR: !\REF:		
NC5H12+O<=>C5H11-2+OH	5.620E+013	0.000
5200.0 !\AUTHOR: !\REF: J. V. MICHAEL, D. G. KEIL, R. B. KLEMM, INT. J. CHEM. KINET., 15, 1983, 705-719		
NC5H12+O<=>C5H11-3+OH	2.810E+013	0.000
5200.0 !\AUTHOR: !\REF: J. V. MICHAEL, D. G. KEIL, R. B. KLEMM, INT. J. CHEM. KINET., 15, 1983, 705-719		
NC5H12+H<=>C5H11-2+H2	2.600E+006	2.400
4471.0 !\AUTHOR: !\REF: W. TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951		
NC5H12+H<=>C5H11-3+H2	1.300E+006	2.400
4471.0 !\AUTHOR: !\REF: W. TSANG, J. PHYS. CHEM. REF. DATA, 17, 1988, 887-951		
NC5H12+OH<=>C5H11-2+H2O	1.411E+10	0.935
504.7 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060		
NC5H12+OH<=>C5H11-3+H2O	5.721E+006	1.811
-1015.5 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060		
NC5H12+HO2<=>C5H11-2+H2O2	1.264E+002	3.370
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M. SIMMIE, J. PHYS. CHEM. A, 112, 2008, 7047-7054		
NC5H12+HO2<=>C5H11-3+H2O2	6.320E+001	3.370
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, H. J. CURRAN, W. KLOPPER, J. M. SIMMIE, J. PHYS. CHEM. A, 112, 2008, 7047-7054		
NC5H12+CH3<=>C5H11-2+CH4	1.680E+005	2.133
7574.0 !\AUTHOR: !\REF:		
NC5H12+CH3<=>C5H11-3+CH4	8.400E+004	2.133
7574.0 !\AUTHOR: !\REF:		
NC5H12+CH3O<=>C5H11-2+CH3OH	2.200E+011	0.000
5000.0 !\AUTHOR: !\REF:		
NC5H12+CH3O<=>C5H11-3+CH3OH	1.100E+011	0.000
5000.0 !\AUTHOR: !\REF:		
NC5H12+CH3O2<=>C5H11-2+CH3O2H	2.037E+001	3.580
14810.0 !\AUTHOR: !\REF:		

NC5H12+CH3O2<=>C5H11-3+CH3O2H	1.019E+001	3.580
14810.0 !\AUTHOR: !\REF:		
NC5H12+C2H5<=>C5H11-2+C2H6	1.000E+011	0.000
10400.0 !\AUTHOR: !\REF:		
NC5H12+C2H5<=>C5H11-3+C2H6	5.000E+010	0.000
10400.0 !\AUTHOR: !\REF:		
NC5H12+C2H3<=>C5H11-2+C2H4	8.000E+011	0.000
16800.0 !\AUTHOR: !\REF: K. M. SUNDARAM, G. F. FROMENT, IND. ENG. CHEM. FUNDAM., 17, 1978, 174-182		
NC5H12+C2H3<=>C5H11-3+C2H4	4.000E+011	0.000
16800.0 !\AUTHOR: !\REF: K. M. SUNDARAM, G. F. FROMENT, IND. ENG. CHEM. FUNDAM., 17, 1978, 174-182		
NC5H12+O2CHO<=>C5H11-2+HO2CHO	2.037E+001	3.580
14810.0 !\AUTHOR: !\REF:		
NC5H12+O2CHO<=>C5H11-3+HO2CHO	1.019E+001	3.580
14810.0 !\AUTHOR: !\REF:		
NC5H12+C5H11-1<=>C5H11-2+NC5H12	1.000E+011	0.000
10400.0 !\AUTHOR: !\REF:		
NC5H12+C5H11-1<=>C5H11-3+NC5H12	5.000E+010	0.000
10400.0 !\AUTHOR: !\REF:		
NC5H12+C5H11-2<=>C5H11-3+NC5H12	5.000E+010	0.000
12300.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \RADICAL_BETA_SCISSION \A \N

\EA

!

C5H11-1<=>C2H4+NC3H7	3.236E+12	0.323
28808.4 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26		
PLOG/ 0.1 4.410E+03 2.192 18827.0 /		
PLOG/ 1.0 8.060E+20 -2.628 29232.0 /		
PLOG/ 10.0 2.170E+28 -4.578 34864.0 /		
PLOG/ 100.0 6.470E+24 -3.383 34388.0 /		
PLOG/ 1000.0 2.340E+17 -1.123 31176.0 /		
C5H11-1<=>H+C5H10-1	2.042E+10	0.950
33810.2 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26		
PLOG/ 0.1 3.240E-14 7.022 15354.0 /		
PLOG/ 1.0 5.100E+12 -0.402 29991.0 /		
PLOG/ 10.0 4.070E+27 -4.483 39814.0 /		
PLOG/ 100.0 1.020E+26 -3.794 40806.0 /		
PLOG/ 1000.0 6.520E+16 -0.987 36957.0 /		
C5H11-2<=>C3H6+C2H5	4.074E+12	0.272
29140.3 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26		
PLOG/ 0.1 8.540E+25 -4.241 31303.0 /		
PLOG/ 1.0 2.340E+31 -5.581 35992.0 /		
PLOG/ 10.0 4.630E+28 -4.592 36186.0 /		
PLOG/ 100.0 3.770E+20 -2.108 32927.0 /		
PLOG/ 1000.0 3.560E+14 -0.301 30124.0 /		
C5H11-2<=>C5H10-1+H	2.239E+08	1.517
34750.2 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26		
PLOG/ 0.1 8.260E+10 -0.118 29715.0 /		
PLOG/ 1.0 6.920E+26 -4.456 39997.0 /		
PLOG/ 10.0 3.810E+29 -4.969 43662.0 /		

PLOG/	100.0	4.220E+20	-2.160	40523.0 /	
PLOG/	1000.0	5.050E+11	0.526	36461.0 /	
C5H11-2<=>C5H10-2+H					2.710E+09 1.193
34513.5 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26					
PLOG/	0.1	2.797E+13	-0.833	30422.7 /	
PLOG/	1.0	9.922E+27	-4.775	39987.0 /	
PLOG/	10.0	8.504E+29	-5.063	43150.6 /	
PLOG/	100.0	1.026E+21	-2.275	39953.2 /	
PLOG/	1000.0	3.141E+12	0.287	36068.2 /	
C5H11-3<=>C4H8-1+CH3					2.951E+10 0.928
30048.5 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26					
PLOG/	0.1	1.310E+16	-1.137	29671.0 /	
PLOG/	1.0	1.850E+25	-3.643	35787.0 /	
PLOG/	10.0	1.010E+24	-3.130	36363.0 /	
PLOG/	100.0	1.980E+16	-0.793	33017.0 /	
PLOG/	1000.0	2.100E+11	0.685	30583.0 /	
C5H11-3<=>C5H10-2+H					1.274E+09 1.330
34417.9 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26					
PLOG/	0.1	5.119E+06	1.511	29138.7 /	
PLOG/	1.0	4.068E+22	-2.949	38765.5 /	
PLOG/	10.0	2.298E+25	-3.569	41777.2 /	
PLOG/	100.0	8.104E+16	-0.983	38322.3 /	
PLOG/	1000.0	1.214E+10	1.047	35008.7 /	

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

C5H11-1+O2<=>C5H10-1+HO2					8.370E-001 3.590
11960.0 !\AUTHOR: !\REF: J. D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427					
C5H11-2+O2<=>C5H10-1+HO2					5.350E-001 3.710
9322.0 !\AUTHOR: !\REF: J. D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427					
C5H11-2+O2<=>C5H10-2+HO2					1.070E+000 3.710
9322.0 !\AUTHOR: !\REF: J. D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427					
C5H11-3+O2<=>C5H10-2+HO2					2.140E+000 3.710
9322.0 !\AUTHOR: !\REF: J. D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A. TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427					

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

C5H11-1<=>C5H11-2					1.148E+01 3.033
15313.4 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM. PHYS. LETT., 552, 2012, 20-26					
PLOG/	0.1	1.610E+10	-0.128	16305.0 /	
PLOG/	1.0	2.880E+17	-2.073	21414.0 /	
PLOG/	10.0	5.090E+18	-2.284	23337.0 /	
PLOG/	100.0	1.380E+14	-0.838	21871.0 /	
PLOG/	1000.0	1.600E+08	0.954	19221.0 /	

C5H11-1<=>C5H11-3 3.890E-12 6.843
 18781.0 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM.
 PHYS. LETT., 552, 2012, 20-26
 PLOG/ 0.1 6.080E-15 6.876 11901.0 /
 PLOG/ 1.0 7.680E+07 0.667 25012.0 /
 PLOG/ 10.0 1.260E+19 -2.350 32938.0 /
 PLOG/ 100.0 1.160E+16 -1.256 33072.0 /
 PLOG/ 1000.0 6.060E+06 1.570 29120.0 /
 C5H11-2<=>C5H11-3 2.754E+10 0.712
 41872.3 !\AUTHOR: !\REF: A. COMANDINI, I. A. AWAN, J. A. MANION, CHEM.
 PHYS. LETT., 552, 2012, 20-26
 PLOG/ 0.1 4.800E-04 3.725 28298.0 /
 PLOG/ 1.0 3.410E+22 -3.517 42976.0 /
 PLOG/ 10.0 1.570E+32 -6.005 50425.0 /
 PLOG/ 100.0 3.120E+24 -3.514 48305.0 /
 PLOG/ 1000.0 1.590E+14 -0.404 43709.0 /
 !

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

C5H11-1+O2<=>C5H11O2-1 6.865E+016 -1.627
 198.7 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H11-2+O2<=>C5H11O2-2 3.487E+014 -0.816
 -536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H11-3+O2<=>C5H11O2-3 3.487E+014 -0.816
 -536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 !

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

C5H11-1+HO2<=>C5H11O-1+OH 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-2+HO2<=>C5H11O-2+OH 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-3+HO2<=>C5H11O-3+OH 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-1+CH3O2<=>C5H11O-1+CH3O 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-2+CH3O2<=>C5H11O-2+CH3O 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-3+CH3O2<=>C5H11O-3+CH3O 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-1+C5H11O2-1<=>C5H11O-1+C5H11O-1 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-1+C5H11O2-2<=>C5H11O-1+C5H11O-2 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-1+C5H11O2-3<=>C5H11O-1+C5H11O-3 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-2+C5H11O2-1<=>C5H11O-2+C5H11O-1 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-2+C5H11O2-2<=>C5H11O-2+C5H11O-2 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
 C5H11-2+C5H11O2-3<=>C5H11O-2+C5H11O-3 9.000E+012 0.000
 -1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS

C5H11-3+C5H11O2-1<=>C5H11O-3+C5H11O-1 9.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
C5H11-3+C5H11O2-2<=>C5H11O-3+C5H11O-2 9.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
C5H11-3+C5H11O2-3<=>C5H11O-3+C5H11O-3 9.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: HJC ESTIMATE BASED ON CH3+HO2<=>PRODUCTS
!

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

C5H11O2-1<=>C5H10OOH1-2 4.009E+008 1.100
30100.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-1<=>C5H10OOH1-3 1.360E+007 1.300
18200.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-1<=>C5H10OOH1-4 3.718E+006 1.200
16600.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-1<=>C5H10OOH1-5 2.941E+005 1.500
19900.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-2<=>C5H10OOH2-1 7.290E+008 1.100
33500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-2<=>C5H10OOH2-3 1.716E+009 0.900
29500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-2<=>C5H10OOH2-4 7.033E+010 0.200
19500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-2<=>C5H10OOH2-5 6.170E+005 1.500
20000.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-3<=>C5H10OOH3-1 2.877E+007 1.400
20800.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-3<=>C5H10OOH3-2 3.432E+009 0.900
30500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-1<=>PC4H9CHO+OH 1.984E+009 1.200
39700.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-2<=>NC3H7COCH3+OH 5.300E+009 1.000
38500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
C5H11O2-3<=>C2H5COC2H5+OH 5.300E+009 1.000
38500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN, J. PHYS. CHEM.
A, 114, 2010, 5689-5701
!

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

C5H11O2-1<=>C5H10-1+HO2	3.870E+007	1.580
28500.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H11O2-2<=>C5H10-1+HO2	3.605E+009	1.130
30100.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H11O2-2<=>C5H10-2+HO2	5.140E+009	1.010
29362.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H11O2-3<=>C5H10-2+HO2	7.200E+010	0.730
30883.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		

!

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

!

C5H11O2H-1+O2<=>C5H11O2-1+HO2	3.746E+013	-0.791
33620.0 !\AUTHOR: !\REF:		
C5H11O2H-2+O2<=>C5H11O2-2+HO2	4.380E+013	-0.812
33640.0 !\AUTHOR: !\REF:		
C5H11O2H-3+O2<=>C5H11O2-3+HO2	4.380E+013	-0.812
33640.0 !\AUTHOR: !\REF:		

!

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

!

C5H11O2H-1+HO2<=>C5H11O2-1+H2O2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		
C5H11O2H-2+HO2<=>C5H11O2-2+H2O2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		
C5H11O2H-3+HO2<=>C5H11O2-3+H2O2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		

!

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

!

!\SITE: \PRIMARY		
NC5H12+C5H11O2-1<=>C5H11-1+C5H11O2H-1	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
NC5H12+C5H11O2-2<=>C5H11-1+C5H11O2H-2	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
NC5H12+C5H11O2-3<=>C5H11-1+C5H11O2H-3	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
!\SITE: \SECONDARY		
NC5H12+C5H11O2-1<=>C5H11-2+C5H11O2H-1	8.064E+012	0.000
17700.0 !\AUTHOR: !\REF:		
NC5H12+C5H11O2-2<=>C5H11-2+C5H11O2H-2	8.064E+012	0.000
17700.0 !\AUTHOR: !\REF:		
NC5H12+C5H11O2-3<=>C5H11-2+C5H11O2H-3	8.064E+012	0.000
17700.0 !\AUTHOR: !\REF:		
NC5H12+C5H11O2-1<=>C5H11-3+C5H11O2H-1	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		

NC5H12+C5H11O2-2<=>C5H11-3+C5H11O2H-2	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		
NC5H12+C5H11O2-3<=>C5H11-3+C5H11O2H-3	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		

!

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

!

C5H11O2-1+CH3O2=>C5H11O-1+CH3O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-2+CH3O2=>C5H11O-2+CH3O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-3+CH3O2=>C5H11O-3+CH3O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		

!

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

!

C5H11O2-1+C5H11O2-1=>C5H11O-1+C5H11O-1+O2	1.400E+016	-1.610
1860.0 !\AUTHOR:		
C5H11O2-1+C5H11O2-2=>C5H11O-1+C5H11O-2+O2	1.400E+016	-1.610
1860.0 !\AUTHOR:		
C5H11O2-1+C5H11O2-3=>C5H11O-1+C5H11O-3+O2	1.400E+016	-1.610
1860.0 !\AUTHOR:		
C5H11O2-2+C5H11O2-2=>C5H11O-2+C5H11O-2+O2	1.400E+016	-1.610
1860.0 !\AUTHOR:		
C5H11O2-2+C5H11O2-3=>C5H11O-2+C5H11O-3+O2	1.400E+016	-1.610
1860.0 !\AUTHOR:		
C5H11O2-3+C5H11O2-3=>C5H11O-3+C5H11O-3+O2	1.400E+016	-1.610
1860.0 !\AUTHOR:		

!

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

!

C5H11O2-1+CH3O2=>PC4H9CHO+CH3OH+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-1+CH3O2=>NC5H11OH+CH2O+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-2+CH3O2=>NC3H7COCH3+CH3OH+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-3+CH3O2=>C2H5COC2H5+CH3OH+O2	1.400E+016	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-1+C2H5O2=>PC4H9CHO+C2H5OH+O2	3.500E+015	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-1+C2H5O2=>NC5H11OH+CH3CHO+O2	3.500E+015	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-2+C2H5O2=>NC3H7COCH3+C2H5OH+O2	3.500E+015	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-3+C2H5O2=>C2H5COC2H5+C2H5OH+O2	3.500E+015	-1.610
1860.0 !\AUTHOR: !\REF:		
C5H11O2-1+C5H11O2-1=>PC4H9CHO+NC5H11OH+O2	3.500E+015	-1.610
1860.0 !\AUTHOR: !\REF:		

!

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

C5H11O2H-1<=>C5H11O-1+OH 7.303E+018 -0.890
45630.0 !\AUTHOR: !\REF: ESTIMATED BY BY USING REVERSE OF
CH3O2H<=>CH3O+OH FOR REVERSE OF THIS REACTION AND DERIVING FORWARD FROM
THERMOCHEMISTRY
C5H11O2H-2<=>C5H11O-2+OH 4.232E+020 -1.400
45750.0 !\AUTHOR: !\REF: ESTIMATED BY BY USING REVERSE OF
CH3O2H<=>CH3O+OH FOR REVERSE OF THIS REACTION AND DERIVING FORWARD FROM
THERMOCHEMISTRY
C5H11O2H-3<=>C5H11O-3+OH 1.422E+020 -1.340
45690.0 !\AUTHOR: !\REF: ESTIMATED BY BY USING REVERSE OF
CH3O2H<=>CH3O+OH FOR REVERSE OF THIS REACTION AND DERIVING FORWARD FROM
THERMOCHEMISTRY

!

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

C5H11O2H-1+OH=>PC4H9CHO+H2O+OH 2.000E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED TO BE 1E+12 PER H-ATOM BY
C5H11O2H-2+OH=>NC3H7COCH3+H2O+OH 1.000E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED TO BE 1E+12 PER H-ATOM BY
C5H11O2H-3+OH=>C2H5COC2H5+H2O+OH 1.000E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED TO BE 1E+12 PER H-ATOM BY

!

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

CH2O+PC4H9<=>C5H11O-1 5.000E+010 0.000
3457.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006,
250-275
CH3CHO+NC3H7<=>C5H11O-2 3.330E+010 0.000
6397.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006,
250-275
C2H5+C2H5CHO<=>C5H11O-3 1.670E+010 0.000
6193.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006,
250-275

!

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

C5H10OOH1-2<=>C5H10O1-2+OH 4.667E+012 0.250
12840.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
PLOG / 1.000E-002 3.900E+007 -0.19 1871. / !FIT FROM: 500-1100 K
ERROR IN FIT: 10%
PLOG / 1.000E-001 3.120E+015 -2.19 5978. / !FIT FROM: 500-1100 K
ERROR IN FIT: 10%

PLOG / 1.000E+000 3.240E+024 -4.48 11337. / !FIT FROM: 500-1100 K
ERROR IN FIT: 10%
PLOG / 2.000E+000 7.600E+026 -5.06 12972. / !FIT FROM: 500-1100 K
ERROR IN FIT: 9%
PLOG / 5.000E+000 1.800E+029 -5.59 14912. / !FIT FROM: 500-1100 K
ERROR IN FIT: 8%
PLOG / 1.000E+001 1.520E+030 -5.73 16062. / !FIT FROM: 500-1100 K
ERROR IN FIT: 7%
PLOG / 2.000E+001 1.320E+030 -5.57 16802. / !FIT FROM: 500-1100 K
ERROR IN FIT: 6%
PLOG / 5.000E+001 2.460E+028 -4.89 17020. / !FIT FROM: 500-1100 K
ERROR IN FIT: 4%
PLOG / 1.000E+002 1.150E+026 -4.09 16650. / !FIT FROM: 500-1100 K
ERROR IN FIT: 3%
C5H10OOH1-3<=>C5H10O1-3+OH 1.275E+005 1.830
14460.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
PLOG / 1.000E-002 4.240E+040 -9.57 25269. / !FIT FROM: 500-1100 K
ERROR IN FIT: 5%
PLOG / 1.000E-001 2.430E+026 -4.87 21713. / !FIT FROM: 500-1100 K
ERROR IN FIT: 2%
PLOG / 1.000E+000 2.900E+012 -0.48 16944. / !FIT FROM: 500-1100 K
ERROR IN FIT: 1%
PLOG / 2.000E+000 3.680E+010 0.11 16258. / !FIT FROM: 500-1100 K
ERROR IN FIT: 1%
PLOG / 5.000E+000 1.710E+009 0.52 15773. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 1.000E+001 5.610E+008 0.68 15596. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 2.000E+001 3.150E+008 0.75 15504. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 5.000E+001 2.210E+008 0.80 15448. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 1.000E+002 1.960E+008 0.82 15429. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
C5H10OOH1-4<=>C5H10O1-4+OH 4.728E+005 1.240
8130.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
PLOG / 1.000E-002 1.470E+018 -3.06 10191. / !FIT FROM: 500-1100 K
ERROR IN FIT: 4%
PLOG / 1.000E-001 2.800E+014 -1.59 10655. / !FIT FROM: 500-1100 K
ERROR IN FIT: 1%
PLOG / 1.000E+000 5.970E+009 -0.07 9377. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 2.000E+000 2.060E+009 0.08 9236. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 5.000E+000 1.040E+009 0.18 9144. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 1.000E+001 8.200E+008 0.21 9112. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 2.000E+001 7.280E+008 0.23 9096. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 5.000E+001 6.770E+008 0.24 9086. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 1.000E+002 6.610E+008 0.24 9083. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
C5H10OOH1-5<=>C5H10O1-5+OH 2.314E+004 1.310
8550.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
PLOG / 1.000E-002 1.330E+012 -1.19 10872. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%

PLOG / 1.000E-001 1.860E+008 0.06 9760. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+000 4.680E+007 0.26 9574. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+000 4.320E+007 0.27 9563. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+000 4.110E+007 0.27 9556. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+001 4.040E+007 0.28 9554. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+001 4.010E+007 0.28 9553. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+001 3.990E+007 0.28 9552. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 3.980E+007 0.28 9552. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 C5H10OOH2-1<=>C5H10O1-2+OH 2.567E+009 1.040
 11340.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 2.800E+005 0.52 1289. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 9%
 PLOG / 1.000E-001 6.620E+015 -2.20 6879. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 9%
 PLOG / 1.000E+000 1.950E+025 -4.60 13023. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 8%
 PLOG / 2.000E+000 4.990E+026 -4.88 14402. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 7%
 PLOG / 5.000E+000 5.550E+026 -4.71 15465. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 5%
 PLOG / 1.000E+001 2.070E+025 -4.16 15596. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 3%
 PLOG / 2.000E+001 8.130E+022 -3.33 15213. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 2%
 PLOG / 5.000E+001 1.540E+019 -2.10 14271. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+002 5.360E+016 -1.31 13545. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 C5H10OOH2-3<=>C5H10O2-3+OH 4.663E+008 1.090
 9850.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 7.380E-002 2.49 -1612. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 7%
 PLOG / 1.000E-001 2.870E+009 -0.29 4045. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 8%
 PLOG / 1.000E+000 2.110E+018 -2.51 9989. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 6%
 PLOG / 2.000E+000 7.990E+018 -2.55 11002. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 5%
 PLOG / 5.000E+000 3.740E+017 -1.98 11395. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 3%
 PLOG / 1.000E+001 2.230E+015 -1.21 11062. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 2%
 PLOG / 2.000E+001 5.530E+012 -0.35 10430. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 5.000E+001 5.710E+009 0.62 9572. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 1.690E+008 1.11 9099. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 DUP

C5H10OOH2-3<=>C5H10O2-3+OH 7.464E+008 0.700
 9270.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 8.820E+002 1.33 904. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 6%
 PLOG / 1.000E-001 4.380E+012 -1.16 6812. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 6%
 PLOG / 1.000E+000 5.110E+013 -1.08 9522. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 2%
 PLOG / 2.000E+000 1.050E+012 -0.48 9319. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 5.000E+000 4.760E+009 0.30 8791. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+001 2.170E+008 0.74 8430. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+001 2.920E+007 1.02 8181. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+001 7.120E+006 1.22 8001. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 4.260E+006 1.29 7934. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%

DUP

C5H10OOH2-4<=>C5H10O2-4+OH 3.835E+006 1.260
 14970.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 1.570E+032 -7.03 22485. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 4%
 PLOG / 1.000E-001 2.910E+016 -1.95 17872. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+000 3.480E+006 1.17 14400. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+000 3.330E+005 1.48 14031. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+000 7.180E+004 1.69 13788. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+001 4.200E+004 1.76 13704. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+001 3.200E+004 1.80 13660. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+001 2.710E+004 1.82 13634. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 2.570E+004 1.83 13625. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%

DUP

C5H10OOH2-4<=>C5H10O2-4+OH 1.392E+006 1.490
 15210.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 1.140E+036 -8.19 23953. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 4%
 PLOG / 1.000E-001 2.240E+020 -3.08 19618. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+000 2.860E+007 0.97 15137. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 2.000E+000 7.110E+005 1.47 14555. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+000 5.640E+004 1.82 14153. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+001 2.270E+004 1.94 14008. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+001 1.420E+004 2.00 13933. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%

PLOG / 5.000E+001 1.070E+004 2.04 13887. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 9.710E+003 2.06 13872. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 DUP
 C5H10OOH2-5<=>C5H10O1-4+OH 3.785E+005 1.280
 10220.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 2.520E+020 -3.62 13849. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 4%
 PLOG / 1.000E-001 1.090E+012 -0.82 11988. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+000 9.190E+007 0.48 10691. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+000 4.390E+007 0.58 10585. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+000 2.770E+007 0.64 10518. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+001 2.370E+007 0.66 10496. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+001 2.190E+007 0.67 10484. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+001 2.090E+007 0.68 10477. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 2.060E+007 0.68 10475. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 C5H10OOH3-1<=>C5H10O1-3+OH 2.398E+006 1.520
 17240.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 2.630E+042 -9.99 28572. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 4%
 PLOG / 1.000E-001 4.280E+025 -4.56 23726. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 1.000E+000 1.020E+012 -0.29 18930. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+000 1.760E+010 0.26 18283. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+000 1.040E+009 0.64 17830. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+001 3.750E+008 0.78 17665. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 2.000E+001 2.210E+008 0.85 17580. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+001 1.600E+008 0.90 17528. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 1.000E+002 1.430E+008 0.91 17510. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 C5H10OOH3-2<=>C5H10O2-3+OH 2.814E+009 0.350
 9860.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY
 PLOG / 1.000E-002 7.370E+008 -0.39 4687. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 7%
 PLOG / 1.000E-001 3.620E+014 -1.67 9295. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 4%
 PLOG / 1.000E+000 5.600E+010 -0.22 9449. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 1%
 PLOG / 2.000E+000 2.080E+009 0.25 9104. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%
 PLOG / 5.000E+000 1.180E+008 0.66 8769. / !FIT FROM: 500-1100 K
 ERROR IN FIT: 0%

PLOG / 1.000E+001 3.610E+007 0.83 8623. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 2.000E+001 1.880E+007 0.92 8542. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 5.000E+001 1.250E+007 0.98 8490. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%
PLOG / 1.000E+002 1.080E+007 1.00 8472. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%

DUP

C5H10OOH3-2<=>C5H10O2-3+OH 4.195E+009 0.710

10050.0 !\AUTHOR: !\REF: NEWLY CALCULATED BY

PLOG / 1.000E-002 1.570E+000 2.10 -841. / !FIT FROM: 500-1100 K
ERROR IN FIT: 7%

PLOG / 1.000E-001 3.250E+010 -0.59 4837. / !FIT FROM: 500-1100 K
ERROR IN FIT: 7%

PLOG / 1.000E+000 3.930E+017 -2.28 10081. / !FIT FROM: 500-1100 K
ERROR IN FIT: 5%

PLOG / 2.000E+000 3.220E+017 -2.12 10773. / !FIT FROM: 500-1100 K
ERROR IN FIT: 4%

PLOG / 5.000E+000 4.630E+015 -1.42 10845. / !FIT FROM: 500-1100 K
ERROR IN FIT: 2%

PLOG / 1.000E+001 3.340E+013 -0.69 10443. / !FIT FROM: 500-1100 K
ERROR IN FIT: 1%

PLOG / 2.000E+001 2.470E+011 0.01 9905. / !FIT FROM: 500-1100 K
ERROR IN FIT: 1%

PLOG / 5.000E+001 1.910E+009 0.69 9301. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%

PLOG / 1.000E+002 2.070E+008 1.00 9009. / !FIT FROM: 500-1100 K
ERROR IN FIT: 0%

DUP

!

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

!

C5H10OOH1-2<=>C5H10-1+HO2 1.040E+010 0.940

15100.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089

C5H10OOH2-1<=>C5H10-1+HO2 2.210E+012 0.230

15600.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089

C5H10OOH2-3<=>C5H10-2+HO2 4.543E+010 0.751

15100.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089

C5H10OOH3-2<=>C5H10-2+HO2 4.066E+010 0.678

15034.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089

!

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

!

C5H10OOH1-3=>OH+CH2O+C4H8-1 9.100E+008 1.400

25500.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089

C5H10OOH2-4=>OH+CH3CHO+C3H6 1.180E+009 1.200
 22700.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
 M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089
 C5H10OOH3-1=>OH+C2H5CHO+C2H4 3.096E+018 -1.730
 26820.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
 M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089
 C5H10OOH1-2<=>C2H5+AC3H5OOH 2.410E+010 1.020
 28200.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
 M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089
 C5H10OOH1-4<=>C3H6+C2H4O2H 5.080E+011 0.700
 28700.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
 M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089
 C5H10OOH2-5<=>C2H4+C3H6OOH2-1 6.860E+013 0.100
 29000.0 !\AUTHOR: !\REF:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A.
 M. DEAN, J. PHYS. CHEM. A, 116, 2012, 5068-5089
 !

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

C5H10OOH1-2+O2<=>C5H10OOH1-2O2 1.569E+014 -0.816
 -536.5 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH1-3+O2<=>C5H10OOH1-3O2 1.569E+014 -0.816
 -536.5 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH1-4+O2<=>C5H10OOH1-4O2 1.569E+014 -0.816
 -536.5 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH1-5+O2<=>C5H10OOH1-5O2 3.089E+016 -1.627
 198.7 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH2-1+O2<=>C5H10OOH2-1O2 3.089E+016 -1.627
 198.7 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH2-3+O2<=>C5H10OOH2-3O2 1.569E+014 -0.816
 -536.5 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH2-4+O2<=>C5H10OOH2-4O2 1.569E+014 -0.816
 -536.5 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH2-5+O2<=>C5H10OOH2-5O2 3.089E+016 -1.627
 198.7 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH3-1+O2<=>C5H10OOH3-1O2 3.089E+016 -1.627
 198.7 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 C5H10OOH3-2+O2<=>C5H10OOH3-2O2 1.569E+014 -0.816
 -536.5 !\AUTHOR: !\REF:A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
 !

!\REACTIONCLASS: \O2QOOH=EROOH+HO2 \A \N
 \EA
 !

C5H10OOH1-2O2<=>C5H92-1OOH+HO2 5.140E+009 1.010
 29362.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN,
 A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442
 C5H10OOH1-3O2<=>C5H92-1OOH+HO2 3.600E+010 0.730
 29883.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN,
 A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442
 C5H10OOH1-3O2<=>C5H92-5OOH+HO2 3.600E+010 0.730
 29883.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN,
 A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442

C5H10OOH1-4O2<=>C5H91-5OOH+HO2	3.605E+009	1.130
30100.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH1-4O2<=>C5H92-5OOH+HO2	5.140E+009	1.010
29362.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH1-5O2<=>C5H91-5OOH+HO2	3.870E+007	1.580
28500.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH2-3O2<=>C5H92-4OOH+HO2	3.600E+010	0.730
29883.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH2-4O2<=>C5H92-4OOH+HO2	5.140E+009	1.010
29362.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH2-4O2<=>C5H91-4OOH+HO2	3.605E+009	1.130
30100.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH2-5O2<=>C5H91-4OOH+HO2	3.870E+007	1.580
28500.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH3-1O2<=>C5H91-3OOH+HO2	3.870E+007	1.580
28500.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
C5H10OOH3-2O2<=>C5H91-3OOH+HO2	3.605E+009	1.130
30100.0 !\AUTHOR: !\REF: S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN, J. PHYS. CHEM. A, 115, 2011, 13425-13442		
!		

!\REACTIONCLASS: \O2QOOH=P(OOH)2	\A	\N
\EA		
!		

C5H10OOH1-2O2<=>C5H93-1,2OOH	1.716E+09	0.900
29500.0 !\AUTHOR: !\REF:		
C5H10OOH1-2O2<=>C5H92-4,5OOH	7.033E+10	0.200
18500.0 !\AUTHOR: !\REF:		
C5H10OOH1-2O2<=>C5H91-4,5OOH	1.233E+06	1.500
20000.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2<=>C5H92-1,3OOH	3.432E+09	0.900
29500.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2<=>C5H92-3,5OOH	3.432E+09	0.900
29500.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2<=>C5H91-3,5OOH	2.877E+07	1.400
20800.0 !\AUTHOR: !\REF:		
C5H10OOH1-4O2<=>C5H92-1,4OOH	7.033E+10	0.200
18500.0 !\AUTHOR: !\REF:		
C5H10OOH1-4O2<=>C5H93-1,4OOH	1.716E+09	0.900
29500.0 !\AUTHOR: !\REF:		
C5H10OOH1-4O2<=>C5H91-2,5OOH	7.290E+08	1.100
33500.0 !\AUTHOR: !\REF:		
C5H10OOH1-5O2<=>C5H92-1,5OOH	3.718E+06	1.200
16600.0 !\AUTHOR: !\REF:		
DUP		
C5H10OOH1-5O2<=>C5H93-1,5OOH	1.360E+07	1.300
18200.0 !\AUTHOR: !\REF:		
C5H10OOH1-5O2<=>C5H92-1,5OOH	4.009E+08	1.100
30100.0 !\AUTHOR: !\REF:		

DUP		
C5H10OOH2-1O2<=>C5H93-1,2OOH	1.360E+07	1.300
18200.0 !\AUTHOR: !\REF:		
C5H10OOH2-1O2<=>C5H92-4,5OOH	3.718E+06	1.200
16600.0 !\AUTHOR: !\REF:		
C5H10OOH2-1O2<=>C5H91-4,5OOH	2.941E+05	1.500
19900.0 !\AUTHOR: !\REF:		
C5H10OOH2-3O2<=>C5H91-2,3OOH	2.877E+07	1.400
20800.0 !\AUTHOR: !\REF:		
C5H10OOH2-3O2<=>C5H92-3,4OOH	3.432E+09	0.900
29500.0 !\AUTHOR: !\REF:		
C5H10OOH2-3O2<=>C5H91-3,4OOH	2.877E+07	1.400
20800.0 !\AUTHOR: !\REF:		
C5H10OOH2-4O2<=>C5H91-2,4OOH	1.233E+06	1.500
20000.0 !\AUTHOR: !\REF:		
DUP		
C5H10OOH2-4O2<=>C5H93-2,4OOH	1.716E+09	0.900
29500.0 !\AUTHOR: !\REF:		
C5H10OOH2-4O2<=>C5H91-2,4OOH	7.290E+08	1.100
33500.0 !\AUTHOR: !\REF:		
DUP		
C5H10OOH2-5O2<=>C5H91-2,5OOH	2.941E+05	1.500
19900.0 !\AUTHOR: !\REF:		
C5H10OOH2-5O2<=>C5H93-1,4OOH	1.360E+07	1.300
18200.0 !\AUTHOR: !\REF:		
C5H10OOH2-5O2<=>C5H92-1,4OOH	4.009E+08	1.100
30100.0 !\AUTHOR: !\REF:		
C5H10OOH3-1O2<=>C5H92-1,3OOH	4.009E+08	1.100
30100.0 !\AUTHOR: !\REF:		
C5H10OOH3-1O2<=>C5H92-3,5OOH	3.718E+06	1.200
16600.0 !\AUTHOR: !\REF:		
C5H10OOH3-1O2<=>C5H91-3,5OOH	2.941E+05	1.500
19900.0 !\AUTHOR: !\REF:		
C5H10OOH3-2O2<=>C5H91-2,3OOH	7.290E+08	1.100
33500.0 !\AUTHOR: !\REF:		
C5H10OOH3-2O2<=>C5H92-3,4OOH	7.033E+10	0.200
18500.0 !\AUTHOR: !\REF:		
C5H10OOH3-2O2<=>C5H91-3,4OOH	1.233E+06	1.500
20000.0 !\AUTHOR: !\REF:		
!		

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

C5H10OOH1-2O2<=>NC5KET12+OH	2.441E+07	1.600
27900.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH1-3O2<=>NC5KET13+OH	1.098E+04	2.400
19900.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH1-4O2<=>NC5KET14+OH	1.256E+03	2.200
17400.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH1-5O2<=>NC5KET15+OH	1.115E+03	1.800
16600.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		

C5H10OOH2-1O2<=>NC5KET21+OH	2.763E+08	1.200
25700.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH2-3O2<=>NC5KET23+OH	1.748E+08	1.700
26000.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH2-4O2<=>NC5KET24+OH	1.754E+02	3.100
17500.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH2-5O2<=>NC5KET25+OH	3.768E+02	2.200
15300.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH3-1O2<=>NC5KET31+OH	5.786E+01	2.900
17000.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
C5H10OOH3-2O2<=>NC5KET32+OH	1.748E+08	1.700
26000.0 !\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	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2+C5H10OOH2-4O2=>NC5KET31+C5H10OOH2-4OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2+C5H10OOH2-4O2=>NC5KET24+C5H10OOH1-3OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2+C5H10OOH3-1O2=>NC5KET31+C5H10OOH3-1OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH1-3O2+C5H10OOH3-1O2=>NC5KET13+C5H10OOH1-3OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH2-4O2+C5H10OOH2-4O2=>NC5KET24+C5H10OOH2-4OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH2-4O2+C5H10OOH3-1O2=>NC5KET24+C5H10OOH3-1OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH2-4O2+C5H10OOH3-1O2=>NC5KET13+C5H10OOH2-4OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		
C5H10OOH3-1O2+C5H10OOH3-1O2=>NC5KET13+C5H10OOH3-1OH+O2	1.400E+016	-
1.610 1860.0 !\AUTHOR: !\REF:		

!

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

!

C5H91-3,4OOH=>C3KET12+C2H4+OH	3.096E+018	-1.730
26820.0 !\AUTHOR: !\REF:		
C5H91-3,5OOH=>C3KET13+C2H4+OH	3.096E+018	-1.730
26820.0 !\AUTHOR: !\REF:		
C5H91-4,5OOH=>AC3H5OOH+C2H4+HO2	6.860E+013	0.100
29000.0 !\AUTHOR: !\REF:		
C5H92-1,4OOH=>AC3H5OOH+CH3CHO+OH	2.410E+010	1.020
28200.0 !\AUTHOR: !\REF:		
C5H92-1,5OOH<=>AC3H5OOH+C2H4O2H	2.410E+010	1.020
28200.0 !\AUTHOR: !\REF:		

C5H92-4, 5OOH=>HO2CH2CHO+C3H6+OH	1.180E+009	1.200
22700.0 !\AUTHOR: !\REF:		
C5H93-1, 4OOH=>CH2O+C4H71-3OOH+OH	9.100E+008	1.400
25500.0 !\AUTHOR: !\REF:		
C5H93-1, 5OOH=>CH2O+C4H71-4OOH+OH	1.820E+009	1.400
25500.0 !\AUTHOR: !\REF:		

!

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

!

NC5KET12<=>NC5KET12O+OH	1.050E+016	0.000
42600.0 !\AUTHOR: !\REF:		
NC5KET13<=>NC5KET13O+OH	1.050E+016	0.000
42600.0 !\AUTHOR: !\REF:		
NC5KET14<=>NC5KET14O+OH	1.050E+016	0.000
42600.0 !\AUTHOR: !\REF:		
NC5KET15<=>NC5KET15O+OH	1.500E+016	0.000
43000.0 !\AUTHOR: !\REF:		
NC5KET21<=>NC5KET21O+OH	1.500E+016	0.000
43000.0 !\AUTHOR: !\REF:		
NC5KET23<=>NC5KET23O+OH	1.050E+016	0.000
42600.0 !\AUTHOR: !\REF:		
NC5KET24<=>NC5KET24O+OH	1.050E+016	0.000
42600.0 !\AUTHOR: !\REF:		
NC5KET25<=>NC5KET25O+OH	1.500E+016	0.000
43000.0 !\AUTHOR: !\REF:		
NC5KET31<=>NC5KET31O+OH	1.500E+016	0.000
43000.0 !\AUTHOR: !\REF:		
NC5KET32<=>NC5KET32O+OH	1.050E+016	0.000
42600.0 !\AUTHOR: !\REF:		
NC5KET12O<=>NC3H7CHO+HCO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET13O<=>C2H5CHO+CH2CHO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET14O<=>CH3CHO+CH2CH2CHO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET15O<=>CH2O+C3H6CHO-1	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET21O<=>CH2O+NC3H7CO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET23O<=>C2H5CHO+CH3CO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET24O<=>CH3CHO+CH3COCH2	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		
NC5KET25O<=>CH2O+CH2CH2COCH3	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,		
3455-3471		

NC5KET31O<=>C2H5COCH2+CH2O 2.900E+012 0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,
3455-3471
NC5KET32O<=>CH3CHO+C2H5CO 2.900E+012 0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,
3455-3471
!

!\REACTIONCLASS: \KORCEK MECHANISM \A \N
\EA
!

NC5KET13<=>NC5CYCPER13 2.100E+008 0.000
28000.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
NC5KET24<=>NC5CYCPER24 2.100E+008 0.000
28000.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
NC5KET31<=>NC5CYCPER31 2.100E+008 0.000
28000.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
NC5CYCPER13<=>HOCHO+C2H5COCH3 3.400E+013 0.000
34400.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
NC5CYCPER13<=>CH3COOH+C2H5CHO 3.700E+013 0.000
36800.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
NC5CYCPER24<=>CH3COOH+CH3COCH3 3.400E+013 0.000
34400.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
NC5CYCPER31<=>C2H5COOH+CH3CHO 3.400E+013 0.000
34400.0 !\AUTHOR: !\REF: A. JALAN ET AL., J. AM. CHEM. SOC., 2013, 135,
11100-11114
!

!\REACTIONCLASS: \OHQOOH_DECOMPOSITION \A \N
\EA
!

C5H10OOH1-3OH=>CH2O+SC4H8OH-1+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: H. J. CURRAN, P. GAFFURI, W. J. PITZ, C. K.
WESTBROOK, COMBUST. FLAME, 1998, 114, 149-177
C5H10OOH2-4OH=>CH3CHO+C3H6OH2-1+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: H. J. CURRAN, P. GAFFURI, W. J. PITZ, C. K.
WESTBROOK, COMBUST. FLAME, 1998, 114, 149-177
C5H10OOH3-1OH=>C2H5CHO+PC2H4OH+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: H. J. CURRAN, P. GAFFURI, W. J. PITZ, C. K.
WESTBROOK, COMBUST. FLAME, 1998, 114, 149-177
!

!\REACTIONCLASS: \DIONE FORMATION \A \N
\EA
!

NC5KET13+OH=>NC5DIONE13+OH+H2O 1.000E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED TO BE 1E+12 PER H-ATOM BY
NC5KET24+OH=>NC5DIONE24+OH+H2O 1.000E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED TO BE 1E+12 PER H-ATOM BY

NC5KET31+OH=>NC5DIONE13+OH+H2O 2.000E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED TO BE 1E+12 PER H-ATOM BY
!

!\REACTIONCLASS: \P(OOH)2=EROOH+HO2 \A \N
\EA
!

C5H91-2,3OOH<=>C5H91-3OOH+HO2 2.210E+012 0.230
15600.0 !\AUTHOR: !\REF:
C5H91-2,4OOH<=>C5H91-4OOH+HO2 2.210E+012 0.230
15600.0 !\AUTHOR: !\REF:
C5H91-2,5OOH<=>C5H91-5OOH+HO2 2.210E+012 0.230
15600.0 !\AUTHOR: !\REF:
C5H92-1,3OOH<=>C5H91-3OOH+HO2 1.040E+010 0.940
15100.0 !\AUTHOR: !\REF:
C5H92-1,3OOH<=>C5H92-1OOH+HO2 4.066E+010 0.678
15034.0 !\AUTHOR: !\REF:
C5H92-1,4OOH<=>C5H91-4OOH+HO2 1.040E+010 0.940
15100.0 !\AUTHOR: !\REF:
C5H92-1,5OOH<=>C5H91-5OOH+HO2 1.040E+010 0.940
15100.0 !\AUTHOR: !\REF:
C5H92-3,4OOH<=>C5H92-4OOH+HO2 4.066E+010 0.678
15034.0 !\AUTHOR: !\REF:
C5H92-3,5OOH<=>C5H92-5OOH+HO2 4.066E+010 0.678
15034.0 !\AUTHOR: !\REF:
C5H93-1,2OOH<=>C5H92-1OOH+HO2 4.543E+010 0.751
15100.0 !\AUTHOR: !\REF:
C5H93-1,4OOH<=>C5H92-5OOH+HO2 4.543E+010 0.751
15100.0 !\AUTHOR: !\REF:
C5H93-2,4OOH<=>C5H92-4OOH+HO2 9.086E+010 0.751
15100.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \EROOH_DECOMPOSITION \A \N
\EA
!

C5H91-3OOH=>C2H5CHO+C2H3+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C5H91-3OOH=>C2H3CHO+C2H5+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C5H91-4OOH=>CH3CHO+C3H5-A+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C5H91-4OOH=>SC3H5CHO+CH3+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C5H91-5OOH=>CH2O+C4H71-4+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C5H92-1OOH=>CH2O+C4H71-1+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C5H92-4OOH=>CH3CHO+C3H5-S+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C5H92-4OOH=>SC3H5CHO+CH3+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C5H92-5OOH=>CH2O+C4H71-3+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \P(OOH)2=CETH-OOH+OH \EA !	\A	\N
C5H91-2,300H<=>C5H901-200H-3+OH 10700.0 !\AUTHOR: !\REF:	5.800E+010	0.430
C5H91-2,300H<=>C5H901-300H-2+OH 17700.0 !\AUTHOR: !\REF:	1.015E+010	0.460
C5H91-2,400H<=>C5H901-200H-4+OH 10700.0 !\AUTHOR: !\REF:	5.800E+010	0.430
C5H91-2,400H<=>C5H901-400H-2+OH 11200.0 !\AUTHOR: !\REF:	1.240E+009	0.350
C5H91-2,500H<=>C5H901-200H-5+OH 10700.0 !\AUTHOR: !\REF:	5.800E+010	0.430
C5H91-2,500H<=>C5H901-500H-2+OH 11300.0 !\AUTHOR: !\REF:	1.445E+007	0.760
C5H91-3,400H<=>C5H901-300H-4+OH 17700.0 !\AUTHOR: !\REF:	1.015E+010	0.460
C5H91-3,400H<=>C5H901-400H-3+OH 11200.0 !\AUTHOR: !\REF:	1.240E+009	0.350
C5H91-3,500H<=>C5H901-300H-5+OH 17700.0 !\AUTHOR: !\REF:	1.015E+010	0.460
C5H91-3,500H<=>C5H901-500H-3+OH 11300.0 !\AUTHOR: !\REF:	1.445E+007	0.760
C5H91-4,500H<=>C5H901-400H-5+OH 11200.0 !\AUTHOR: !\REF:	1.240E+009	0.350
C5H91-4,500H<=>C5H901-500H-2+OH 11300.0 !\AUTHOR: !\REF:	1.445E+007	0.760
C5H92-1,300H<=>C5H901-200H-3+OH 10900.0 !\AUTHOR: !\REF:	3.670E+009	0.930
C5H92-1,300H<=>C5H902-300H-1+OH 9591.0 !\AUTHOR: !\REF:	7.040E+009	0.784
C5H92-1,400H<=>C5H901-200H-4+OH 10900.0 !\AUTHOR: !\REF:	3.670E+009	0.930
C5H92-1,400H<=>C5H902-400H-1+OH 16415.0 !\AUTHOR: !\REF:	1.340E+009	0.700
C5H92-1,500H<=>C5H901-200H-5+OH 10900.0 !\AUTHOR: !\REF:	3.670E+009	0.930
C5H92-1,500H<=>C5H901-400H-5+OH 10000.0 !\AUTHOR: !\REF:	2.410E+007	0.940
C5H92-3,400H<=>C5H902-300H-4+OH 9591.0 !\AUTHOR: !\REF:	7.040E+009	0.784
C5H92-3,400H<=>C5H902-400H-3+OH 16415.0 !\AUTHOR: !\REF:	1.340E+009	0.700
C5H92-3,500H<=>C5H902-300H-5+OH 9591.0 !\AUTHOR: !\REF:	7.040E+009	0.784
C5H92-3,500H<=>C5H901-400H-3+OH 10000.0 !\AUTHOR: !\REF:	2.410E+007	0.940
C5H92-4,500H<=>C5H902-400H-1+OH 16415.0 !\AUTHOR: !\REF:	1.340E+009	0.700
C5H92-4,500H<=>C5H901-400H-2+OH 10000.0 !\AUTHOR: !\REF:	2.410E+007	0.940
C5H93-1,200H<=>C5H901-300H-2+OH 15300.0 !\AUTHOR: !\REF:	4.225E+008	0.900
C5H93-1,200H<=>C5H902-300H-1+OH 9403.0 !\AUTHOR: !\REF:	2.441E+009	0.900
C5H93-1,400H<=>C5H901-300H-4+OH 15300.0 !\AUTHOR: !\REF:	4.225E+008	0.900

C5H93-1, 4OOH<=>C5H9O2-3OOH-5+OH 9403.0 !\AUTHOR: !\REF:	2.441E+009	0.900
C5H93-1, 5OOH<=>C5H9O1-3OOH-5+OH 15300.0 !\AUTHOR: !\REF:	4.225E+008	0.900
C5H93-2, 4OOH<=>C5H9O2-3OOH-4+OH 9403.0 !\AUTHOR: !\REF:	4.881E+009	0.900

!\REACTIONCLASS: \CETH-OOH_DECOMPOSITION \EA	\A	\N
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C5H9O1-2OOH-3=>C2H5CHO+CH2CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-3OOH-2=>C2H5CHO+CH2CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-3OOH-2=>CH2O+C3H6CHO-3+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-2OOH-4=>CH3CHO+C3H5O+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-4OOH-2=>CH2O+C3H6CHO-2+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-4OOH-2=>C3H6+OCH2CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-2OOH-5<=>C5H9O1-2O-5+OH 45700.0 !\AUTHOR: !\REF:	4.151E+019	-1.310
C5H9O1-5OOH-2=>CH2O+C3H6CHO-1+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-5OOH-2=>C2H4+CH2OCH2CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-3OOH-4=>CH3CHO+CH2CH2CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-4OOH-3=>C2H4+C2H4OCHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-3OOH-5=>CH2O+C4H7O1-4+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9O1-5OOH-3<=>CH2CH2OCH2CH2CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O1-4OOH-5=>CH2O+C3H6CHO-1+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9O2-3OOH-1=>CH2O+C3H6CHO-3+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9O2-4OOH-1=>CH2O+C3H6CHO-2+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9O2-4OOH-3=>CH3CHO+CH3CHCHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9O2-3OOH-5=>CH2O+C4H71-O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000

!\REACTIONCLASS: \CETH_DECOMPOSITION \EA	\A	\N
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C5H10O1-2+OH=>CH2CO+NC3H7+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H10O1-3+OH=>C2H4+C2H5CO+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730

C5H1001-4+OH=>CH3COCH2+C2H4+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1001-5+OH=>CH2CH2CHO+C2H4+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1002-3+OH=>CH3CHCO+C2H5+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1002-4+OH=>CH3CO+C3H6+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1001-2+OH=>C2H3CHO+C2H5+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1001-3+OH=>HCO+C4H8-1+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1001-4+OH=>CH2CHO+C3H6+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1001-5+OH=>CH2O+C4H71-3+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1002-3+OH=>C2H3COCH3+CH3+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1002-4+OH=>CH3CHO+C3H5-S+H2O -4688.6 !\AUTHOR: !\REF:	2.260E+003	2.730
C5H1001-2+HO2=>CH2CO+NC3H7+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-3+HO2=>C2H4+C2H5CO+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-4+HO2=>CH3COCH2+C2H4+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-5+HO2=>CH2CH2CHO+C2H4+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1002-3+HO2=>CH3CHCO+C2H5+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1002-4+HO2=>CH3CO+C3H6+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-2+HO2=>C2H3CHO+C2H5+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-3+HO2=>HCO+C4H8-1+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-4+HO2=>CH2CHO+C3H6+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1001-5+HO2=>CH2O+C4H71-3+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1002-3+HO2=>C2H3COCH3+CH3+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460
C5H1002-4+HO2=>CH3CHO+C3H5-S+H2O2 9733.3 !\AUTHOR: !\REF:	1.720E+001	3.460

!

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

C5H81-3+OH<=>CH2O+C4H71-3 0.0 !\AUTHOR: !\REF:	1.000E+012	0.000
C5H81-3+OH<=>C2H3CHO+C2H5 0.0 !\AUTHOR: !\REF:	1.000E+012	0.000
C5H81-3+OH<=>CH3CHO+C3H5-S 0.0 !\AUTHOR: !\REF:	1.000E+012	0.000
OCH2CHO<=>CH2O+HCO 11080.0 !\AUTHOR: !\REF:	2.900E+012	0.380

C5H9O1-2O-5=>CH2O+CH2CHO+C2H4	1.326E+021	-2.349
25084.0 !\AUTHOR: !\REF:		
CH2OCH2CHO<=>CH2O+CH2CHO	1.600E+013	0.000
25500.0 !\AUTHOR: !\REF:		
C2H4OCHO<=>CH3CHO+HCO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:		
C4H7O1-4<=>CH2O+C3H5-A	1.326E+021	-2.349
25084.0 !\AUTHOR: !\REF:		
CH2CH2OCH2CH2CHO=>CH2O+C2H4+CH2CHO	1.600E+013	0.000
25500.0 !\AUTHOR: !\REF:		
NC5DIONE13+OH=>CH3CHCO+CH2CHO+H2O	2.360E+002	3.150
3050.0 !\AUTHOR: !\REF: PELUCCHI ET AL., COMBUST. FLAME, 162, 2015, 265-286		
NC5DIONE24+OH=>CH2CO+CH3COCH2+H2O	1.720E+005	2.400
815.0 !\AUTHOR: !\REF: PELUCCHI ET AL., COMBUST. FLAME, 162, 2015, 265-286		

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!-----
!-----
!\ENDSUBMECH: \NC5H12
!-----
!-----
!\SUBMECH: \IC5H12
!-----
!-----
!-----

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

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IC5H12<=>IC3H7+C2H5 1.469E+026 -2.659 86860.0 !\AUTHOR: !\REF: 7/10/2013
PLOG / 1.000E-002 4.070E+095 -23.37 121614. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG / 1.000E-001 2.800E+090 -21.55 122339. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E+000 8.580E+079 -18.27 119001. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+000 3.960E+075 -16.97 117015. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 1.410E+069 -15.06 113723. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 7.290E+063 -13.51 110811. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+001 2.460E+058 -11.91 107645. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+001 1.550E+051 -9.83 103292. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
IC5H12<=>SC4H9+CH3 8.694E+023 -2.019 87290.0 !\AUTHOR: !\REF: 7/10/2013
PLOG / 1.000E-002 1.050E+093 -22.64 121641. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG / 1.000E-001 1.310E+088 -20.89 122563. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E+000 6.800E+077 -17.67 119420. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+000 3.550E+073 -16.39 117484. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

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PLOG / 5.000E+000 1.430E+067 -14.49 114248. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 7.810E+061 -12.94 111365. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+001 2.700E+056 -11.35 108218. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+001 1.660E+049 -9.26 103871. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
IC5H12<=>IC4H9+CH3 1.067E+021 -1.460 89070.0 !\AUTHOR: !\REF: 7/10/2013
PLOG / 1.000E-002 2.910E+088 -21.68 121666. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG / 1.000E-001 4.790E+084 -20.23 123421. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 1.000E+000 2.450E+075 -17.28 121108. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+000 2.210E+071 -16.05 119391. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 1.560E+065 -14.22 116397. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 1.120E+060 -12.70 113651. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+001 4.350E+054 -11.12 110591. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+001 2.490E+047 -9.02 106282. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
IC5H12<=>AC5H11+H 5.090E+017 -0.417 101180.0 !\AUTHOR: !\REF: 7/10/2013
PLOG / 1.000E-002 8.010E+067 -16.14 118712. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 7%
PLOG / 1.000E-001 1.480E+072 -16.92 125626. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 5%
PLOG / 1.000E+000 7.250E+070 -16.14 129319. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 2.000E+000 9.570E+068 -15.50 129394. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 5.000E+000 2.140E+065 -14.33 128592. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 4.960E+061 -13.21 127269. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+001 2.300E+057 -11.91 125334. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+001 5.700E+050 -9.95 121933. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 1%
IC5H12<=>BC5H11+H 6.342E+018 -0.784 96250.0 !\AUTHOR: !\REF: 7/10/2013
PLOG / 1.000E-002 1.240E+077 -18.65 120361. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 6%
PLOG / 1.000E-001 1.430E+078 -18.53 125424. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 4%
PLOG / 1.000E+000 2.480E+073 -16.81 126657. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 3%
PLOG / 2.000E+000 3.390E+070 -15.90 125951. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 5.000E+000 4.900E+065 -14.41 124153. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 1.000E+001 1.950E+061 -13.09 122150. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%
PLOG / 2.000E+001 2.310E+056 -11.63 119644. / !FIT FROM: 1000-2000 K
ERROR IN FIT: 2%

IC5H12+OH<=>DC5H11+H2O	1.366E+007	1.813
868.4 !\AUTHOR: !\REF:R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM.		
A, 2009, 113, 5047-5060		
IC5H12+HO2<=>AC5H11+H2O2	4.080E+001	3.590
17160.0		
IC5H12+HO2<=>DC5H11+H2O2	2.040E+001	3.590
17160.0		
IC5H12+CH3<=>AC5H11+CH4	9.040E-001	3.650
7154.0		
IC5H12+CH3<=>DC5H11+CH4	4.520E-001	3.650
7154.0		
IC5H12+CH3O<=>AC5H11+CH3OH	3.000E+011	0.000
7000.0		
IC5H12+CH3O<=>DC5H11+CH3OH	1.500E+011	0.000
7000.0		
IC5H12+CH3O2<=>AC5H11+CH3O2H	1.386E+000	3.970
18280.0		
IC5H12+CH3O2<=>DC5H11+CH3O2H	6.930E-001	3.970
18280.0		
IC5H12+C2H5<=>AC5H11+C2H6	1.000E+011	0.000
13400.0		
IC5H12+C2H5<=>DC5H11+C2H6	5.000E+010	0.000
13400.0		
IC5H12+C2H3<=>AC5H11+C2H4	1.000E+012	0.000
18000.0		
IC5H12+C2H3<=>DC5H11+C2H4	5.000E+011	0.000
18000.0		
IC5H12+O2CHO<=>AC5H11+HO2CHO	1.680E+013	0.000
20440.0		
IC5H12+O2CHO<=>DC5H11+HO2CHO	8.400E+012	0.000
20440.0		
IC5H12+AC5H11<=>DC5H11+IC5H12	7.500E+010	0.000
12300.0		
IC5H12+BC5H11<=>DC5H11+IC5H12	7.500E+010	0.000
12300.0		
IC5H12+CC5H11<=>DC5H11+IC5H12	7.500E+010	0.000
12300.0		
!\SITE: \SECONDARY		
IC5H12+O2<=>CC5H11+HO2	1.400E+013	0.000
50160.0		
IC5H12+O<=>CC5H11+OH	5.946E+005	2.439
2846.0		
IC5H12+H<=>CC5H11+H2	1.300E+006	2.400
4471.0		
IC5H12+OH<=>CC5H11+H2O	7.053E+009	0.935
504.7 !\AUTHOR: !\REF:R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM.		
A, 2009, 113, 5047-5060		
IC5H12+HO2<=>CC5H11+H2O2	6.320E+001	3.370
13720.0		
IC5H12+CH3<=>CC5H11+CH4	8.400E+004	2.133
7574.0		
IC5H12+CH3O<=>CC5H11+CH3OH	1.100E+011	0.000
5000.0		
IC5H12+CH3O2<=>CC5H11+CH3O2H	1.019E+001	3.580
14810.0		
IC5H12+C2H5<=>CC5H11+C2H6	5.000E+010	0.000
10400.0		

IC5H12+C2H3<=>CC5H11+C2H4 16800.0	4.000E+011	0.000
IC5H12+O2CHO<=>CC5H11+HO2CHO 17690.0	5.600E+012	0.000
IC5H12+AC5H11<=>CC5H11+IC5H12 10400.0	5.000E+010	0.000
IC5H12+BC5H11<=>CC5H11+IC5H12 10400.0	5.000E+010	0.000
!\SITE: \TERTIARY		
IC5H12+O2<=>BC5H11+HO2 48000.0	7.000E+012	0.000
IC5H12+O<=>BC5H11+OH 1150.0	3.968E+005	2.401
IC5H12+H<=>BC5H11+H2 2583.0	6.020E+005	2.400
IC5H12+OH<=>BC5H11+H2O -999.6	4.844E+006	1.840
!\AUTHOR: !\REF:R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
IC5H12+HO2<=>BC5H11+H2O2 12090.0	6.504E+002	3.010
IC5H12+CH3<=>BC5H11+CH4 893.0	6.010E-010	6.360
IC5H12+CH3O<=>BC5H11+CH3OH 2800.0	1.900E+010	0.000
IC5H12+CH3O2<=>BC5H11+CH3O2H 11100.0	2.620E+002	3.120
IC5H12+C2H5<=>BC5H11+C2H6 7900.0	1.000E+011	0.000
IC5H12+C2H3<=>BC5H11+C2H4 14300.0	2.000E+011	0.000
IC5H12+O2CHO<=>BC5H11+HO2CHO 12260.0	1.500E+004	2.500
IC5H12+AC5H11<=>BC5H11+IC5H12 7900.0	2.500E+010	0.000

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!\REACTIONCLASS: \RADICAL_BETA_SCISSION

\A

\N

\EA

!

C3H6+C2H5<=>AC5H11 6850.0	1.420E+003	2.670
C4H8-1+CH3<=>AC5H11 6850.0	1.890E+003	2.670
AC5H10+H<=>AC5H11 2620.0	6.250E+011	0.510
IC4H8+CH3<=>BC5H11 6130.0	4.400E+004	2.480
AC5H10+H<=>BC5H11 1230.0	1.060E+012	0.510
BC5H10+H<=>BC5H11 2620.0	6.250E+011	0.510
C4H8-2+CH3<=>CC5H11 6850.0	1.890E+003	2.670
BC5H10+H<=>CC5H11 2620.0	2.500E+011	0.510
CC5H10+H<=>CC5H11 2620.0	6.250E+011	0.510

C2H4+IC3H7<=>DC5H11 6130.0	8.800E+003	2.480
CC5H10+H<=>DC5H11 2620.0	2.500E+011	0.510

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!\REACTIONCLASS: \R+O2=E+HO2 \EA	\A	\N
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AC5H11+O2<=>AC5H10+HO2 11960.0	8.370E-001	3.590
BC5H11+O2<=>AC5H10+HO2 9322.0	5.350E-001	3.710
BC5H11+O2<=>BC5H10+HO2 9322.0	1.070E+000	3.710
CC5H11+O2<=>BC5H10+HO2 9322.0	1.070E+000	3.710
CC5H11+O2<=>CC5H10+HO2 9322.0	5.350E-001	3.710
DC5H11+O2<=>CC5H10+HO2 11960.0	8.370E-001	3.590

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!\REACTIONCLASS: \RADICAL_ISOMERISATION \EA	\A	\N
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AC5H11<=>DC5H11 21100.0	3.000E+011	0.000
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!\REACTIONCLASS: \R+O2=RO2 \EA	\A	\N
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AC5H11+O2<=>AC5H11O2 198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74	6.865E+016	-1.627
BC5H11+O2<=>BC5H11O2 -417.3 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74	9.756E+011	0.325
CC5H11+O2<=>CC5H11O2 -536.5 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74	3.487E+014	-0.816
DC5H11+O2<=>DC5H11O2 198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74	6.865E+016	-1.627

!

!\REACTIONCLASS: \R+R'O2=RO+R'O \EA	\A	\N
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AC5H11+HO2<=>AC5H11O+OH -1000.0	9.000E+012	0.000
BC5H11+HO2<=>BC5H11O+OH -1000.0	9.000E+012	0.000
CC5H11+HO2<=>CC5H11O+OH -1000.0	9.000E+012	0.000
DC5H11+HO2<=>DC5H11O+OH -1000.0	9.000E+012	0.000

AC5H11+CH3O2<=>AC5H11O+CH3O -1000.0	9.000E+012	0.000
BC5H11+CH3O2<=>BC5H11O+CH3O -1000.0	9.000E+012	0.000
CC5H11+CH3O2<=>CC5H11O+CH3O -1000.0	9.000E+012	0.000
DC5H11+CH3O2<=>DC5H11O+CH3O -1000.0	9.000E+012	0.000
AC5H11+AC5H11O2<=>AC5H11O+AC5H11O -1000.0	9.000E+012	0.000
AC5H11+BC5H11O2<=>AC5H11O+BC5H11O -1000.0	9.000E+012	0.000
AC5H11+CC5H11O2<=>AC5H11O+CC5H11O -1000.0	9.000E+012	0.000
AC5H11+DC5H11O2<=>AC5H11O+DC5H11O -1000.0	9.000E+012	0.000
BC5H11+AC5H11O2<=>BC5H11O+AC5H11O -1000.0	9.000E+012	0.000
BC5H11+BC5H11O2<=>BC5H11O+BC5H11O -1000.0	9.000E+012	0.000
BC5H11+CC5H11O2<=>BC5H11O+CC5H11O -1000.0	9.000E+012	0.000
BC5H11+DC5H11O2<=>BC5H11O+DC5H11O -1000.0	9.000E+012	0.000
CC5H11+AC5H11O2<=>CC5H11O+AC5H11O -1000.0	9.000E+012	0.000
CC5H11+BC5H11O2<=>CC5H11O+BC5H11O -1000.0	9.000E+012	0.000
CC5H11+CC5H11O2<=>CC5H11O+CC5H11O -1000.0	9.000E+012	0.000
CC5H11+DC5H11O2<=>CC5H11O+DC5H11O -1000.0	9.000E+012	0.000
DC5H11+AC5H11O2<=>DC5H11O+AC5H11O -1000.0	9.000E+012	0.000
DC5H11+BC5H11O2<=>DC5H11O+BC5H11O -1000.0	9.000E+012	0.000
DC5H11+CC5H11O2<=>DC5H11O+CC5H11O -1000.0	9.000E+012	0.000
DC5H11+DC5H11O2<=>DC5H11O+DC5H11O -1000.0	9.000E+012	0.000

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

AC5H11O2<=>AC5H10OOH-A 21500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	4.910E+007	1.300
AC5H11O2<=>AC5H10OOH-B 27100.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	2.309E+009	0.800
AC5H11O2<=>AC5H10OOH-C 18200.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	1.360E+007	1.300
AC5H11O2<=>AC5H10OOH-D 20000.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	1.233E+006	1.500

BC5H11O2<=>BC5H10OOH-A	3.014E+009	1.200
33500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
BC5H11O2<=>BC5H10OOH-C	6.513E+009	0.700
30100.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
BC5H11O2<=>BC5H10OOH-D	1.504E+008	1.100
21900.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
CC5H11O2<=>CC5H10OOH-A	2.877E+007	1.400
20800.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
CC5H11O2<=>CC5H10OOH-B	7.449E+009	0.600
27300.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
CC5H11O2<=>CC5H10OOH-D	1.458E+009	1.100
33500.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
DC5H11O2<=>DC5H10OOH-A	2.467E+006	1.500
20000.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
DC5H11O2<=>DC5H10OOH-B	1.231E+007	1.200
15400.0 !\AUTHOR: !\REF: S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701		
DC5H11O2<=>DC5H10OOH-C	4.009E+008	1.100
30100.0 !\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	1.260E+008	1.320
28900.0 !\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	2.448E+010	0.890
29500.0 !\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	1.124E+011	0.580
29600.0 !\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	3.500E+010	0.710
30100.0 !\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	1.476E+009	1.210
29800.0 !\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	1.518E+007	1.660
28400.0 !\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	1.750E+010	0.000
-3275.0 !\AUTHOR: !\REF:		
BC5H11O2+HO2<=>BC5H11O2H+O2	1.750E+010	0.000
-3275.0 !\AUTHOR: !\REF:		
CC5H11O2+HO2<=>CC5H11O2H+O2	1.750E+010	0.000
-3275.0 !\AUTHOR: !\REF:		
DC5H11O2+HO2<=>DC5H11O2H+O2	1.750E+010	0.000
-3275.0 !\AUTHOR: !\REF:		

!

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

!

AC5H11O2+H2O2<=>AC5H11O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		
BC5H11O2+H2O2<=>BC5H11O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		
CC5H11O2+H2O2<=>CC5H11O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		
DC5H11O2+H2O2<=>DC5H11O2H+HO2	2.400E+012	0.000
10000.0 !\AUTHOR: !\REF:		

!

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

!

!\SITE: \PRIMARY		
IC5H12+AC5H11O2<=>AC5H11+AC5H11O2H	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+BC5H11O2<=>AC5H11+BC5H11O2H	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+CC5H11O2<=>AC5H11+CC5H11O2H	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+DC5H11O2<=>AC5H11+DC5H11O2H	1.210E+013	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+AC5H11O2<=>DC5H11+AC5H11O2H	6.048E+012	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+BC5H11O2<=>DC5H11+BC5H11O2H	6.048E+012	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+CC5H11O2<=>DC5H11+CC5H11O2H	6.048E+012	0.000
20430.0 !\AUTHOR: !\REF:		
IC5H12+DC5H11O2<=>DC5H11+DC5H11O2H	6.048E+012	0.000
20430.0 !\AUTHOR: !\REF:		
!\SITE: \SECONDARY		
IC5H12+AC5H11O2<=>CC5H11+AC5H11O2H	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		
IC5H12+BC5H11O2<=>CC5H11+BC5H11O2H	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		
IC5H12+CC5H11O2<=>CC5H11+CC5H11O2H	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		
IC5H12+DC5H11O2<=>CC5H11+DC5H11O2H	4.032E+012	0.000
17700.0 !\AUTHOR: !\REF:		
!\SITE: \TERTIARY		
IC5H12+AC5H11O2<=>BC5H11+AC5H11O2H	2.016E+012	0.000
16000.0 !\AUTHOR: !\REF:		

IC5H12+BC5H11O2<=>BC5H11+BC5H11O2H 16000.0 !\AUTHOR: !\REF:	2.016E+012	0.000
IC5H12+CC5H11O2<=>BC5H11+CC5H11O2H 16000.0 !\AUTHOR: !\REF:	2.016E+012	0.000
IC5H12+DC5H11O2<=>BC5H11+DC5H11O2H 16000.0 !\AUTHOR: !\REF:	2.016E+012	0.000

!\REACTIONCLASS: \RO2+CH3O2=RO+CH3O+O2 \EA	\A	\N
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AC5H11O2+CH3O2=>AC5H11O+CH3O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
BC5H11O2+CH3O2=>BC5H11O+CH3O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
CC5H11O2+CH3O2=>CC5H11O+CH3O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
DC5H11O2+CH3O2=>DC5H11O+CH3O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610

!\REACTIONCLASS: \RO2+R'O2=RO+R'O+O2 \EA	\A	\N
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AC5H11O2+AC5H11O2=>AC5H11O+AC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
AC5H11O2+BC5H11O2=>AC5H11O+BC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
AC5H11O2+CC5H11O2=>AC5H11O+CC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
AC5H11O2+DC5H11O2=>AC5H11O+DC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
BC5H11O2+BC5H11O2=>BC5H11O+BC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
BC5H11O2+CC5H11O2=>BC5H11O+CC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
BC5H11O2+DC5H11O2=>BC5H11O+DC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
CC5H11O2+CC5H11O2=>CC5H11O+CC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
CC5H11O2+DC5H11O2=>CC5H11O+DC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610
DC5H11O2+DC5H11O2=>DC5H11O+DC5H11O+O2 1860.0 !\AUTHOR: !\REF:	1.400E+016	-1.610

!\REACTIONCLASS: \RO2H=RO+OH \EA	\A	\N
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AC5H11O2H<=>AC5H11O+OH 46072.1 !\AUTHOR: !\REF:	3.031E+020	-1.414
BC5H11O2H<=>BC5H11O+OH 45155.6 !\AUTHOR: !\REF:	8.618E+020	-1.641
CC5H11O2H<=>CC5H11O+OH 45777.4 !\AUTHOR: !\REF:	1.129E+021	-1.555

DC5H11O2H<=>DC5H11O+OH 3.591E+020 -1.436
46103.7 !\AUTHOR: !\REF:
!

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

CH2O+SC4H9<=>AC5H11O 5.000E+010 0.000
2330.0 !\AUTHOR: !\REF:
C2H5+CH3COCH3<=>BC5H11O 8.330E+009 0.000
7240.0 !\AUTHOR: !\REF:
CH3CHO+IC3H7<=>CC5H11O 1.665E+010 0.000
5230.0 !\AUTHOR: !\REF:
CH2O+IC4H9<=>DC5H11O 5.000E+010 0.000
2330.0 !\AUTHOR: !\REF:
!

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

AC5H10OOH-A<=>A-AC5H10O+OH 4.100E+010 0.360
17200.0 !\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 7.190E+009 0.880
9600.0 !\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 1.701E+009 0.734
14983.0 !\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 5.200E+008 0.670
10500.0 !\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 1.050E+012 0.150
9600.0 !\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 4.270E+010 0.520
8800.0 !\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 1.030E+010 0.550
16200.0 !\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 3.792E+007 1.517
16033.0 !\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 5.360E+010 0.540
8900.0 !\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 1.530E+010 0.640
10500.0 !\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 5.200E+008 0.670
10500.0 !\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 2.850E+008 0.920
13400.0 !\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 1.120E+010 0.820
10900.0 !\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 8.380E+009 0.920
14500.0 !\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 3.890E+013 -0.150
15500.0 !\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 3.010E+011 0.350
15200.0 !\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 9.790E+012 0.040
15400.0 !\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 6.830E+009 0.920
15100.0 !\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 6.240E+010 0.720
15000.0 !\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 1.960E+009 1.200
23400.0 !\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 8.283E+013 -0.170
30090.0 !\AUTHOR: !\REF:
BC5H10OOH-D=>OH+CH3COCH3+C2H4 1.182E+020 -2.060
24210.0 !\AUTHOR: !\REF:
CC5H10OOH-A=>OH+CH3CHO+C3H6 3.530E+009 1.200
21900.0 !\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 6.270E+008 1.400
23600.0 !\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 3.089E+016 -1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
!A*0.45
AC5H10OOH-B+O2<=>AC5H10OOH-BO2 4.390E+011 0.325
-417.3 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
!A*0.45

AC5H10OOH-C+O2<=>AC5H10OOH-CO2	1.569E+014	-0.816
-536.5 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
AC5H10OOH-D+O2<=>AC5H10OOH-DO2	3.089E+016	-1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
BC5H10OOH-A+O2<=>BC5H10OOH-AO2	3.089E+016	-1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
BC5H10OOH-C+O2<=>BC5H10OOH-CO2	1.569E+014	-0.816
-536.5 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
BC5H10OOH-D+O2<=>BC5H10OOH-DO2	3.089E+016	-1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
CC5H10OOH-A+O2<=>CC5H10OOH-AO2	3.089E+016	-1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
CC5H10OOH-B+O2<=>CC5H10OOH-BO2	4.390E+011	0.325
-417.3 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
CC5H10OOH-D+O2<=>CC5H10OOH-DO2	3.089E+016	-1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
DC5H10OOH-A+O2<=>DC5H10OOH-AO2	3.089E+016	-1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
DC5H10OOH-B+O2<=>DC5H10OOH-BO2	4.390E+011	0.325
-417.3 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74		
!A*0.45		
DC5H10OOH-C+O2<=>DC5H10OOH-CO2	1.569E+014	-0.816
-536.5 !\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	1.260E+008	1.320
28900.0 !\AUTHOR: !\REF:		
AC5H10OOH-BO2<=>C5H9A-AOOH+HO2	2.448E+010	0.890
29500.0 !\AUTHOR: !\REF:		
AC5H10OOH-BO2<=>C5H9B-AOOH+HO2	1.124E+011	0.580
29600.0 !\AUTHOR: !\REF:		
AC5H10OOH-CO2<=>C5H9B-AOOH+HO2	3.500E+010	0.710
30100.0 !\AUTHOR: !\REF:		
AC5H10OOH-CO2<=>C5H9C-AOOH+HO2	1.476E+009	1.210
29800.0 !\AUTHOR: !\REF:		
AC5H10OOH-DO2<=>C5H9C-AOOH+HO2	1.518E+007	1.660
28400.0 !\AUTHOR: !\REF:		
BC5H10OOH-CO2<=>C5H9C-BOOH+HO2	1.476E+009	1.210
29800.0 !\AUTHOR: !\REF:		
BC5H10OOH-DO2<=>C5H9C-BOOH+HO2	1.518E+007	1.660
28400.0 !\AUTHOR: !\REF:		
CC5H10OOH-AO2<=>C5H9A-COOH+HO2	1.260E+008	1.320
28900.0 !\AUTHOR: !\REF:		

CC5H10OOH-BO2<=>C5H9A-COOH+HO2 29500.0 !\AUTHOR: !\REF:	2.448E+010	0.890
DC5H10OOH-AO2<=>C5H9A-DOOH+HO2 28900.0 !\AUTHOR: !\REF:	1.260E+008	1.320
DC5H10OOH-BO2<=>C5H9A-DOOH+HO2 29500.0 !\AUTHOR: !\REF:	2.448E+010	0.890
DC5H10OOH-BO2<=>C5H9B-DOOH+HO2 29600.0 !\AUTHOR: !\REF:	1.124E+011	0.580
DC5H10OOH-CO2<=>C5H9B-DOOH+HO2 30100.0 !\AUTHOR: !\REF:	3.500E+010	0.710

!

!\REACTIONCLASS: \O2QOOH=P(OOH)2 \EA	\A	\N
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!

AC5H10OOH-AO2<=>C5H9B-A,AOOH 27100.0 !\AUTHOR: !\REF:	2.309E+009	0.800
AC5H10OOH-AO2<=>C5H9C-A,AOOH 18200.0 !\AUTHOR: !\REF:	1.360E+007	1.300
AC5H10OOH-AO2<=>C5H9D-A,AOOH 20000.0 !\AUTHOR: !\REF:	1.233E+006	1.500
AC5H10OOH-BO2<=>C5H9A-A,BOOH 33500.0 !\AUTHOR: !\REF:	3.014E+009	1.200
AC5H10OOH-BO2<=>C5H9C-A,BOOH 30100.0 !\AUTHOR: !\REF:	6.513E+009	0.700
AC5H10OOH-BO2<=>C5H9D-A,BOOH 21900.0 !\AUTHOR: !\REF:	1.504E+008	1.100
AC5H10OOH-CO2<=>C5H9A-A,COOH 20800.0 !\AUTHOR: !\REF:	2.877E+007	1.400
AC5H10OOH-CO2<=>C5H9B-A,COOH 27300.0 !\AUTHOR: !\REF:	7.449E+009	0.600
AC5H10OOH-CO2<=>C5H9D-A,COOH 33500.0 !\AUTHOR: !\REF:	1.458E+009	1.100
AC5H10OOH-DO2<=>C5H9A-A,DOOH 20000.0 !\AUTHOR: !\REF:	2.467E+006	1.500
AC5H10OOH-DO2<=>C5H9B-A,DOOH 15400.0 !\AUTHOR: !\REF:	1.231E+007	1.200
AC5H10OOH-DO2<=>C5H9C-A,DOOH 30100.0 !\AUTHOR: !\REF:	4.009E+008	1.100
BC5H10OOH-AO2<=>C5H9A-A,BOOH 21500.0 !\AUTHOR: !\REF:	4.910E+007	1.300
BC5H10OOH-AO2<=>C5H9C-A,BOOH 18200.0 !\AUTHOR: !\REF:	1.360E+007	1.300
BC5H10OOH-AO2<=>C5H9D-A,BOOH 20000.0 !\AUTHOR: !\REF:	1.233E+006	1.500
BC5H10OOH-CO2<=>C5H9A-B,COOH 20800.0 !\AUTHOR: !\REF:	2.877E+007	1.400
BC5H10OOH-CO2<=>C5H9D-B,COOH 33500.0 !\AUTHOR: !\REF:	1.458E+009	1.100
BC5H10OOH-DO2<=>C5H9A-B,DOOH 20000.0 !\AUTHOR: !\REF:	2.467E+006	1.500
BC5H10OOH-DO2<=>C5H9C-B,DOOH 30100.0 !\AUTHOR: !\REF:	4.009E+008	1.100
CC5H10OOH-AO2<=>C5H9A-A,COOH 21500.0 !\AUTHOR: !\REF:	4.910E+007	1.300
CC5H10OOH-AO2<=>C5H9B-A,COOH 27100.0 !\AUTHOR: !\REF:	2.309E+009	0.800

CC5H10OOH-AO2<=>C5H9D-A, COOH 20000.0 !\AUTHOR: !\REF:	1.233E+006	1.500
CC5H10OOH-BO2<=>C5H9A-B, COOH 33500.0 !\AUTHOR: !\REF:	3.014E+009	1.200
CC5H10OOH-BO2<=>C5H9D-B, COOH 21900.0 !\AUTHOR: !\REF:	1.504E+008	1.100
CC5H10OOH-DO2<=>C5H9A-C, DOOH 20000.0 !\AUTHOR: !\REF:	2.467E+006	1.500
CC5H10OOH-DO2<=>C5H9B-C, DOOH 15400.0 !\AUTHOR: !\REF:	1.231E+007	1.200
DC5H10OOH-AO2<=>C5H9A-A, DOOH 21500.0 !\AUTHOR: !\REF:	4.910E+007	1.300
DC5H10OOH-AO2<=>C5H9B-A, DOOH 27100.0 !\AUTHOR: !\REF:	2.309E+009	0.800
DC5H10OOH-AO2<=>C5H9C-A, DOOH 18200.0 !\AUTHOR: !\REF:	1.360E+007	1.300
DC5H10OOH-BO2<=>C5H9A-B, DOOH 33500.0 !\AUTHOR: !\REF:	3.014E+009	1.200
DC5H10OOH-BO2<=>C5H9C-B, DOOH 30100.0 !\AUTHOR: !\REF:	6.513E+009	0.700
DC5H10OOH-CO2<=>C5H9A-C, DOOH 20800.0 !\AUTHOR: !\REF:	2.877E+007	1.400
DC5H10OOH-CO2<=>C5H9B-C, DOOH 27300.0 !\AUTHOR: !\REF:	7.449E+009	0.600

!

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

!

AC5H10OOH-AO2<=>IC5KETAA+OH 18800.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	5.188E+004	1.900
AC5H10OOH-BO2<=>IC5KETAB+OH 27900.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	2.441E+007	1.600
AC5H10OOH-CO2<=>IC5KETAC+OH 19900.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	1.098E+004	2.400
AC5H10OOH-DO2<=>IC5KETAD+OH 16600.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	4.766E+003	1.700
CC5H10OOH-AO2<=>IC5KETCA+OH 17000.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	5.786E+001	2.900
CC5H10OOH-BO2<=>IC5KETCB+OH 26000.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	1.747E+008	1.700
CC5H10OOH-DO2<=>IC5KETCD+OH 25700.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	2.763E+008	1.200
DC5H10OOH-AO2<=>IC5KETDA+OH 16600.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	4.766E+003	1.700
DC5H10OOH-BO2<=>IC5KETDB+OH 19900.0 !\AUTHOR: !\REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114, 5689-5701	1.098E+004	2.400

DC5H10OOH-CO2<=>IC5KETDC+OH 2.441E+007 1.600
27900.0 !\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 1.978E+008 1.521
21890.0 !\AUTHOR: !\REF:
C5H9A-A, DOOH<=>AC3H5OOH+C2H4O2H 1.978E+008 1.521
21890.0 !\AUTHOR: !\REF:
C5H9A-C, DOOH=>C3H6+HO2CH2CHO+OH 3.530E+009 1.200
21900.0 !\AUTHOR: !\REF:
C5H9C-A, AOOH=>C4H72-1OOH+CH2O+OH 1.960E+009 1.200
23400.0 !\AUTHOR: !\REF:
C5H9D-A, AOOH=>AC3H5OOH+C2H4+HO2 1.978E+008 1.521
21890.0 !\AUTHOR: !\REF:
C5H9D-A, BOOH=>IC3H5Q+C2H4+HO2 1.960E+009 1.200
23400.0 !\AUTHOR: !\REF:

!

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

!

IC5KETAA<=>IC5KETAAO+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
IC5KETAB<=>IC5KETABO+OH 6.000E+015 0.000
41200.0 !\AUTHOR: !\REF:
IC5KETAC<=>IC5KETACO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
IC5KETAD<=>IC5KETADO+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
IC5KETCA<=>IC5KETCAO+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
IC5KETCB<=>IC5KETCBO+OH 6.000E+015 0.000
41200.0 !\AUTHOR: !\REF:
IC5KETCD<=>IC5KETCDO+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
IC5KETDA<=>IC5KETDAO+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
IC5KETDB<=>IC5KETDBO+OH 6.000E+015 0.000
41200.0 !\AUTHOR: !\REF:
IC5KETDC<=>IC5KETDCO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
IC5KETAAO<=>CH2O+C3H6CHO-3 2.900E+012 0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,
3455-3471
IC5KETABO<=>C2H5COCH3+HCO 2.900E+012 0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,
3455-3471
IC5KETACO<=>CH3CHO+CH3CHCHO 2.900E+012 0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159,
3455-3471

IC5KETADO<=>CH2O+IC3H6CHO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159, 3455-3471		
IC5KETCAO<=>CH2O+CH3CHCOCH3	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159, 3455-3471		
IC5KETCBO<=>CH3COCH3+CH3CO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159, 3455-3471		
IC5KETCDO<=>CH2O+IC3H7CO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159, 3455-3471		
IC5KETDAO<=>CH2O+C3H6CHO-2	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159, 3455-3471		
IC5KETDBO<=>CH3COCH3+CH2CHO	2.900E+012	0.380
11080.0 !\AUTHOR: !\REF:O. Herbinet et al. Combust. Flame 2012, 159, 3455-3471		
IC5KETDCO<=>IC3H7CHO+HCO	2.900E+012	0.380
11080.0 !\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	3.890E+013	-0.150
15500.0 !\AUTHOR: !\REF:		
C5H9A-B, COOH<=>C5H9A-COOH+HO2	3.890E+013	-0.150
15500.0 !\AUTHOR: !\REF:		
C5H9A-B, DOOH<=>C5H9A-DOOH+HO2	3.890E+013	-0.150
15500.0 !\AUTHOR: !\REF:		
C5H9B-A, AOOH<=>C5H9A-AOOH+HO2	1.676E+010	0.920
14500.0 !\AUTHOR: !\REF:		
C5H9B-A, COOH<=>C5H9A-COOH+HO2	8.380E+009	0.920
14500.0 !\AUTHOR: !\REF:		
C5H9B-A, COOH<=>C5H9B-AOOH+HO2	9.790E+012	0.040
15400.0 !\AUTHOR: !\REF:		
C5H9B-A, DOOH<=>C5H9A-DOOH+HO2	8.380E+009	0.920
14500.0 !\AUTHOR: !\REF:		
C5H9B-C, DOOH<=>C5H9B-DOOH+HO2	9.790E+012	0.040
15400.0 !\AUTHOR: !\REF:		
C5H9C-A, BOOH<=>C5H9B-AOOH+HO2	3.010E+011	0.350
15200.0 !\AUTHOR: !\REF:		
C5H9C-A, DOOH<=>C5H9C-AOOH+HO2	6.240E+010	0.720
15000.0 !\AUTHOR: !\REF:		
C5H9C-B, DOOH<=>C5H9B-DOOH+HO2	3.010E+011	0.350
15200.0 !\AUTHOR: !\REF:		
C5H9C-B, DOOH<=>C5H9C-BOOH+HO2	6.240E+010	0.720
15000.0 !\AUTHOR: !\REF:		
C5H9D-A, COOH<=>C5H9C-AOOH+HO2	6.830E+009	0.920
15100.0 !\AUTHOR: !\REF:		
C5H9D-B, COOH<=>C5H9C-BOOH+HO2	6.830E+009	0.920
15100.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \EROOH_DECOMPOSITION \EA !	\A	\N
C5H9A-AOOH=>CH2O+C4H71-2+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9A-COOH=>CH3CHO+C3H5-T+OH 42600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9A-DOOH=>CH2O+IC4H7+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9B-AOOH=>CH2O+C4H72-2+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9B-DOOH=>CH2O+IC4H7+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9C-AOOH=>CH2O+C4H71-3+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9C-BOOH=>CH3COCH3+C2H3+OH 42200.0 !\AUTHOR: !\REF:	6.000E+015	0.000

!\REACTIONCLASS: \P(OOH)2=CETH-OOH+OH \EA !	\A	\N
C5H9A-A, BOOH<=>C5H9OA-AOOH-B+OH 17200.0 !\AUTHOR: !\REF:	4.100E+010	0.360
C5H9A-A, BOOH<=>C5H9OA-BOOH-A+OH 9600.0 !\AUTHOR: !\REF:	1.050E+012	0.150
C5H9A-A, COOH<=>C5H9OA-AOOH-C+OH 17200.0 !\AUTHOR: !\REF:	4.100E+010	0.360
C5H9A-A, COOH<=>C5H9OA-COOH-A+OH 16033.0 !\AUTHOR: !\REF:	3.792E+007	1.517
C5H9A-A, DOOH<=>C5H9OA-AOOH-D+OH 17200.0 !\AUTHOR: !\REF:	4.100E+010	0.360
C5H9A-A, DOOH<=>C5H9OA-DOOH-A+OH 10500.0 !\AUTHOR: !\REF:	5.200E+008	0.670
C5H9A-B, COOH<=>C5H9OA-BOOH-C+OH 9600.0 !\AUTHOR: !\REF:	1.050E+012	0.150
C5H9A-B, COOH<=>C5H9OA-COOH-B+OH 16033.0 !\AUTHOR: !\REF:	3.792E+007	1.517
C5H9A-B, DOOH<=>C5H9OA-BOOH-D+OH 9600.0 !\AUTHOR: !\REF:	1.050E+012	0.150
C5H9A-B, DOOH<=>C5H9OA-DOOH-B+OH 10500.0 !\AUTHOR: !\REF:	5.200E+008	0.670
C5H9A-C, DOOH<=>C5H9OA-COOH-D+OH 16033.0 !\AUTHOR: !\REF:	3.792E+007	1.517
C5H9A-C, DOOH<=>C5H9OA-DOOH-C+OH 10500.0 !\AUTHOR: !\REF:	5.200E+008	0.670
C5H9B-A, AOOH<=>C5H9OA-BOOH-A+OH 9600.0 !\AUTHOR: !\REF:	7.190E+009	0.880
C5H9B-A, COOH<=>C5H9OA-BOOH-C+OH 9600.0 !\AUTHOR: !\REF:	7.190E+009	0.880
C5H9B-A, COOH<=>C5H9OB-COOH-A+OH 8900.0 !\AUTHOR: !\REF:	5.360E+010	0.540
C5H9B-A, DOOH<=>C5H9OA-BOOH-D+OH 9600.0 !\AUTHOR: !\REF:	7.190E+009	0.880
C5H9B-A, DOOH<=>C5H9OB-DOOH-A+OH 13400.0 !\AUTHOR: !\REF:	2.850E+008	0.920

C5H9B-C, DOOH<=>C5H9OB-COOH-D+OH 8900.0 !\AUTHOR: !\REF:	5.360E+010	0.540
C5H9B-C, DOOH<=>C5H9OB-DOOH-C+OH 13400.0 !\AUTHOR: !\REF:	2.850E+008	0.920
C5H9C-A, AOOH<=>C5H9OA-COOH-A+OH 14983.0 !\AUTHOR: !\REF:	1.701E+009	0.734
C5H9C-A, BOOH<=>C5H9OA-COOH-B+OH 14983.0 !\AUTHOR: !\REF:	1.701E+009	0.734
C5H9C-A, BOOH<=>C5H9OB-COOH-A+OH 8800.0 !\AUTHOR: !\REF:	4.270E+010	0.520
C5H9C-A, DOOH<=>C5H9OA-COOH-D+OH 14983.0 !\AUTHOR: !\REF:	1.701E+009	0.734
C5H9C-A, DOOH<=>C5H9OC-DOOH-A+OH 10900.0 !\AUTHOR: !\REF:	1.120E+010	0.820
C5H9C-B, DOOH<=>C5H9OB-COOH-D+OH 8800.0 !\AUTHOR: !\REF:	4.270E+010	0.520
C5H9C-B, DOOH<=>C5H9OC-DOOH-B+OH 10900.0 !\AUTHOR: !\REF:	1.120E+010	0.820
C5H9D-A, AOOH<=>C5H9OA-DOOH-A+OH 10500.0 !\AUTHOR: !\REF:	5.200E+008	0.670
C5H9D-A, BOOH<=>C5H9OA-DOOH-B+OH 10500.0 !\AUTHOR: !\REF:	5.200E+008	0.670
C5H9D-A, BOOH<=>C5H9OB-DOOH-A+OH 16200.0 !\AUTHOR: !\REF:	1.030E+010	0.550
C5H9D-A, COOH<=>C5H9OA-DOOH-C+OH 10500.0 !\AUTHOR: !\REF:	5.200E+008	0.670
C5H9D-A, COOH<=>C5H9OC-DOOH-A+OH 10500.0 !\AUTHOR: !\REF:	1.530E+010	0.640
C5H9D-B, COOH<=>C5H9OB-DOOH-C+OH 16200.0 !\AUTHOR: !\REF:	1.030E+010	0.550
C5H9D-B, COOH<=>C5H9OC-DOOH-B+OH 10500.0 !\AUTHOR: !\REF:	1.530E+010	0.640

!

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

!

C5H9OA-AOOH-B=>CH2O+C2H5COCH2+OH 42200.0 !\AUTHOR: !\REF:	6.000E+015	0.000
C5H9OA-BOOH-A=>CH2O+C2H5COCH2+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OA-AOOH-C=>CH3CHO+C3H5O+OH 42600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9OA-COOH-A=>CH2O+C4H71-O+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OA-AOOH-D=>CH2O+AC3H5OCH2+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OA-DOOH-A=>CH2O+C4H7O1-4+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OA-BOOH-C=>CH3CHO+CH3COCH2+OH 42600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9OA-COOH-B=>CH3CHO+CH3COCH2+OH 42200.0 !\AUTHOR: !\REF:	6.000E+015	0.000
C5H9OA-BOOH-D=>CH2O+IC4H7O+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OA-DOOH-B<=>CH3COCH2OCH2CH2+OH 42200.0 !\AUTHOR: !\REF:	6.000E+015	0.000

C5H9OA-COOH-D=>CH2O+IC3H6CHO+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OA-DOOH-C=>CH2O+IC3H6CHO+OH 42600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9OB-COOH-A=>CH2O+CH3CHCOCH3+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OB-DOOH-A=>CH2O+CH2CH2COCH3+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OB-COOH-D=>CH2O+TC3H6CHO+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OB-DOOH-C=>CH3COCH3+CH2CHO+OH 42600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C5H9OC-DOOH-A=>CH2O+C4H7O2-1+OH 43000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C5H9OC-DOOH-B=>CH3COCH3+CH2CHO+OH 42200.0 !\AUTHOR: !\REF:	6.000E+015	0.000
CH3COCH2OCH2CH2=>CH2O+C2H4+CH3CO 25500.0 !\AUTHOR: !\REF:	1.600E+013	0.000

!

!\REACTIONCLASS: \CETH_DECOMPOSITION

\A

\N

\EA

!

A-AC5H10O+OH=>CH2O+C4H71-2+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-BC5H10O+OH=>IC3H5CHO+CH3+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-CC5H10O+OH=>C3H6+CH3CO+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-DC5H10O+OH=>C3H6+CH2CHO+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
B-CC5H10O+OH=>IC3H5COCH3+H+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
B-DC5H10O+OH=>IC4H8+HCO+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
C-DC5H10O+OH=>CH2CO+IC3H7+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-AC5H10O+OH=>C2H3CHO+C2H5+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-BC5H10O+OH=>CH2O+C4H72-2+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-CC5H10O+OH=>C3H5-T+CH3CHO+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-DC5H10O+OH=>CH3CHCHO+C2H4+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
B-CC5H10O+OH=>IC3H5CHO+CH3+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
B-DC5H10O+OH=>CH3COCH3+C2H3+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
C-DC5H10O+OH=>SC3H5CHO+CH3+H2O 0.0 !\AUTHOR: !\REF:	2.500E+012	0.000
A-AC5H10O+HO2=>CH2O+C4H71-2+H2O2 17700.0 !\AUTHOR: !\REF:	5.000E+012	0.000
A-BC5H10O+HO2=>IC3H5CHO+CH3+H2O2 17700.0 !\AUTHOR: !\REF:	5.000E+012	0.000
A-CC5H10O+HO2=>C3H6+CH3CO+H2O2 17700.0 !\AUTHOR: !\REF:	5.000E+012	0.000

A-DC5H10O+HO2=>C3H6+CH2CHO+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
B-CC5H10O+HO2=>IC3H5COCH3+H+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
B-DC5H10O+HO2=>IC4H8+HCO+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
C-DC5H10O+HO2=>CH2CO+IC3H7+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
A-AC5H10O+HO2=>C2H3CHO+C2H5+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
A-BC5H10O+HO2=>CH2O+C4H7-2+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
A-CC5H10O+HO2=>C3H5-T+CH3CHO+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
A-DC5H10O+HO2=>CH3CHCHO+C2H4+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
B-CC5H10O+HO2=>IC3H5CHO+CH3+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
B-DC5H10O+HO2=>CH3COCH3+C2H3+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		
C-DC5H10O+HO2=>SC3H5CHO+CH3+H2O2	5.000E+012	0.000
17700.0 !\AUTHOR: !\REF:		

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!\SUBSPECIES: \IC3H5COCH3

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!

!\REACTIONCLASS: \MISC

\A

\N

\EA

!

IC3H5COCH3<=>IC3H5CO+CH3	1.903E+022	-1.752
83625.5 !\AUTHOR: !\REF:		
IC3H5COCH3<=>C3H5-T+CH3CO	6.070E+024	-2.210
96960.0 !\AUTHOR: !\REF:		
IC3H5COCH3+OH<=>IC3H5COCH2+H2O	5.100E+011	0.000
1192.0 !\AUTHOR: !\REF:		
IC3H5COCH3+O<=>IC3H5COCH2+OH	5.000E+012	0.000
5962.0 !\AUTHOR: !\REF:		
IC3H5COCH3+H<=>IC3H5COCH2+H2	9.300E+012	0.000
6357.0 !\AUTHOR: !\REF:		
IC3H5COCH3+CH3<=>IC3H5COCH2+CH4	1.620E+011	0.000
9630.0 !\AUTHOR: !\REF:		
IC3H5COCH3+HO2<=>IC3H5COCH2+H2O2	8.500E+012	0.000
20460.0 !\AUTHOR: !\REF:		
IC3H5COCH3+O2<=>IC3H5COCH2+HO2	6.000E+013	0.000
46000.0 !\AUTHOR: !\REF:		
IC3H5COCH2<=>C3H5-T+CH2CO	5.972E+014	0.188
51272.0 !\AUTHOR: !\REF:		
IC3H5COCH3+OH<=>AC3H4COCH3+H2O	3.120E+006	2.000
-298.0 !\AUTHOR: !\REF:		
IC3H5COCH3+O<=>AC3H4COCH3+OH	6.030E+010	0.700
7633.0 !\AUTHOR: !\REF:		
IC3H5COCH3+H<=>AC3H4COCH3+H2	1.730E+005	2.500
2492.0 !\AUTHOR: !\REF:		

PLOG / 3.000E-001 2.930E+083 -20.44 128998. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 8%
 PLOG / 1.000E+000 7.740E+081 -19.79 129931. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%
 PLOG / 2.000E+000 2.900E+080 -19.26 130191. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 5%
 PLOG / 5.000E+000 9.040E+077 -18.40 130162. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 5%
 PLOG / 1.000E+001 3.440E+075 -17.60 129792. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 4%
 PLOG / 2.000E+001 4.170E+072 -16.67 129063. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 4%
 PLOG / 5.000E+001 9.620E+067 -15.22 127494. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 5%
 PLOG / 1.000E+002 8.760E+063 -13.99 125858. / !FIT FROM: 800-2000 K
 ERROR IN FIT: 6%

!

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

!

!\SITE: \PRIMARY
 NEOC5H12+O2<=>NEOC5H11+HO2 8.400E+013 0.000
 52800.0 !\AUTHOR: !\REF:
 NEOC5H12+O<=>NEOC5H11+OH 2.260E+014 0.000
 7850.0 !\AUTHOR: !\REF:
 NEOC5H12+H<=>NEOC5H11+H2 6.980E+005 2.690
 6450.0 !\AUTHOR: !\REF:
 NEOC5H12+OH<=>NEOC5H11+H2O 6.567E+007 1.763
 743.2 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM.
 A, 2009, 113, 5047-5060
 NEOC5H12+HO2<=>NEOC5H11+H2O2 8.160E+001 3.590
 17160.0 !\AUTHOR: !\REF:
 NEOC5H12+CH3<=>NEOC5H11+CH4 1.808E+000 3.650
 7154.0 !\AUTHOR: !\REF:
 NEOC5H12+CH3O<=>NEOC5H11+CH3OH 6.000E+011 0.000
 7000.0 !\AUTHOR: !\REF:
 NEOC5H12+CH3O2<=>NEOC5H11+CH3O2H 2.772E+000 3.970
 18280.0 !\AUTHOR: !\REF:
 NEOC5H12+C2H5<=>NEOC5H11+C2H6 2.000E+011 0.000
 13400.0 !\AUTHOR: !\REF:
 NEOC5H12+C2H3<=>NEOC5H11+C2H4 2.000E+012 0.000
 18000.0 !\AUTHOR: !\REF:
 NEOC5H12+O2CHO<=>NEOC5H11+HO2CHO 2.772E+000 3.970
 18280.0 !\AUTHOR: !\REF:
 NEOC5H12+IC4H6OH<=>NEOC5H11+IC4H7OH 9.400E+002 3.300
 19840.0 !\AUTHOR: !\REF:
 NEOC5H12+IC4H7O<=>NEOC5H11+IC4H7OH 5.400E+011 0.000
 4000.0 !\AUTHOR: !\REF:
 NEOC5H12+TC3H6CHO<=>NEOC5H11+IC3H7CHO 9.400E+002 3.300
 19840.0 !\AUTHOR: !\REF:
 NEOC5H12+CH2CCH2OH<=>NEOC5H11+C3H5OH 1.590E+012 0.000
 20500.0 !\AUTHOR: !\REF:

!

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

!
NEOC5H11<=>IC4H8+CH3 3.652E+018 -1.337 33461.5 !\AUTHOR: !\REF:H. J. CURRAN INT. J. CHEM. KIN. 2006, 38, 4, 250-275
PLOG / 1.000E-002 2.750E+032 -6.66 31143. / !FIT FROM: 800-2000 K
ERROR IN FIT: 4%
PLOG / 1.000E-001 2.650E+037 -7.68 36912. / !FIT FROM: 800-2000 K
ERROR IN FIT: 5%
PLOG / 1.000E+000 6.530E+039 -7.98 41554. / !FIT FROM: 800-2000 K
ERROR IN FIT: 6%
PLOG / 2.000E+000 1.050E+040 -7.94 42640. / !FIT FROM: 800-2000 K
ERROR IN FIT: 6%
PLOG / 5.000E+000 1.190E+040 -7.83 43859. / !FIT FROM: 800-2000 K
ERROR IN FIT: 7%
PLOG / 1.000E+001 1.130E+040 -7.75 44627. / !FIT FROM: 800-2000 K
ERROR IN FIT: 8%
PLOG / 2.000E+001 1.150E+040 -7.69 45269. / !FIT FROM: 800-2000 K
ERROR IN FIT: 10%
PLOG / 5.000E+001 1.440E+040 -7.66 45920. / !FIT FROM: 800-2000 K
ERROR IN FIT: 11%
PLOG / 1.000E+002 1.810E+040 -7.67 46255. / !FIT FROM: 800-2000 K
ERROR IN FIT: 12%

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

NEOC5H11+O2<=>NEOC5H11O2 6.865E+016 -1.627
198.7 !\AUTHOR: !\REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
!

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

NEOC5H11+HO2<=>NEOC5H11O+OH 9.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:
NEOC5H11+CH3O2<=>NEOC5H11O+CH3O 9.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:
NEOC5H11+NEOC5H11O2<=>NEOC5H11O+NEOC5H11O 9.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:

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

NEOC5H11O2<=>NEOC5H10OOH 1.198E+009 1.200
21600.0 !\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 -3275.0 !\AUTHOR: !\REF: !	1.750E+010	0.000
!\REACTIONCLASS: \RO2+H2O2=RO2H+HO2 \EA !	\A	\N
NEOC5H11O2+H2O2<=>NEOC5H11O2H+HO2 10000.0 !\AUTHOR: !\REF: !	2.400E+012	0.000
!\REACTIONCLASS: \RO2+F=RO2H+R' \EA !	\A	\N
!\SITE: \PRIMARY NEOC5H12+NEOC5H11O2<=>NEOC5H11+NEOC5H11O2H 20430.0 !\AUTHOR: !\REF: !	2.419E+013	0.000
!\REACTIONCLASS: \RO2+CH3O2=RO+CH3O+O2 \EA !	\A	\N
NEOC5H11O2+CH3O2=>NEOC5H11O+CH3O+O2 1860.0 !\AUTHOR: !\REF: !	1.400E+016	-1.610
!\REACTIONCLASS: \RO2+R'O2=RO+R'O+O2 \EA !	\A	\N
NEOC5H11O2+NEOC5H11O2=>NEOC5H11O+NEOC5H11O+O2 1860.0 !\AUTHOR: !\REF: !	1.400E+016	-1.610
!\REACTIONCLASS: \RO2H=RO+OH \EA !	\A	\N
NEOC5H11O2H<=>NEOC5H11O+OH 45110.0 !\AUTHOR: !\REF: !	2.094E+017	-0.400
!\REACTIONCLASS: \RO_DECOMPOSITION \EA !	\A	\N
CH2O+TC4H9<=>NEOC5H11O 2330.0 !\AUTHOR: !\REF:H. J. CURRAN INT. J. CHEM. KIN. 2006, 38, 4, 250- 275 !	5.000E+010	0.000
!\REACTIONCLASS: \QOOH=CETH+OH \EA !	\A	\N

NEOC5H10OOH<=>NEO-C5H10O+OH 3.710E+009 0.700
15900.0 !\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 3.640E+009 1.300
23700.0 !\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 1.640E+007 2.000
28300.0 !\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 3.433E+016 -1.627
198.7 !\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 7.987E+008 1.200
21600.0
!

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

NEOC5H10OOH-O2<=>NEOC5KET+OH 5.188E+004 1.900
18800.0 !\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 3.640E+009 1.300
23700.0 !\AUTHOR: !\REF:
NEOC5H9Q2<=>IC4H6Q2-II+CH3 1.640E+007 2.000
28300.0 !\AUTHOR: !\REF:
!

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

NEOC5KET<=>NEOC5KETOX+OH 1.500E+016 0.000
43000.0 !\AUTHOR: !\REF:
NEOC5KETOX<=>TC3H6CHO+CH2O 2.475E+021 -2.540
15830.0 !\AUTHOR: !\REF:

!

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

!

NEOC5H9Q2<=>NEOC5H9O-OOH+OH 3.710E+009 0.700
15900.0 !\AUTHOR: !\REF:

!

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

!

NEOC5H9O-OOH=>C3H5-T+CH2O+CH2O+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF:

!

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

!

NEO-C5H10O+OH<=>TC4H8CHO+H2O 2.500E+012 0.000
0.0 !\AUTHOR: !\REF:
NEO-C5H10O+OH=>IC4H7+CH2O+H2O 2.500E+012 0.000
0.0 !\AUTHOR: !\REF:
NEO-C5H10O+HO2<=>TC4H8CHO+H2O2 5.000E+012 0.000
17700.0 !\AUTHOR: !\REF:
NEO-C5H10O+HO2=>IC4H7+CH2O+H2O2 5.000E+012 0.000
17700.0 !\AUTHOR: !\REF:
NEO-C5H10O+H<=>TC4H8CHO+H2 3.544E+007 2.000
5000.0 !\AUTHOR: !\REF:
NEO-C5H10O+H=>IC4H7+CH2O+H2 1.330E+006 2.540
6756.0 !\AUTHOR: !\REF:
NEO-C5H10O<=>IC4H8+CH2O 3.800E+015 0.000
60700.0 !\AUTHOR: !\REF:

!

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

!

NEOC5KETOX<=>NEOC5KEJOL 1.203E+09 1.199
13600.7 !\AUTHOR: !\REF:
NEOC5KEJOL<=>IC4H8OH+CO 2.273E+21 -2.340
11020.0 !\AUTHOR: !\REF:

!

!\ENDSUBMECH: \NEOC5H12

!

!

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

!-----

!

!\REACTIONCLASS: \E_UNIMOL	\A	\N
!\EA		
!		
C5H10-1<=>C2H5+C3H5-A	9.864E+021	-2.086
75060.0 !\AUTHOR: !\REF:		
!ANALOGY WITH C3H5-A+CH3		
C4H71-3+CH3 (+M) <=>C5H10-2 (+M)	1.000E+014	-0.320
-262.3		
LOW/	3.910E+060	-12.810
6250.0/		
TROE/ 1.040E-001 1.606E+003 6.000E+004 6.118E+003/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/		
0.70/		
!		

!\REACTIONCLASS: \E_R_ABSTRACTION	\A	\N
-----------------------------------	----	----

!\EA

!

!\SITE: \PRIMARY		
C5H10-1+O2<=>C5H91-5+HO2	3.000E+013	0.000
52290.0 !\AUTHOR: !\REF:		
C5H10-1+O<=>C5H91-5+OH	9.800E+005	2.430
4750.0 !\AUTHOR: !\REF:		
C5H10-1+H<=>C5H91-5+H2	6.650E+005	2.540
6756.0 !\AUTHOR: !\REF:		
C5H10-1+OH<=>C5H91-5+H2O	5.270E+009	0.970
1586.0 !\AUTHOR: !\REF:		
C5H10-1+HO2<=>C5H91-5+H2O2	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:		
C5H10-1+CH3<=>C5H91-5+CH4	4.521E-001	3.650
7154.0 !\AUTHOR: !\REF:		
C5H10-1+CH3O<=>C5H91-5+CH3OH	2.170E+011	0.000
6458.0 !\AUTHOR: !\REF:		
C5H10-1+CH3O2<=>C5H91-5+CH3O2H	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:		
C5H10-2+O2<=>C5H92-5+HO2	3.000E+013	0.000
52290.0 !\AUTHOR: !\REF:		
C5H10-2+O<=>C5H92-5+OH	9.800E+005	2.430
4750.0 !\AUTHOR: !\REF:		
C5H10-2+H<=>C5H92-5+H2	6.651E+005	2.540
6756.0 !\AUTHOR: !\REF:		
C5H10-2+OH<=>C5H92-5+H2O	5.270E+009	0.970
1586.0 !\AUTHOR: !\REF:		
C5H10-2+HO2<=>C5H92-5+H2O2	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:		
C5H10-2+CH3<=>C5H92-5+CH4	4.521E-001	3.650
7154.0 !\AUTHOR: !\REF:		
C5H10-2+CH3O<=>C5H92-5+CH3OH	2.170E+011	0.000
6458.0 !\AUTHOR: !\REF:		
C5H10-2+CH3O2<=>C5H92-5+CH3O2H	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:		
!\SITE: \SECONDARY		

C5H10-1+O2<=>C5H91-4+HO2	2.000E+013	0.000
49640.0 !\AUTHOR: !\REF:		
C5H10-1+O<=>C5H91-4+OH	5.510E+005	2.450
2830.0 !\AUTHOR: !\REF:		
C5H10-1+H<=>C5H91-4+H2	1.300E+006	2.400
4471.0 !\AUTHOR: !\REF:		
C5H10-1+OH<=>C5H91-4+H2O	4.670E+007	1.610
-35.0 !\AUTHOR: !\REF:		
C5H10-1+HO2<=>C5H91-4+H2O2	9.640E+003	2.600
13910.0 !\AUTHOR: !\REF:		
C5H10-1+CH3<=>C5H91-4+CH4	1.510E+000	3.460
5481.0 !\AUTHOR: !\REF:		
C5H10-1+CH3O<=>C5H91-4+CH3OH	1.450E+011	0.000
4571.0 !\AUTHOR: !\REF:		
C5H10-1+CH3O2<=>C5H91-4+CH3O2H	9.640E+003	2.600
13910.0 !\AUTHOR: !\REF:		
!\SITE: \ALLYLIC_PRIMARY		
C5H10-2+O2<=>C5H91-3+HO2	3.300E+012	0.000
39900.0 !\AUTHOR: !\REF:		
C5H10-2+O<=>C5H91-3+OH	4.410E+005	2.420
3150.0 !\AUTHOR: !\REF:		
C5H10-2+H<=>C5H91-3+H2	1.730E+005	2.500
2492.0 !\AUTHOR: !\REF:		
C5H10-2+OH<=>C5H91-3+H2O	3.120E+006	2.000
-298.0 !\AUTHOR: !\REF:		
C5H10-2+HO2<=>C5H91-3+H2O2	9.639E+003	2.600
13910.0 !\AUTHOR: !\REF:		
C5H10-2+CH3<=>C5H91-3+CH4	2.210E+000	3.500
5675.0 !\AUTHOR: !\REF:		
C5H10-2+CH3O<=>C5H91-3+CH3OH	9.000E+001	2.950
11990.0 !\AUTHOR: !\REF:		
C5H10-2+CH3O2<=>C5H91-3+CH3O2H	9.639E+003	2.600
13910.0 !\AUTHOR: !\REF:		
!\SITE: \ALLYLIC_SECONDARY		
C5H10-1+O2<=>C5H91-3+HO2	2.200E+012	0.000
37220.0 !\AUTHOR: !\REF:		
C5H10-1+O<=>C5H91-3+OH	6.600E+005	2.430
1210.0 !\AUTHOR: !\REF:		
C5H10-1+H<=>C5H91-3+H2	3.376E+005	2.360
207.0 !\AUTHOR: !\REF:		
C5H10-1+OH<=>C5H91-3+H2O	2.764E+004	2.640
-1919.0 !\AUTHOR: !\REF:		
C5H10-1+HO2<=>C5H91-3+H2O2	4.820E+003	2.550
10530.0 !\AUTHOR: !\REF:		
C5H10-1+CH3<=>C5H91-3+CH4	3.690E+000	3.310
4002.0 !\AUTHOR: !\REF:		
C5H10-1+CH3O<=>C5H91-3+CH3OH	4.000E+001	2.900
8609.0 !\AUTHOR: !\REF:		
C5H10-1+CH3O2<=>C5H91-3+CH3O2H	4.820E+003	2.550
10530.0 !\AUTHOR: !\REF:		
C5H10-2+O2<=>C5H92-4+HO2	2.200E+012	0.000
37220.0 !\AUTHOR: !\REF:		
C5H10-2+O<=>C5H92-4+OH	9.900E+005	2.430
1210.0 !\AUTHOR: !\REF:		
C5H10-2+H<=>C5H92-4+H2	3.376E+005	2.360
207.0 !\AUTHOR: !\REF:		
C5H10-2+OH<=>C5H92-4+H2O	2.764E+004	2.640
-1919.0 !\AUTHOR: !\REF:		

C5H10-2+HO2<=>C5H92-4+H2O2 10530.0 !\AUTHOR: !\REF:	4.820E+003	2.550
C5H10-2+CH3<=>C5H92-4+CH4 4002.0 !\AUTHOR: !\REF:	3.690E+000	3.310
C5H10-2+CH3O<=>C5H92-4+CH3OH 8609.0 !\AUTHOR: !\REF:	4.000E+001	2.900
C5H10-2+CH3O2<=>C5H92-4+CH3O2H 10530.0 !\AUTHOR: !\REF:	4.820E+003	2.550

!

!\REACTIONCLASS: \WADDINGTON \EA	\A	\N
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!

C5H10-1+OH<=>C5H10OH12 -782.0 !\AUTHOR: !\REF:	4.750E+012	0.000
C5H10-2+OH<=>C5H10OH23 -782.0 !\AUTHOR: !\REF:	4.750E+012	0.000
C5H10OH-2O2=>NC3H7CHO+CH2O+OH 18860.0 !\AUTHOR: !\REF:	2.500E+010	0.000
C5H10OH23+O2<=>O2C5H10OH23 0.0 !\AUTHOR: !\REF:	2.000E+012	0.000
O2C5H10OH23=>C2H5CHO+CH3CHO+OH 18860.0 !\AUTHOR: !\REF:	2.500E+010	0.000

!

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

!

C4H6+CH3<=>C5H91-3 7800.0 !\AUTHOR: !\REF:	1.000E+011	0.000
C5H81-3+H<=>C5H91-3 2620.0 !\AUTHOR: !\REF:	2.500E+011	0.510
C3H6+C2H3<=>C5H91-4 7800.0 !\AUTHOR: !\REF:	1.000E+011	0.000
C2H4+C3H5-A<=>C5H91-5 7800.0 !\AUTHOR: !\REF:	1.000E+011	0.000
C5H81-3+H<=>C5H92-4 1230.0 !\AUTHOR: !\REF:	4.240E+011	0.510
C2H4+C3H5-S<=>C5H92-5 7800.0 !\AUTHOR: !\REF:	2.000E+011	0.000

!

!\REACTIONCLASS: \PEROXYL_ADDITION \EA	\A	\N
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!

C5H901-3+OH<=>C5H91-3+HO2 15720.0 !\AUTHOR: !\REF:	6.088E+015	-1.070
C5H901-3+CH3O<=>C5H91-3+CH3O2 20480.0 !\AUTHOR: !\REF:	5.946E+017	-1.650
C5H901-3+C2H5O<=>C5H91-3+C2H5O2 18330.0 !\AUTHOR: !\REF:	3.893E+014	-0.720
C5H902-4+OH<=>C5H92-4+HO2 15890.0 !\AUTHOR: !\REF:	7.027E+015	-1.240
C5H902-4+CH3O<=>C5H92-4+CH3O2 20650.0 !\AUTHOR: !\REF:	6.863E+017	-1.820

C5H9O2-4+C2H5O<=>C5H92-4+C2H5O2 4.493E+014 -0.890
18490.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \ALLYLOXY_RADICAL_BETA_SCISSION \A \N
\EA
!

C5H9O1-3<=>C2H3CHO+C2H5 3.131E+019 -1.850
10670.0 !\AUTHOR: !\REF:
C5H9O1-3<=>C2H5CHO+C2H3 1.417E+018 -1.560
23340.0 !\AUTHOR: !\REF:
C5H9O2-4<=>SC3H5CHO+CH3 5.983E+015 -1.130
9941.0 !\AUTHOR: !\REF:
C5H9O2-4<=>CH3CHO+C3H5-S 1.073E+022 -2.660
29650.0 !\AUTHOR: !\REF:

!-----
!\ENDSUBMECH: \C5H10-1\C5H10-2
!-----

!-----

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

!

!\REACTIONCLASS: \E_UNIMOL \A \N
\EA
!

BC5H10<=>C4H72-2+CH3 1.217E+023 -1.926
101400.0 !\AUTHOR: !\REF:
BC5H10<=>IC4H7+CH3 2.610E+019 -1.017
79020.0 !\AUTHOR: !\REF:
!ANALOGY WITH C3H5-A+CH3
C4H71-3+CH3 (+M) <=>CC5H10 (+M) 1.000E+014 -0.320
-262.3
LOW/ 3.910E+060 -12.810
6250.0/
TROE/ 1.040E-001 1.606E+003 6.000E+004 6.118E+003/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/
!

!\REACTIONCLASS: \E_R_ABSTRACTION \A \N
\EA
!

!\SITE: \PRIMARY
CC5H10+H<=>CC5H9-A+H2 3.900E+006 2.400
4471.0 !\AUTHOR: !\REF:
CC5H10+OH<=>CC5H9-A+H2O 1.400E+008 1.610
-35.0 !\AUTHOR: !\REF:
CC5H10+HO2<=>CC5H9-A+H2O2 2.892E+004 2.600
13910.0 !\AUTHOR: !\REF:

CC5H10+CH3<=>CC5H9-A+CH4	4.530E+000	3.460
5481.0 !\AUTHOR: !\REF:		
CC5H10+CH3O<=>CC5H9-A+CH3OH	4.350E+011	0.000
4571.0 !\AUTHOR: !\REF:		
CC5H10+CH3O2<=>CC5H9-A+CH3O2H	2.892E+004	2.600
13910.0 !\AUTHOR: !\REF:		
!\SITE: \ALLYLIC_PRIMARY		
BC5H10+H<=>AC5H9-C+H2	3.460E+005	2.500
2492.0 !\AUTHOR: !\REF:		
BC5H10+H<=>CC5H9-B+H2	1.730E+005	2.500
2492.0 !\AUTHOR: !\REF:		
BC5H10+OH<=>AC5H9-C+H2O	6.240E+006	2.000
-298.0 !\AUTHOR: !\REF:		
BC5H10+OH<=>CC5H9-B+H2O	3.120E+006	2.000
-298.0 !\AUTHOR: !\REF:		
BC5H10+HO2<=>AC5H9-C+H2O2	1.928E+004	2.600
13910.0 !\AUTHOR: !\REF:		
BC5H10+HO2<=>CC5H9-B+H2O2	9.639E+003	2.600
13910.0 !\AUTHOR: !\REF:		
BC5H10+CH3<=>AC5H9-C+CH4	4.420E+000	3.500
5675.0 !\AUTHOR: !\REF:		
BC5H10+CH3<=>CC5H9-B+CH4	2.210E+000	3.500
5675.0 !\AUTHOR: !\REF:		
BC5H10+CH3O<=>AC5H9-C+CH3OH	1.800E+002	2.950
11990.0 !\AUTHOR: !\REF:		
BC5H10+CH3O<=>CC5H9-B+CH3OH	9.000E+001	2.950
11990.0 !\AUTHOR: !\REF:		
BC5H10+CH3O2<=>AC5H9-C+CH3O2H	1.928E+004	2.600
13910.0 !\AUTHOR: !\REF:		
BC5H10+CH3O2<=>CC5H9-B+CH3O2H	9.639E+003	2.600
13910.0 !\AUTHOR: !\REF:		
!\SITE: \ALLYLIC_TERTIARY		
CC5H10+H<=>CC5H9-B+H2	2.650E+006	2.200
0.0 !\AUTHOR: !\REF:		
CC5H10+OH<=>CC5H9-B+H2O	6.140E+002	3.200
-3500.0 !\AUTHOR: !\REF:		
CC5H10+HO2<=>CC5H9-B+H2O2	1.810E+003	2.500
7154.0 !\AUTHOR: !\REF:		
CC5H10+CH3<=>CC5H9-B+CH4	4.613E+000	3.100
2330.0 !\AUTHOR: !\REF:		
CC5H10+CH3O<=>CC5H9-B+CH3OH	1.000E+001	2.850
5231.0 !\AUTHOR: !\REF:		
CC5H10+CH3O2<=>CC5H9-B+CH3O2H	1.810E+003	2.500
7154.0 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \WADDINGTON
 \EA
 !

BC5H10+OH<=>BC5H10OH	1.000E+012	0.000
-1042.0 !\AUTHOR: !\REF:		
BC5H10OH+O2<=>BO2C5H10OH	2.000E+012	0.000
0.0 !\AUTHOR: !\REF:		
BO2C5H10OH=>CH3COCH3+CH3CHO+OH	2.500E+010	0.000
18860.0 !\AUTHOR: !\REF:		
CC5H10+OH<=>CC5H10OH	1.000E+012	0.000
-1042.0 !\AUTHOR: !\REF:		

CC5H10OH+O2<=>CO2C5H10OH	2.000E+012	0.000
0.0 !\AUTHOR: !\REF:		
CO2C5H10OH=>IC3H7CHO+CH2O+OH	2.500E+010	0.000
18860.0 !\AUTHOR: !\REF:		
BC5H10+OH<=>IC3H7+CH3CHO	2.000E+010	0.000
4000.0 !\AUTHOR: !\REF:		
CC5H10+OH<=>IC4H9+CH2O	2.000E+010	0.000
4000.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \E_RADICAL_BETA_SCISSION \A \N
 \EA

!

!

!\REACTIONCLASS: \PEROXYL_ADDITION \A \N
 \EA

!

AC5H9-A2+HO2<=>AC5H9O-A2+OH	9.640E+012	0.000
0.0 !\AUTHOR: !\REF:		
AC5H9-A2+CH3O2<=>AC5H9O-A2+CH3O	9.640E+012	0.000
0.0 !\AUTHOR: !\REF:		
AC5H9-A2+C2H5O2<=>AC5H9O-A2+C2H5O	9.640E+012	0.000
0.0 !\AUTHOR: !\REF:		
CC5H9-B+HO2<=>CC5H9O-B+OH	7.000E+012	0.000
-1000.0		
CC5H9-B+CH3O2<=>CC5H9O-B+CH3O	7.000E+012	0.000
-1000.0		
CC5H9-B+C2H5O2<=>CC5H9O-B+C2H5O	9.640E+012	0.000
0.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \ALLYLOXY_RADICAL_BETA_SCISSION \A \N
 \EA

!

AC5H9O-A2<=>C4H71-2+CH2O	9.210E+017	-1.430
30330.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \ALLYLOXY_RADICAL_BETA_SCISSION \A \N
 \EA

!

AC5H9-D<=>AC5H9-A2	1.113E+012	0.000
31700.0 !\AUTHOR: !\REF:		

!

!\ENDSUBMECH: \BC5H10\CC5H10

!

!\SUBMECH: \AC5H10

!

!

```

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

```

AC5H10<=>C3H5-T+C2H5                    8.922E+24 -
2.409 100500.0 !\AUTHOR:
IC4H7+CH3(+M)<=>AC5H10(+M)              1.500E+014  -0.320
-262.3          !\AUTHOR:
LOW/                                         5.865E+060  -12.810
6250.0/
TROE/ 1.040E-001 1.606E+003 6.000E+004 6.118E+003/
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/
0.70/
!
```

```

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

```

AC5H10+H<=>AC5H9-A2+H2                    1.730E+05
2.500 2492.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+O<=>AC5H9-A2+OH                    3.700E+05
2.56  -1.130E+03 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+OH<=>AC5H9-A2+H2O                  3.120E+06
2.000 -298.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+HO2<=>AC5H9-A2+H2O2                9.639E+03
2.600 13910.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3<=>AC5H9-A2+CH4                 2.210E+00
3.500 5675.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3O2<=>AC5H9-A2+CH3O2H            9.639E+03
2.600 13910.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3O<=>AC5H9-A2+CH3OH              9.000E+01
2.950 11990.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH

AC5H10+H<=>AC5H9-C+H2                    3.376E+05
2.360 207.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+OH<=>AC5H9-C+H2O                   2.764E+04
2.640 -1919.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+HO2<=>AC5H9-C+H2O2                 4.820E+03
2.550 10530.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3<=>AC5H9-C+CH4                  3.690E+00
3.310 4002.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3O2<=>AC5H9-C+CH3O2H             4.820E+03
2.550 10530.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3O<=>AC5H9-C+CH3OH               4.000E+01
2.900 8609.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+H<=>AC5H9-D+H2                    1.950E+06
2.400 4471.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+OH<=>AC5H9-D+H2O                   7.010E+07
1.610 -35.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3<=>AC5H9-D+CH4                  2.270E+00
3.460 5481.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+HO2<=>AC5H9-D+H2O2                 1.450E+04
2.600 13910.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+CH3O<=>AC5H9-D+CH3OH               2.180E+11
0.000 4571.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
```

AC5H10+CH3O2<=>AC5H9-D+CH3O2H 1.450E+04
2.600 13910.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A
\N \EA
!

AC5H9-A2<=>C3H4-A+C2H5 1.983E+20 -1.63
5.924E+04 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
B13DE2M+H<=>AC5H9-C 4.000E+013 0.000
1300.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
C4H612+CH3<=>AC5H9-C 1.76E+04 2.48
6130 !\AUTHOR: !\REF:H.J. CURRAN, INT. J. CHEM. KIN. 38 (4) (2006)
250-275. EXTERNAL CH3 ATOM ADDITION TO PROPENE
B13DE2M+H<=>AC5H9-D 2.50E+11 0.51
2620 !\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 1.22E12 0.64
29370 !\AUTHOR: !\REF:CURRAN IJCK, 2006, 38, 250-275.
!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA
!

AC5H10+OH<=>SC4H9+CH2O 2.000E+10 0.000
4000.0 !\AUTHOR:
AC5H10+OH<=>AC5H10OH 1.000E+012 0.000
-1042.0 !\AUTHOR:
AC5H10OH+O2<=>AO2C5H10OH 2.000E+012 0.000
0.0 !\AUTHOR:
AO2C5H10OH=>C2H5COCH3+CH2O+OH 2.500E+010 0.000
18860.0 !\AUTHOR:
AC5H10+O<=>SC4H9+HCO 7.230E+05 2.340
-1050.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+O<=>IC3H7+CH3CO 7.230E+05 2.340
-1050.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
AC5H10+O<=>IC4H9+HCO 7.230E+05 2.340
-1050.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH
!

!\REACTIONCLASS: \R_RO2 \A \N
\EA
!

AC5H9-C+HO2<=>AC5H9O-C+OH 7.000E+012 0.000
-1000.0 !\AUTHOR:
AC5H9-C+CH3O2<=>AC5H9O-C+CH3O 7.000E+012
0.000 -1000.0 !\AUTHOR:
AC5H9-C+C2H5O2<=>AC5H9O-C+C2H5O 9.640E+012 0.000
0.0 !\AUTHOR:
CH3CHO+C3H5-T<=>AC5H9O-C 9.45E+02 2.67
6850 !\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 7.000E+012
0.000 -1000.0 !\AUTHOR: !\REF:FROM LLNL C8-C16 N-ALKANES MECH

AC5H9-C+CH3O2<=>B2E2M1OJ+CH3O 7.000E+012
0.000 -1000.0 !\AUTHOR: !\REF: FROM LLNL C8-C16 N-ALKANES MECH
CH2O+C4H72-2<=>B2E2M1OJ 8.80E+03 2.48
6.1E+03 !\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: \AC5H10

!-----

!-----

!\SUBMECH: \B13DE2M

!-----

!-----

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!-----

C2H3+C3H5-T<=>B13DE2M 8E+12 0.0 0.0 !\AUTHOR:

!\REF:

H+B13DE2MJ<=>B13DE2M 1E+14 0.0 0.0 !\AUTHOR:

!\REF:

!-----

!\REACTIONCLASS: \RH_R_ABSTRACTION \A \N

\EA

!-----

B13DE2M+H<=>B13DE2MJ+H2 3.644E+005 2.455

4361.2 !\AUTHOR: !\REF:

B13DE2M+O2<=>B13DE2MJ+HO2 5.960E+019 -1.670

46192.1 !\AUTHOR: !\REF:

B13DE2M+OH<=>B13DE2MJ+H2O 4.460E+006 2.072

1050.8 !\AUTHOR: !\REF:

B13DE2M+HO2<=>B13DE2MJ+H2O2 3.070E-002 4.403

13547.2 !\AUTHOR: !\REF:

B13DE2M+CH3<=>B13DE2MJ+CH4 2.210E+000 3.500

5675.0 !\AUTHOR: !\REF:

B13DE2M+CH3O2<=>B13DE2MJ+CH3O2H 7.680E-002 4.403

13547.2 !\AUTHOR: !\REF:

!-----

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N

\EA

!-----

C2H3+C3H4-A<=>B13DE2MJ 9.45E+02 2.67 6850 !\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


```

!
-----
TC4H8CHO+O2<=>O2C4H8CHO                2.000E+012    0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
O2C4H8CHO<=>O2HC4H8CO                    2.160E+011    0.000
15360.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
IC4H8O2H-T+CO<=>O2HC4H8CO                1.500E+011    0.000
4809.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
!-----
-----
!\ENDSUBMECH:  \TC4H8CHO
!-----
-----
!\SUBMECH:  \PC4H8CHO-1\PC4H8CHO-2\PC4H8CHO-3
!-----
-----
!
-----
!\REACTIONCLASS:  \1. F_UNIMOLECULAR_DECOMPOSITION  \A          \N
\EA
!
-----
C2H5+C2H3CHO<=>PC4H8CHO-1                1.000E+11     0.0000
7800.0 !\AUTHOR: !\REF:
CH3+AC3H5CHO<=>PC4H8CHO-2                1.000E+11     0.0000
7800.0 !\AUTHOR: !\REF:
C4H8-1+HCO<=>PC4H8CHO-2                  1.000E+11     0.0000
6000.0 !\AUTHOR: !\REF:
C3H6+CH2CHO<=>PC4H8CHO-3                 1.000E+11     0.0000
7800.0 !\AUTHOR: !\REF:
C2H4+CH2CH2CHO<=>PC4H8CHO-4              1.000E+11     0.0000
7800.0 !\AUTHOR: !\REF:
C3H5-A+HCO<=>AC3H5CHO                    1.810E+13     0.0000
0.0 !\AUTHOR: !\REF:
!
-----
!\REACTIONCLASS:  \2. F_H_ABSTRACTION          \A          \N
\EA
!
-----
PC4H9CHO+O2<=>PC4H9CO+HO2                3.010E+013
0.000 39150.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+O<=>PC4H9CO+OH                  5.940E+012
0.000 1868.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+H<=>PC4H9CO+H2                  1.310E+005
2.580 1220.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+OH<=>PC4H9CO+H2O                3.370E+012
0.000 -619.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+HO2<=>PC4H9CO+H2O2              3.010E+012
0.000 11920.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+CH3<=>PC4H9CO+CH4               7.080E-004
4.580 1966.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+CH3O2<=>PC4H9CO+CH3O2H          3.010E+012
0.000 11920.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO
PC4H9CHO+OH<=>PC4H8CHO-1+H2O              5.520E+02     3.1200
-1176.0 !\AUTHOR: !\REF:

```

PC4H9CHO+OH<=>PC4H8CHO-2+H2O	4.680E+07	1.6100
-35.0 !\AUTHOR: !\REF:		
PC4H9CHO+OH<=>PC4H8CHO-3+H2O	4.680E+07	1.6100
-35.0 !\AUTHOR: !\REF:		
PC4H9CHO+OH<=>PC4H8CHO-4+H2O	5.280E+09	0.9700
1586.0 !\AUTHOR: !\REF:		
PC4H9CHO+HO2<=>PC4H8CHO-1+H2O2	3.440E+12	0.0500
17880.0 !\AUTHOR: !\REF:		
PC4H9CHO+HO2<=>PC4H8CHO-2+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
PC4H9CHO+HO2<=>PC4H8CHO-3+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
PC4H9CHO+HO2<=>PC4H8CHO-4+H2O2	2.379E+04	2.5500
16490.0 !\AUTHOR: !\REF:		
PC4H9CHO+CH3O2<=>PC4H8CHO-1+CH3O2H	3.440E+12	0.0500
17880.0 !\AUTHOR: !\REF:		
PC4H9CHO+CH3O2<=>PC4H8CHO-2+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
PC4H9CHO+CH3O2<=>PC4H8CHO-3+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
PC4H9CHO+CH3O2<=>PC4H8CHO-4+CH3O2H	2.379E+04	2.5500
16490.0 !\AUTHOR: !\REF:		

!

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

!

PC4H9CO<=>NC3H7+CH2CO	1.000E+11	0.0000
9600.0 !\AUTHOR: !\REF:		
PC4H9CO<=>PC4H9+CO	5.780E+14	0.000
16843.5 !\AUTHOR: !\REF: J. M. SIMMIE, J. PHYS. CHEM. A, 116, 2012, 4528-4538		

!

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

!

PC4H8CHO-1+O2<=>PC4H8CHO-1O2	1.000E+011	0.000
0.0 !\AUTHOR: !\REF: ESTIMATED BY		
PC4H8CHO-2+O2<=>PC4H8CHO-2O2	3.487E+014	-0.816
-536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74		
PC4H8CHO-3+O2<=>PC4H8CHO-3O2	3.487E+014	-0.816
-536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74		
PC4H8CHO-4+O2<=>PC4H8CHO-4O2	6.865E+016	-1.627
198.7 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74		

!

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

!

PC4H8CHO-1O2<=>C4H7CHO-2+HO2	2.885E+009	0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527		

PC4H8CHO-2O2<=>C4H7CHO-2+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
PC4H8CHO-2O2<=>C4H7CHO-3+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
PC4H8CHO-3O2<=>C4H7CHO-3+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
PC4H8CHO-3O2<=>C4H7CHO-4+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
PC4H8CHO-4O2<=>C4H7CHO-4+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527

!

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

!

C4H7CHO-2+OH=>C4H7-1+CO+H2O 1.700E+012 0.000
-619.0 !\AUTHOR: !\REF: M. PELUCCHI, K. P. SOMERS, K. YASUNAGA, U. BURKE,
A. FRASSOLDATI, E. RANZI, H. J. CURRAN, T. FARAVELLI, COMBUST. FLAME,
2015, 162, 265;\S286
C4H7CHO-3+OH=>C4H7-2+CO+H2O 1.700E+012 0.000
-619.0 !\AUTHOR: !\REF: M. PELUCCHI, K. P. SOMERS, K. YASUNAGA, U. BURKE,
A. FRASSOLDATI, E. RANZI, H. J. CURRAN, T. FARAVELLI, COMBUST. FLAME,
2015, 162, 265;\S286
C4H7CHO-3+OH=>C4H6+HCO+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556
C4H7CHO-4+OH=>C4H7-4+CO+H2O 1.700E+012 0.000
-619.0 !\AUTHOR: !\REF: M. PELUCCHI, K. P. SOMERS, K. YASUNAGA, U. BURKE,
A. FRASSOLDATI, E. RANZI, H. J. CURRAN, T. FARAVELLI, COMBUST. FLAME,
2015, 162, 265;\S286
C4H7CHO-4+OH=>C4H6+HCO+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556

!

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

!

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

!

C3H5O+C2H4<=>C5H9O12-5 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
CH2CH2CHO+C2H4<=>C5H9O13-5 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
CH2O+C4H7-4<=>C5H9O14-5 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
C2H3CHO+C2H5<=>C5H9O23-1 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:

CH3CHCHO+C2H4<=>C5H9O23-5	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
CH3CHO+C3H5-A<=>C5H9O24-1	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
!-----		
!-----		
!\ENDSUBMECH: \C5H9O12-5\C5H9O13-5\C5H9O14-5\C5H9O23-1\C5H9O23-5\C5H9O24-1		
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!-----		
!-----		
!\SUBMECH: \NC3H7COCH3\C2H5COC2H5		
!-----		
!-----		
!		

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

CH3CO+NC3H7<=>NC3H7COCH3	2.000E+013	0.000
0.0 !\AUTHOR: !\REF:		
NC3H7COCH3+OH<=>NC3H7COCH2+H2O	3.990E+002	3.080
944.0 !\AUTHOR: !\REF: C. -W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011, 11175-11192		
NC3H7COCH3+HO2<=>NC3H7COCH2+H2O2	4.140E-002	4.070
16253.3 !\AUTHOR: !\REF: J. MENDES, C. -W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525		
NC3H7COCH3+OH<=>CH3CH2CHCOCH3+H2O	2.360E+002	3.150
3050.4 !\AUTHOR: !\REF: C. -W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011, 11175-11192		
NC3H7COCH3+HO2<=>CH3CH2CHCOCH3+H2O2	3.560E-001	3.690
13099.6 !\AUTHOR: !\REF: J. MENDES, C. -W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525		
NC3H7COCH3+OH<=>CH3CHCH2COCH3+H2O	4.140E+002	3.000
2440.0 !\AUTHOR: !\REF: ESTIMATED BY		
NC3H7COCH3+HO2<=>CH3CHCH2COCH3+H2O2	1.150E-003	4.430
11364.8 !\AUTHOR: !\REF: J. MENDES, C. -W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525		
NC3H7COCH3+OH<=>CH2CH2CH2COCH3+H2O	2.732E+007	1.813
868.4 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 113, 2009, 5047-5060		
NC3H7COCH3+HO2<=>CH2CH2CH2COCH3+H2O2	4.440E-001	3.880
15814.1 !\AUTHOR: !\REF: J. MENDES, C. -W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525		
C2H5COC2H5+OH<=>CH2CH2COC2H5+H2O	2.700E+000	3.810
2899.3 !\AUTHOR: !\REF: C. -W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011, 11175-11192		
C2H5COC2H5+HO2<=>CH2CH2COC2H5+H2O2	6.180E-005	4.910
14081.3 !\AUTHOR: !\REF: J. MENDES, C. -W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525		
C2H5COC2H5+OH<=>CH3CHCOC2H5+H2O	2.360E+002	3.150
3050.4 !\AUTHOR: !\REF: C. -W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011, 11175-11192		
C2H5COC2H5+HO2<=>CH3CHCOC2H5+H2O2	8.420E-002	3.930
13389.8 !\AUTHOR: !\REF: J. MENDES, C. -W. ZHOU, H. J. CURRAN, J. PHYS. CHEM. A, 117, 2013, 4515-4525		

!\REACTIONCLASS: \RADICAL_BETA_SCISSION \EA	\A	\N
NC3H7+CH2CO<=>NC3H7COCH2 8960.0 !\AUTHOR: !\REF: FROM PRAJACTA PARAB'S CALCULATIONS FOR KETENE + METHYL = ACETONYL RADICAL	3.630E+003	2.430
C2H3COCH3+CH3<=>CH3CH2CHCOCH3 6130.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275	1.760E+004	2.480
C3H6+CH3CO<=>CH3CHCH2COCH3 6130.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275	8.800E+003	2.480
C2H4+CH3COCH2<=>CH2CH2CH2COCH3 6130.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275	1.320E+004	2.480
C2H4+C2H5CO<=>CH2CH2COC2H5 6130.0 !\AUTHOR: !\REF: H. J. CURRAN, INT. J. CHEM. KINET., 38, 2006, 250-275	8.800E+003	2.480
CH3CHCO+C2H5<=>CH3CHCOC2H5 8960.0 !\AUTHOR: !\REF: FROM PRAJACTA PARAB'S CALCULATIONS FOR KETENE + METHYL = ACETONYL RADICAL	3.630E+003	2.430
!\REACTIONCLASS: \R+O2=RO2 \EA	\A	\N
CH3CH2CHCOCH3+O2<=>NC52ONEO2-3 0.0 !\AUTHOR: !\REF: ESTIMATED BY	1.000E+011	0.000
CH3CHCH2COCH3+O2<=>NC52ONEO2-4 -536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74	3.487E+014	-0.816
CH2CH2CH2COCH3+O2<=>NC52ONEO2-5 198.7 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74	6.865E+016	-1.627
CH2CH2COC2H5+O2<=>NC53ONEO2-1 198.7 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74	6.865E+016	-1.627
CH3CHCOC2H5+O2<=>NC53ONEO2-2 0.0 !\AUTHOR: !\REF: ESTIMATED BY	1.000E+011	0.000
!\REACTIONCLASS: \RO2=E+HO2 \EA	\A	\N
NC52ONEO2-3<=>NC52ONE-3+HO2 29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527	2.885E+009	0.930
NC52ONEO2-4<=>NC52ONE-3+HO2 29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527	2.885E+009	0.930
NC52ONEO2-4<=>NC52ONE-4+HO2 29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527	2.885E+009	0.930
NC52ONEO2-5<=>NC52ONE-4+HO2 29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527	2.885E+009	0.930

NC53ONEO2-1<=>NC53ONE-1+HO2	2.885E+009	0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527		
NC53ONEO2-2<=>NC53ONE-1+HO2	2.885E+009	0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J. CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527		

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

!

NC52ONE-3+OH=>CH2CO+C3H5-S+H2O	4.460E+006	2.072
1050.8 !\AUTHOR: !\REF: ANALOGY TO C3H6+OH<=>C3H5-A+H2O		
NC52ONE-4+OH=>CH2CO+C3H5-A+H2O	1.010E+006	2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115, 2549;§C2556		
NC53ONE-1+OH=>CH3CHCO+C2H3+H2O	2.360E+002	3.150
3050.4 !\AUTHOR: !\REF: C. -W. ZHOU, J. M. SIMMIE, H. J. CURRAN, PHYS. CHEM. CHEM. PHYS., 13, 2011, 11175-11192		

!

!\ENDSUBMECH: \NC3H7COCH3\C2H5COC2H5

!

!\SUBMECH: \NC5H11OH

!

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

!

NC5H11OH+OH<=>C5H10OH15+H2O	5.280E+09	0.970
1590.0		
NC5H11OH+HO2<=>C5H10OH15+H2O2	2.040E+01	3.590
17160.0		
NC5H11OH+OH<=>C5H10OH14+H2O	4.670E+07	1.610
-35.0		
NC5H11OH+HO2<=>C5H10OH14+H2O2	6.320E+01	3.370
13720.0		
NC5H11OH+OH<=>C5H10OH13+H2O	1.141E+03	2.870
-2926.0		
NC5H11OH+HO2<=>C5H10OH13+H2O2	2.760E-04	4.760
11850.0		
NC5H11OH+OH<=>C5H10OH12+H2O	1.540E+00	3.700
-3736.0		
NC5H11OH+HO2<=>C5H10OH12+H2O2	7.510E-03	4.520
14710.0		
NC5H11OH+OH<=>C5H10OH11+H2O	3.610E+03	2.890
-2291.0		
NC5H11OH+HO2<=>C5H10OH11+H2O2	3.500E-05	5.260
8268.0		
NC5H11OH+OH<=>C5H11O-1+H2O	5.880E+02	2.820
-585.0		

NC5H11OH+HO2<=>C5H11O-1+H2O2 6.470E-07 5.300
10530.0
!

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

C5H10OH15=>C2H4+C2H4+CH2OH 5.168E+13 0.103
29083.8
C3H6+PC2H4OH<=>C5H10OH14 8.800E+03 2.480
6130.0
C4H71-4OH+CH3<=>C5H10OH13 1.760E+04 2.480
6130.0
C4H8-1+CH2OH<=>C5H10OH13 8.800E+03 2.480
6130.0
C3H5OH+C2H5<=>C5H10OH12 8.800E+03 2.480
6130.0
C2H3OH+NC3H7<=>C5H10OH11 8.800E+03 2.480
6130.0
!

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

C5H10OH11+O2<=>C5H10OH-1O2 5.000E+011 0.000
0.0 !\AUTHOR: !\REF: ESTIMATED BY
C5H10OH12+O2<=>C5H10OH-2O2 3.487E+014 -0.816
-536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
C5H10OH13+O2<=>C5H10OH-3O2 3.487E+014 -0.816
-536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
C5H10OH14+O2<=>C5H10OH-4O2 3.487E+014 -0.816
-536.5 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
C5H10OH15+O2<=>C5H10OH-5O2 6.865E+016 -1.627
198.7 !\AUTHOR: !\REF: A. MIYOSHI, INT. J. CHEM. KIN., 44, 2012, 59-74
!

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

C5H10OH-1O2<=>C5H9OH1-1+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
C5H10OH-2O2<=>C5H9OH1-1+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
C5H10OH-2O2<=>C5H9OH1-2+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
C5H10OH-3O2<=>C5H9OH1-2+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
C5H10OH-3O2<=>C5H9OH1-3+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527

C5H10OH-4O2<=>C5H9OH1-3+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
C5H10OH-4O2<=>C5H9OH1-4+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
C5H10OH-5O2<=>C5H9OH1-4+HO2 2.885E+009 0.930
29800.0 !\AUTHOR: !\REF: J. BUGLER, K. P. SOMERS, E. J. SILKE, H. J.
CURRAN, J. PHYS. CHEM. A, 119, 2015, 7510-7527
!

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

C5H9OH1-1+OH=>C4H7CHO-2+H+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556
C5H9OH1-2+OH=>C4H7CHO-2+H+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556
C5H9OH1-2+OH=>C5H81-3+OH+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556
C5H9OH1-3+OH=>C5H81-3+OH+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556
C5H9OH1-4+OH=>C4H6+CH2OH+H2O 1.010E+006 2.200
-437.2 !\AUTHOR: !\REF: S. S. VASU ET AL. J. PHYS. CHEM. A, 2011, 115,
2549;\S2556

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!\ENDSUBMECH: \NC5H11OH
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!\END_KINETICS_MODULE: \C5

!++++
++++
++++
!\KINETICS_MODULE: \C6

!\MODSUBMECHS: \NC6H14 \C6H12-1 \C6H12-2 \C6H12-3 \NC5H11CHO \C6H10-15

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!\SUBMECH: \NC6H14
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!\REACTIONCLASS: \1. F_UNIMOLECULAR_DECOMPOSITION \A \N
 \EA !REF:CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
 MILLER. COMBUST. FLAME (2013)
 !

NC6H14<=>CH3+C5H11-1	1.450E+51	-9.9800
105372.0 !\AUTHOR: !\REF:		
PLOG / 1.000E-002 1.92E+94 -23.05 124349. /		
PLOG / 1.000E-001 7.10E+83 -19.75 121206. /		
PLOG / 1.000E+000 3.98E+68 -15.14 114401. /		
PLOG / 2.000E+000 2.52E+63 -13.59 111809. /		
PLOG / 5.000E+000 2.51E+56 -11.52 108177. /		
PLOG / 1.000E+001 1.45E+51 -9.98 105372. /		
PLOG / 2.000E+001 1.30E+46 -8.50 102608. /		
PLOG / 5.000E+001 8.78E+39 -6.70 99154. /		
NC6H14<=>C2H5+PC4H9	4.380E+52	-10.2100
103971.0 !\AUTHOR: !\REF:		
PLOG / 1.000E-002 3.84E+96 -23.49 123675. /		
PLOG / 1.000E-001 3.95E+85 -20.04 120116. /		
PLOG / 1.000E+000 1.16E+70 -15.35 113057. /		
PLOG / 2.000E+000 6.94E+64 -13.80 110428. /		
PLOG / 5.000E+000 7.03E+57 -11.74 106773. /		
PLOG / 1.000E+001 4.38E+52 -10.21 103971. /		
PLOG / 2.000E+001 4.45E+47 -8.74 101224. /		
PLOG / 5.000E+001 3.73E+41 -6.97 97811. /		
NC6H14<=>NC3H7+NC3H7	3.000E+54	-10.7400
104866.0 !\AUTHOR: !\REF:		
PLOG / 1.000E-002 8.73E+97 -23.89 124152. /		
PLOG / 1.000E-001 1.93E+87 -20.53 120839. /		
PLOG / 1.000E+000 8.22E+71 -15.89 113924. /		
PLOG / 2.000E+000 5.07E+66 -14.34 111315. /		
PLOG / 5.000E+000 5.06E+59 -12.27 107672. /		
PLOG / 1.000E+001 3.00E+54 -10.74 104866. /		
PLOG / 2.000E+001 2.82E+49 -9.26 102108. /		
PLOG / 5.000E+001 2.07E+43 -7.47 98669. /		
NC6H14<=>C6H13-1+H	9.880E+51	-10.5100
119684.0 !\AUTHOR: !\REF:		
PLOG / 1.000E-002 1.14E+82 -20.07 128443. /		
PLOG / 1.000E-001 4.84E+78 -18.72 130156. /		
PLOG / 1.000E+000 1.57E+68 -15.39 127126. /		
PLOG / 2.000E+000 5.74E+63 -14.04 125268. /		
PLOG / 5.000E+000 1.75E+57 -12.08 122267. /		
PLOG / 1.000E+001 9.88E+51 -10.51 119684. /		
PLOG / 2.000E+001 4.44E+46 -8.93 116936. /		
PLOG / 5.000E+001 5.14E+39 -6.89 113232. /		
NC6H14<=>C6H13-2+H	3.070E+51	-10.3500
115970.0 !\AUTHOR: !\REF:		
PLOG / 1.000E-002 7.12E+85 -21.09 127902. /		
PLOG / 1.000E-001 2.57E+80 -19.16 128267. /		
PLOG / 1.000E+000 2.05E+68 -15.39 124032. /		
PLOG / 2.000E+000 3.71E+63 -13.95 121912. /		
PLOG / 5.000E+000 6.39E+56 -11.93 118663. /		
PLOG / 1.000E+001 3.07E+51 -10.35 115970. /		
PLOG / 2.000E+001 1.46E+46 -8.78 113177. /		
PLOG / 5.000E+001 2.41E+39 -6.79 109502. /		
NC6H14<=>C6H13-3+H	3.070E+51	-10.3500
115970.0 !\AUTHOR: !\REF:		
PLOG / 1.000E-002 7.12E+85 -21.09 127902. /		

PLOG / 1.000E-001 2.57E+80 -19.16 128267. /
PLOG / 1.000E+000 2.05E+68 -15.39 124032. /
PLOG / 2.000E+000 3.71E+63 -13.95 121912. /
PLOG / 5.000E+000 6.39E+56 -11.93 118663. /
PLOG / 1.000E+001 3.07E+51 -10.35 115970. /
PLOG / 2.000E+001 1.46E+46 -8.78 113177. /
PLOG / 5.000E+001 2.41E+39 -6.79 109502. /

!

!\REACTIONCLASS: \2. F_H_ABSTRACTION	\A	\N
\EA !REF:ANOLOGY TO NC5H12		

NC6H14+H<=>C6H13-1+H2	3.490E+05	2.7000
6450.0 !\AUTHOR: !\REF:		
NC6H14+H<=>C6H13-2+H2	2.600E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
NC6H14+H<=>C6H13-3+H2	2.600E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
NC6H14+O<=>C6H13-1+OH	1.130E+14	0.0000
7850.0 !\AUTHOR: !\REF:		
NC6H14+O<=>C6H13-2+OH	5.620E+13	0.0000
5200.0 !\AUTHOR: !\REF:		
NC6H14+O<=>C6H13-3+OH	5.620E+13	0.0000
5200.0 !\AUTHOR: !\REF:		
NC6H14+OH<=>C6H13-1+H2O	2.731E+07	1.8130
818.1 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC6H14+OH<=>C6H13-2+H2O	1.410E+10	0.9350
475.5 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC6H14+OH<=>C6H13-3+H2O	1.144E+07	1.8110
-956.6 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC6H14+O2<=>C6H13-1+HO2	4.200E+13	0.0000
52800.0 !\AUTHOR: !\REF:		
NC6H14+O2<=>C6H13-2+HO2	2.800E+13	0.0000
50160.0 !\AUTHOR: !\REF:		
NC6H14+O2<=>C6H13-3+HO2	2.800E+13	0.0000
50160.0 !\AUTHOR: !\REF:		
NC6H14+HO2<=>C6H13-1+H2O2	4.080E+01	3.5900
17160.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC6H14+HO2<=>C6H13-2+H2O2	1.264E+02	3.3700
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC6H14+HO2<=>C6H13-3+H2O2	1.264E+02	3.3700
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC6H14+CH3<=>C6H13-1+CH4	9.040E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
NC6H14+CH3<=>C6H13-2+CH4	1.680E+05	2.1000
7574.0 !\AUTHOR: !\REF:		
NC6H14+CH3<=>C6H13-3+CH4	1.680E+05	2.1000
7574.0 !\AUTHOR: !\REF:		
NC6H14+CH3O<=>C6H13-1+CH3OH	3.000E+11	0.0000
7000.0 !\AUTHOR: !\REF:		

NC6H14+CH3O<=>C6H13-2+CH3OH	2.200E+11	0.0000
5000.0 !\AUTHOR: !\REF:		
NC6H14+CH3O<=>C6H13-3+CH3OH	2.200E+11	0.0000
5000.0 !\AUTHOR: !\REF:		
NC6H14+CH3O2<=>C6H13-1+CH3O2H	1.440E+01	3.7000
16800.0 !\AUTHOR: !\REF:		
NC6H14+CH3O2<=>C6H13-2+CH3O2H	1.050E+02	3.4900
13400.0 !\AUTHOR: !\REF:		
NC6H14+CH3O2<=>C6H13-3+CH3O2H	1.050E+02	3.4900
13400.0 !\AUTHOR: !\REF:		
NC6H14+O2CHO<=>C6H13-1+HO2CHO	1.440E+01	3.7000
16800.0 !\AUTHOR: !\REF:		
NC6H14+O2CHO<=>C6H13-2+HO2CHO	1.050E+02	3.4900
13400.0 !\AUTHOR: !\REF:		
NC6H14+O2CHO<=>C6H13-3+HO2CHO	1.050E+02	3.4900
13400.0 !\AUTHOR: !\REF:		
NC6H14+C2H3<=>C6H13-1+C2H4	1.000E+12	0.0000
18000.0 !\AUTHOR: !\REF:		
NC6H14+C2H3<=>C6H13-2+C2H4	8.000E+11	0.0000
16800.0 !\AUTHOR: !\REF:		
NC6H14+C2H3<=>C6H13-3+C2H4	8.000E+11	0.0000
16800.0 !\AUTHOR: !\REF:		
NC6H14+C2H5<=>C6H13-1+C2H6	1.000E+11	0.0000
13400.0 !\AUTHOR: !\REF:		
NC6H14+C2H5<=>C6H13-2+C2H6	1.000E+11	0.0000
10400.0 !\AUTHOR: !\REF:		
NC6H14+C2H5<=>C6H13-3+C2H6	1.000E+11	0.0000
10400.0 !\AUTHOR: !\REF:		
!		

!\REACTIONCLASS: \3. R_DECOMPOSITION \A \N
\EA !REF:W. Tsang, J. A. Walker, and J. A. Manion, Proc. Combust.
Inst., 31, (2007) 141-148.
!

C6H13-1<=>C2H4+PC4H9	1.023E+12	0.3000
27276.3 !\AUTHOR: !\REF:		
C6H13-2<=>C3H6+NC3H7	4.467E+11	0.5700
28047.3 !\AUTHOR: !\REF:		
C6H13-3<=>C2H5+C4H8-1	3.548E+12	0.2900
28299.7 !\AUTHOR: !\REF:		
C6H13-3<=>CH3+C5H10-1	8.128E+10	0.7800
29651.0 !\AUTHOR: !\REF:		
!		

!\REACTIONCLASS: \4. R+O2=E+HO2 \A \N
\EA !REF:J. D. DESAIN, S. J. KLIPPENSTEIN, J. A. MILLER, C. A.
TAATJES, J. PHYS. CHEM. A, 107, 2003, 4415-4427
!

C6H13-1+O2<=>C6H12-1+HO2	8.370E-01	3.6000
11960.0 !\AUTHOR: !\REF:		
C6H13-2+O2<=>C6H12-1+HO2	5.350E-01	3.7000
9322.0 !\AUTHOR: !\REF:		
C6H13-2+O2<=>C6H12-2+HO2	1.070E+00	3.7000
9322.0 !\AUTHOR: !\REF:		
C6H13-3+O2<=>C6H12-2+HO2	1.070E+00	3.7000
9322.0 !\AUTHOR: !\REF:		

C6H13-3+O2<=>C6H12-3+HO2 1.070E+00 3.7000
9322.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \5. R_ISOMERIZATION \A \N
\EA !REF:W. Tsang, J. A. Walker, and J. A. Manion, Proc. Combust.
Inst., 31, (2007) 141-148.
!

C6H13-2<=>C6H13-3 2.750E+10 0.7000
41872.3 !\AUTHOR: !\REF:
C6H13-1<=>C6H13-2 1.820E+02 2.5500
10961.4 !\AUTHOR: !\REF:
C6H13-1<=>C6H13-3 6.918E+00 3.2000
16559.3 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \10. R+O2=RO2 \A \N
\EA !REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74
!

C6H13-1+O2<=>C6H13O2-1 6.863E+16 -1.6270
198.7 !\AUTHOR: !\REF:
C6H13-2+O2<=>C6H13O2-2 3.486E+14 -0.8160
-536.5 !\AUTHOR: !\REF:
C6H13-3+O2<=>C6H13O2-3 3.486E+14 -0.8160
-536.5 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \11. R+R'O2=RO+R'O \A \N
\EA !REF:ESTIMATED
!

C6H13-1+HO2<=>C6H13O-1+OH 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-2+HO2<=>C6H13O-2+OH 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-3+HO2<=>C6H13O-3+OH 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-1+CH3O2<=>C6H13O-1+CH3O 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-2+CH3O2<=>C6H13O-2+CH3O 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-3+CH3O2<=>C6H13O-3+CH3O 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-1+C6H13O2-1<=>C6H13O-1+C6H13O-1 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-1+C6H13O2-2<=>C6H13O-1+C6H13O-2 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-1+C6H13O2-3<=>C6H13O-1+C6H13O-3 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-2+C6H13O2-1<=>C6H13O-2+C6H13O-1 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:
C6H13-2+C6H13O2-2<=>C6H13O-2+C6H13O-2 9.000E+12 0.0000
-1000.0 !\AUTHOR: !\REF:

C6H13-2+C6H13O2-3<=>C6H13O-2+C6H13O-3	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13-3+C6H13O2-1<=>C6H13O-3+C6H13O-1	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13-3+C6H13O2-2<=>C6H13O-3+C6H13O-2	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13-3+C6H13O2-3<=>C6H13O-3+C6H13O-3	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \12. RO2=QOOH \A \N
 \EA !REF:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A 2010, 114,
 5689-5701

C6H13O2-1<=>C6H12OOH1-2	4.009E+08	1.1000
30100.0 !\AUTHOR: !\REF:		
C6H13O2-1<=>C6H12OOH1-3	1.360E+07	1.3000
18200.0 !\AUTHOR: !\REF:		
C6H13O2-1<=>C6H12OOH1-4	3.718E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C6H13O2-1<=>C6H12OOH1-5	2.600E+06	1.0000
18200.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12OOH2-1	2.110E+11	0.2000
34200.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12OOH2-3	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12OOH2-4	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12OOH2-5	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12OOH2-6	1.471E+05	1.5000
19900.0 !\AUTHOR: !\REF:		
C6H13O2-3<=>C6H12OOH3-1	1.439E+07	1.4000
20800.0 !\AUTHOR: !\REF:		
C6H13O2-3<=>C6H12OOH3-2	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H13O2-3<=>C6H12OOH3-4	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H13O2-3<=>C6H12OOH3-5	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H13O2-3<=>C6H12OOH3-6	1.233E+06	1.5000
20000.0 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \12A.RO2=E+HO2 \A \N
 \EA !REF:BASED ON:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M.
 DEAN. J. PHYS. CHEM. A 2011, 115, 13425-13442

C6H13O2-1<=>C6H12-1+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12-1+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C6H13O2-2<=>C6H12-2+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H13O2-3<=>C6H12-2+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		

C6H13O2-3<=>C6H12-3+HO2 7.710E+09 1.0100
29362.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \13. RO2+HO2=ROOH+O2 \A \N
\EA !REF:ANOLOGY TO NC5H12
!

C6H13OOH-1+O2<=>C6H13O2-1+HO2 3.750E+13 -0.8000
33620.0 !\AUTHOR: !\REF:
C6H13OOH-2+O2<=>C6H13O2-2+HO2 4.380E+13 -0.8000
33640.0 !\AUTHOR: !\REF:
C6H13OOH-3+O2<=>C6H13O2-3+HO2 4.380E+13 -0.8000
33640.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \14. RO2+H2O2=ROOH+HO2 \A \N
\EA !REF:ANOLOGY TO NC5H12
!

C6H13OOH-1+HO2<=>C6H13O2-1+H2O2 2.400E+12 0.0000
10000.0 !\AUTHOR: !\REF:
C6H13OOH-2+HO2<=>C6H13O2-2+H2O2 2.400E+12 0.0000
10000.0 !\AUTHOR: !\REF:
C6H13OOH-3+HO2<=>C6H13O2-3+H2O2 2.400E+12 0.0000
10000.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \14A. RO2+F=ROOH+R' \A \N
\EA !REF:ANOLOGY TO NC5H12
!

C6H13O2-1+NC6H14<=>C6H13OOH-1+C6H13-1 1.210E+13 0.0000
20430.0 !\AUTHOR: !\REF:
C6H13O2-1+NC6H14<=>C6H13OOH-1+C6H13-2 8.060E+12 0.0000
17700.0 !\AUTHOR: !\REF:
C6H13O2-1+NC6H14<=>C6H13OOH-1+C6H13-3 8.060E+12 0.0000
17700.0 !\AUTHOR: !\REF:
C6H13O2-2+NC6H14<=>C6H13OOH-2+C6H13-1 1.210E+13 0.0000
20430.0 !\AUTHOR: !\REF:
C6H13O2-2+NC6H14<=>C6H13OOH-2+C6H13-2 8.060E+12 0.0000
17700.0 !\AUTHOR: !\REF:
C6H13O2-2+NC6H14<=>C6H13OOH-2+C6H13-3 8.060E+12 0.0000
17700.0 !\AUTHOR: !\REF:
C6H13O2-3+NC6H14<=>C6H13OOH-3+C6H13-1 1.210E+13 0.0000
20430.0 !\AUTHOR: !\REF:
C6H13O2-3+NC6H14<=>C6H13OOH-3+C6H13-2 8.060E+12 0.0000
17700.0 !\AUTHOR: !\REF:
C6H13O2-3+NC6H14<=>C6H13OOH-3+C6H13-3 8.060E+12 0.0000
17700.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \15. RO2+CH3O2=RO+CH3O+O2 \A \N
\EA !REF:ANOLOGY TO NC5H12
!

C6H13O2-1+CH3O2=>C6H13O-1+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:

C6H13O2-2+CH3O2=>C6H13O-2+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C6H13O2-3+CH3O2=>C6H13O-3+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:

!

!\REACTIONCLASS: \16. RO2+R'O2=RO+R'O+O2 \A \N
\EA !REF:ESTIMATED

!

C6H13O2-1+C6H13O2-1=>C6H13O-1+C6H13O-1+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C6H13O2-1+C6H13O2-2=>C6H13O-1+C6H13O-2+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C6H13O2-1+C6H13O2-3=>C6H13O-1+C6H13O-3+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C6H13O2-2+C6H13O2-2=>C6H13O-2+C6H13O-2+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C6H13O2-2+C6H13O2-3=>C6H13O-2+C6H13O-3+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C6H13O2-3+C6H13O2-3=>C6H13O-3+C6H13O-3+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:

!

!\REACTIONCLASS: \17. ROOH=RO+OH \A \N
\EA !REF:ESTIMATED

!

C6H13OOH-1<=>C6H13O-1+OH 1.500E+16 0.0000
42000.0 !\AUTHOR: !\REF:
C6H13OOH-2<=>C6H13O-2+OH 1.050E+16 0.0000
41600.0 !\AUTHOR: !\REF:
C6H13OOH-3<=>C6H13O-3+OH 1.050E+16 0.0000
41600.0 !\AUTHOR: !\REF:

!

!\REACTIONCLASS: \18. RO_DECOMPOSITION \A \N
\EA !REF:ESTIMATED

!

CH2O+C5H11-1<=>C6H13O-1 6.250E+10 0.0000
11900.0 !\AUTHOR: !\REF:
CH3CHO+PC4H9<=>C6H13O-2 7.500E+10 0.0000
11900.0 !\AUTHOR: !\REF:
C2H5CHO+NC3H7<=>C6H13O-3 8.500E+10 0.0000
11900.0 !\AUTHOR: !\REF:

!

!\REACTIONCLASS: \19. QOOH=CETH+OH \A \N
\EA !REF:BASED ON:S. M. VILLANO, L. K. HUYNH, H. -H. CARSTENSEN, A. M. DEAN. J. PHYS. CHEM. A 2012, 116, 5068-5089

!

C6H12OOH1-2<=>C6H12O1-2+OH 1.775E+12 0.0000
13376.0 !\AUTHOR: !\REF:
C6H12OOH1-3<=>C6H12O1-3+OH 3.170E+11 0.0000
18292.0 !\AUTHOR: !\REF:

C6H12OOH2-5<=>C3H6OOH2-1+C3H6	1.392E+14	0.0000
28247.6 !\AUTHOR: !\REF:		
C6H12OOH3-6<=>C4H8OOH2-1+C2H4	1.392E+14	0.0000
28123.8 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \22. QOOH+O2=O2QOOH	\A	\N
\EA !REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.5		

!

C6H12OOH1-2+O2<=>C6H12OOH1-2O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH1-3+O2<=>C6H12OOH1-3O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH1-4+O2<=>C6H12OOH1-4O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH1-5+O2<=>C6H12OOH1-5O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH2-1+O2<=>C6H12OOH2-1O2	3.430E+16	-1.6270
198.7 !\AUTHOR: !\REF:		
C6H12OOH2-3+O2<=>C6H12OOH2-3O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH2-4+O2<=>C6H12OOH2-4O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH2-5+O2<=>C6H12OOH2-5O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH2-6+O2<=>C6H12OOH2-6O2	3.430E+16	-1.6270
198.7 !\AUTHOR: !\REF:		
C6H12OOH3-1+O2<=>C6H12OOH3-1O2	3.430E+16	-1.6270
198.7 !\AUTHOR: !\REF:		
C6H12OOH3-2+O2<=>C6H12OOH3-2O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH3-4+O2<=>C6H12OOH3-4O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH3-5+O2<=>C6H12OOH3-5O2	1.740E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C6H12OOH3-6+O2<=>C6H12OOH3-6O2	3.430E+16	-1.6270
198.7 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \23A. O2QOOH=EROOH+HO2	\A	\N
\EA !REF:ANALOGY TO RO2=E+HO2		

!

C6H12OOH1-2O2<=>C6H11-2D1OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2<=>C6H11-2D1OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2<=>C6H11-3D1OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2<=>C6H11-3D1OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2<=>C6H11-2D6OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH1-5O2<=>C6H11-2D6OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH1-5O2<=>C6H11-1D6OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		

C6H12OOH2-3O2<=>C6H11-3D2OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2<=>C6H11-3D2OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2<=>C6H11-2D5OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH2-5O2<=>C6H11-2D5OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH2-5O2<=>C6H11-1D5OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C6H12OOH2-6O2<=>C6H11-1D5OOH+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		
C6H12OOH3-1O2<=>C6H11-1D3OOH+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		
C6H12OOH3-2O2<=>C6H11-1D3OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C6H12OOH3-4O2<=>C6H11-2D4OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH3-5O2<=>C6H11-2D4OOH+HO2	5.140E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C6H12OOH3-5O2<=>C6H11-1D4OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C6H12OOH3-6O2<=>C6H11-1D4OOH+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \23B. O2QOOH=HOOPOOH	\A	\N
\EA !REF:BASED ON:S. SHARMA, S. RAMAN, W. H. GREEN. J. PHYS. CHEM. A		
2010, 114, 5689-5701		

!

C6H12OOH1-2O2<=>C6H11Q12-3	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH1-2O2<=>C6H11Q12-4	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H12OOH1-2O2<=>C6H11Q12-5	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C6H12OOH1-2O2<=>C6H11Q12-6	1.470E+05	1.5000
19900.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2<=>C6H11Q13-2	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2<=>C6H11Q13-4	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2<=>C6H11Q13-5	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2<=>C6H11Q13-6	6.166E+05	1.5000
20000.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2<=>C6H11Q14-2	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2<=>C6H11Q14-3	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2<=>C6H11Q14-5	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2<=>C6H11Q14-6	1.439E+07	1.4000
20800.0 !\AUTHOR: !\REF:		
C6H12OOH1-5O2<=>C6H11Q15-2	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		

C6H12OOH1-5O2<=>C6H11Q15-3	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H12OOH1-5O2<=>C6H11Q15-4	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH1-5O2<=>C6H11Q15-6	2.110E+11	0.2000
34200.0 !\AUTHOR: !\REF:		
C6H12OOH2-1O2<=>C6H11Q12-3	1.360E+07	1.3000
18200.0 !\AUTHOR: !\REF:		
C6H12OOH2-1O2<=>C6H11Q12-4	3.718E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C6H12OOH2-1O2<=>C6H11Q12-5	2.600E+06	1.0000
18200.0 !\AUTHOR: !\REF:		
C6H12OOH2-3O2<=>C6H11Q23-1	1.439E+07	1.4000
20800.0 !\AUTHOR: !\REF:		
C6H12OOH2-3O2<=>C6H11Q23-4	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH2-3O2<=>C6H11Q23-5	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H12OOH2-3O2<=>C6H11Q23-6	6.166E+05	1.5000
20000.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2<=>C6H11Q24-1	6.166E+05	1.5000
20000.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2<=>C6H11Q24-3	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2<=>C6H11Q24-5	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2<=>C6H11Q24-6	1.439E+07	1.4000
20800.0 !\AUTHOR: !\REF:		
C6H12OOH2-5O2<=>C6H11Q25-1	1.470E+05	1.5000
19900.0 !\AUTHOR: !\REF:		
DUP		
C6H12OOH2-5O2<=>C6H11Q25-3	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
DUP		
C6H12OOH2-5O2<=>C6H11Q25-3	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
DUP		
C6H12OOH2-5O2<=>C6H11Q25-1	2.110E+11	0.2000
34200.0 !\AUTHOR: !\REF:		
DUP		
C6H12OOH2-6O2<=>C6H11Q15-4	3.718E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C6H12OOH2-6O2<=>C6H11Q15-3	1.360E+07	1.3000
18200.0 !\AUTHOR: !\REF:		
C6H12OOH2-6O2<=>C6H11Q15-2	4.009E+08	1.1000
30100.0 !\AUTHOR: !\REF:		
C6H12OOH3-1O2<=>C6H11Q13-2	4.009E+08	1.1000
30100.0 !\AUTHOR: !\REF:		
C6H12OOH3-1O2<=>C6H11Q13-4	3.718E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C6H12OOH3-1O2<=>C6H11Q13-5	2.600E+06	1.0000
18200.0 !\AUTHOR: !\REF:		
C6H12OOH3-2O2<=>C6H11Q23-1	2.110E+11	0.2000
34200.0 !\AUTHOR: !\REF:		
C6H12OOH3-2O2<=>C6H11Q23-4	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C6H12OOH3-2O2<=>C6H11Q23-5	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		

C6H12OOH3-4O2<=>C6KET34+OH	1.750E+08	1.7000
26000.0 !\AUTHOR: !\REF:		
C6H12OOH3-5O2<=>C6KET35+OH	1.750E+02	3.1000
17500.0 !\AUTHOR: !\REF:		
C6H12OOH3-6O2<=>C6KET36+OH	3.770E+02	2.2000
15300.0 !\AUTHOR: !\REF:		
!		

!\REACTIONCLASS: \23C. HOOPOOH_DECOMPOSITION	\A	\N
\EA !REF:ANALOGY TO QOOH DECOMPOSITION		
!		

C6H11Q12-3=>PC4H8CHO-1+CH2O+2OH	3.081E+13	0.0000
33871.4 !\AUTHOR: !\REF:		
C6H11Q12-4=>C4H8-1+HO2CH2CHO+OH	3.081E+13	0.0000
2316.3 !\AUTHOR: !\REF:		
C6H11Q12-5<=>C3H51-2,3OOH+C3H6	1.392E+14	0.0000
25866.6 !\AUTHOR: !\REF:		
C6H11Q13-5=>C3KET13+C3H6+OH	3.081E+13	0.0000
24186.1 !\AUTHOR: !\REF:		
C6H11Q14-6=>NC4KET14+C2H4+OH	3.081E+13	0.0000
24608.4 !\AUTHOR: !\REF:		
C6H11Q15-3=>C4H71-4OOH+CH3CHO+OH	3.081E+13	0.0000
24638.9 !\AUTHOR: !\REF:		
C6H11Q15-3=>C5H91-4OOH+CH2O+OH	3.081E+13	0.0000
27282.9 !\AUTHOR: !\REF:		
C6H11Q23-5=>C3KET12+C3H6+OH	3.081E+13	0.0000
23942.2 !\AUTHOR: !\REF:		
C6H11Q24-6=>NC4KET13+C2H4+OH	3.081E+13	0.0000
24608.4 !\AUTHOR: !\REF:		
C6H11Q34-1=>NC4KET12+C2H4+OH	3.081E+13	0.0000
26362.9 !\AUTHOR: !\REF:		
!		

!\REACTIONCLASS: \24. KET_DECOMPOSITION	\A	\N
\EA !REF:ESTIMATED		
!		

C6KET12<=>C6KET12O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET13<=>C6KET13O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET14<=>C6KET14O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET15<=>C6KET15O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET21<=>C6KET21O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		
C6KET23<=>C6KET23O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET24<=>C6KET24O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET25<=>C6KET25O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET26<=>C6KET26O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		
C6KET31<=>C6KET31O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		

C6KET32<=>C6KET32O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET34<=>C6KET34O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET35<=>C6KET35O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C6KET36<=>C6KET36O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		
C6KET120<=>PC4H9CHO+HCO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET130<=>NC3H7CHO+CH2CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET140<=>C2H5CHO+CH2CH2CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET150<=>CH3CHO+C3H6CHO-1	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET210<=>CH2O+PC4H9CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET230<=>NC3H7CHO+CH3CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET240<=>C2H5CHO+CH3COCH2	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET250<=>CH3CHO+CH2CH2COCH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET260<=>CH2O+CH2CH2CH2COCH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET310<=>CH2O+NC3H7COCH2	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET320<=>CH3CHO+NC3H7CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET340<=>C2H5CHO+C2H5CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET350<=>CH3CHO+C2H5COCH2	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6KET360<=>CH2O+CH2CH2COC2H5	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \24A. HOOPOOH=EROOH+HO2

\A

\N

\EA !REF:ANALOGY TO QOOH=E+HO2

!

C6H11Q12-3<=>C6H11-2D1OOH+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C6H11Q13-2<=>C6H11-1D3OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C6H11Q13-2<=>C6H11-2D1OOH+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C6H11Q13-4<=>C6H11-3D1OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C6H11Q14-2<=>C6H11-1D4OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C6H11Q14-3<=>C6H11-3D1OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C6H11Q14-5<=>C6H11-2D6OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C6H11Q15-2<=>C6H11-1D5OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		

C6H11Q15-4<=>C6H11-2D6OOH+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C6H11Q15-6<=>C6H11-1D6OOH+HO2	1.780E+12	0.2400
15700.0 !\AUTHOR: !\REF:		
C6H11Q23-1<=>C6H11-1D3OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C6H11Q23-4<=>C6H11-3D2OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C6H11Q24-1<=>C6H11-1D4OOH+HO2	1.780E+12	0.2400
15700.0 !\AUTHOR: !\REF:		
C6H11Q24-3<=>C6H11-2D4OOH+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C6H11Q24-3<=>C6H11-3D2OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C6H11Q24-5<=>C6H11-2D5OOH+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C6H11Q25-1<=>C6H11-1D5OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C6H11Q25-3<=>C6H11-2D5OOH+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C6H11Q34-2<=>C6H11-2D4OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \24B. EROOH_DECOMPOSITION	\A	\N
\EA !REF:ANALOGY TO QOOH=E+HO2		

!

C6H11-1D3OOH=>C2H3CHO+NC3H7+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-1D4OOH=>AC3H5CHO+C2H5+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-1D4OOH=>C3H5-A+C2H5CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-1D5OOH=>C4H71-4+CH3CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-1D6OOH=>C5H91-5+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11-2D1OOH=>C5H91-1+CH2O+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-2D4OOH=>SC3H5CHO+C2H5+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-2D4OOH=>C3H5-S+C2H5CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11-2D6OOH=>C5H92-5+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11-3D1OOH=>C5H91-3+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11-3D2OOH=>CH3CHO+C4H71-1+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C2H2+NC3H7<=>C5H91-1	2.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \24C. HOPOOH=CETH-OOH+OH	\A	\N
\EA !REF:ANALOGY TO QOOH=CETH+OH		

!

C6H11Q12-3<=>C6H11O13-2OOH+OH 18003.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q12-3<=>C6H11O23-1OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q12-4<=>C6H11O14-2OOH+OH 11501.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q12-4<=>C6H11O24-1OOH+OH 17284.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q12-5<=>C6H11O15-2OOH+OH 11137.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q12-5<=>C6H11O25-1OOH+OH 11490.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q12-6<=>C6H11O15-6OOH+OH 11908.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q13-2<=>C6H11O12-3OOH+OH 13376.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q13-2<=>C6H11O23-1OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q13-4<=>C6H11O14-3OOH+OH 11068.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q13-4<=>C6H11O34-1OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q13-5<=>C6H11O15-3OOH+OH 11137.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q13-5<=>C6H11O24-6OOH+OH 17284.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q13-6<=>C6H11O14-6OOH+OH 11573.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q14-2<=>C6H11O12-4OOH+OH 13376.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q14-2<=>C6H11O24-1OOH+OH 16995.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q14-3<=>C6H11O13-4OOH+OH 18003.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q14-3<=>C6H11O34-1OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q14-5<=>C6H11O15-4OOH+OH 10825.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q14-5<=>C6H11O23-6OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q14-6<=>C6H11O13-6OOH+OH 19006.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q15-2<=>C6H11O12-5OOH+OH 13376.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q15-2<=>C6H11O25-1OOH+OH 11056.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q15-3<=>C6H11O13-5OOH+OH 18292.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q15-3<=>C6H11O24-6OOH+OH 17284.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q15-4<=>C6H11O14-5OOH+OH 11068.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q15-4<=>C6H11O23-6OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q15-6<=>C6H11O12-6OOH+OH 15034.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q23-1<=>C6H11O12-3OOH+OH 15034.0 !\AUTHOR: !\REF:	1.780E+12	0.0000

C6H11Q23-1<=>C6H11O13-2OOH+OH 19044.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q23-4<=>C6H11O24-3OOH+OH 16995.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q23-4<=>C6H11O34-2OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q23-5<=>C6H11O25-3OOH+OH 11490.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q23-5<=>C6H11O24-5OOH+OH 17284.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q23-6<=>C6H11O15-4OOH+OH 11908.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q23-6<=>C6H11O14-5OOH+OH 11573.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q24-1<=>C6H11O12-4OOH+OH 15034.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q24-1<=>C6H11O14-2OOH+OH 12630.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q24-3<=>C6H11O23-4OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q24-3<=>C6H11O34-2OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q24-5<=>C6H11O25-3OOH+OH 11056.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q24-5<=>C6H11O23-5OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q24-6<=>C6H11O15-3OOH+OH 11908.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q24-6<=>C6H11O13-5OOH+OH 19006.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q25-1<=>C6H11O12-5OOH+OH 15034.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q25-1<=>C6H11O15-2OOH+OH 11949.0 !\AUTHOR: !\REF:	5.200E+09	0.0000
C6H11Q25-3<=>C6H11O23-5OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q25-3<=>C6H11O24-5OOH+OH 16995.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q34-1<=>C6H11O13-4OOH+OH 19006.0 !\AUTHOR: !\REF:	3.170E+11	0.0000
C6H11Q34-1<=>C6H11O14-3OOH+OH 11573.0 !\AUTHOR: !\REF:	2.770E+10	0.0000
C6H11Q34-2<=>C6H11O23-4OOH+OH 13364.0 !\AUTHOR: !\REF:	1.780E+12	0.0000
C6H11Q34-2<=>C6H11O24-3OOH+OH 16995.0 !\AUTHOR: !\REF:	3.170E+11	0.0000

!

!\REACTIONCLASS: \24D. CETH-OOH_DECOMPOSITION
\EA !REF:ESTIMATED

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C6H11O12-3OOH=>CH2CHO+NC3H7CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+16	0.0000
C6H11O12-4OOH=>C3H5O+C2H5CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+16	0.0000
C6H11O12-5OOH=>C4H7O12-4+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+16	0.0000

C6H11O12-6OOH=>C5H9O12-5+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O13-2OOH=>CH2CHO+NC3H7CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O13-4OOH=>CH2CH2CHO+C2H5CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O13-5OOH=>C4H7O13-4+CH3CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O13-6OOH=>C5H9O13-5+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O14-2OOH=>CH2O+PC4H8CHO-2+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O14-3OOH=>CH2CH2CHO+C2H5CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O14-5OOH=>C3H6CHO-1+CH3CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O14-6OOH=>C5H9O14-5+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O15-2OOH=>CH2O+PC4H8CHO-3+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O15-3OOH=>C3H6+CH2CHO+CH2O+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O15-4OOH=>C3H6CHO-1+CH3CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O15-6OOH=>PC4H8CHO-4+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O23-1OOH=>CH2O+PC4H8CHO-1+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O23-4OOH=>CH3CHCHO+C2H5CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O23-5OOH=>C4H7O23-1+CH3CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O23-6OOH=>C5H9O23-5+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O24-1OOH=>CH2O+PC4H8CHO-2+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O24-3OOH=>CH3CHCHO+C2H5CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O24-5OOH=>C3H6CHO-2+CH3CHO+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O24-6OOH=>C5H9O24-1+CH2O+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O25-1OOH=>CH2O+PC4H8CHO-3+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O25-3OOH=>CH3CHO+C3H6CHO-2+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		
C6H11O34-1OOH=>CH2O+C5H9O23-1+OH	1.500E+16	0.0000
42000.0 !\AUTHOR: !\REF:		
C6H11O34-2OOH=>CH3CHO+C3H6CHO-3+OH	1.050E+16	0.0000
41600.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \25. CETH_DECOMPOSTION

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\EA !REF:ANOLOGY TO NC5H12

!

C6H12O1-2+OH=>CH2CO+PC4H9+H2O

2.500E+12

0.0000

0.0 !\AUTHOR: !\REF:

!

C6KET13=>HOCHO+NC3H7COCH3	1.700E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
C6KET13=>CH3COOH+NC3H7CHO	5.100E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
C6KET24=>CH3COOH+C2H5COCH3	1.700E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
C6KET35=>C2H5COOH+CH3COCH3	3.400E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
CH3COOH<=>CH4+CO2	1.500E+13	0.0000
70000.0 !\AUTHOR: !\REF:		
CH3COOH<=>H2O+CH2CO	1.400E+12	0.0000
65000.0 !\AUTHOR: !\REF:		
CH3COOH=>CO+OH+CH3	7.500E+15	0.0000
91600.0 !\AUTHOR: !\REF:		
CH3COOH=>CH3+CO2+H	2.500E+14	0.0000
88000.0 !\AUTHOR: !\REF:		
C2H5COOH=>C2H6+CO2	1.500E+13	0.0000
70000.0 !\AUTHOR: !\REF:		
C2H5COOH=>H2O+CH3CHCO	1.400E+12	0.0000
65000.0 !\AUTHOR: !\REF:		
C2H5COOH=>CO+OH+C2H5	7.500E+15	0.0000
91600.0 !\AUTHOR: !\REF:		
C2H5COOH=>CO2+C2H5+H	2.500E+14	0.0000
88000.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \X2. O2QOOH+R'=OQOOH+R'O,ETC	\A	\N
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\EA !REF:ESTIMATED

!

C6H13O2-1+CH3<=>C6H13O-1+CH3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13O2-2+CH3<=>C6H13O-2+CH3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13O2-3+CH3<=>C6H13O-3+CH3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13O2-1+C2H5<=>C6H13O-1+C2H5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13O2-2+C2H5<=>C6H13O-2+C2H5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H13O2-3+C2H5<=>C6H13O-3+C2H5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH1-2O2+CH3=>CH3O+C6H12OOH1-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH1-3O2+CH3=>CH3O+C6H12OOH1-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH1-4O2+CH3=>CH3O+C6H12OOH1-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH1-5O2+CH3=>CH3O+C6H12OOH1-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH2-1O2+CH3=>CH3O+C6H12OOH2-1O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH2-3O2+CH3=>CH3O+C6H12OOH2-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C6H12OOH2-4O2+CH3=>CH3O+C6H12OOH2-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		

C6H12OOH2-5O2+CH3=>CH3O+C6H12OOH2-5O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-6O2+CH3=>CH3O+C6H12OOH2-6O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-1O2+CH3=>CH3O+C6H12OOH3-1O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-2O2+CH3=>CH3O+C6H12OOH3-2O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-4O2+CH3=>CH3O+C6H12OOH3-4O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-5O2+CH3=>CH3O+C6H12OOH3-5O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-6O2+CH3=>CH3O+C6H12OOH3-6O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-2O=>HO2CH2CHO+PC4H9 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-3O=>C3KET13+NC3H7 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-4O=>NC4KET14+C2H5 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-5O=>NC5KET15+CH3 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-1O=>CH2O+PC4H9CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-3O=>C3KET12+NC3H7 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-4O=>NC4KET13+C2H5 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-5O=>NC5KET14+CH3 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-6O=>CH2O+C5H10OOH2-5 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-1O=>CH2O+C5H10OOH2-1 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-2O=>CH3+NC5KET12 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-4O=>NC4KET12+C2H5 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-5O=>CH3+NC5KET13 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-6O=>CH2O+C5H10OOH3-1 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-2O=>CH2O2H+PC4H9CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-3O=>C2H4O2H+NC3H7CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-4O=>C3H6OOH1-3+C2H5CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-5O=>C4H8OOH1-4+CH3CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-3O=>CH3CHO+NC3H7CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-4O=>C3H6OOH2-1+C2H5CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH2-5O=>C4H8OOH2-4+CH3CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-2O=>CH3CHO+NC3H7CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000

C6H12OOH3-4O=>C2H5CHO+C2H5CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH3-5O=>C4H8OOH2-1+CH3CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C6H12OOH1-2O2+C6H13-1=>C6H13O-1+C6H12OOH1-2O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-3O2+C6H13-1=>C6H13O-1+C6H12OOH1-3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-4O2+C6H13-1=>C6H13O-1+C6H12OOH1-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-5O2+C6H13-1=>C6H13O-1+C6H12OOH1-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-1O2+C6H13-1=>C6H13O-1+C6H12OOH2-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-3O2+C6H13-1=>C6H13O-1+C6H12OOH2-3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-4O2+C6H13-1=>C6H13O-1+C6H12OOH2-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-5O2+C6H13-1=>C6H13O-1+C6H12OOH2-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-6O2+C6H13-1=>C6H13O-1+C6H12OOH2-6O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-1O2+C6H13-1=>C6H13O-1+C6H12OOH3-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-2O2+C6H13-1=>C6H13O-1+C6H12OOH3-2O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-4O2+C6H13-1=>C6H13O-1+C6H12OOH3-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-5O2+C6H13-1=>C6H13O-1+C6H12OOH3-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-6O2+C6H13-1=>C6H13O-1+C6H12OOH3-6O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-2O2+C6H13-2=>C6H13O-2+C6H12OOH1-2O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-3O2+C6H13-2=>C6H13O-2+C6H12OOH1-3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-4O2+C6H13-2=>C6H13O-2+C6H12OOH1-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-5O2+C6H13-2=>C6H13O-2+C6H12OOH1-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-1O2+C6H13-2=>C6H13O-2+C6H12OOH2-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-3O2+C6H13-2=>C6H13O-2+C6H12OOH2-3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-4O2+C6H13-2=>C6H13O-2+C6H12OOH2-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-5O2+C6H13-2=>C6H13O-2+C6H12OOH2-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-6O2+C6H13-2=>C6H13O-2+C6H12OOH2-6O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-1O2+C6H13-2=>C6H13O-2+C6H12OOH3-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-2O2+C6H13-2=>C6H13O-2+C6H12OOH3-2O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-4O2+C6H13-2=>C6H13O-2+C6H12OOH3-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-5O2+C6H13-2=>C6H13O-2+C6H12OOH3-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000

C6H12OOH3-6O2+C6H13-2=>C6H13O-2+C6H12OOH3-6O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-2O2+C6H13-3=>C6H13O-3+C6H12OOH1-2O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-3O2+C6H13-3=>C6H13O-3+C6H12OOH1-3O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-4O2+C6H13-3=>C6H13O-3+C6H12OOH1-4O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH1-5O2+C6H13-3=>C6H13O-3+C6H12OOH1-5O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-1O2+C6H13-3=>C6H13O-3+C6H12OOH2-1O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-3O2+C6H13-3=>C6H13O-3+C6H12OOH2-3O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-4O2+C6H13-3=>C6H13O-3+C6H12OOH2-4O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-5O2+C6H13-3=>C6H13O-3+C6H12OOH2-5O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH2-6O2+C6H13-3=>C6H13O-3+C6H12OOH2-6O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-1O2+C6H13-3=>C6H13O-3+C6H12OOH3-1O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-2O2+C6H13-3=>C6H13O-3+C6H12OOH3-2O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-4O2+C6H13-3=>C6H13O-3+C6H12OOH3-4O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-5O2+C6H13-3=>C6H13O-3+C6H12OOH3-5O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C6H12OOH3-6O2+C6H13-3=>C6H13O-3+C6H12OOH3-6O-1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000

!-----

!\ENDSUBMECH: \C6H14

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!-----

!\SUBMECH: \C6H12-1\C6H12-2\C6H12-3

!-----

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!\REACTIONCLASS: \9. E_UNIMOLECULAR_DECOMPOSITION \A \N
 \EA !REF: H. J. Curran, et al., Combust. Flame, 114, (1998) 149-177.
 !-----

C6H12-1<=>NC3H7+C3H5-A 75330.0 !\AUTHOR: !\REF:	3.170E+21	-1.6200
C6H12-2<=>C2H5+C4H71-3 75710.0 !\AUTHOR: !\REF:	3.735E+21	-1.7400
C6H12-3<=>CH3+C5H91-3 76790.0 !\AUTHOR: !\REF:	5.947E+21	-1.8500

!-----

!\REACTIONCLASS: \6. E_H_ABSTRACTION \A \N
 \EA !REF:ANALOGY TO PENTENES
 !-----

!-----

C6H12-1+H<=>C6H111-3+H2	3.380E+05	2.4000
207.0 !\AUTHOR: !\REF:		
C6H12-1+H<=>C6H111-4+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C6H12-1+H<=>C6H111-5+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C6H12-1+H<=>C6H111-6+H2	6.650E+05	2.5000
6756.0 !\AUTHOR: !\REF:		
C6H12-1+O<=>C6H111-3+OH	6.600E+05	2.4000
1210.0 !\AUTHOR: !\REF:		
C6H12-1+O<=>C6H111-4+OH	5.510E+05	2.5000
2830.0 !\AUTHOR: !\REF:		
C6H12-1+O<=>C6H111-5+OH	5.510E+05	2.5000
2830.0 !\AUTHOR: !\REF:		
C6H12-1+O<=>C6H111-6+OH	9.800E+05	2.4000
4750.0 !\AUTHOR: !\REF:		
C6H12-1+OH<=>C6H111-3+H2O	2.760E+04	2.6000
-1919.0 !\AUTHOR: !\REF:		
C6H12-1+OH<=>C6H111-4+H2O	4.670E+07	1.6000
-35.0 !\AUTHOR: !\REF:		
C6H12-1+OH<=>C6H111-5+H2O	4.670E+07	1.6000
-35.0 !\AUTHOR: !\REF:		
C6H12-1+OH<=>C6H111-6+H2O	5.270E+09	1.0000
1586.0 !\AUTHOR: !\REF:		
C6H12-1+O2<=>C6H111-3+HO2	2.200E+12	0.0000
37220.0 !\AUTHOR: !\REF:		
C6H12-1+O2<=>C6H111-4+HO2	2.000E+13	0.0000
49640.0 !\AUTHOR: !\REF:		
C6H12-1+O2<=>C6H111-5+HO2	2.000E+13	0.0000
49640.0 !\AUTHOR: !\REF:		
C6H12-1+O2<=>C6H111-6+HO2	3.000E+13	0.0000
52290.0 !\AUTHOR: !\REF:		
C6H12-1+HO2<=>C6H111-3+H2O2	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C6H12-1+HO2<=>C6H111-4+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C6H12-1+HO2<=>C6H111-5+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C6H12-1+HO2<=>C6H111-6+H2O2	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C6H12-1+CH3<=>C6H111-3+CH4	3.690E+00	3.3000
4002.0 !\AUTHOR: !\REF:		
C6H12-1+CH3<=>C6H111-4+CH4	1.510E+00	3.5000
5481.0 !\AUTHOR: !\REF:		
C6H12-1+CH3<=>C6H111-5+CH4	1.510E+00	3.5000
5481.0 !\AUTHOR: !\REF:		
C6H12-1+CH3<=>C6H111-6+CH4	4.520E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
C6H12-1+CH3O<=>C6H111-3+CH3OH	4.000E+01	2.9000
8609.0 !\AUTHOR: !\REF:		
C6H12-1+CH3O<=>C6H111-4+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C6H12-1+CH3O<=>C6H111-5+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C6H12-1+CH3O<=>C6H111-6+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C6H12-1+CH3O2<=>C6H111-3+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		

C6H12-1+CH3O2<=>C6H111-4+CH3O2H 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C6H12-1+CH3O2<=>C6H111-5+CH3O2H 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C6H12-1+CH3O2<=>C6H111-6+CH3O2H 16490.0 !\AUTHOR: !\REF:	2.380E+04	2.5000
C6H12-2+H<=>C6H111-3+H2 2492.0 !\AUTHOR: !\REF:	1.730E+05	2.5000
C6H12-2+H<=>C6H112-4+H2 207.0 !\AUTHOR: !\REF:	3.380E+05	2.4000
C6H12-2+H<=>C6H112-5+H2 4471.0 !\AUTHOR: !\REF:	1.300E+06	2.4000
C6H12-2+H<=>C6H112-6+H2 6756.0 !\AUTHOR: !\REF:	6.650E+05	2.5000
C6H12-2+O<=>C6H111-3+OH 3150.0 !\AUTHOR: !\REF:	4.410E+05	2.4000
C6H12-2+O<=>C6H112-4+OH 1210.0 !\AUTHOR: !\REF:	6.600E+05	2.4000
C6H12-2+O<=>C6H112-5+OH 2830.0 !\AUTHOR: !\REF:	5.510E+05	2.5000
C6H12-2+O<=>C6H112-6+OH 4750.0 !\AUTHOR: !\REF:	9.800E+05	2.4000
C6H12-2+OH<=>C6H111-3+H2O -298.0 !\AUTHOR: !\REF:	3.120E+06	2.0000
C6H12-2+OH<=>C6H112-4+H2O -1919.0 !\AUTHOR: !\REF:	2.760E+04	2.6000
C6H12-2+OH<=>C6H112-5+H2O -35.0 !\AUTHOR: !\REF:	4.670E+07	1.6000
C6H12-2+OH<=>C6H112-6+H2O 1586.0 !\AUTHOR: !\REF:	5.270E+09	1.0000
C6H12-2+O2<=>C6H111-3+HO2 39900.0 !\AUTHOR: !\REF:	3.300E+12	0.0000
C6H12-2+O2<=>C6H112-4+HO2 37220.0 !\AUTHOR: !\REF:	2.200E+12	0.0000
C6H12-2+O2<=>C6H112-5+HO2 49640.0 !\AUTHOR: !\REF:	2.000E+13	0.0000
C6H12-2+O2<=>C6H112-6+HO2 52290.0 !\AUTHOR: !\REF:	3.000E+13	0.0000
C6H12-2+HO2<=>C6H111-3+H2O2 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C6H12-2+HO2<=>C6H112-4+H2O2 10530.0 !\AUTHOR: !\REF:	4.820E+03	2.5000
C6H12-2+HO2<=>C6H112-5+H2O2 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C6H12-2+HO2<=>C6H112-6+H2O2 16490.0 !\AUTHOR: !\REF:	2.380E+04	2.5000
C6H12-2+CH3<=>C6H111-3+CH4 5675.0 !\AUTHOR: !\REF:	2.210E+00	3.5000
C6H12-2+CH3<=>C6H112-4+CH4 4002.0 !\AUTHOR: !\REF:	3.690E+00	3.3000
C6H12-2+CH3<=>C6H112-5+CH4 5481.0 !\AUTHOR: !\REF:	1.510E+00	3.5000
C6H12-2+CH3<=>C6H112-6+CH4 7154.0 !\AUTHOR: !\REF:	4.520E-01	3.6000
C6H12-2+CH3O<=>C6H111-3+CH3OH 11990.0 !\AUTHOR: !\REF:	9.000E+01	3.0000
C6H12-2+CH3O<=>C6H112-4+CH3OH 8609.0 !\AUTHOR: !\REF:	4.000E+01	2.9000

C6H12-2+CH3O<=>C6H112-5+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C6H12-2+CH3O<=>C6H112-6+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C6H12-2+CH3O2<=>C6H111-3+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C6H12-2+CH3O2<=>C6H112-4+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C6H12-2+CH3O2<=>C6H112-5+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C6H12-2+CH3O2<=>C6H112-6+CH3O2H	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C6H12-3+H<=>C6H112-4+H2	3.380E+05	2.4000
207.0 !\AUTHOR: !\REF:		
C6H12-3+H<=>C6H113-1+H2	6.650E+05	2.5000
6756.0 !\AUTHOR: !\REF:		
C6H12-3+O<=>C6H112-4+OH	6.600E+05	2.4000
1210.0 !\AUTHOR: !\REF:		
C6H12-3+O<=>C6H113-1+OH	9.800E+05	2.4000
4750.0 !\AUTHOR: !\REF:		
C6H12-3+OH<=>C6H112-4+H2O	2.760E+04	2.6000
-1919.0 !\AUTHOR: !\REF:		
C6H12-3+OH<=>C6H113-1+H2O	5.270E+09	1.0000
1586.0 !\AUTHOR: !\REF:		
C6H12-3+O2<=>C6H112-4+HO2	2.200E+12	0.0000
37220.0 !\AUTHOR: !\REF:		
C6H12-3+O2<=>C6H113-1+HO2	3.000E+13	0.0000
52290.0 !\AUTHOR: !\REF:		
C6H12-3+HO2<=>C6H112-4+H2O2	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C6H12-3+HO2<=>C6H113-1+H2O2	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C6H12-3+CH3<=>C6H112-4+CH4	3.690E+00	3.3000
4002.0 !\AUTHOR: !\REF:		
C6H12-3+CH3<=>C6H113-1+CH4	4.520E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
C6H12-3+CH3O<=>C6H112-4+CH3OH	4.000E+01	2.9000
8609.0 !\AUTHOR: !\REF:		
C6H12-3+CH3O<=>C6H113-1+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C6H12-3+CH3O2<=>C6H112-4+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C6H12-3+CH3O2<=>C6H113-1+CH3O2H	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		

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!\REACTIONCLASS: \7. E_H_ADDITION

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\EA !REF:

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C6H12-1+H<=>C6H13-1	1.200E+09	1.3000
1049.2 !\AUTHOR: !\REF:		
C6H12-1+H<=>C6H13-2	6.610E+08	1.4000
-677.6 !\AUTHOR: !\REF:		
C6H12-2+H<=>C6H13-2	3.890E+08	1.6000
579.9 !\AUTHOR: !\REF:		
C6H12-2+H<=>C6H13-3	3.890E+08	1.6000
579.9 !\AUTHOR: !\REF:		

C6H12-3+H<=>C6H13-3 7.780E+08 1.6000
579.9 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \7A. E_WADDINGTON \A \N
\EA !REF:ANALOGY TO PENTENES
!

C6H12-1+OH<=>C6H12OH-1J2 4.750E+12 0.0000
-782.0 !\AUTHOR: !\REF:
C6H12-1+OH<=>C6H12OH-2J1 4.750E+12 0.0000
-782.0 !\AUTHOR: !\REF:
C6H12-2+OH<=>C6H12OH-2J3 4.750E+12 0.0000
-782.0 !\AUTHOR: !\REF:
C6H12-2+OH<=>C6H12OH-3J2 4.750E+12 0.0000
-782.0 !\AUTHOR: !\REF:
C6H12-3+OH<=>C6H12OH-3J4 4.750E+12 0.0000
-782.0 !\AUTHOR: !\REF:
C6H12OH-1J2+O2<=>C6H12OH-1O2-2 2.000E+12 0.0000
0.0 !\AUTHOR: !\REF:
C6H12OH-2J1+O2<=>C6H12OH-2O2-1 2.000E+12 0.0000
0.0 !\AUTHOR: !\REF:
C6H12OH-2J3+O2<=>C6H12OH-2O2-3 2.000E+12 0.0000
0.0 !\AUTHOR: !\REF:
C6H12OH-3J2+O2<=>C6H12OH-3O2-2 2.000E+12 0.0000
0.0 !\AUTHOR: !\REF:
C6H12OH-3J4+O2<=>C6H12OH-3O2-4 2.000E+12 0.0000
0.0 !\AUTHOR: !\REF:
C6H12OH-1O2-2=>CH2O+PC4H9CHO+OH 2.500E+10 0.0000
18860.0 !\AUTHOR: !\REF:
C6H12OH-2O2-1=>CH2O+PC4H9CHO+OH 2.500E+10 0.0000
18860.0 !\AUTHOR: !\REF:
C6H12OH-2O2-3=>CH3CHO+NC3H7CHO+OH 2.500E+10 0.0000
18860.0 !\AUTHOR: !\REF:
C6H12OH-3O2-2=>CH3CHO+NC3H7CHO+OH 2.500E+10 0.0000
18860.0 !\AUTHOR: !\REF:
C6H12OH-3O2-4=>C2H5CHO+C2H5CHO+OH 2.500E+10 0.0000
18860.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \8. ER_DECOMPOSITION \A \N
\EA !REF:ANALOGY TO PENTENES
!

C4H6+C2H5<=>C6H111-3 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
C3H6+C3H5-A<=>C6H111-5 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
C4H71-4+C2H4<=>C6H111-6 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
C5H81-3+CH3<=>C6H112-4 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
C4H71-3+C2H4<=>C6H112-6 1.000E+11 0.0000
7800.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \8A. ER+HO2=ERO+OH \A \N
\EA !REF:ANALOGY TO PENTENES

!

C6H11-1D30+OH<=>C6H111-3+HO2	6.090E+15	-1.1000
15720.0 !\AUTHOR: !\REF:		
C6H11-1D40+OH<=>C6H111-4+HO2	6.090E+15	-1.1000
15720.0 !\AUTHOR: !\REF:		
C6H11-1D50+OH<=>C6H111-5+HO2	6.090E+15	-1.1000
15720.0 !\AUTHOR: !\REF:		
C6H11-1D60+OH<=>C6H111-6+HO2	6.090E+15	-1.1000
15720.0 !\AUTHOR: !\REF:		
C6H11-2D40+OH<=>C6H112-4+HO2	7.030E+15	-1.2000
15890.0 !\AUTHOR: !\REF:		
C6H11-2D50+OH<=>C6H112-5+HO2	7.030E+15	-1.2000
15890.0 !\AUTHOR: !\REF:		
C6H11-2D60+OH<=>C6H112-6+HO2	7.030E+15	-1.2000
15890.0 !\AUTHOR: !\REF:		
C6H11-3D10+OH<=>C6H113-1+HO2	7.030E+15	-1.2000
15890.0 !\AUTHOR: !\REF:		
C6H11-1D30+CH3O<=>C6H111-3+CH3O2	5.950E+17	-1.6000
20480.0 !\AUTHOR: !\REF:		
C6H11-1D40+CH3O<=>C6H111-4+CH3O2	5.950E+17	-1.6000
20480.0 !\AUTHOR: !\REF:		
C6H11-1D50+CH3O<=>C6H111-5+CH3O2	5.950E+17	-1.6000
20480.0 !\AUTHOR: !\REF:		
C6H11-1D60+CH3O<=>C6H111-6+CH3O2	5.950E+17	-1.6000
20480.0 !\AUTHOR: !\REF:		
C6H11-2D40+CH3O<=>C6H112-4+CH3O2	6.860E+17	-1.8000
20650.0 !\AUTHOR: !\REF:		
C6H11-2D50+CH3O<=>C6H112-5+CH3O2	6.860E+17	-1.8000
20650.0 !\AUTHOR: !\REF:		
C6H11-2D60+CH3O<=>C6H112-6+CH3O2	6.860E+17	-1.8000
20650.0 !\AUTHOR: !\REF:		
C6H11-3D10+CH3O<=>C6H113-1+CH3O2	6.860E+17	-1.8000
20650.0 !\AUTHOR: !\REF:		
C6H11-1D30+C2H5O<=>C6H111-3+C2H5O2	3.890E+14	-0.7000
18330.0 !\AUTHOR: !\REF:		
C6H11-2D10+C2H5O<=>C6H111-3+C2H5O2	3.890E+14	-0.7000
18330.0 !\AUTHOR: !\REF:		
C6H11-1D40+C2H5O<=>C6H111-4+C2H5O2	3.890E+14	-0.7000
18330.0 !\AUTHOR: !\REF:		
C6H11-1D50+C2H5O<=>C6H111-5+C2H5O2	3.890E+14	-0.7000
18330.0 !\AUTHOR: !\REF:		
C6H11-1D60+C2H5O<=>C6H111-6+C2H5O2	3.890E+14	-0.7000
18330.0 !\AUTHOR: !\REF:		
C6H11-2D40+C2H5O<=>C6H112-4+C2H5O2	4.490E+14	-0.9000
18490.0 !\AUTHOR: !\REF:		
C6H11-3D20+C2H5O<=>C6H112-4+C2H5O2	4.490E+14	-0.9000
18490.0 !\AUTHOR: !\REF:		
C6H11-2D50+C2H5O<=>C6H112-5+C2H5O2	4.490E+14	-0.9000
18490.0 !\AUTHOR: !\REF:		
C6H11-2D60+C2H5O<=>C6H112-6+C2H5O2	4.490E+14	-0.9000
18490.0 !\AUTHOR: !\REF:		
C6H11-3D10+C2H5O<=>C6H113-1+C2H5O2	4.490E+14	-0.9000
18490.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \8B. ERO_DECOMPOSITION
\EA !REF:ESTIMATED

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C6H11-1D3O<=>C2H3CHO+NC3H7	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6H11-1D4O<=>C2H5CHO+C3H5-A	3.130E+19	-1.9000
10670.0 !\AUTHOR: !\REF:		
C6H11-1D5O<=>CH3CHO+C4H71-4	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6H11-1D6O<=>CH2O+C5H91-5	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6H11-2D4O<=>SC3H5CHO+C2H5	3.130E+19	-1.9000
10670.0 !\AUTHOR: !\REF:		
C6H11-2D5O<=>CH3CHO+C4H71-3	3.130E+19	-1.9000
10670.0 !\AUTHOR: !\REF:		
C6H11-2D6O<=>CH2O+C5H92-5	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C6H11-3D1O<=>CH2O+C5H91-3	5.980E+15	-1.1000
9941.0 !\AUTHOR: !\REF:		

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 !-----
 !\ENDSUBMECH: \C6H12-1\C6H12-2\C6H12-3
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 !-----
 !-----
 !\SUBMECH: \NC5H11CHO
 !-----
 !-----
 !

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

NC5H11CHO+O2<=>NC5H11CO+HO2	3.010E+013	0.000
39150.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+O<=>NC5H11CO+OH	5.940E+012	0.000
1868.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+H<=>NC5H11CO+H2	1.310E+005	2.580
1220.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+OH<=>NC5H11CO+H2O	3.370E+012	0.000
-619.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+HO2<=>NC5H11CO+H2O2	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+CH3<=>NC5H11CO+CH4	7.080E-004	4.580
1966.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+CH3O2<=>NC5H11CO+CH3O2H	3.010E+012	0.000
11920.0 !\AUTHOR: !\REF:!ANALOGY TO CH3CHO		
NC5H11CHO+OH<=>NC5H10CHO-1+H2O	5.520E+02	3.1200
-1176.0 !\AUTHOR: !\REF:		
NC5H11CHO+OH<=>NC5H10CHO-2+H2O	4.680E+07	1.6100
-35.0 !\AUTHOR: !\REF:		
NC5H11CHO+OH<=>NC5H10CHO-3+H2O	4.680E+07	1.6100
-35.0 !\AUTHOR: !\REF:		
NC5H11CHO+OH<=>NC5H10CHO-4+H2O	4.680E+07	1.6100
-35.0 !\AUTHOR: !\REF:		
NC5H11CHO+OH<=>NC5H10CHO-5+H2O	4.680E+07	1.6100
-35.0 !\AUTHOR: !\REF:		

NC5H11CHO+HO2<=>NC5H10CHO-1+H2O2	3.440E+12	0.0500
17880.0 !\AUTHOR: !\REF:		
NC5H11CHO+HO2<=>NC5H10CHO-2+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+HO2<=>NC5H10CHO-3+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+HO2<=>NC5H10CHO-4+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+HO2<=>NC5H10CHO-5+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+CH3O2<=>NC5H10CHO-1+CH3O2H	3.440E+12	0.0500
17880.0 !\AUTHOR: !\REF:		
NC5H11CHO+CH3O2<=>NC5H10CHO-2+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+CH3O2<=>NC5H10CHO-3+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+CH3O2<=>NC5H10CHO-4+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CHO+CH3O2<=>NC5H10CHO-5+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
NC5H11CO<=>C5H11-1+CO	1.000E+11	0.0000
9600.0 !\AUTHOR: !\REF:		
C2H3CHO+NC3H7<=>NC5H10CHO-1	1.230E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
HCO+C5H10-1<=>NC5H10CHO-2	1.000E+11	0.0000
6000.0 !\AUTHOR: !\REF:		
NC5H10CHO-3<=>CH2CHO+C4H8-1	7.400E+11	0.0000
21970.0 !\AUTHOR: !\REF:		
NC5H10CHO-4<=>CH2CH2CHO+C3H6	7.400E+11	0.0000
21970.0 !\AUTHOR: !\REF:		
NC5H10CHO-5<=>C3H6CHO-1+C2H4	7.400E+11	0.0000
21970.0 !\AUTHOR: !\REF:		

!-----

!\ENDSUBMECH: \NC5H11CHO

!-----

!-----

!\SUBMECH: \C6H10D13\C6H10D24

!-----

C6H111-3+O2<=>C6H10D13+HO2	2.000E+12	0.0000
----------------------------	-----------	--------

5000.0 !\AUTHOR: !\REF:

C6H112-4+O2<=>C6H10D24+HO2	2.000E+12	0.0000
----------------------------	-----------	--------

5000.0 !\AUTHOR: !\REF:

!-----

!\ENDSUBMECH: \C6H10D13\C6H10D24

!-----

!-----

!\SUBMECH: \C6H10-15

!-----

!-----

```

!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
-----
C6H101-5<=>C3H5-A+C3H5-A                4.900E+022        -2.060
63355.5 !\AUTHOR: !\REF:
PLOG/      1.0000      5.070E+047      -9.700      72680.0/
PLOG/      4.0000      4.220E+039      -7.300      69390.0/
PLOG/     10.0000      2.120E+035      -6.000      67620.0/
!

```

```

!\REACTIONCLASS: \RH_R_ABSTRACTION      \A                \N
\EA
!
-----
C6H101-5+H<=>C6H9-A+H2                    6.752E+005         2.360
207.0 !\AUTHOR: !\REF:
C6H101-5+O2<=>C6H9-A+HO2                  4.000E+014         0.000
38890.0 !\AUTHOR: !\REF:
C6H101-5+O<=>C6H9-A+OH                    1.320E+006         2.430
1210.0 !\AUTHOR: !\REF:
C6H101-5+OH<=>C6H9-A+H2O                  5.528E+004         2.640
-1919.0 !\AUTHOR: !\REF:
C6H101-5+CH3<=>C6H9-A+CH4                 7.380E+000         3.310
4002.0 !\AUTHOR: !\REF:
!

```

```

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A                \N
\EA
!
-----
C4H6+C2H3<=>C6H9-A                        8.800E+005         2.500
6130.0 !\AUTHOR: !\REF:
!

```

```

!\REACTIONCLASS: \RADICAL_ADDITION\H     \A                \N
\EA
!
-----
C6H101-5+H=>C3H4-A+C3H5-A+H2              1.000E+012         0.000
0.0 !\AUTHOR: !\REF:
C6H101-5+H<=>C3H5-A+C3H6                  1.000E+013         0.000
0.0 !\AUTHOR: !\REF:
!-----

```

```

!\ENDSUBMECH: \C6H10-15
!-----

```

```

!+++++
+++++
+++++
!\END_KINETICS_MODULE: \C6
!+++++
+++++
+++++
!+++++
+++++
+++++

```

```

!\KINETICS_MODULE: \C7
!\MODSUBMECHS: \NC7H16
!+++++
!-----
!-----
!\SUBMECH: \NC7H16
!-----
!-----
!
```

```

!\REACTIONCLASS: \1. F_UNIMOLECULAR_DECOMPOSITION \A \N
\EA !REF: CALCULATED BASED ON LJ PARAMETERS FROM A. W. JASPER, J. A.
MILLER. COMBUST. FLAME (2013)
!
```

NC7H16<=>C6H13-1+CH3	5.73E+35	-5.68	96525.
PLOG / 1.000E-002 3.21E+84	-20.20	120586. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001 1.98E+69	-15.58	114157. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000 5.48E+51	-10.36	105321. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000 3.58E+46	-8.84	102532. /	!\AUTHOR: !\REF:
PLOG / 5.000E+000 1.36E+40	-6.96	98990. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001 5.73E+35	-5.68	96525. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001 8.09E+31	-4.56	94324. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001 5.41E+27	-3.35	91903. /	!\AUTHOR: !\REF:
NC7H16<=>C5H11-1+C2H5	2.11E+28	-3.39	91711.
PLOG / 1.000E-002 5.31E+77	-18.03	116934. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001 2.48E+61	-13.11	109490. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000 4.62E+43	-7.87	100282. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000 4.04E+38	-6.39	97509. /	!\AUTHOR: !\REF:
PLOG / 5.000E+000 2.82E+32	-4.59	94062. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001 2.11E+28	-3.39	91711. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001 5.56E+24	-2.35	89645. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001 8.45E+20	-1.24	87414. /	!\AUTHOR: !\REF:
NC7H16<=>PC4H9+NC3H7	1.04E+39	-6.31	95823.
PLOG / 1.000E-002 8.03E+87	-20.87	120084. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001 3.26E+72	-16.19	113496. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000 8.14E+54	-10.97	104592. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000 5.51E+49	-9.45	101803. /	!\AUTHOR: !\REF:
PLOG / 5.000E+000 2.27E+43	-7.58	98272. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001 1.04E+39	-6.31	95823. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001 1.60E+35	-5.20	93640. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001 1.21E+31	-4.01	91246. /	!\AUTHOR: !\REF:
NC7H16<=>C7H15-1+H	5.41E+114	-29.17	154079.
PLOG / 1.000E-002 7.75E+101	-26.74	136707. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001 1.58E+109	-28.45	142837. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000 2.70E+116	-30.07	150954. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000 1.34E+117	-30.14	152681. /	!\AUTHOR: !\REF:
PLOG / 5.000E+000 2.87E+116	-29.78	153956. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001 5.41E+114	-29.17	154079. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001 1.18E+112	-28.31	153502. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001 2.96E+107	-26.88	151838. /	!\AUTHOR: !\REF:
NC7H16<=>C7H15-2+H	6.16E+114	-29.08	151369.
PLOG / 1.000E-002 1.12E+104	-27.26	134548. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001 1.21E+112	-29.16	141621. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000 1.82E+118	-30.48	149382. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000 2.58E+118	-30.39	150791. /	!\AUTHOR: !\REF:

PLOG / 5.000E+000	1.04E+117	-29.83	151596. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001	6.16E+114	-29.08	151369. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001	5.15E+111	-28.11	150481. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001	5.42E+106	-26.58	148505. /	!\AUTHOR: !\REF:
NC7H16<=>C7H15-3+H		6.16E+114	-29.08	151369.
PLOG / 1.000E-002	1.12E+104	-27.26	134548. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001	1.21E+112	-29.16	141621. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000	1.82E+118	-30.48	149382. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000	2.58E+118	-30.39	150791. /	!\AUTHOR: !\REF:
PLOG / 5.000E+000	1.04E+117	-29.83	151596. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001	6.16E+114	-29.08	151369. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001	5.15E+111	-28.11	150481. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001	5.42E+106	-26.58	148505. /	!\AUTHOR: !\REF:
NC7H16<=>C7H15-4+H		3.08E+114	-29.08	151369.
PLOG / 1.000E-002	5.59E+103	-27.26	134548. /	!\AUTHOR: !\REF:
PLOG / 1.000E-001	6.06E+111	-29.16	141621. /	!\AUTHOR: !\REF:
PLOG / 1.000E+000	9.11E+117	-30.48	149382. /	!\AUTHOR: !\REF:
PLOG / 2.000E+000	1.29E+118	-30.39	150791. /	!\AUTHOR: !\REF:
PLOG / 5.000E+000	5.18E+116	-29.83	151596. /	!\AUTHOR: !\REF:
PLOG / 1.000E+001	3.08E+114	-29.08	151369. /	!\AUTHOR: !\REF:
PLOG / 2.000E+001	2.57E+111	-28.11	150481. /	!\AUTHOR: !\REF:
PLOG / 5.000E+001	2.71E+106	-26.58	148505. /	!\AUTHOR: !\REF:

!

!\REACTIONCLASS: \2. F_H ABSTRACTION	\A	\N
\EA !REF: H. J. Curran, et al., Combust. Flame, 114, (1998)	149-177.	

!

NC7H16+H<=>C7H15-1+H2	3.490E+05	2.7000
6450.0 !\AUTHOR: !\REF:		
NC7H16+H<=>C7H15-2+H2	2.600E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
NC7H16+H<=>C7H15-3+H2	2.600E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
NC7H16+H<=>C7H15-4+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
NC7H16+O<=>C7H15-1+OH	1.130E+14	0.0000
7850.0 !\AUTHOR: !\REF:		
NC7H16+O<=>C7H15-2+OH	5.620E+13	0.0000
5200.0 !\AUTHOR: !\REF:		
NC7H16+O<=>C7H15-3+OH	5.620E+13	0.0000
5200.0 !\AUTHOR: !\REF:		
NC7H16+O<=>C7H15-4+OH	2.810E+13	0.0000
5200.0 !\AUTHOR: !\REF:		
NC7H16+OH<=>C7H15-1+H2O	2.731E+07	1.8130
868.4 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC7H16+OH<=>C7H15-2+H2O	1.410E+10	0.9350
504.7 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC7H16+OH<=>C7H15-3+H2O	1.144E+07	1.8110
-1015.5 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC7H16+OH<=>C7H15-4+H2O	5.617E+11	0.3200
846.5 !\AUTHOR: !\REF: R. SIVARAMAKRISHNAN, J. V. MICHAEL, J. PHYS. CHEM. A, 2009, 113, 5047-5060		
NC7H16+O2<=>C7H15-1+HO2	4.200E+13	0.0000
52800.0 !\AUTHOR: !\REF:		

NC7H16+O2<=>C7H15-2+HO2	2.800E+13	0.0000
50160.0 !\AUTHOR: !\REF:		
NC7H16+O2<=>C7H15-3+HO2	2.800E+13	0.0000
50160.0 !\AUTHOR: !\REF:		
NC7H16+O2<=>C7H15-4+HO2	1.400E+13	0.0000
50160.0 !\AUTHOR: !\REF:		
NC7H16+HO2<=>C7H15-1+H2O2	4.080E+01	3.6000
17160.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC7H16+HO2<=>C7H15-2+H2O2	1.260E+02	3.4000
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC7H16+HO2<=>C7H15-3+H2O2	1.260E+02	3.4000
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC7H16+HO2<=>C7H15-4+H2O2	6.320E+01	3.4000
13720.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE, ET AL, J. PHYS. CHEM. A, 2008, 112, 7047-7054		
NC7H16+CH3<=>C7H15-1+CH4	9.040E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
NC7H16+CH3<=>C7H15-2+CH4	1.680E+05	2.1000
7574.0 !\AUTHOR: !\REF:		
NC7H16+CH3<=>C7H15-3+CH4	1.680E+05	2.1000
7574.0 !\AUTHOR: !\REF:		
NC7H16+CH3<=>C7H15-4+CH4	8.400E+04	2.1000
7574.0 !\AUTHOR: !\REF:		
NC7H16+CH3O<=>C7H15-1+CH3OH	3.160E+11	0.0000
7000.0 !\AUTHOR: !\REF:		
NC7H16+CH3O<=>C7H15-2+CH3OH	2.190E+11	0.0000
5000.0 !\AUTHOR: !\REF:		
NC7H16+CH3O<=>C7H15-3+CH3OH	2.190E+11	0.0000
5000.0 !\AUTHOR: !\REF:		
NC7H16+CH3O<=>C7H15-4+CH3OH	1.095E+11	0.0000
5000.0 !\AUTHOR: !\REF:		
NC7H16+CH3O2<=>C7H15-1+CH3O2H	1.390E+00	4.0000
18280.0 !\AUTHOR: !\REF:		
NC7H16+CH3O2<=>C7H15-2+CH3O2H	2.040E+01	3.6000
14810.0 !\AUTHOR: !\REF:		
NC7H16+CH3O2<=>C7H15-3+CH3O2H	2.040E+01	3.6000
14810.0 !\AUTHOR: !\REF:		
NC7H16+CH3O2<=>C7H15-4+CH3O2H	1.020E+01	3.6000
14810.0 !\AUTHOR: !\REF:		
NC7H16+O2CHO<=>C7H15-1+HO2CHO	1.390E+00	4.0000
18280.0 !\AUTHOR: !\REF:		
NC7H16+O2CHO<=>C7H15-2+HO2CHO	2.040E+01	3.6000
14810.0 !\AUTHOR: !\REF:		
NC7H16+O2CHO<=>C7H15-3+HO2CHO	2.040E+01	3.6000
14810.0 !\AUTHOR: !\REF:		
NC7H16+O2CHO<=>C7H15-4+HO2CHO	1.020E+01	3.6000
14810.0 !\AUTHOR: !\REF:		
NC7H16+C2H3<=>C7H15-1+C2H4	1.000E+12	0.0000
18000.0 !\AUTHOR: !\REF:		
NC7H16+C2H3<=>C7H15-2+C2H4	8.000E+11	0.0000
16800.0 !\AUTHOR: !\REF:		
NC7H16+C2H3<=>C7H15-3+C2H4	8.000E+11	0.0000
16800.0 !\AUTHOR: !\REF:		
NC7H16+C2H3<=>C7H15-4+C2H4	4.000E+11	0.0000
16800.0 !\AUTHOR: !\REF:		

NC7H16+C2H5<=>C7H15-1+C2H6	1.000E+11	0.0000
13400.0 !\AUTHOR: !\REF:		
NC7H16+C2H5<=>C7H15-2+C2H6	1.000E+11	0.0000
10400.0 !\AUTHOR: !\REF:		
NC7H16+C2H5<=>C7H15-3+C2H6	1.000E+11	0.0000
10400.0 !\AUTHOR: !\REF:		
NC7H16+C2H5<=>C7H15-4+C2H6	5.000E+10	0.0000
10400.0 !\AUTHOR: !\REF:		
!		

!\REACTIONCLASS: \3. R_DECOMPOSITION \A \N
\EA !REF: W. Tsang, et al., "Soot precursor from real fuels: the
unimolecular reaction of fuel radicals", 2009, ISBN: 978-3-86644-441-6
!

C7H15-1(+M)<=>C2H4+C5H11-1(+M)	7.94E+11	0.33
27210.0 !\AUTHOR: !\REF:		
LOW /	2.80E-44	18.729
-602.5 /		
TROE / -14.66 219.0 28.0 50000.0 /		
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/		
C7H15-2(+M)<=>PC4H9+C3H6(+M)	5.01E+11	0.56
28092.2 !\AUTHOR: !\REF:		
LOW /	8.90E-39	16.934
-602.5 /		
TROE / -25.27 223.0 28.0 50000.0 /		
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/		
C7H15-3(+M)<=>NC3H7+C4H8-1(+M)	2.95E+12	0.31
28257.1 !\AUTHOR: !\REF:		
LOW /	2.00E-38	16.814
-602.4 /		
TROE / -20.96 221.0 28.0 50000.0 /		
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/		
C7H15-3(+M)<=>C6H12-1+CH3(+M)	1.10E+11	0.75
29401.6 !\AUTHOR: !\REF:		
LOW /	1.06E-42	18.004
-602.4 /		
TROE / -20.94 217.0 28.0 50000.0 /		
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/		
C7H15-4(+M)<=>C2H5+C5H10-1(+M)	5.89E+12	0.31
28257.1 !\AUTHOR: !\REF:		
LOW /	2.10E-38	16.897
-602.5 /		
TROE / -27.54 224.0 28.0 50000.0 /		
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/		
!		

!\REACTIONCLASS: \4. R+O2=E+HO2 \A \N
\EA !REF: J. D. DESAIN, ET AL., J. PHYS. CHEM. A, 107, 2003, 4415-4427
!

C7H15-1+O2<=>C7H14-1+HO2	8.370E-01	3.6000
11960.0		
C7H15-2+O2<=>C7H14-1+HO2	5.350E-01	3.7000
9322.0		
C7H15-2+O2<=>C7H14-2+HO2	1.070E+00	3.7000
9322.0		

C7H15-3+O2<=>C7H14-2+HO2 9322.0	1.070E+00	3.7000
C7H15-3+O2<=>C7H14-3+HO2 9322.0	1.070E+00	3.7000
C7H15-4+O2<=>C7H14-3+HO2 9322.0	2.140E+00	3.7000

!

!\REACTIONCLASS: \5. R_ISOMERIZATION \A \N
 \EA !REF: H. J. Curran, et al., Combust. Flame, 114, (1998) 149-177.

!

C7H15-1<=>C7H15-3 33760.0 !\AUTHOR: !\REF:	1.386E+09	0.9800
C7H15-1<=>C7H15-4 19760.0 !\AUTHOR: !\REF:	2.541E+09	0.3500
C7H15-2<=>C7H15-3 39700.0 !\AUTHOR: !\REF:	9.587E+08	1.3900
C7H15-1<=>C7H15-2 38760.0 !\AUTHOR: !\REF:	5.478E+08	1.6200

!

!\REACTIONCLASS: \10. R+O2=RO2 \A \N
 \EA !REF: A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74

!

C7H15-1+O2<=>C7H15-1O2 198.7 !\AUTHOR: !\REF:	6.863E+16	-1.6270
C7H15-2+O2<=>C7H15-2O2 -536.5 !\AUTHOR: !\REF:	3.486E+14	-0.8160
C7H15-3+O2<=>C7H15-3O2 -536.5 !\AUTHOR: !\REF:	3.486E+14	-0.8160
C7H15-4+O2<=>C7H15-4O2 -536.5 !\AUTHOR: !\REF:	3.486E+14	-0.8160

!

!\REACTIONCLASS: \11. R+R'O2=RO+R'O \A \N
 \EA !REF: ESTIMATED

!

C7H15-1+HO2<=>C7H15-1O+OH -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-2+HO2<=>C7H15-2O+OH -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-3+HO2<=>C7H15-3O+OH -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-4+HO2<=>C7H15-4O+OH -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-1+CH3O2<=>C7H15-1O+CH3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-2+CH3O2<=>C7H15-2O+CH3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-3+CH3O2<=>C7H15-3O+CH3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-4+CH3O2<=>C7H15-4O+CH3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H15-1+C7H15-1O2<=>C7H15-1O+C7H15-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000

C7H15OOH-1+O2<=>C7H15-1O2+HO2	3.750E+13	-0.8000
33620.0 !\AUTHOR: !\REF:		
C7H15OOH-2+O2<=>C7H15-2O2+HO2	4.380E+13	-0.8000
33640.0 !\AUTHOR: !\REF:		
C7H15OOH-3+O2<=>C7H15-3O2+HO2	4.380E+13	-0.8000
33640.0 !\AUTHOR: !\REF:		
C7H15OOH-4+O2<=>C7H15-4O2+HO2	4.380E+13	-0.8000
33640.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \14. RO2+H2O2=ROOH+HO2	\A	\N
\EA !REF: ANOLOGY TO N-HEXANE		

!

C7H15OOH-1+HO2<=>C7H15-1O2+H2O2	2.400E+12	0.0000
10000.0 !\AUTHOR: !\REF:		
C7H15OOH-2+HO2<=>C7H15-2O2+H2O2	2.400E+12	0.0000
10000.0 !\AUTHOR: !\REF:		
C7H15OOH-3+HO2<=>C7H15-3O2+H2O2	2.400E+12	0.0000
10000.0 !\AUTHOR: !\REF:		
C7H15OOH-4+HO2<=>C7H15-4O2+H2O2	2.400E+12	0.0000
10000.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \14A. RO2+F=ROOH+R'	\A	\N
\EA !REF: ANOLOGY TO N-HEXANE		

!

C7H15-1O2+NC7H16<=>C7H15OOH-1+C7H15-1	1.210E+13	0.0000
20430.0 !\AUTHOR: !\REF:		
C7H15-1O2+NC7H16<=>C7H15OOH-1+C7H15-2	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-1O2+NC7H16<=>C7H15OOH-1+C7H15-3	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-1O2+NC7H16<=>C7H15OOH-1+C7H15-4	4.030E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-2O2+NC7H16<=>C7H15OOH-2+C7H15-1	1.210E+13	0.0000
20430.0 !\AUTHOR: !\REF:		
C7H15-2O2+NC7H16<=>C7H15OOH-2+C7H15-2	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-2O2+NC7H16<=>C7H15OOH-2+C7H15-3	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-2O2+NC7H16<=>C7H15OOH-2+C7H15-4	4.030E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-3O2+NC7H16<=>C7H15OOH-3+C7H15-1	1.210E+13	0.0000
20430.0 !\AUTHOR: !\REF:		
C7H15-3O2+NC7H16<=>C7H15OOH-3+C7H15-2	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-3O2+NC7H16<=>C7H15OOH-3+C7H15-3	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-3O2+NC7H16<=>C7H15OOH-3+C7H15-4	4.030E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-4O2+NC7H16<=>C7H15OOH-4+C7H15-1	1.210E+13	0.0000
20430.0 !\AUTHOR: !\REF:		
C7H15-4O2+NC7H16<=>C7H15OOH-4+C7H15-2	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H15-4O2+NC7H16<=>C7H15OOH-4+C7H15-3	8.060E+12	0.0000
17700.0 !\AUTHOR: !\REF:		

C7H15-4O2+NC7H16<=>C7H15OOH-4+C7H15-4 4.030E+12 0.0000
17700.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \15. RO2+CH3O2=RO+CH3O+O2 \A \N
\EA !REF: ANOLOGY TO N-HEXANE
!

C7H15-1O2+CH3O2=>C7H15-1O+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-2O2+CH3O2=>C7H15-2O+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-3O2+CH3O2=>C7H15-3O+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-4O2+CH3O2=>C7H15-4O+CH3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \16. RO2+R'O2=RO+R'O+O2 \A \N
\EA !REF: ANOLOGY TO N-HEXANE
!

C7H15-1O2+C7H15-1O2=>C7H15-1O+C7H15-1O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-1O2+C7H15-2O2=>C7H15-1O+C7H15-2O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-1O2+C7H15-3O2=>C7H15-1O+C7H15-3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-1O2+C7H15-4O2=>C7H15-1O+C7H15-4O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-2O2+C7H15-2O2=>C7H15-2O+C7H15-2O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-2O2+C7H15-3O2=>C7H15-2O+C7H15-3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-2O2+C7H15-4O2=>C7H15-2O+C7H15-4O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-3O2+C7H15-3O2=>C7H15-3O+C7H15-3O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-3O2+C7H15-4O2=>C7H15-3O+C7H15-4O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
C7H15-4O2+C7H15-4O2=>C7H15-4O+C7H15-4O+O2 1.400E+16 -1.6000
1860.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \17. ROOH=RO+OH \A \N
\EA !REF: ESTIMATED
!

C7H15OOH-1<=>C7H15-1O+OH 1.500E+16 0.0000
42000.0 !\AUTHOR: !\REF:
C7H15OOH-2<=>C7H15-2O+OH 1.050E+16 0.0000
41600.0 !\AUTHOR: !\REF:
C7H15OOH-3<=>C7H15-3O+OH 1.050E+16 0.0000
41600.0 !\AUTHOR: !\REF:
C7H15OOH-4<=>C7H15-4O+OH 1.050E+16 0.0000
41600.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \18. RO_DECOMPOSITION \A \N
\EA !REF: ESTIMATED
!

C7H15-1O=>PC4H9+C2H4+CH2O	2.000E+13	0.0000
15000.0 !\AUTHOR: !\REF:		
C7H15-2O=>CH3CHO+C2H4+NC3H7	2.000E+13	0.0000
15000.0 !\AUTHOR: !\REF:		
C7H15-3O=>NC3H7+CH3CO+C2H5	2.000E+13	0.0000
15000.0 !\AUTHOR: !\REF:		
C7H15-4O=>HCO+NC3H7+NC3H7	2.000E+13	0.0000
15000.0 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \19. QOOH=CETH+OH \A \N
\EA !REF: BASED ON:S. M. VILLANO, ET AL., J. PHYS. CHEM. A 2012, 116,
5068-5089
!

C7H14OOH1-2<=>C7H14O1-2+OH	1.780E+12	0.0000
13376.0 !\AUTHOR: !\REF:		
C7H14OOH1-3<=>C7H14O1-3+OH	3.170E+11	0.0000
18292.0 !\AUTHOR: !\REF:		
C7H14OOH1-4<=>C7H14O1-4+OH	2.770E+10	0.0000
11501.0 !\AUTHOR: !\REF:		
C7H14OOH1-5<=>C7H14O1-5+OH	5.200E+09	0.0000
11137.0 !\AUTHOR: !\REF:		
C7H14OOH2-1<=>C7H14O1-2+OH	1.780E+12	0.0000
15034.0 !\AUTHOR: !\REF:		
C7H14OOH2-3<=>C7H14O2-3+OH	1.780E+12	0.0000
13364.0 !\AUTHOR: !\REF:		
C7H14OOH2-4<=>C7H14O2-4+OH	3.170E+11	0.0000
17284.0 !\AUTHOR: !\REF:		
C7H14OOH2-5<=>C7H14O2-5+OH	2.770E+10	0.0000
11490.0 !\AUTHOR: !\REF:		
C7H14OOH2-6<=>C7H14O2-6+OH	5.200E+09	0.0000
11129.0 !\AUTHOR: !\REF:		
C7H14OOH3-1<=>C7H14O1-3+OH	3.170E+11	0.0000
19006.0 !\AUTHOR: !\REF:		
C7H14OOH3-2<=>C7H14O2-3+OH	1.780E+12	0.0000
13364.0 !\AUTHOR: !\REF:		
C7H14OOH3-4<=>C7H14O3-4+OH	1.780E+12	0.0000
13364.0 !\AUTHOR: !\REF:		
C7H14OOH3-5<=>C7H14O3-5+OH	3.170E+11	0.0000
17284.0 !\AUTHOR: !\REF:		
C7H14OOH3-6<=>C7H14O2-5+OH	2.770E+10	0.0000
11490.0 !\AUTHOR: !\REF:		
C7H14OOH3-7<=>C7H14O1-5+OH	5.200E+09	0.0000
11908.0 !\AUTHOR: !\REF:		
C7H14OOH4-1<=>C7H14O1-4+OH	2.770E+10	0.0000
11573.0 !\AUTHOR: !\REF:		
C7H14OOH4-2<=>C7H14O2-4+OH	3.170E+11	0.0000
17284.0 !\AUTHOR: !\REF:		
C7H14OOH4-3<=>C7H14O3-4+OH	1.780E+12	0.0000
13364.0 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \20. QOOH=E+HO2 \A \N
\EA !REF:S. M. VILLANO, ET AL., J. PHYS. CHEM. A 2012, 116, 5068-5089
!

C7H14OOH1-2<=>C7H14-1+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C7H14OOH2-1<=>C7H14-1+HO2	1.780E+12	0.2400
15700.0 !\AUTHOR: !\REF:		
C7H14OOH2-3<=>C7H14-2+HO2	2.650E+11	0.3800
14800.0 !\AUTHOR: !\REF:		
C7H14OOH3-2<=>C7H14-2+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C7H14OOH3-4<=>C7H14-3+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C7H14OOH4-3<=>C7H14-3+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \21. QOOH_DECOMPOSITION \A \N
\EA !REF:S. M. VILLANO, ET AL., J. PHYS. CHEM. A 2012, 116, 5068-5089
!

C7H14OOH1-3=>CH2O+C6H12-1+OH	3.081E+13	0.0000
27330.6 !\AUTHOR: !\REF:		
C7H14OOH1-4<=>C2H4O2H+C5H10-1	1.392E+14	0.0000
28080.6 !\AUTHOR: !\REF:		
C7H14OOH2-4=>CH3CHO+C5H10-1+OH	3.081E+13	0.0000
24904.0 !\AUTHOR: !\REF:		
C7H14OOH2-5<=>C3H6OOH2-1+C4H8-1	1.392E+14	0.0000
28406.1 !\AUTHOR: !\REF:		
C7H14OOH3-1=>PC4H9CHO+C2H4+OH	3.081E+13	0.0000
24608.4 !\AUTHOR: !\REF:		
C7H14OOH3-5=>C2H5CHO+C4H8-1+OH	3.081E+13	0.0000
25136.0 !\AUTHOR: !\REF:		
C7H14OOH3-6<=>C4H8OOH2-1+C3H6	1.392E+14	0.0000
28415.1 !\AUTHOR: !\REF:		
C7H14OOH4-1<=>C5H10OOH2-1+C2H4	1.392E+14	0.0000
28105.2 !\AUTHOR: !\REF:		
C7H14OOH4-2=>NC3H7CHO+C3H6+OH	3.081E+13	0.0000
24774.4 !\AUTHOR: !\REF:		

!\REACTIONCLASS: \22. QOOH+O2=O2QOOH \A \N
\EA !REF:A. MIYOSHI. INT. J. CHEM. KIN. 2012, 44, 1, 59-74 !A*0.5
!

C7H14OOH1-2+O2<=>C7H14OOH1-2O2	1.742E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C7H14OOH1-3+O2<=>C7H14OOH1-3O2	1.742E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C7H14OOH1-4+O2<=>C7H14OOH1-4O2	1.742E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C7H14OOH1-5+O2<=>C7H14OOH1-5O2	1.742E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		
C7H14OOH2-1+O2<=>C7H14OOH2-1O2	3.432E+16	-1.6270
198.7 !\AUTHOR: !\REF:		
C7H14OOH2-3+O2<=>C7H14OOH2-3O2	1.742E+14	-0.8160
-536.5 !\AUTHOR: !\REF:		

C7H14OOH2-4+O2<=>C7H14OOH2-4O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH2-5+O2<=>C7H14OOH2-5O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH2-6+O2<=>C7H14OOH2-6O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH3-1+O2<=>C7H14OOH3-1O2 198.7 !\AUTHOR: !\REF:	3.432E+16	-1.6270
C7H14OOH3-2+O2<=>C7H14OOH3-2O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH3-4+O2<=>C7H14OOH3-4O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH3-5+O2<=>C7H14OOH3-5O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH3-6+O2<=>C7H14OOH3-6O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH3-7+O2<=>C7H14OOH3-7O2 198.7 !\AUTHOR: !\REF:	3.432E+16	-1.6270
C7H14OOH4-1+O2<=>C7H14OOH4-1O2 198.7 !\AUTHOR: !\REF:	3.432E+16	-1.6270
C7H14OOH4-2+O2<=>C7H14OOH4-2O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160
C7H14OOH4-3+O2<=>C7H14OOH4-3O2 -536.5 !\AUTHOR: !\REF:	1.742E+14	-0.8160

!

!\REACTIONCLASS: \23. O2QOOH=KET+OH	\A	\N
\EA !REF: BASED ON:S. SHARMA, ET AL., J. PHYS. CHEM. A 2010, 114, 5689-5701		

!

C7H14OOH1-2O2=>C7KET12+OH 27900.0 !\AUTHOR: !\REF:	2.441E+07	1.6000
C7H14OOH1-3O2=>C7KET13+OH 19900.0 !\AUTHOR: !\REF:	1.098E+04	2.4000
C7H14OOH1-4O2=>C7KET14+OH 17400.0 !\AUTHOR: !\REF:	1.256E+03	2.2000
C7H14OOH1-5O2=>C7KET15+OH 16600.0 !\AUTHOR: !\REF:	1.115E+03	1.8000
C7H14OOH2-1O2=>C7KET21+OH 25700.0 !\AUTHOR: !\REF:	2.763E+08	1.2000
C7H14OOH2-3O2=>C7KET23+OH 26000.0 !\AUTHOR: !\REF:	1.748E+08	1.7000
C7H14OOH2-4O2=>C7KET24+OH 17500.0 !\AUTHOR: !\REF:	1.754E+02	3.1000
C7H14OOH2-5O2=>C7KET25+OH 16200.0 !\AUTHOR: !\REF:	2.536E+02	2.6000
C7H14OOH2-6O2=>C7KET26+OH 14900.0 !\AUTHOR: !\REF:	1.995E+03	1.9000
C7H14OOH3-1O2=>C7KET31+OH 17000.0 !\AUTHOR: !\REF:	5.786E+01	2.9000
C7H14OOH3-2O2=>C7KET32+OH 26000.0 !\AUTHOR: !\REF:	1.748E+08	1.7000
C7H14OOH3-4O2=>C7KET34+OH 26000.0 !\AUTHOR: !\REF:	1.748E+08	1.7000
C7H14OOH3-5O2=>C7KET35+OH 17500.0 !\AUTHOR: !\REF:	1.754E+02	3.1000

C7H14OOH3-6O2=>C7KET36+OH	2.536E+02	2.6000
16200.0 !\AUTHOR: !\REF:		
C7H14OOH3-7O2=>C7KET37+OH	1.995E+03	1.9000
14900.0 !\AUTHOR: !\REF:		
C7H14OOH4-1O2=>C7KET41+OH	3.768E+02	2.2000
15300.0 !\AUTHOR: !\REF:		
C7H14OOH4-2O2=>C7KET42+OH	1.754E+02	3.1000
17500.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O2=>C7KET43+OH	1.748E+08	1.7000
26000.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \23A. O2QOOH=EROOH+HO2	\A	\N
\EA !REF: ANALOGY TO RO2=E+HO2		

!

C7H14OOH1-2O2<=>C7H13-2D1OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13-2D1OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13-3D1OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13-3D1OOH+HO2	1.080E+11	0.7300
29883.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13-3D7OOH+HO2	1.080E+11	0.7300
29883.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13-3D7OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13-2D7OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH2-3O2<=>C7H13-3D2OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH2-4O2<=>C7H13-3D2OOH+HO2	1.080E+11	0.7300
29883.0 !\AUTHOR: !\REF:		
C7H14OOH2-4O2<=>C7H13-3D6OOH+HO2	1.080E+11	0.7300
29883.0 !\AUTHOR: !\REF:		
C7H14OOH2-5O2<=>C7H13-3D6OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH2-5O2<=>C7H13-2D6OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH2-6O2<=>C7H13-2D6OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH2-6O2<=>C7H13-1D6OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C7H14OOH3-1O2<=>C7H13-1D3OOH+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		
C7H14OOH3-2O2<=>C7H13-1D3OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C7H14OOH3-4O2<=>C7H13-3D5OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH3-5O2<=>C7H13-3D5OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH3-5O2<=>C7H13-2D5OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH3-6O2<=>C7H13-2D5OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH3-6O2<=>C7H13-1D5OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		

C7H14OOH3-7O2<=>C7H13-1D5OOH+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		
C7H14OOH4-1O2<=>C7H13-1D4OOH+HO2	3.870E+07	1.5800
28500.0 !\AUTHOR: !\REF:		
C7H14OOH4-2O2<=>C7H13-1D4OOH+HO2	3.605E+09	1.1300
30100.0 !\AUTHOR: !\REF:		
C7H14OOH4-2O2<=>C7H13-2D4OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O2<=>C7H13-2D4OOH+HO2	7.710E+09	1.0100
29362.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \23B. O2QOOH=HOOPOOH	\A	\N
\EA !REF: BASED ON:S. SHARMA, ET AL., J. PHYS. CHEM. A 2010, 114,		
5689-5701		

!

C7H14OOH1-2O2<=>C7H13Q12-3	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-2O2<=>C7H13Q12-4	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C7H14OOH1-2O2<=>C7H13Q12-5	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C7H14OOH1-2O2<=>C7H13Q12-6	1.300E+06	1.0000
18200.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13Q13-2	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13Q13-4	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13Q13-5	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13Q13-6	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2<=>C7H13Q13-7	1.470E+05	1.5000
19900.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13Q14-2	1.407E+11	0.2000
18500.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13Q14-3	3.432E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13Q14-5	3.432E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13Q14-6	1.407E+11	0.2000
18500.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2<=>C7H13Q14-7	1.233E+06	1.5000
20000.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13Q15-2	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13Q15-3	7.033E+10	0.2000
18500.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13Q15-4	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13Q15-6	1.716E+09	0.9000
29500.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2<=>C7H13Q15-7	1.439E+07	1.4000
20800.0 !\AUTHOR: !\REF:		
C7H14OOH2-1O2<=>C7H13Q12-3	1.360E+07	1.3000
18200.0 !\AUTHOR: !\REF:		

C7H14OOH2-1O2<=>C7H13Q12-4 16600.0 !\AUTHOR: !\REF:	3.718E+06	1.2000
C7H14OOH2-1O2<=>C7H13Q12-5 18200.0 !\AUTHOR: !\REF:	2.600E+06	1.0000
C7H14OOH2-3O2<=>C7H13Q23-1 20800.0 !\AUTHOR: !\REF:	1.439E+07	1.4000
C7H14OOH2-3O2<=>C7H13Q23-4 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH2-3O2<=>C7H13Q23-5 18500.0 !\AUTHOR: !\REF:	7.033E+10	0.2000
C7H14OOH2-3O2<=>C7H13Q23-6 16600.0 !\AUTHOR: !\REF:	1.859E+06	1.2000
C7H14OOH2-3O2<=>C7H13Q23-7 19900.0 !\AUTHOR: !\REF:	1.470E+05	1.5000
C7H14OOH2-4O2<=>C7H13Q24-1 20000.0 !\AUTHOR: !\REF:	1.233E+06	1.5000
C7H14OOH2-4O2<=>C7H13Q24-3 29500.0 !\AUTHOR: !\REF:	3.432E+09	0.9000
C7H14OOH2-4O2<=>C7H13Q24-5 29500.0 !\AUTHOR: !\REF:	3.432E+09	0.9000
C7H14OOH2-4O2<=>C7H13Q24-6 18500.0 !\AUTHOR: !\REF:	1.407E+11	0.2000
C7H14OOH2-4O2<=>C7H13Q24-7 20000.0 !\AUTHOR: !\REF:	1.233E+06	1.5000
C7H14OOH2-5O2<=>C7H13Q25-1 19900.0 !\AUTHOR: !\REF:	1.470E+05	1.5000
C7H14OOH2-5O2<=>C7H13Q25-3 18500.0 !\AUTHOR: !\REF:	7.033E+10	0.2000
C7H14OOH2-5O2<=>C7H13Q25-4 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH2-5O2<=>C7H13Q25-6 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH2-5O2<=>C7H13Q25-7 20800.0 !\AUTHOR: !\REF:	1.439E+07	1.4000
C7H14OOH2-6O2<=>C7H13Q26-4 18500.0 !\AUTHOR: !\REF:	7.033E+10	0.2000
C7H14OOH2-6O2<=>C7H13Q26-3 29500.0 !\AUTHOR: !\REF:	8.580E+08	0.9000
DUP		
C7H14OOH2-6O2<=>C7H13Q26-3 16600.0 !\AUTHOR: !\REF:	1.859E+06	1.2000
DUP		
C7H14OOH2-6O2<=>C7H13Q26-1 34200.0 !\AUTHOR: !\REF:	2.110E+11	0.2000
C7H14OOH3-1O2<=>C7H13Q13-2 30100.0 !\AUTHOR: !\REF:	4.009E+08	1.1000
C7H14OOH3-1O2<=>C7H13Q13-4 16600.0 !\AUTHOR: !\REF:	3.718E+06	1.2000
C7H14OOH3-1O2<=>C7H13Q13-5 18200.0 !\AUTHOR: !\REF:	2.600E+06	1.0000
C7H14OOH3-2O2<=>C7H13Q23-1 34200.0 !\AUTHOR: !\REF:	2.110E+11	0.2000
C7H14OOH3-2O2<=>C7H13Q23-4 18500.0 !\AUTHOR: !\REF:	7.033E+10	0.2000
C7H14OOH3-2O2<=>C7H13Q23-5 16600.0 !\AUTHOR: !\REF:	1.859E+06	1.2000
C7H14OOH3-2O2<=>C7H13Q23-6 18200.0 !\AUTHOR: !\REF:	1.300E+06	1.0000

C7H14OOH3-4O2<=>C7H13Q34-1 20000.0 !\AUTHOR: !\REF:	1.233E+06	1.5000
C7H14OOH3-4O2<=>C7H13Q34-2 18500.0 !\AUTHOR: !\REF:	1.407E+11	0.2000
C7H14OOH3-4O2<=>C7H13Q34-5 29500.0 !\AUTHOR: !\REF:	3.432E+09	0.9000
C7H14OOH3-4O2<=>C7H13Q34-6 18500.0 !\AUTHOR: !\REF:	1.407E+11	0.2000
C7H14OOH3-4O2<=>C7H13Q34-7 20000.0 !\AUTHOR: !\REF:	1.233E+06	1.5000
C7H14OOH3-5O2<=>C7H13Q35-1 19900.0 !\AUTHOR: !\REF:	1.470E+05	1.5000
DUP		
C7H14OOH3-5O2<=>C7H13Q35-2 16600.0 !\AUTHOR: !\REF:	1.859E+06	1.2000
DUP		
C7H14OOH3-5O2<=>C7H13Q35-4 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH3-5O2<=>C7H13Q35-2 16600.0 !\AUTHOR: !\REF:	1.859E+06	1.2000
DUP		
C7H14OOH3-5O2<=>C7H13Q35-1 19900.0 !\AUTHOR: !\REF:	1.470E+05	1.5000
DUP		
C7H14OOH3-6O2<=>C7H13Q25-6 18200.0 !\AUTHOR: !\REF:	1.300E+06	1.0000
C7H14OOH3-6O2<=>C7H13Q25-4 18500.0 !\AUTHOR: !\REF:	7.033E+10	0.2000
C7H14OOH3-6O2<=>C7H13Q25-3 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH3-6O2<=>C7H13Q25-1 34200.0 !\AUTHOR: !\REF:	2.110E+11	0.2000
C7H14OOH3-7O2<=>C7H13Q15-4 16600.0 !\AUTHOR: !\REF:	3.718E+06	1.2000
C7H14OOH3-7O2<=>C7H13Q15-3 18200.0 !\AUTHOR: !\REF:	1.360E+07	1.3000
C7H14OOH3-7O2<=>C7H13Q15-2 30100.0 !\AUTHOR: !\REF:	4.009E+08	1.1000
C7H14OOH4-1O2<=>C7H13Q14-2 30100.0 !\AUTHOR: !\REF:	4.009E+08	1.1000
C7H14OOH4-1O2<=>C7H13Q14-3 18200.0 !\AUTHOR: !\REF:	1.360E+07	1.3000
C7H14OOH4-1O2<=>C7H13Q14-5 18200.0 !\AUTHOR: !\REF:	2.600E+06	1.0000
C7H14OOH4-2O2<=>C7H13Q24-1 34200.0 !\AUTHOR: !\REF:	2.110E+11	0.2000
C7H14OOH4-2O2<=>C7H13Q24-3 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH4-2O2<=>C7H13Q24-5 16600.0 !\AUTHOR: !\REF:	1.859E+06	1.2000
C7H14OOH4-2O2<=>C7H13Q24-6 18200.0 !\AUTHOR: !\REF:	1.300E+06	1.0000
C7H14OOH4-3O2<=>C7H13Q34-1 20800.0 !\AUTHOR: !\REF:	1.439E+07	1.4000
C7H14OOH4-3O2<=>C7H13Q34-2 29500.0 !\AUTHOR: !\REF:	1.716E+09	0.9000
C7H14OOH4-3O2<=>C7H13Q34-5 18500.0 !\AUTHOR: !\REF:	7.033E+10	0.2000

C7H14OOH4-3O2<=>C7H13Q34-6	1.859E+06	1.2000
16600.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O2<=>C7H13Q34-7	1.470E+05	1.5000
19900.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \23C. HOOPOOH_DECOMPOSITION	\A	\N
\EA !REF: ANALOGY TO QOOH_DECOMPOSITION		

!

C7H13Q12-3=>NC5H10CHO-1+CH2O2H+OH	3.081E+13	0.0000
55888.8 !\AUTHOR: !\REF:		
C7H13Q12-4=>C5H10-1+HO2CH2CHO+OH	3.081E+13	0.0000
3964.8 !\AUTHOR: !\REF:		
C7H13Q12-5<=>C4H8-1+C3H51-2,3OOH	1.392E+14	0.0000
26025.1 !\AUTHOR: !\REF:		
C7H13Q13-4=>C2H4O2H+PC4H8CHO-1+OH	1.392E+14	0.0000
47820.9 !\AUTHOR: !\REF:		
C7H13Q13-5=>C3KET13+C4H8-1+OH	3.081E+13	0.0000
24276.4 !\AUTHOR: !\REF:		
C7H13Q13-6=>C4H71-4OOH+C3H6+HO2	1.392E+14	0.0000
28415.1 !\AUTHOR: !\REF:		
C7H13Q14-2=>AC3H5OOH+NC3H7CHO+OH	3.081E+13	0.0000
26500.4 !\AUTHOR: !\REF:		
C7H13Q14-3=>C6H11-1D3OOH+CH2O+OH	3.081E+13	0.0000
28968.4 !\AUTHOR: !\REF:		
C7H13Q14-6=>NC4KET14+C3H6+OH	3.081E+13	0.0000
24774.4 !\AUTHOR: !\REF:		
C7H13Q14-7<=>C5H91-2,5OOH+C2H4	1.392E+14	0.0000
27547.1 !\AUTHOR: !\REF:		
C7H13Q15-2<=>AC3H5OOH+C4H8OOH2-1	1.392E+14	0.0000
31443.6 !\AUTHOR: !\REF:		
C7H13Q15-3=>C6H11-1D4OOH+CH2O+OH	3.081E+13	0.0000
27330.6 !\AUTHOR: !\REF:		
C7H13Q15-3=>C4H71-4OOH+C2H5CHO+OH	3.081E+13	0.0000
24886.9 !\AUTHOR: !\REF:		
C7H13Q15-4<=>C2H4O2H+C5H91-3OOH	1.392E+14	0.0000
27615.6 !\AUTHOR: !\REF:		
C7H13Q15-7=>NC5KET15+C2H4+OH	3.081E+13	0.0000
24062.5 !\AUTHOR: !\REF:		
C7H13Q23-1=>CH2CHO+PC4H9CHO+2OH	3.081E+13	0.0000
31595.2 !\AUTHOR: !\REF:		
C7H13Q23-4=>CH3CHO+PC4H8CHO-1+2OH	3.081E+13	0.0000
31428.9 !\AUTHOR: !\REF:		
C7H13Q23-5=>C3KET12+C4H8-1+OH	3.081E+13	0.0000
24032.6 !\AUTHOR: !\REF:		
C7H13Q23-6=>C4H71-3OOH+C3H6+HO2	1.392E+14	0.0000
28415.1 !\AUTHOR: !\REF:		
C7H13Q24-1=>CH2CHO+C5H10OOH2-1+OH	1.392E+14	0.0000
48655.8 !\AUTHOR: !\REF:		
C7H13Q24-6=>NC4KET13+C3H6+OH	3.081E+13	0.0000
24774.4 !\AUTHOR: !\REF:		
C7H13Q24-7<=>C5H91-2,4OOH+C2H4	1.392E+14	0.0000
27863.4 !\AUTHOR: !\REF:		
C7H13Q25-3=>C2H5CHO+C4H71-3OOH+OH	3.081E+13	0.0000
24865.7 !\AUTHOR: !\REF:		
C7H13Q25-4=>CH3CHO+C5H91-3OOH+OH	3.081E+13	0.0000
24638.9 !\AUTHOR: !\REF:		

C7H13Q25-7=>NC5KET14+C2H4+OH	3.081E+13	0.0000
24242.7 !\AUTHOR: !\REF:		
C7H13Q26-3<=>C4H71-3OOH+C3H6OOH2-1	1.392E+14	0.0000
27931.8 !\AUTHOR: !\REF:		
C7H13Q26-4=>CH3CHO+C5H91-4OOH+OH	3.081E+13	0.0000
24840.3 !\AUTHOR: !\REF:		
C7H13Q34-1=>NC5KET12+C2H4+OH	3.081E+13	0.0000
25467.1 !\AUTHOR: !\REF:		
C7H13Q34-2=>CH3CHCHO+NC3H7CHO+2OH	3.081E+13	0.0000
31087.6 !\AUTHOR: !\REF:		
C7H13Q34-5=>C2H5CHO+C3H6CHO-3+2OH	3.081E+13	0.0000
31676.9 !\AUTHOR: !\REF:		
C7H13Q34-6=>NC4KET12+C3H6+OH	3.081E+13	0.0000
26528.9 !\AUTHOR: !\REF:		
C7H13Q34-7<=>C5H91-2,3OOH+C2H4	1.392E+14	0.0000
27863.4 !\AUTHOR: !\REF:		
C7H13Q35-1=>NC5KET13+C2H4+OH	3.081E+13	0.0000
24242.7 !\AUTHOR: !\REF:		
C7H13Q35-2=>CH3CHCHO+C4H8OOH2-1+OH	1.392E+14	0.0000
47783.7 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \24. KET_DECOMPOSITION	\A	\N
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\EA !REF: ESTIMATED

!

C7KET12<=>C7KET12O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET13<=>C7KET13O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET14<=>C7KET14O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET15<=>C7KET15O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET21<=>C7KET21O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		
C7KET23<=>C7KET23O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET24<=>C7KET24O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET25<=>C7KET25O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET26<=>C7KET26O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET31<=>C7KET31O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		
C7KET32<=>C7KET32O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET34<=>C7KET34O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET35<=>C7KET35O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET36<=>C7KET36O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET37<=>C7KET37O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		
C7KET41<=>C7KET41O+OH	1.500E+16	0.0000
42300.0 !\AUTHOR: !\REF:		

C7KET42<=>C7KET42O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET43<=>C7KET43O+OH	1.050E+16	0.0000
41900.0 !\AUTHOR: !\REF:		
C7KET120<=>NC5H11CHO+HCO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET130<=>PC4H9CHO+CH2CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET140<=>NC3H7CHO+CH2CH2CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET150<=>C2H5CHO+C3H6CHO-1	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET210<=>CH2O+NC5H11CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET230<=>PC4H9CHO+CH3CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET240<=>NC3H7CHO+CH3COCH2	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET250<=>C2H5CHO+CH2CH2COCH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET260<=>CH3CHO+CH2CH2CH2COCH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET310<=>CH2O+C6Y2-1J	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET320<=>CH3CHO+PC4H9CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET340<=>NC3H7CHO+C2H5CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET350<=>C2H5CHO+C2H5COCH2	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET360<=>CH3CHO+CH2CH2COC2H5	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET370<=>C6Y3-6J+CH2O	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET410<=>C6Y3-1J+CH2O	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET420<=>CH3CHO+NC3H7COCH2	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7KET430<=>C2H5CHO+NC3H7CO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \24A. HOOPHOH=EROOH+HO2

\A

\N

\EA !REF: ANALOGY TO QOOH=E+HO2

!

C7H13Q12-3<=>C7H13-2D1OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C7H13Q13-2<=>C7H13-1D3OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C7H13Q13-2<=>C7H13-2D1OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C7H13Q13-4<=>C7H13-3D1OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		
C7H13Q14-2<=>C7H13-1D4OOH+HO2	5.630E+09	0.9700
15000.0 !\AUTHOR: !\REF:		
C7H13Q14-3<=>C7H13-3D1OOH+HO2	3.500E+11	0.3700
14900.0 !\AUTHOR: !\REF:		

C7H13Q14-5<=>C7H13-3D7OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q15-2<=>C7H13-1D5OOH+HO2 15000.0 !\AUTHOR: !\REF:	5.630E+09	0.9700
C7H13Q15-4<=>C7H13-3D7OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q15-6<=>C7H13-2D7OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q23-1<=>C7H13-1D3OOH+HO2 15700.0 !\AUTHOR: !\REF:	1.780E+12	0.2400
C7H13Q23-4<=>C7H13-3D2OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q24-1<=>C7H13-1D4OOH+HO2 15700.0 !\AUTHOR: !\REF:	1.780E+12	0.2400
C7H13Q24-3<=>C7H13-2D4OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q24-3<=>C7H13-3D2OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q24-5<=>C7H13-3D6OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q25-1<=>C7H13-1D5OOH+HO2 15700.0 !\AUTHOR: !\REF:	1.780E+12	0.2400
C7H13Q25-3<=>C7H13-2D5OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q25-4<=>C7H13-3D6OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q25-6<=>C7H13-2D6OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q26-1<=>C7H13-1D6OOH+HO2 15700.0 !\AUTHOR: !\REF:	1.780E+12	0.2400
C7H13Q26-3<=>C7H13-2D6OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q34-2<=>C7H13-2D4OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q34-5<=>C7H13-3D5OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q35-2<=>C7H13-2D5OOH+HO2 14900.0 !\AUTHOR: !\REF:	3.500E+11	0.3700
C7H13Q35-4<=>C7H13-3D5OOH+HO2 14900.0 !\AUTHOR: !\REF:	7.000E+11	0.3700

!

!\REACTIONCLASS: \24B. EROOH_DECOMPOSITION

\A

\N

\EA !REF: ESTIMATED

!

C7H13-1D3OOH=>C2H3CHO+PC4H9+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-1D4OOH=>C3H5-A+NC3H7CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-1D5OOH=>C4H71-4+C2H5CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-1D6OOH=>C5H91-5+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-2D1OOH=>C2H2+PC4H9+CH2O2H 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-2D4OOH=>SC3H5CHO+NC3H7+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000

C7H13-2D5OOH=>C4H71-3+C2H5CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-2D6OOH=>C5H92-5+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-2D7OOH=>C6H112-6+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13-3D1OOH=>C6H111-3+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13-3D2OOH=>C6D2Y1+CH3+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13-3D5OOH=>C5D2Y1+C2H5+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-3D6OOH=>C5H91-3+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13-3D7OOH=>C6H113-1+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000

!\REACTIONCLASS: \24C. HOOPOOH=CETH-OOH+OH \EA !REF: ANALOGY TO QOOH=CETH+OH	\A	\N
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C7H13Q12-3<=>C7H13O13-2OOH+OH 18002.9 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q12-3<=>C7H13O23-1OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q12-4<=>C7H13O14-2OOH+OH 11501.1 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q12-4<=>C7H13O24-1OOH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q12-5<=>C7H13O15-2OOH+OH 11137.0 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q12-5<=>C7H13O25-1OOH+OH 10489.7 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q12-6<=>C7H13O26-1OOH+OH 11128.8 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q13-2<=>C7H13O12-3OOH+OH 13376.0 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q13-2<=>C7H13O23-1OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q13-4<=>C7H13O14-3OOH+OH 11067.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q13-4<=>C7H13O34-1OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q13-5<=>C7H13O15-3OOH+OH 11137.0 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q13-5<=>C7H13O35-1OOH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q13-6<=>C7H13O25-7OOH+OH 11489.7 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q13-7<=>C7H13O15-7OOH+OH 11907.9 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q14-2<=>C7H13O12-4OOH+OH 13376.0 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q14-2<=>C7H13O24-1OOH+OH 16995.3 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q14-3<=>C7H13O13-4OOH+OH 18002.9 !\AUTHOR: !\REF:	3.170E+11	0.000

C7H13Q14-3<=>C7H13O34-10OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q14-5<=>C7H13O15-40OH+OH 10825.4 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q14-5<=>C7H13O34-70OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q14-6<=>C7H13O24-70OH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q14-7<=>C7H13O14-70OH+OH 12572.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q15-2<=>C7H13O12-50OH+OH 13376.0 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q15-2<=>C7H13O25-10OH+OH 11056.4 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q15-3<=>C7H13O13-50OH+OH 18291.7 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q15-3<=>C7H13O35-10OH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q15-4<=>C7H13O14-50OH+OH 11067.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q15-4<=>C7H13O34-70OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q15-6<=>C7H13O23-70OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q15-7<=>C7H13O13-70OH+OH 19006.2 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q23-1<=>C7H13O12-30OH+OH 15033.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q23-1<=>C7H13O13-20OH+OH 19044.2 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q23-4<=>C7H13O24-30OH+OH 16995.3 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q23-4<=>C7H13O34-20OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q23-5<=>C7H13O25-30OH+OH 11489.7 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q23-5<=>C7H13O35-20OH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q23-6<=>C7H13O26-30OH+OH 11128.8 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q23-6<=>C7H13O25-60OH+OH 11489.7 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q23-7<=>C7H13O15-60OH+OH 11907.9 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q24-1<=>C7H13O12-40OH+OH 15033.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q24-1<=>C7H13O14-20OH+OH 12629.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q24-3<=>C7H13O23-40OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q24-3<=>C7H13O34-20OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q24-5<=>C7H13O25-40OH+OH 11056.4 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q24-5<=>C7H13O34-60OH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q24-6<=>C7H13O26-40OH+OH 11128.8 !\AUTHOR: !\REF:	5.200E+09	0.000

C7H13Q24-6<=>C7H13O24-6OOH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q24-7<=>C7H13O14-6OOH+OH 12572.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q25-1<=>C7H13O12-5OOH+OH 15033.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q25-1<=>C7H13O15-2OOH+OH 11948.9 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q25-3<=>C7H13O23-5OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q25-3<=>C7H13O35-2OOH+OH 16995.3 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q25-4<=>C7H13O24-5OOH+OH 16995.3 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q25-4<=>C7H13O34-6OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q25-6<=>C7H13O26-3OOH+OH 10817.2 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q25-6<=>C7H13O23-6OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q25-7<=>C7H13O13-6OOH+OH 19006.2 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q26-1<=>C7H13O12-6OOH+OH 15033.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q26-3<=>C7H13O23-6OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q26-3<=>C7H13O25-6OOH+OH 11056.4 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q26-4<=>C7H13O24-6OOH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q34-1<=>C7H13O13-4OOH+OH 19006.2 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q34-1<=>C7H13O14-3OOH+OH 12572.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q34-2<=>C7H13O23-4OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q34-2<=>C7H13O24-3OOH+OH 16995.3 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q34-5<=>C7H13O35-4OOH+OH 16995.3 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q34-5<=>C7H13O34-5OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q34-6<=>C7H13O25-4OOH+OH 11489.7 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q34-6<=>C7H13O24-5OOH+OH 17284.1 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q34-7<=>C7H13O15-4OOH+OH 11907.9 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q34-7<=>C7H13O14-5OOH+OH 12572.8 !\AUTHOR: !\REF:	2.770E+10	0.000
C7H13Q35-1<=>C7H13O13-5OOH+OH 19006.2 !\AUTHOR: !\REF:	3.170E+11	0.000
C7H13Q35-1<=>C7H13O15-3OOH+OH 11907.9 !\AUTHOR: !\REF:	5.200E+09	0.000
C7H13Q35-2<=>C7H13O23-5OOH+OH 13363.9 !\AUTHOR: !\REF:	1.775E+12	0.000
C7H13Q35-2<=>C7H13O25-3OOH+OH 11056.4 !\AUTHOR: !\REF:	2.770E+10	0.000

C7H13Q35-4<=>C7H13O34-5OOH+OH 1.775E+12 0.000
13363.9 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \24D. CETH-OOH_DECOMPOSITION \A \N
\EA !REF: ESTIMATED
!

C7H13O12-3OOH=>CH2CHO+PC4H9CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O12-4OOH=>C3H5O+NC3H7CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O12-5OOH=>C4H7O12-4+C2H5CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O12-6OOH=>C5H9O12-5+CH3CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O13-2OOH=>CH2CHO+PC4H9CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O13-4OOH=>CH2CH2CHO+NC3H7CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O13-5OOH=>C4H7O13-4+C2H5CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O13-6OOH=>C5H9O13-5+CH3CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O13-7OOH=>C6H11O13-6+CH2O+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O14-2OOH=>CH2O+NC5H10CHO-2+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O14-3OOH=>CH2CH2CHO+NC3H7CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O14-5OOH=>C3H6CHO-1+C2H5CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O14-6OOH=>C5H9O14-5+CH3CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O14-7OOH=>C6H11O14-6+CH2O+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O15-2OOH=>CH2O+NC5H10CHO-3+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O15-3OOH=>C4H8-1+C3Y1-3OR+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O15-4OOH=>C3H6CHO-1+C2H5CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O15-6OOH=>PC4H8CHO-4+CH3CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O15-7OOH=>C6H11O15-6+CH2O+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O23-1OOH=>CH2O+NC5H10CHO-1+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O23-4OOH=>CH3CHCHO+NC3H7CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O23-5OOH=>C4H7O23-1+C2H5CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O23-6OOH=>C5H9O23-5+CH3CHO+OH 1.050E+016 0.000
41600.0 !\AUTHOR: !\REF:
C7H13O23-7OOH=>C6H11O23-6+CH2O+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:
C7H13O24-1OOH=>CH2O+NC5H10CHO-2+OH 1.500E+016 0.000
42000.0 !\AUTHOR: !\REF:

C7H13O24-3OOH=>CH3CHCHO+NC3H7CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O24-5OOH=>C3H6CHO-2+C2H5CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O24-6OOH=>C5H9O24-1+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O24-7OOH=>C6H11O24-6+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O25-1OOH=>CH2O+NC5H10CHO-3+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O25-3OOH=>CH3CHO+PC4H8CHO-2+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O25-4OOH=>C3H6CHO-2+C2H5CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O25-6OOH=>PC4H8CHO-3+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O25-7OOH=>C6H11-1D5O+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O26-1OOH=>CH2O+NC5H10CHO-4+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O26-3OOH=>CH3CHO+PC4H8CHO-3+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O26-4OOH=>C3H6+C4Y1-3OR+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O34-1OOH=>C6H11O23-1+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O34-2OOH=>CH3CHO+PC4H8CHO-1+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O34-5OOH=>C3H6CHO-3+C2H5CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O34-6OOH=>C5H9O23-1+CH3CHO+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O34-7OOH=>C6H11O34-1+CH2O+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O35-1OOH=>CH2O+C6H11O24-1+OH 42000.0 !\AUTHOR: !\REF:	1.500E+016	0.000
C7H13O35-2OOH=>CH3CHO+PC4H8CHO-2+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000
C7H13O35-4OOH=>C2H5CHO+C3H6CHO-1+OH 41600.0 !\AUTHOR: !\REF:	1.050E+016	0.000

!

!\REACTIONCLASS: \25. CETH_DECOMPOSTION

\A

\N

\EA !REF: ANOLOGY TO N-HEXANE

!

C7H14O1-2+OH=>CH2CO+C5H11-1+H2O 0.0 !\AUTHOR: !\REF:	2.500E+12	0.0000
C7H14O1-2+OH=>C2H3CHO+PC4H9+H2O 0.0 !\AUTHOR: !\REF:	2.500E+12	0.0000
C7H14O1-3+OH=>C2H4+PC4H9CO+H2O 0.0 !\AUTHOR: !\REF:	2.500E+12	0.0000
C7H14O1-3+OH=>HCO+C6H12-1+H2O 0.0 !\AUTHOR: !\REF:	2.500E+12	0.0000
C7H14O1-4+OH=>NC3H7COCH2+C2H4+H2O 0.0 !\AUTHOR: !\REF:	2.500E+12	0.0000
C7H14O1-4+OH=>CH2CHO+C5H10-1+H2O 0.0 !\AUTHOR: !\REF:	2.500E+12	0.0000

C7H14O1-5+OH=>CH2CH2CHO+C4H8-1+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O1-5+OH=>CH2CH2COC2H5+C2H4+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-3+OH=>C2H3COCH3+NC3H7+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-3+OH=>PC4H9CO+C2H4+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-4+OH=>C3H6+NC3H7CO+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-4+OH=>CH3CO+C5H10-1+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-5+OH=>C2H5COCH2+C3H6+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-5+OH=>CH3COCH2+C4H8-1+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O2-6+OH=>C3H6+CH2CH2COCH3+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O3-4+OH=>C2H5+NC53ONE-1+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O3-4+OH=>C2H5CHCO+NC3H7+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O3-5+OH=>C2H5CO+C4H8-1+H2O	2.500E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14O1-2+HO2=>CH2CO+C5H11-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-2+HO2=>C2H3CHO+PC4H9+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-3+HO2=>C2H4+PC4H9CO+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-3+HO2=>HCO+C6H12-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-4+HO2=>NC3H7COCH2+C2H4+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-4+HO2=>CH2CHO+C5H10-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-5+HO2=>CH2CH2CHO+C4H8-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O1-5+HO2=>CH2CH2COC2H5+C2H4+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-3+HO2=>C2H3COCH3+NC3H7+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-3+HO2=>PC4H9CO+C2H4+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-4+HO2=>C3H6+NC3H7CO+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-4+HO2=>CH3CO+C5H10-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-5+HO2=>C2H5COCH2+C3H6+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-5+HO2=>CH3COCH2+C4H8-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O2-6+HO2=>C3H6+CH2CH2COCH3+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O3-4+HO2=>C2H5+NC53ONE-1+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		
C7H14O3-4+HO2=>C2H5CHCO+NC3H7+H2O2	5.000E+12	0.0000
17700.0 !\AUTHOR: !\REF:		

C7H14O3-5+HO2=>C2H5CO+C4H8-1+H2O2 5.000E+12 0.0000
17700.0 !\AUTHOR: !\REF:
!

!\REACTIONCLASS: \X1. DIONE_FORMATION \A \N
\EA !REF:
!

C7KET24=>H2O+C7Y24 1.280E+07 2.2500
44950.0 !\AUTHOR: !\REF:
C7KET13=>H2O+C7Y13 1.280E+07 2.2500
44950.0 !\AUTHOR: !\REF:
C7KET42=>H2O+C7Y24 1.280E+07 2.2500
44950.0 !\AUTHOR: !\REF:
C7KET35=>H2O+C7Y35 1.280E+07 2.2500
44950.0 !\AUTHOR: !\REF:
C7KET24O=>C7Y24+H 2.430E+09 1.4200
19380.0 !\AUTHOR: !\REF:
DUP
C7KET13O=>C7Y13+H 2.430E+09 1.4200
19380.0 !\AUTHOR: !\REF:
DUP
C7KET42O=>C7Y24+H 2.430E+09 1.4200
19380.0 !\AUTHOR: !\REF:
DUP
C7KET35O=>C7Y35+H 2.430E+09 1.4200
19380.0 !\AUTHOR: !\REF:
DUP
C7KET24O=>C7Y24+H 7.492E+01 3.4900
19800.0 !\AUTHOR: !\REF:
DUP
C7KET13O=>C7Y13+H 7.492E+01 3.4900
19800.0 !\AUTHOR: !\REF:
DUP
C7KET42O=>C7Y24+H 7.492E+01 3.4900
19800.0 !\AUTHOR: !\REF:
DUP
C7KET35O=>C7Y35+H 7.492E+01 3.4900
19800.0 !\AUTHOR: !\REF:
DUP
C7KET24O+O2=>C7Y24+HO2 9.040E+09 0.0000
0.0 !\AUTHOR: !\REF:
C7KET13O+O2=>C7Y13+HO2 9.040E+09 0.0000
0.0 !\AUTHOR: !\REF:
C7KET42O+O2=>C7Y24+HO2 9.040E+09 0.0000
0.0 !\AUTHOR: !\REF:
C7KET35O+O2=>C7Y35+HO2 9.040E+09 0.0000
0.0 !\AUTHOR: !\REF:
C7KET24+OH=>H2O+OH+C7Y24 1.190E+10 0.0000
1680.0 !\AUTHOR: !\REF:
C7KET13+OH=>H2O+OH+C7Y13 1.190E+10 0.0000
1680.0 !\AUTHOR: !\REF:
C7KET42+OH=>H2O+OH+C7Y24 1.190E+10 0.0000
1680.0 !\AUTHOR: !\REF:
C7KET35+OH=>H2O+OH+C7Y35 1.190E+10 0.0000
1680.0 !\AUTHOR: !\REF:
C7KET13=>HOCHO+C6Y2 1.700E+05 1.1300
26100.0 !\AUTHOR: !\REF:

C7KET13=>CH3COOH+PC4H9CHO	5.100E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
C7KET24=>CH3COOH+NC3H7COCH3	1.700E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
C7KET35=>C2H5COOH+C2H5COCH3	3.400E+05	1.1300
26100.0 !\AUTHOR: !\REF:		
CH3CO+PC4H9<=>C6Y2	2.000E+13	0.0000
0.0 !\AUTHOR: !\REF:		
!		

!\REACTIONCLASS: \X2. O2QOOH+R'=OQOOH+R'O,ETC	\A	\N
\EA !REF:		
!		

C7H14OOH1-2O2+CH3=>CH3O+C7H14OOH1-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2+CH3=>CH3O+C7H14OOH1-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2+CH3=>CH3O+C7H14OOH1-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2+CH3=>CH3O+C7H14OOH1-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-1O2+CH3=>CH3O+C7H14OOH2-1O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-3O2+CH3=>CH3O+C7H14OOH2-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-4O2+CH3=>CH3O+C7H14OOH2-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-5O2+CH3=>CH3O+C7H14OOH2-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-6O2+CH3=>CH3O+C7H14OOH2-6O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-1O2+CH3=>CH3O+C7H14OOH3-1O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-2O2+CH3=>CH3O+C7H14OOH3-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-4O2+CH3=>CH3O+C7H14OOH3-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-5O2+CH3=>CH3O+C7H14OOH3-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-6O2+CH3=>CH3O+C7H14OOH3-6O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-7O2+CH3=>CH3O+C7H14OOH3-7O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH4-1O2+CH3=>CH3O+C7H14OOH4-1O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH4-2O2+CH3=>CH3O+C7H14OOH4-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O2+CH3=>CH3O+C7H14OOH4-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-2O2+C2H5=>C2H5O+C7H14OOH1-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2+C2H5=>C2H5O+C7H14OOH1-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2+C2H5=>C2H5O+C7H14OOH1-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2+C2H5=>C2H5O+C7H14OOH1-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		

C7H14OOH2-1O2+C2H5=>C2H5O+C7H14OOH2-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH2-3O2+C2H5=>C2H5O+C7H14OOH2-3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH2-4O2+C2H5=>C2H5O+C7H14OOH2-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH2-5O2+C2H5=>C2H5O+C7H14OOH2-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH2-6O2+C2H5=>C2H5O+C7H14OOH2-6O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH3-1O2+C2H5=>C2H5O+C7H14OOH3-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH3-2O2+C2H5=>C2H5O+C7H14OOH3-2O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH3-4O2+C2H5=>C2H5O+C7H14OOH3-4O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH3-5O2+C2H5=>C2H5O+C7H14OOH3-5O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH3-6O2+C2H5=>C2H5O+C7H14OOH3-6O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH3-7O2+C2H5=>C2H5O+C7H14OOH3-7O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH4-1O2+C2H5=>C2H5O+C7H14OOH4-1O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH4-2O2+C2H5=>C2H5O+C7H14OOH4-2O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH4-3O2+C2H5=>C2H5O+C7H14OOH4-3O -1000.0 !\AUTHOR: !\REF:	9.000E+12	0.0000
C7H14OOH1-2O=>CH2O+NC5H11CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-2O=>HO2CH2CHO+C5H11-1 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-3O=>C3KET13+PC4H9 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-3O=>C2H4O2H+PC4H9CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-4O=>NC4KET14+NC3H7 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-4O=>C3H6OOH1-3+NC3H7CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-5O=>NC5KET15+C2H5 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH1-5O=>C4H8OOH1-4+C2H5CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-1O=>CH2O+NC5H11CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-3O=>CH3CHO+PC4H9CHO+OH 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-3O=>C3KET12+PC4H9 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-4O=>NC4KET13+NC3H7 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-4O=>C3H6OOH2-1+NC3H7CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-5O=>NC5KET14+C2H5 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000
C7H14OOH2-5O=>C4H8OOH2-4+C2H5CHO 11080.0 !\AUTHOR: !\REF:	2.900E+12	0.4000

C7H14OOH2-6O=>C6KET15+CH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH2-6O=>C5H10OOH2-5+CH3CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-1O=>CH2O+C6H12OOH2-1	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-2O=>CH3CHO+PC4H9CHO+OH	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-2O=>C6KET12+CH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-4O=>NC4KET12+NC3H7	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-4O=>C2H5CHO+NC3H7CHO+OH	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-5O=>NC5KET13+C2H5	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-5O=>C4H8OOH2-1+C2H5CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-6O=>C6KET14+CH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-6O=>C5H10OOH3-1+CH3CHO	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH3-7O=>C6H12OOH3-6+CH2O	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH4-1O=>C6H12OOH3-1+CH2O	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH4-2O=>C6KET13+CH3	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH4-2O=>CH3CHO+C5H10OOH2-1	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O=>NC5KET12+C2H5	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O=>C2H5CHO+NC3H7CHO+OH	2.900E+12	0.4000
11080.0 !\AUTHOR: !\REF:		
C7H14OOH1-2O2+C7H15-1=>C7H15-1O+C7H14OOH1-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-3O2+C7H15-1=>C7H15-1O+C7H14OOH1-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-4O2+C7H15-1=>C7H15-1O+C7H14OOH1-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH1-5O2+C7H15-1=>C7H15-1O+C7H14OOH1-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-1O2+C7H15-1=>C7H15-1O+C7H14OOH2-1O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-3O2+C7H15-1=>C7H15-1O+C7H14OOH2-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-4O2+C7H15-1=>C7H15-1O+C7H14OOH2-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-5O2+C7H15-1=>C7H15-1O+C7H14OOH2-5O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH2-6O2+C7H15-1=>C7H15-1O+C7H14OOH2-6O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-1O2+C7H15-1=>C7H15-1O+C7H14OOH3-1O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-2O2+C7H15-1=>C7H15-1O+C7H14OOH3-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH3-4O2+C7H15-1=>C7H15-1O+C7H14OOH3-4O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		

C7H14OOH4-2O2+C7H15-4=>C7H15-4O+C7H14OOH4-2O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		
C7H14OOH4-3O2+C7H15-4=>C7H15-4O+C7H14OOH4-3O	9.000E+12	0.0000
-1000.0 !\AUTHOR: !\REF:		

!-----
 !\ENDSUBMECH: \NC7H16
 !-----

CH2CO+PC4H9<=>C6Y2-1J	1.760E+004	2.480
6130.0 !REF: ANALOGY TO CH3COCH2		
C6Y3-6J<=>C2H5COCH2+C2H4	2.340E+17	-1.123
31176.0 !REF: ANALOGY TO C5H11-1		
C6Y3-1J<=>NC3H7CO+C2H4	1.000E+014	0.000
18000.0 !REF: ANALOGY TO CH2CH2COCH3		

!-----
 !\SUBMECH: \C7H14-1\C7H14-2\C7H14-3
 !-----

!\REACTIONCLASS: \6. E_H ABSTRACTION	\A	\N
\EA !REF: ANALOGY TO HEXENES		

C7H14-1+H<=>C7H131-3+H2	3.380E+05	2.4000
207.0 !\AUTHOR: !\REF:		
C7H14-1+H<=>C7H131-4+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C7H14-1+H<=>C7H131-5+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C7H14-1+H<=>C7H131-6+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C7H14-1+H<=>C7H131-7+H2	6.650E+05	2.5000
6756.0 !\AUTHOR: !\REF:		
C7H14-1+O<=>C7H131-3+OH	6.600E+05	2.4000
1210.0 !\AUTHOR: !\REF:		
C7H14-1+O<=>C7H131-4+OH	5.510E+05	2.5000
2830.0 !\AUTHOR: !\REF:		
C7H14-1+O<=>C7H131-5+OH	5.510E+05	2.5000
2830.0 !\AUTHOR: !\REF:		
C7H14-1+O<=>C7H131-6+OH	5.510E+05	2.5000
2830.0 !\AUTHOR: !\REF:		
C7H14-1+O<=>C7H131-7+OH	9.800E+05	2.4000
4750.0 !\AUTHOR: !\REF:		
C7H14-1+OH<=>C7H131-3+H2O	2.760E+04	2.6000
-1919.0 !\AUTHOR: !\REF:		
C7H14-1+OH<=>C7H131-4+H2O	4.670E+07	1.6000
-35.0 !\AUTHOR: !\REF:		
C7H14-1+OH<=>C7H131-5+H2O	4.670E+07	1.6000
-35.0 !\AUTHOR: !\REF:		
C7H14-1+OH<=>C7H131-6+H2O	4.670E+07	1.6000
-35.0 !\AUTHOR: !\REF:		
C7H14-1+OH<=>C7H131-7+H2O	5.270E+09	1.0000
1586.0 !\AUTHOR: !\REF:		
C7H14-1+O2<=>C7H131-3+HO2	2.200E+12	0.0000
37220.0 !\AUTHOR: !\REF:		

C7H14-1+O2<=>C7H131-4+HO2	2.000E+13	0.0000
49640.0 !\AUTHOR: !\REF:		
C7H14-1+O2<=>C7H131-5+HO2	2.000E+13	0.0000
49640.0 !\AUTHOR: !\REF:		
C7H14-1+O2<=>C7H131-6+HO2	2.000E+13	0.0000
49640.0 !\AUTHOR: !\REF:		
C7H14-1+O2<=>C7H131-7+HO2	3.000E+13	0.0000
52290.0 !\AUTHOR: !\REF:		
C7H14-1+HO2<=>C7H131-3+H2O2	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C7H14-1+HO2<=>C7H131-4+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-1+HO2<=>C7H131-5+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-1+HO2<=>C7H131-6+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-1+HO2<=>C7H131-7+H2O2	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C7H14-1+CH3<=>C7H131-3+CH4	3.690E+00	3.3000
4002.0 !\AUTHOR: !\REF:		
C7H14-1+CH3<=>C7H131-4+CH4	1.510E+00	3.5000
5481.0 !\AUTHOR: !\REF:		
C7H14-1+CH3<=>C7H131-5+CH4	1.510E+00	3.5000
5481.0 !\AUTHOR: !\REF:		
C7H14-1+CH3<=>C7H131-6+CH4	1.510E+00	3.5000
5481.0 !\AUTHOR: !\REF:		
C7H14-1+CH3<=>C7H131-7+CH4	4.520E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O<=>C7H131-3+CH3OH	4.000E+01	2.9000
8609.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O<=>C7H131-4+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O<=>C7H131-5+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O<=>C7H131-6+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O<=>C7H131-7+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O2<=>C7H131-3+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O2<=>C7H131-4+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O2<=>C7H131-5+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O2<=>C7H131-6+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-1+CH3O2<=>C7H131-7+CH3O2H	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H131-3+H2	1.730E+05	2.5000
2492.0 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H132-4+H2	3.380E+05	2.4000
207.0 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H132-5+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H132-6+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H132-7+H2	6.650E+05	2.5000
6756.0 !\AUTHOR: !\REF:		

C7H14-2+O<=>C7H131-3+OH 3150.0 !\AUTHOR: !\REF:	4.410E+05	2.4000
C7H14-2+O<=>C7H132-4+OH 1210.0 !\AUTHOR: !\REF:	6.600E+05	2.4000
C7H14-2+O<=>C7H132-5+OH 2830.0 !\AUTHOR: !\REF:	5.510E+05	2.5000
C7H14-2+O<=>C7H132-6+OH 2830.0 !\AUTHOR: !\REF:	5.510E+05	2.5000
C7H14-2+O<=>C7H132-7+OH 4750.0 !\AUTHOR: !\REF:	9.800E+05	2.4000
C7H14-2+OH<=>C7H131-3+H2O -298.0 !\AUTHOR: !\REF:	3.120E+06	2.0000
C7H14-2+OH<=>C7H132-4+H2O -1919.0 !\AUTHOR: !\REF:	2.760E+04	2.6000
C7H14-2+OH<=>C7H132-5+H2O -35.0 !\AUTHOR: !\REF:	4.670E+07	1.6000
C7H14-2+OH<=>C7H132-6+H2O -35.0 !\AUTHOR: !\REF:	4.670E+07	1.6000
C7H14-2+OH<=>C7H132-7+H2O 1586.0 !\AUTHOR: !\REF:	5.270E+09	1.0000
C7H14-2+O2<=>C7H131-3+HO2 39900.0 !\AUTHOR: !\REF:	3.300E+12	0.0000
C7H14-2+O2<=>C7H132-4+HO2 37220.0 !\AUTHOR: !\REF:	2.200E+12	0.0000
C7H14-2+O2<=>C7H132-5+HO2 49640.0 !\AUTHOR: !\REF:	2.000E+13	0.0000
C7H14-2+O2<=>C7H132-6+HO2 49640.0 !\AUTHOR: !\REF:	2.000E+13	0.0000
C7H14-2+O2<=>C7H132-7+HO2 52290.0 !\AUTHOR: !\REF:	3.000E+13	0.0000
C7H14-2+HO2<=>C7H131-3+H2O2 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C7H14-2+HO2<=>C7H132-4+H2O2 10530.0 !\AUTHOR: !\REF:	4.820E+03	2.5000
C7H14-2+HO2<=>C7H132-5+H2O2 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C7H14-2+HO2<=>C7H132-6+H2O2 13910.0 !\AUTHOR: !\REF:	9.640E+03	2.6000
C7H14-2+HO2<=>C7H132-7+H2O2 16490.0 !\AUTHOR: !\REF:	2.380E+04	2.5000
C7H14-2+CH3<=>C7H131-3+CH4 5675.0 !\AUTHOR: !\REF:	2.210E+00	3.5000
C7H14-2+CH3<=>C7H132-4+CH4 4002.0 !\AUTHOR: !\REF:	3.690E+00	3.3000
C7H14-2+CH3<=>C7H132-5+CH4 5481.0 !\AUTHOR: !\REF:	1.510E+00	3.5000
C7H14-2+CH3<=>C7H132-6+CH4 5481.0 !\AUTHOR: !\REF:	1.510E+00	3.5000
C7H14-2+CH3<=>C7H132-7+CH4 7154.0 !\AUTHOR: !\REF:	4.520E-01	3.6000
C7H14-2+CH3O<=>C7H131-3+CH3OH 11990.0 !\AUTHOR: !\REF:	9.000E+01	3.0000
C7H14-2+CH3O<=>C7H132-4+CH3OH 8609.0 !\AUTHOR: !\REF:	4.000E+01	2.9000
C7H14-2+CH3O<=>C7H132-5+CH3OH 4571.0 !\AUTHOR: !\REF:	1.450E+11	0.0000
C7H14-2+CH3O<=>C7H132-6+CH3OH 4571.0 !\AUTHOR: !\REF:	1.450E+11	0.0000

C7H14-2+CH3O<=>C7H132-7+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C7H14-2+CH3O2<=>C7H131-3+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-2+CH3O2<=>C7H132-4+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C7H14-2+CH3O2<=>C7H132-5+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-2+CH3O2<=>C7H132-6+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-2+CH3O2<=>C7H132-7+CH3O2H	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H133-1+H2	6.650E+05	2.5000
6756.0 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H132-4+H2	3.380E+05	2.4000
207.0 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H133-5+H2	3.380E+05	2.4000
207.0 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H133-6+H2	1.300E+06	2.4000
4471.0 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H133-7+H2	6.650E+05	2.5000
6756.0 !\AUTHOR: !\REF:		
C7H14-3+O<=>C7H133-1+OH	9.800E+05	2.4000
4750.0 !\AUTHOR: !\REF:		
C7H14-3+O<=>C7H132-4+OH	6.600E+05	2.4000
1210.0 !\AUTHOR: !\REF:		
C7H14-3+O<=>C7H133-5+OH	6.600E+05	2.4000
1210.0 !\AUTHOR: !\REF:		
C7H14-3+O<=>C7H133-6+OH	5.510E+05	2.5000
2830.0 !\AUTHOR: !\REF:		
C7H14-3+O<=>C7H133-7+OH	9.800E+05	2.4000
4750.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H133-1+H2O	5.270E+09	1.0000
1586.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H132-4+H2O	2.760E+04	2.6000
-1919.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H133-5+H2O	2.760E+04	2.6000
-1919.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H133-6+H2O	4.670E+07	1.6000
-35.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H133-7+H2O	5.270E+09	1.0000
1586.0 !\AUTHOR: !\REF:		
C7H14-3+O2<=>C7H133-1+HO2	3.000E+13	0.0000
52290.0 !\AUTHOR: !\REF:		
C7H14-3+O2<=>C7H132-4+HO2	2.200E+12	0.0000
37220.0 !\AUTHOR: !\REF:		
C7H14-3+O2<=>C7H133-5+HO2	2.200E+12	0.0000
37220.0 !\AUTHOR: !\REF:		
C7H14-3+O2<=>C7H133-6+HO2	2.000E+13	0.0000
49640.0 !\AUTHOR: !\REF:		
C7H14-3+O2<=>C7H133-7+HO2	3.000E+13	0.0000
52290.0 !\AUTHOR: !\REF:		
C7H14-3+HO2<=>C7H133-1+H2O2	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C7H14-3+HO2<=>C7H132-4+H2O2	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C7H14-3+HO2<=>C7H133-5+H2O2	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		

C7H14-3+HO2<=>C7H133-6+H2O2	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-3+HO2<=>C7H133-7+H2O2	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C7H14-3+CH3<=>C7H133-1+CH4	4.520E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
C7H14-3+CH3<=>C7H132-4+CH4	3.690E+00	3.3000
4002.0 !\AUTHOR: !\REF:		
C7H14-3+CH3<=>C7H133-5+CH4	3.690E+00	3.3000
4002.0 !\AUTHOR: !\REF:		
C7H14-3+CH3<=>C7H133-6+CH4	1.510E+00	3.5000
5481.0 !\AUTHOR: !\REF:		
C7H14-3+CH3<=>C7H133-7+CH4	4.520E-01	3.6000
7154.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O<=>C7H133-1+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O<=>C7H132-4+CH3OH	4.000E+01	2.9000
8609.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O<=>C7H133-5+CH3OH	4.000E+01	2.9000
8609.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O<=>C7H133-6+CH3OH	1.450E+11	0.0000
4571.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O<=>C7H133-7+CH3OH	2.170E+11	0.0000
6458.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O2<=>C7H133-1+CH3O2H	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O2<=>C7H132-4+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O2<=>C7H133-5+CH3O2H	4.820E+03	2.5000
10530.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O2<=>C7H133-6+CH3O2H	9.640E+03	2.6000
13910.0 !\AUTHOR: !\REF:		
C7H14-3+CH3O2<=>C7H133-7+CH3O2H	2.380E+04	2.5000
16490.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \7. E_H ADDITION
 \EA !REF:ANALOGY TO HEXENES

\A

\N

!

C7H14-1+H<=>C7H15-1	1.200E+09	1.3000
1049.2 !\AUTHOR: !\REF:		
C7H14-1+H<=>C7H15-2	6.610E+08	1.4000
-677.6 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H15-2	3.890E+08	1.6000
579.9 !\AUTHOR: !\REF:		
C7H14-2+H<=>C7H15-3	3.890E+08	1.6000
579.9 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H15-3	3.890E+08	1.6000
579.9 !\AUTHOR: !\REF:		
C7H14-3+H<=>C7H15-4	3.890E+08	1.6000
579.9 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \7A. E_WADDINGTON
 \EA !REF:ANALOGY TO HEXENES

\A

\N

!

C7H14-1+OH<=>C7H14OH-1J2	4.750E+12	0.0000
-782.0 !\AUTHOR: !\REF:		
C7H14-1+OH<=>C7H14OH-2J1	4.750E+12	0.0000
-782.0 !\AUTHOR: !\REF:		
C7H14-2+OH<=>C7H14OH-2J3	4.750E+12	0.0000
-782.0 !\AUTHOR: !\REF:		
C7H14-2+OH<=>C7H14OH-3J2	4.750E+12	0.0000
-782.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H14OH-3J4	4.750E+12	0.0000
-782.0 !\AUTHOR: !\REF:		
C7H14-3+OH<=>C7H14OH-4J3	4.750E+12	0.0000
-782.0 !\AUTHOR: !\REF:		
C7H14OH-1J2+O2<=>C7H14OH-1O2-2	2.000E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14OH-2J1+O2<=>C7H14OH-2O2-1	2.000E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14OH-2J3+O2<=>C7H14OH-2O2-3	2.000E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14OH-3J2+O2<=>C7H14OH-3O2-2	2.000E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14OH-4J3+O2<=>C7H14OH-3O2-4	2.000E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14OH-3J4+O2<=>C7H14OH-4O2-3	2.000E+12	0.0000
0.0 !\AUTHOR: !\REF:		
C7H14OH-1O2-2=>CH2O+NC5H11CHO+OH	2.500E+10	0.0000
18860.0 !\AUTHOR: !\REF:		
C7H14OH-2O2-1=>CH2O+NC5H11CHO+OH	2.500E+10	0.0000
18860.0 !\AUTHOR: !\REF:		
C7H14OH-2O2-3=>CH3CHO+PC4H9CHO+OH	2.500E+10	0.0000
18860.0 !\AUTHOR: !\REF:		
C7H14OH-3O2-2=>CH3CHO+PC4H9CHO+OH	2.500E+10	0.0000
18860.0 !\AUTHOR: !\REF:		
C7H14OH-3O2-4=>C2H5CHO+NC3H7CHO+OH	2.500E+10	0.0000
18860.0 !\AUTHOR: !\REF:		
C7H14OH-4O2-3=>C2H5CHO+NC3H7CHO+OH	2.500E+10	0.0000
18860.0 !\AUTHOR: !\REF:		

!

!\REACTIONCLASS: \8. ER_DECOMPOSITION

\A

\N

\EA !REF:ESTIMATED

!

C4H6+NC3H7<=>C7H131-3	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C3H5-A+C4H8-1<=>C7H131-5	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C4H71-4+C3H6<=>C7H131-6	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C5H91-5+C2H4<=>C7H131-7	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C5H81-3+C2H5<=>C7H132-4	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C4H71-3+C3H6<=>C7H132-6	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C5H92-5+C2H4<=>C7H132-7	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		
C5H91-3+C2H4<=>C7H133-7	1.000E+11	0.0000
7800.0 !\AUTHOR: !\REF:		

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!
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!\REACTIONCLASS: \8A. ER+HO2=ERO+OH           \A           \N
\EA      !REF:ANALOGY TO HEXENES
!
-----
C7H13-1D3O+OH<=>C7H131-3+HO2                 6.090E+15      -1.1000
15720.0 !\AUTHOR: !\REF:
C7H13-2D4O+OH<=>C7H132-4+HO2                 7.030E+15      -1.2000
15890.0 !\AUTHOR: !\REF:
C7H13-3D5O+OH<=>C7H133-5+HO2                 7.030E+15      -1.2000
15890.0 !\AUTHOR: !\REF:
C7H13-1D3O+CH3O<=>C7H131-3+CH3O2             5.950E+17      -1.6000
20480.0 !\AUTHOR: !\REF:
C7H13-2D4O+CH3O<=>C7H132-4+CH3O2             6.860E+17      -1.8000
20650.0 !\AUTHOR: !\REF:
C7H13-3D5O+CH3O<=>C7H133-5+CH3O2             6.860E+17      -1.8000
20650.0 !\AUTHOR: !\REF:
C7H13-1D3O+C2H5O<=>C7H131-3+C2H5O2           3.890E+14      -0.7000
18330.0 !\AUTHOR: !\REF:
C7H13-2D4O+C2H5O<=>C7H132-4+C2H5O2           4.490E+14      -0.9000
18490.0 !\AUTHOR: !\REF:
C7H13-3D5O+C2H5O<=>C7H133-5+C2H5O2           4.490E+14      -0.9000
18490.0 !\AUTHOR: !\REF:
!
-----
!\REACTIONCLASS: \8B. ERO_DECOMPOSITION       \A           \N
\EA      !REF:ESTIMIATED
!
-----
C7H13-1D3O<=>C2H3CHO+PC4H9                   3.130E+19      -1.9000
10670.0 !\AUTHOR: !\REF:
C7H13-2D4O<=>SC3H5CHO+NC3H7                 3.130E+19      -1.9000
10670.0 !\AUTHOR: !\REF:
C7H13-3D5O<=>C5D2Y1+C2H5                   3.130E+19      -1.9000
10670.0 !\AUTHOR: !\REF:
!
-----
!\REACTIONCLASS: \9. E_UNIMOLECULAR_DECOMPOSITION \A           \N
\EA      !REF: H. J. Curran, et al., Combust. Flame, 114, (1998) 149-177.
!
-----
C7H14-1<=>PC4H9+C3H5-A                       3.170E+21      -1.6200
75330.0 !\AUTHOR: !\REF:
C7H14-2<=>C4H71-3+NC3H7                     3.735E+21      -1.7400
75710.0 !\AUTHOR: !\REF:
C7H14-3<=>C5H91-3+C2H5                      5.947E+21      -1.8500
75790.0 !\AUTHOR: !\REF:
C7H14-3<=>C6H111-3+CH3                      5.947E+21      -1.8500
76790.0 !\AUTHOR: !\REF:
!-----
-----
!\ENDSUBMECH: \C7H14-1\C7H14-2\C7H14-3
!-----
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!
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!\REACTIONCLASS: \X3. PRD_UNIMOLECULAR_DECOMPOSITION \A \N
\EA !REF: ANALOGY TO SMALL ALDEHYDES
!

C5D2Y1+O2<=>C5D2Y1-1R+HO2 37560.0	1.200E+005	2.500
C5D2Y1+OH<=>C5D2Y1-1R+H2O -1300.0	2.000E+006	1.800
C5D2Y1+H<=>C5D2Y1-1R+H2 2320.0	4.140E+009	1.120
C5D2Y1+O<=>C5D2Y1-1R+OH 1868.0	5.940E+012	0.000
C5D2Y1+HO2<=>C5D2Y1-1R+H2O2 10200.0	4.090E+004	2.500
C5D2Y1+CH3<=>C5D2Y1-1R+CH4 3210.0	2.890E-003	4.620
C5D2Y1+CH3O<=>C5D2Y1-1R+CH3OH 3300.0	1.000E+012	0.000
C5D2Y1+CH3O2<=>C5D2Y1-1R+CH3O2H 10200.0	4.090E+004	2.500
C5D2Y1-1R=>C2H5+CO+C2H2 9600.0	1.000E+011	0.000
C6D2Y1+O2<=>C6D2Y1-1R+HO2 37560.0	1.200E+005	2.500
C6D2Y1+OH<=>C6D2Y1-1R+H2O -1300.0	2.000E+006	1.800
C6D2Y1+H<=>C6D2Y1-1R+H2 2320.0	4.140E+009	1.120
C6D2Y1+O<=>C6D2Y1-1R+OH 1868.0	5.940E+012	0.000
C6D2Y1+HO2<=>C6D2Y1-1R+H2O2 10200.0	4.090E+004	2.500
C6D2Y1+CH3<=>C6D2Y1-1R+CH4 3210.0	2.890E-003	4.620
C6D2Y1+CH3O<=>C6D2Y1-1R+CH3OH 3300.0	1.000E+012	0.000
C6D2Y1+CH3O2<=>C6D2Y1-1R+CH3O2H 10200.0	4.090E+004	2.500
C6D2Y1-1R=>NC3H7+CO+C2H2 9600.0	1.000E+011	0.000
CH2O+CH2CHO<=>C3Y1-3OR 7800.0	1.230E+011	0.000
CH3CHO+CH2CHO<=>C4Y1-3OR 6000.0	1.000E+011	0.000

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!\END_KINETICS_MODULE: \C7

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

!\KINETICS_MODULE: \AROMATIC
!\MODSUBMECHS:

FULVENE<=>C6H5+H 8.511E+24 -2.505 113330.0
!\AUTHOR: !\REF:10ATM/MILLER&KLIPPENSTEIN, J.PHYS.CHEM.A, 2003, PP. 7783-7799
!

!\REACTIONCLASS: \R_CAT_ISO \A \N
\EA
!

C6H6+H<=>FULVENE+H 8.43E+32 -4.95 51244.0
!\AUTHOR: !\REF: 1997BUR/DVI505-514
!

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

C6H6+H<=>C6H5+H2 2.500E+014 0.000
16000.0 !\AUTHOR: !\REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
C6H6+O2<=>C6H5+HO2 6.300E+013 0.000
60000.0 !\AUTHOR: !\REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
C6H6+O<=>C6H5+OH 2.000E+013 0.000
14700.0 !\AUTHOR: !\REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
C6H6+OH<=>C6H5+H2O 1.200E+000 4.100
-301.0 !\AUTHOR: !\REF:CHEN&BOZ J. PHYS. CHEM. A 108: 4632 - 4652 2004
C6H6+HO2<=>C6H5+H2O2 5.500E+012 0.000
28900.0 !\AUTHOR:
C6H6+CH3<=>C6H5+CH4 7.320E+012 0.000
18920.0 !\AUTHOR:
C6H5+CH2O<=>C6H6+HCO 8.550E+004 2.190
38.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

C6H5+HCO<=>C6H6+CO 8.550E+004 2.190
38.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA
!

C6H5=>H+C4H2+C2H2 4.300E+012 0.620
77294.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
!

!\REACTIONCLASS: \R_ADDITION \A \N
\EA
!

C6H6+O<=>C6H5O+H 2.200E+013 0.000
4530.0 !\AUTHOR: !\REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)

C6H6+OH<=>C6H5OH+H 1.320E+002 3.250
5590.0 !\AUTHOR: !\REF:TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA
MIYOSHI J. PHYS. CHEM. A, 2006, 110 (15), 5081-5090

!

!\REACTIONCLASS: \R_HO2 \A \N
\EA

!

C6H5+HO2<=>C6H5O+OH 5.000E+012 0.000
0.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003

!

!\REACTIONCLASS: \R_O2 \A \N
\EA

!

C6H5+O2<=>C6H5O+O 2.600E+013 0.000
6120.0 !\AUTHOR: !\REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25,
833.

C6H5+O2<=>O-C6H4O2+H 3.000E+013 0.000
8980.0 !\AUTHOR: !\REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25,
833.

C6H5+O2<=>C6H5OO 1.860E+013 -0.220
-711.0 !\AUTHOR: !\REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575
C6H5OO<=>C6H5O+O 1.270E+015 -0.246
38536.0 !\AUTHOR: !\REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575
C6H5O+OH<=>C6H5OOH 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:WKM ESTIMATED

!

!\ENDSUBMECH: \C6H6

!

!\SUBMECH: \C6H5OH

!

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

!

C6H5O+H(+M)<=>C6H5OH(+M) 2.000E+014 0.000
0.0 !\AUTHOR: !\REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161
LOW/ 1.000E+094 -21.840
13880.0/

TROE/ 4.300E-002 3.042E+002 6.000E+004 5.896E+003/
C6H4OH+H<=>C6H5OH 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003
C6H5OH<=>C5H6+CO 4.310E+015 -0.610
74115.0 !\AUTHOR: !\REF:WKM A FACTOR *0.5 TO FIT PYROLYSIS DATA

!

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

!

C6H5OH+H<=>C6H5O+H2	1.200E+014	0.000
12400.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+O2<=>C6H5O+HO2	1.000E+013	0.000
38800.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+O<=>C6H5O+OH	1.300E+013	0.000
2900.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+OH<=>C6H5O+H2O	1.400E+008	1.400
-960.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+HO2<=>C6H5O+H2O2	1.000E+012	0.000
10000.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+CH3<=>C6H5O+CH4	1.800E+011	0.000
7700.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+C3H5-A<=>C6H5O+C3H6	4.900E+011	0.000
9400.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+C4H5-I<=>C6H5O+C4H6	4.900E+011	0.000
9400.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+C6H5<=>C6H5O+C6H6	4.900E+012	0.000
4400.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+C6H5OO<=>C6H5O+C6H5OOH	1.330E+011	0.000
14000.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+H<=>C6H4OH+H2	1.700E+014	0.000
16000.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+O<=>C6H4OH+OH	2.000E+013	0.000
14700.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+OH<=>C6H4OH+H2O	1.400E+013	0.000
4600.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+HO2<=>C6H4OH+H2O2	4.000E+011	0.000
28900.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		
C6H5OH+CH3<=>C6H4OH+CH4	2.000E+012	0.000
15000.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		

!

!\REACTIONCLASS: \R_ADDITION\O	\A	\N
\EA		

!

C6H5OH+O<=>OC6H4OH+H	1.600E+013	0.000
3400.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003		

!

!\REACTIONCLASS: \R_DECOMPOSITION	\A	\N
\EA		

!

C6H5O<=>CO+C5H5	2.000E+011	0.000
43900.0 !\AUTHOR: !\REF:WKM A FACTOR REDUCED FROM 2.5E+11 TO 2.0E+11 TO FIT DATA BENZENE FLOW REACTOR DATA (LOVELL)		

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!
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!\REACTIONCLASS: \R_R_PRODUCTS          \A          \N
\EA
!
-----
C6H5O+H<=>CO+C5H6                      1.000E+013    0.000
0.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
C6H5O+O<=>C5H5+CO2                      1.000E+013    0.000
0.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
C6H5O+O<=>OC6H4OH                      2.600E+010    0.470
800.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
!
-----
!\REACTIONCLASS: \R_O2_PRODUCTS          \A          \N
\EA
!
-----
C6H4OH+O2<=>OC6H4OH+O                  2.100E+013    0.000
6100.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003
OC6H4OH<=>C5H4OH+CO                    7.400E+011    0.000
43800.0 !\AUTHOR: !\REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524,
2003
!
-----
!\REACTIONCLASS: \R_O_PRODUCTS           \A          \N
\EA
!
-----
C6H5O+O<=>P-C6H4O2+H                   4.250E+013    0.000
0.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
C6H5O+O<=>O-C6H4O2+H                   8.500E+013    0.000
0.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
!
-----
!\REACTIONCLASS: \R_HO2_PRODUCTS         \A          \N
\EA
!
-----
C6H5O+HO2<=>O-OC6H5OJ+OH              2.000E+012    0.000
0.0 !\AUTHOR: !\REF:UP AND IT IS NOT SEEN IN THE EXPERIMENT
P-C6H4O2+H<=>P-OC6H5OJ                 4.000E+012    0.000
9740.0 !\AUTHOR: !\REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN
INT J CHEM KINET 38: 250-275, 2006
O-C6H4O2+H<=>O-OC6H5OJ                 4.000E+012    0.000
6960.0 !\AUTHOR: !\REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN
INT J CHEM KINET 38: 250-275, 2006
!=====
=====
!\SUBSPECIES: O-C6H4O2\P-C6H4O2
!=====
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!
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!\REACTIONCLASS: \UNIMOL \A \N
\EA
!

O-C6H4O2<=>C5H4O+CO 1.000E+012 0.000
40000.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697,
1998
P-C6H4O2<=>C5H4O+CO 3.700E+011 0.000
59000.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697,
1998
P-C6H3O2+H<=>P-C6H4O2 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
!

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

P-C6H4O2+H<=>P-C6H3O2+H2 2.000E+012 0.000
8100.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
P-C6H4O2+O<=>P-C6H3O2+OH 1.400E+013 0.000
14700.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697,
1998
P-C6H4O2+OH<=>P-C6H3O2+H2O 1.000E+006 2.000
4000.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
!

!\REACTIONCLASS: \RADICAL_ADDITION \A \N
\EA
!

P-C6H4O2+H<=>C5H5O+CO 2.500E+013 0.000
4700.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
P-C6H4O2+O=>2CO+C2H2+CH2CO 3.000E+013 0.000
5000.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
!

!\REACTIONCLASS: \R_R_PRODUCTS \A \N
\EA
!

P-C6H3O2+H<=>2C2H2+2CO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998
P-C6H3O2+O=>C2H2+HCCO+2CO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998

!=====
=====

!\ENDSUBSPECIES: \O-C6H4O2\P-C6H4O2

!=====
=====

!-----

!\ENDSUBMECH: \C6H5OH

!-----

!-----

!\SUBMECH: \C5H6

!

!\REACTIONCLASS: \AROMATIC_GROWTH

\A

\N

\EA

!

C5H6+C2H3<=>C6H6+CH3 2.100E+067 -16.080
42460.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

!

!\REACTIONCLASS: \UNIMOL

\A

\N

\EA

!

C5H5+H(+M)<=>C5H6(+M) 2.600E+014 0.000
0.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007

LOW/ 4.400E+080 -18.280
12994.0/

TROE/ 6.800E-002 4.007E+002 4.136E+003 5.502E+003/

CO/ 1.50/ CO2/ 2.00/ H2O/ 6.00/ H2/ 2.00/ CH4/ 2.00/

C5H6(+M)<=>C3H4-A+C2H2(+M) 3.800E+017 0.000

104000.0 !\AUTHOR: !\REF:MACKIE ET AL. PHYS CHEM CHEM PHYS 3 2467 2001

LOW/ 1.000E+098 -22.250
126321.5/

TROE/ 1.441E-001 5.358E+000 3.284E+003 6.710E+009/

CO/ 1.50/ CO2/ 2.00/ H2O/ 6.00/ H2/ 2.00/ CH4/ 2.00/

C#CCVCCJ+H<=>C5H6 1.000E+014 0.000

0.0 !\AUTHOR: !\REF:LIN J COMPUT CHEM 21 415-425 2000

!

!\REACTIONCLASS: \RH_R_ABSTRACTION

\A

\N

\EA

!

C5H6+H<=>C5H5+H2 7.200E+013 0.000
3500.0 !\AUTHOR: !\REF:ROY AND FRANK, 21ST INTERNATIONAL SYMPOSIUM ON
SHOCKWAVES, 1997 PPER 1560

C5H6+O2<=>C5H5+HO2 4.000E+013 0.000

37150.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+O<=>C5H5+OH 4.800E+004 2.710

1100.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+OH<=>C5H5+H2O 3.080E+006 2.000

0.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+HO2<=>C5H5+H2O2 1.100E+004 2.600

12900.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+CH3<=>C5H5+CH4 1.800E-001 4.000

0.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+HCO<=>C5H5+CH2O 1.080E+008 1.900

16000.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+C2H3<=>C5H5+C2H4 1.200E-001 4.000

0.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

C5H6+C3H5-A<=>C5H5+C3H6 5.50E+10 0.00

5505 !\AUTHOR: !\1997BUR/DVI505-514

C5H6+C4H5-I<=>C5H5+C4H6	6.000E+012	0.000
0.0 !\AUTHOR: !\REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161		
C5H6+C4H5-N<=>C5H5+C4H6	6.000E+012	0.000
0.0 !\AUTHOR:		
C5H6+C6H5<=>C5H5+C6H6	1.000E-001	4.000
0.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H6+C6H5O<=>C5H5+C6H5OH	3.160E+011	0.000
8000.0 !\AUTHOR: !\REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161		
C5H6+C5H5<=>C6H6+C4H5-N	5.000E+009	0.000
0.0 !\AUTHOR: !\REF:ON OTHER CONDITIONS.		

!

!\REACTIONCLASS: \RADICAL_ADDITION	\A	\N
\EA		

!

C5H6+H<=>C2H2+C3H5-A	1.548E+037	-6.180
32890.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H6+H<=>C5H7	2.400E+073	-17.850
31500.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H6+O<=>C5H5O+H	8.900E+012	-0.150
590.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
DUP		
C5H6+O<=>C5H5O+H	5.600E+012	-0.060
200.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
DUP		
C5H6+H<=>CVCCJCVC	1.100E+014	-0.160
3100.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H6+OH<=>CVCCJCVCOH	1.100E+013	-0.070
870.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
CVCCJCVCOH+O2<=>HOCVCCVO+CH2CHO	1.200E+036	-7.250
33600.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		

!=====
=====

!\SUBSPECIES: \C5H7

!=====
=====

!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION	\A	\N
\EA		

!

C5H7<=>CVCCJCVC	3.200E+015	0.000
39500.0 !\AUTHOR: !\REF:ARENDS ET AL. J PHYS CHEM 97: 7914 1993		
CVCCJCVC<=>CVCCVCCJ	5.400E+011	-0.700
60.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
!\ CVCCVCCJ+H<=>CVCCVCC	2.300E+020	-1.600 3020.0
!\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
CVCCVCCJ+H(+M)<=>C5H81-3(+M)	2.00E+14	0.00 0.0
!\AUTHOR:		
LOW / 1.33E+60 -12.00 5967.8 /		
TROE / 0.020 1096.6 1096.6 6859.5 /		
H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/ AR/0.7/		
CVCCJCVC+O2<=>C2H3CHO+CH2CHO	1.200E+036	-7.250
33600.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		

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CVCCJVC+O<=>C2H3CHO+C2H3                2.000E+014    0.000
0.0 !\AUTHOR: !\REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
!=====
=====
!\ENDSUBSPECIES: \C5H7
!=====
=====
!\SUBSPECIES: \CVCCVC
!=====
=====
!\REACTIONCLASS: \UNIMOL_CHEMACT           \A           \N
\EA
!-----

CVCCVCCJ+H<=>C4H5-N+CH3                    2.900E+026    -2.180
36770.0 !\AUTHOR: !\REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
!-----

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

C5H81-3+H<=>CVCCVCCJ+H2                    7.000E+006     2.000
5000.0 !\AUTHOR: !\REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
C5H81-3+OH<=>CVCCVCCJ+H2O                  7.000E+006     2.000
0.0 !\AUTHOR: !\REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996
!-----

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

C5H81-3+H<=>C4H6+CH3                       5.200E+071   -16.380
51000.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
!-----

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

CVCCVCCJ+OH<=>CVCCVCCOH                     1.500E+013     0.000
0.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
CVCCVCCJ+O2<=>CH2CHCHCHO+CH2O               8.200E+010     0.180
9140.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
CVCCVCCOH+H<=>C4H6+CH2OH                    2.500E+034    -6.120
16250.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
!=====
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!\ENDSUBSPECIES: \CVCCVC
!=====
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!\REACTIONCLASS: \RADICAL_OXIDATION \A \N
\EA
!

C5H7+O2<=>OC5H7O 8.900E+024 -3.800
20000.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
OC5H7O+O2<=>OC4H6O+HOCO 6.300E+005 -7.250
33600.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
OC4H6O+H<=>OC4H5O+H2 2.300E+010 1.050
3279.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
OC4H6O+OH<=>OC4H5O+H2O 3.500E+009 1.180
-447.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
OC4H5O+O2<=>O2CCHOOJ+C2H4 1.600E+045 -9.920
20670.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
O2CCHOOJ<=>HOCO+CO2 3.000E+013 0.000
4000.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)

!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

C5H7+H<=>C5H6+H2 3.600E+012 0.000
0.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
C5H7+O<=>C5H6+OH 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
C5H7+OH<=>C5H6+H2O 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
C5H6+HO2<=>C5H7+O2 1.300E+015 -1.070
9530.0 !\AUTHOR: !\REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998

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!\ENDSUBSPECIES: \C5H7
!=====
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!=====
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!\SUBSPECIES: \HOCVCCVO
!=====
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!

!

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

HOCVCCVO+OH<=>HOCVCCJVO+H2O 2.690E+010 0.760
-340.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)

$\text{HOCVCCVO} + \text{HO}_2 \rightleftharpoons \text{HOCVCCJVO} + \text{H}_2\text{O}_2$ 1.000E+012 0.000
 11920.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
 THESIS)
 $\text{HOCVCCVO} + \text{CH}_3 \rightleftharpoons \text{HOCVCCJVO} + \text{CH}_4$ 3.980E+012 0.000
 8700.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
 THESIS)
 $\text{HOCVCCVO} + \text{O} \rightleftharpoons \text{HOCVCCJVO} + \text{OH}$ 7.180E+012 0.000
 1389.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
 THESIS)
 $\text{HOCVCCVO} + \text{O}_2 \rightleftharpoons \text{HOCVCCJVO} + \text{HO}_2$ 2.000E+013 0.000
 40700.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
 THESIS)
 $\text{HOCVCCVO} + \text{H} \rightleftharpoons \text{HOCVCCJVO} + \text{H}_2$ 2.600E+012 0.000
 2600.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
 THESIS)

!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
 \EA

!

$\text{C}_2\text{H}_2\text{OH} + \text{CO} \rightleftharpoons \text{HOCVCCJVO}$ 1.510E+011 0.000
 4810.0 !\AUTHOR: !\REF:WKM ANALOGY TO $\text{C}_2\text{H}_5 + \text{CO} \rightleftharpoons \text{C}_2\text{H}_5\text{CO}$

!=====

!\ENDSUBSPECIES: \HOCVCCVO

!=====

!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
 \EA

!

$\text{C}_5\text{H}_5 \rightleftharpoons \text{C}_3\text{H}_3 + \text{C}_2\text{H}_2$ 1.980E+068 -15.000
 124900.0 !\AUTHOR: !\REF:LIN J COMPUT CHEM 21 415-425 2000
 $\text{C}\#\text{CCVCCJ} \rightleftharpoons \text{C}_5\text{H}_5$ 8.000E+013 0.000
 34058.3 !\AUTHOR: !\REF:LIN J COMPUT CHEM 21 415-425 2000
 $\text{C}_3\text{H}_3 + \text{C}_2\text{H}_2 \rightleftharpoons \text{C}\#\text{CCVCCJ}$ 4.110E+072 -18.200
 45400.0 !\AUTHOR: !\REF:LIN J COMPUT CHEM 21 415-425 2000
 $\text{C}\#\text{CCVCCJ} + \text{H} \rightleftharpoons \text{C}_5\text{H}_6\text{-L}$ 1.000E+010 0.000
 0.0 !\AUTHOR: !\REF:LINDSTEDT C&F 99:551-561 (1994)
 $\text{C}_5\text{H}_6\text{-L} + \text{O} \rightleftharpoons \text{C}\#\text{CCVCCJ} + \text{OH}$ 1.000E+010 0.000
 0.0 !\AUTHOR: !\REF:LINDSTEDT C&F 99:551-561 (1994)
 $\text{C}_5\text{H}_6\text{-L} + \text{OH} \rightleftharpoons \text{C}\#\text{CCVCCJ} + \text{H}_2\text{O}$ 1.000E+010 0.000
 0.0 !\AUTHOR: !\REF:LINDSTEDT C&F 99:551-561 (1994)

!

!\REACTIONCLASS: \RADICAL_OXIDATION \A \N
 \EA

!

$\text{C}_5\text{H}_5 + \text{HO}_2 \rightleftharpoons \text{C}_5\text{H}_5\text{O} + \text{OH}$ 6.300E+029 -4.690
 11650.0 !\AUTHOR: !\REF:RISTORI ET AL. COMBUST. SCI. AND TECH 2001. VOL.
 167. PP. 223-256
 $\text{C}_5\text{H}_5 + \text{O}_2 \rightleftharpoons \text{C}_4\text{H}_4\text{O} + \text{HCO}$ 6.000E+018 -2.480
 10970.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998

C5H5+O<=>C4H5-N+CO	3.200E+013	-0.170
440.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
C5H5+O<=>C5H4O+H	5.800E+013	-0.020
20.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
C5H5+OH<=>C5H5OH	6.500E+014	-0.850
-2730.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
DUP		
C5H5+OH<=>C5H5OH	1.100E+043	-8.760
18730.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
DUP		
C5H5+OH<=>C5H5OH	1.100E+059	-13.080
33450.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
DUP		
C5H5+OH<=>C5H4OH+H	3.500E+057	-12.180
48350.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
C5H5+OH<=>C4H6+CO	4.000E+014	0.000
4500.0 !\AUTHOR: !\REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998		
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!\SUBSPECIES: C5H5OH		
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!		
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!\REACTIONCLASS: \UNIMOL	\A	\N
\EA		
!		
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C5H4OH+H<=>C5H5OH	1.000E+014	0.000
0.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!		
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!\REACTIONCLASS: \RH_R_ABSTRACTION	\A	\N
\EA		
!		
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C5H5OH+H<=>C5H5O+H2	4.000E+013	0.000
6094.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+O<=>C5H5O+OH	1.000E+013	0.000
4683.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+OH<=>C5H5O+H2O	1.000E+013	0.000
1697.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+HO2<=>C5H5O+H2O2	1.000E+013	0.000
15800.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+H<=>C5H4OH+H2	3.200E+012	0.000
0.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+O<=>C5H4OH+OH	4.700E+011	0.000
0.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+OH<=>C5H4OH+H2O	5.500E+012	0.000
1731.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+HO2<=>C5H4OH+H2O2	3.600E+003	2.550
10531.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		

!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA
!

C5H5O<=>C5H4O+H 2.900E+032 -6.500
21220.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
C5H5O<=>C4H5-N+CO 1.100E+079 -19.620
66250.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)
C5H5O<=>CJVCCVCCVO 2.000E+013 0.000
14338.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)

!

!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A \N
\EA
!

C5H5O+O2<=>C5H4O+HO2 6.0E+10 0.0
1600.0 !\AUTHOR:

!=====
=====
!\SUBSPECIES: CJVCCVCCVO
!=====
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CJVCCVCCVO<=>CVCCVCCJVO 4.300E+011 -1.050
4118.0 !\AUTHOR: FROM METHODS DESCRIBED IN CURRAN'S N-HEPTANE C&F 114:
149-177 (1998)
C4H5-N+CO<=>CVCCVCCJVO 1.510E+011 0.000
4810.0 !\AUTHOR: !\REF:WKM ANALOGY TO C2H5+CO<=>C2H5CO
CJVCCVCCVO<=>C2H2+CJVCCVO 3.000E+013 0.000
43710.0 !\AUTHOR: !\REF:SAKAI ET AL PROCEEDINGS OF THE COMBUSTION
INSTITUTE 32 (2009) 411-418
CJVCCVO<=>C2H3CO 1.400E+009 0.980
32100.0 !\AUTHOR: !\REF:SAKAI ET AL PROCEEDINGS OF THE COMBUSTION
INSTITUTE 32 (2009) 411-418
C2H2+HCO<=>CJVCCVO 7.770E+006 1.410
7755.0 !\AUTHOR: !\REF:SAKAI ET AL PROCEEDINGS OF THE COMBUSTION
INSTITUTE 32 (2009) 411-418

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!\ENDSUBSPECIES: CJVCCVCCVO
!=====
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!

!\REACTIONCLASS: \R_R_ABSTRACTION \A \N
\EA
!

C5H4OH+H<=>C5H4O+H2 2.100E+013 0.000
54000.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.
C5H4OH+O2<=>C5H4O+HO2 3.000E+013 0.000
5000.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.


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!\SUBSPECIES: \C5H4O
!
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!
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!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
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C5H4O=>CO+C2H2+C2H2                    5.700E+032    -6.760
68500.0 !\AUTHOR: !\REF:WANG AND BREZINSKY J PHYS CHEM A 102: 1530 1998
DUP
C5H4O=>CO+C2H2+C2H2                    6.200E+041    -7.870
98700.0 !\AUTHOR: !\REF:WANG AND BREZINSKY J PHYS CHEM A 102: 1530 1998
DUP
C5H3O+H<=>C5H4O                        1.000E+014     0.000
0.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.
!
-----
!\REACTIONCLASS: \RH_R_ABSTRACTION      \A                \N
\EA
!
-----
C5H4O+H<=>C5H3O+H2                      2.000E+012     0.000
8100.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.
C5H4O+O<=>C5H3O+OH                      1.400E+013     0.000
1470.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.
C5H4O+OH<=>C5H3O+H2O                    1.100E+008     1.420
1450.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.
!
-----
!\REACTIONCLASS: \RADICAL_DECOMPOSITION \A                \N
\EA
!
-----
C5H3O=>C2H2+CO+C2H                      2.000E+013     0.000
51000.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.
!
-----
!\REACTIONCLASS: \R_O2_PRODUCTS         \A                \N
\EA
!
-----
C5H3O+O2=>CO2+C2H2+HCCO                9.700E+058    -13.470
38180.0 !\AUTHOR: !\REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING
(WESTERN STATES) 2007
!
-----
!\REACTIONCLASS: \RADICAL_ADDITION      \A                \N
\EA
!
-----
C5H4O+H<=>C4H5-N+CO                    2.100E+061    -13.270
40810.0 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S
THESIS)

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C5H4O+O<=>C4H4+CO2          1.000E+013      0.000
2000.0 !\AUTHOR: !\REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.
!=====
=====
!\ENDSUBSPECIES: \C5H4O
!=====
=====
!\ENDSUBSPECIES: \C5H5OH
!=====
=====
!\SUBSPECIES: \C4H4O
!=====
=====
C4H4O+H<=>C3H5-A+CO          6.600E+013      -0.020
2740.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000
DUP
C4H4O+H<=>C3H5-A+CO          5.900E+006       2.000
1300.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000
DUP
C4H4O+O<=>CH2CHO+HCCO        3.000E+008       1.450
-860.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000
C4H4O+OH<=>C3H5-A+CO2        3.000E+012       0.000
0.0 !\AUTHOR: !\REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000
C4H4O+OH=>C2H2+HCCO+H2O     2.02E+13         0.0
5933.0 !\AUTHOR:
!=====
=====
!\ENDSUBSPECIES: \C4H4O
!=====
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!\ENDSUBMECH: \C5H6
!-----
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!
END

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