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#####
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!
###
###
!
###          COLIBRI V2 for
Lignin derived biofuels      ###
*
!
###          *
!
#####
!
#####
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!+++++
+++++
+++++
ELEMENTS
C
H
N
O
AR
HE
!XE
NE
END
```

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!+++++
+++++
+++++
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SPECIES
!-----
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!
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+++++
!
+
!
model : Burke and Curran model ==> +
!
+
!
+++++
```

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!SPECIES_MODULE: DILUENTS
AR
N2
HE
!XE
NE
```

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!SPECIES_MODULE: C0 / MODSUBMECHS: H2 O2 H2O H2O2
H2
H
O2
O
H2O
OH
OH*
H2O2
HO2

```

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!SPECIES_MODULE: C1 / MODSUBMECHS: CO CH4 CH3OH CH2O
CO
CO2
HOCO          ! [C](=O)O
CH4
CH3
CH2
CH2(S)
C
CH
CH*
CH3O2H        ! COO
CH3O2         ! CO[O]
CH2O2H        ! [CH2]OO
CH3OH         ! CO
CH3O          ! C[O]
CH2OH         ! [CH2]O
CH2O          ! C=O
HCO           ! [CH]=O
HCOH          ! singlet[CH]O
HO2CHO        ! O=COO
HOCH2O2H     ! OCOO
HOCH2O2      ! [O]OCO
OCH2O2H      ! [O]COO
HOCH2O       ! [O]CO
O2CHO        ! [O]OC=O
HOCHO        ! O=CO
OCHO         ! [O]C=O

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!SPECIES_MODULE: C2 / MODSUBMECHS: C2H6 CH3CHO CH2CO C2H4 C2H2 C2H5OH
CH3OCH3 CH3OCHO
C2H6          ! CC                      InChI=1S/C2H6/c1-2/h1-2H3
C2H5          ! [C]C                      InChI=1S/C2H5/c1-2/h1H2,2H3
C2H5O2H      ! CCOO                      InChI=1S/C2H6O2/c1-2-4-
3/h3H,2H2,1H3
C2H5O2       ! CCO[O]                    InChI=1S/C2H5O2/c1-2-4-
3/h2H2,1H3
C2H4         ! C=C                      InChI=1S/C2H4/c1-2/h1-2H2
C2H3         ! C=[CH]                   InChI=1S/C2H3/c1-2/h1H,2H2
C2H2         ! C#C                      InChI=1S/C2H2/c1-2/h1-2H
C2H          ! C#[C]                    InChI=1S/C2H/c1-2/h1H
H2CC        ! [C]=C                    InChI=1S/C2H2/c1-2/h1H2
C2H5OH      ! CCO                      InChI=1S/C2H6O/c1-2-
3/h3H,2H2,1H3
C2H5O       ! CC[O]                    InChI=1S/C2H5O/c1-2-
3/h2H2,1H3

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PC2H4OH 2H2	! [CH2]CO	InChI=1S/C2H5O/c1-2-3/h3H,1-
SC2H4OH 3H,1H3	! C[CH]O	InChI=1S/C2H5O/c1-2-3/h2-
O2C2H4OH 4/h3H,1-2H2	! [O]OCCO	InChI=1S/C2H5O3/c3-1-2-5-
C2H4O2H 3/h3H,1-2H2	! [CH2]COO	InChI=1S/C2H5O2/c1-2-4-
C2H4O1-2 2H2	! C1CO1	InChI=1S/C2H4O/c1-2-3-1/h1-
C2H3O1-2 1/h1H,2H2	! [CH]1CO1	InChI=1S/C2H3O/c1-2-3-
CH3CHO	! CC=O	InChI=1S/C2H4O/c1-2-3/h2H,1H3
CH3CO	! C[C]=O	InChI=1S/C2H3O/c1-2-3/h1H3
CH2CHO	! [CH2]C=O	InChI=1S/C2H3O/c1-2-3/h2H,1H2
O2CH2CHO 4/h1H,2H2	! [O]OCC=O	InChI=1S/C2H3O3/c3-1-2-5-
HO2CH2CO 4/h4H,2H2	! O=[C]COO	InChI=1S/C2H3O3/c3-1-2-5-
C2H3OH 3H,1H2	! C=CO	InChI=1S/C2H4O/c1-2-3/h2-
C2H2OH	! OC=[CH]	InChI=1S/C2H3O/c1-2-3/h1-3H
CH2CO	! C=C=O	InChI=1S/C2H2O/c1-2-3/h1H2
HCCO	! [CH]=C=O	InChI=1S/C2HO/c1-2-3/h1H
HCCOH	! C#CO	InChI=1S/C2H2O/c1-2-3/h1,3H
CH3CO3H 4/h4H,1H3	! CC(=O)OO	InChI=1S/C2H4O3/c1-2(3)5-
CH3CO3 4/h1H3	! CC(=O)O[O]	InChI=1S/C2H3O3/c1-2(3)5-
CH3CO2	! CC([O])=O	InChI=1S/C2H3O2/c1-2(3)4/h1H3
CH3OCH3	! COC	InChI=1S/C2H6O/c1-3-2/h1-2H3
CH3OCH2 2/h1H2,2H3	! [CH2]OC	InChI=1S/C2H5O/c1-3-
CH3OCH2O2H 3/h3H,2H2,1H3	! COCOO	InChI=1S/C2H6O3/c1-4-2-5-
CH3OCH2O2 3/h2H2,1H3	! COCO[O]	InChI=1S/C2H5O3/c1-4-2-5-
CH2OCH2O2H 3/h3H,1-2H2	! [CH2]OCOO	InChI=1S/C2H5O3/c1-4-2-5-
O2CH2OCH2O2H 4/h3H,1-2H2	! [O]OCOCOO	InChI=1S/C2H5O5/c3-6-1-5-2-7-
HO2CH2OCHO 4/h1,4H,2H2	! O=COCOO	InChI=1S/C2H4O4/c3-1-5-2-6-
OCH2OCHO 4/h1H,2H2	! [O]COC=O	InChI=1S/C2H3O3/c3-1-5-2-
HOCH2OCO 4/h3H,1H2	! O=[C]OCO	InChI=1S/C2H3O3/c3-1-5-2-
CH3OCH2O 3/h2H2,1H3	! COC[O]	InChI=1S/C2H5O2/c1-4-2-
CH3OCHO 3/h2H,1H3	! COC=O	InChI=1S/C2H4O2/c1-4-2-
CH3OCO	! CO[C]=O	InChI=1S/C2H3O2/c1-4-2-3/h1H3
CH2OCHO 3/h2H,1H2	! [CH2]OC=O	InChI=1S/C2H3O2/c1-4-2-

!SPECIES_MODULE: C3 / MODSUBMECHS: CH3COCH3 C2H3CHO C2H5CHO C3H8 C3H6
C3H4-A C3H4-P

C3H8 2H3	! CCC	InChI=1S/C3H8/c1-3-2/h3H2,1-
IC3H7 2H3	! C[CH]C	InChI=1S/C3H7/c1-3-2/h3H,1-
NC3H7 2/h1,3H2,2H3	! [CH2]CC	InChI=1S/C3H7/c1-3-
NC3H7O2H 4/h4H,2-3H2,1H3	! CCCOO	InChI=1S/C3H8O2/c1-2-3-5-
NC3H7O2 4/h2-3H2,1H3	! CCCO[O]	InChI=1S/C3H7O2/c1-2-3-5-
IC3H7O2H 4/h3-4H,1-2H3	! CC(C)OO	InChI=1S/C3H8O2/c1-3(2)5-
IC3H7O2 4/h3H,1-2H3	! CC(C)O[O]	InChI=1S/C3H7O2/c1-3(2)5-
NC3H7O 3H2,1H3	! CCC[O]	InChI=1S/C3H7O/c1-2-3-4/h2-
IC3H7O 3(2)4/h3H,1-2H3	! CC(C)[O]	InChI=1S/C3H7O/c1-
C3H6OOH1-2 4/h2,4H,3H2,1H3	! C[CH]COO	InChI=1S/C3H7O2/c1-2-3-5-
C3H6OOH1-3 4/h4H,1-3H2	! [CH2]CCOO	InChI=1S/C3H7O2/c1-2-3-5-
C3H6OOH2-1 4/h3-4H,1H2,2H3	! OOC([CH2])C	InChI=1S/C3H7O2/c1-3(2)5-
C3H6OOH1-2O2 4/h3-4H,2H2,1H3	! O OCC(O[O])C	InChI=1S/C3H7O4/c1-3(7-5)2-6-
C3H6OOH1-3O2 5/h4H,1-3H2	! OCCCCO[O]	InChI=1S/C3H7O4/c4-6-2-1-3-7-
C3H6OOH2-1O2 4/h3,5H,2H2,1H3	! [O]OCC(OO)C	InChI=1S/C3H7O4/c1-3(7-5)2-6-
C3KET12 5/h2-3,5H,1H3	! CC(C=O)OO	InChI=1S/C3H6O3/c1-3(2-4)6-
C3KET13 5/h2,5H,1,3H2	! OCCCC=O	InChI=1S/C3H6O3/c4-2-1-3-6-
C3H51-2,3OOH 4/h3-5H,1-2H2	! O OCC(OO)[CH2]	InChI=1S/C3H7O4/c1-3(7-5)2-6-
C3H52-1,3OOH 5/h1,4-5H,2-3H2	! OOC[CH]COO	InChI=1S/C3H7O4/c4-6-2-1-3-7-
C3H5O1-2OOH-3 3/h3-4H,1-2H2	! O OCC1CO1	InChI=1S/C3H6O3/c4-6-2-3-1-5-
C3H5O1-3OOH-2 3/h3-4H,1-2H2	! OOC1COC1	InChI=1S/C3H6O3/c4-6-3-1-5-2-
C3H6O1-2 3/h3H,2H2,1H3	! CC1CO1	InChI=1S/C3H6O/c1-3-2-4-
C3H6O1-3 3H2	! C1CCO1	InChI=1S/C3H6O/c1-2-4-3-1/h1-
C3H6 2/h3H,1H2,2H3	! CC=C	InChI=1S/C3H6/c1-3-
C3H5-A 2H2	! [CH2]C=C	InChI=1S/C3H5/c1-3-2/h3H,1-
C3H5-S 2/h1,3H,2H3	! CC=[CH]	InChI=1S/C3H5/c1-3-
C3H5-T	! C[C]=C	InChI=1S/C3H5/c1-3-2/h1H2,2H3
CC3H6	! C1CC1	InChI=1S/C3H6/c1-2-3-1/h1-3H2
C3H5O 4/h2H,1,3H2	! [O]CC=C	InChI=1S/C3H5O/c1-2-3-
CH2CHOCH2 2/h3H,1-2H2	! C=CO[CH2]	InChI=1S/C3H5O/c1-3-4-

CH3CHCHO 3H, 1H3	! C[CH]C=O	InChI=1S/C3H5O/c1-2-3-4/h2-
AC4H7OOH 2/h3H, 1, 4H2, 2H3	! C=CCOOC	InChI=1S/C4H8O2/c1-3-4-6-5-
C3H6OH1-2 4/h2, 4H, 3H2, 1H3	! C[CH]CO	InChI=1S/C3H7O/c1-2-3-
CH3CHCO 4/h2H, 1H3	! CC=C=O	InChI=1S/C3H4O/c1-2-3-
AC3H5OOH 4/h2, 4H, 1, 3H2	! C=CCOO	InChI=1S/C3H6O2/c1-2-3-5-
C2H3OOH 3H, 1H2	! C=COO	InChI=1S/C2H4O2/c1-2-4-3/h2-
C2H3OO 3/h2H, 1H2	! C=C(O[O])	InChI=1S/C2H3O2/c1-2-4-
CHCHO	! [CH]C=O ?	InChI=1S/C2H2O/c1-2-3/h1-2H
C3H6OH2-1 4H, 1H2, 2H3	! CC(O)[CH2]	InChI=1S/C3H7O/c1-3(2)4/h3-
TQJC3H6OH 5/h3-4H, 2H2, 1H3	! CC(O[O])CO	InChI=1S/C3H7O3/c1-3(2-4)6-
TQC3H6OI 5/h3, 5H, 2H2, 1H3	! CC(OO)C([O])	InChI=1S/C3H7O3/c1-3(2-4)6-
QC3H5OHP 5/h3-5H, 1-2H2	! C(O)C(OO)[CH2]	InChI=1S/C3H7O3/c1-3(2-4)6-
CCY(COC)OH 2/h2-4H, 1H3	! CC1C(O)O1	InChI=1S/C3H6O2/c1-2-3(4)5-
IQJC3H6OH 5/h3-4H, 2H2, 1H3	! C(O[O])C(O)C	InChI=1S/C3H7O3/c1-3(4)2-6-
IQC3H6OT 5/h3, 5H, 2H2, 1H3	! C(OO)C([O])C	InChI=1S/C3H7O3/c1-3(4)2-6-
CY(COC)COH 3/h3-4H, 1-2H2	! C1C(O1)C(O)	InChI=1S/C3H6O2/c4-1-3-2-5-
CHOCOCH3 4/h2-3, 5H, 1H3	! C(=O)C(O)C	InChI=1S/C3H6O2/c1-3(5)2-
CY(CCOC)OH 3/h3-4H, 1-2H2	! C1C(O)CO1	InChI=1S/C3H6O2/c4-3-1-5-2-
TQC3H5OHI 5/h2-5H, 1H3	! [CH](O)C(OO)C	InChI=1S/C3H7O3/c1-3(2-4)6-
TQC3H5OHIO2 5)3(4)8-6/h2-5H, 1H3	! C(O)(O[O])C(OO)C	InChI=1S/C3H7O5/c1-2(7-
TQC3H5OHIOQ-I 5)3(4)8-6/h2-3, 5-6H, 1H3	! C([O])(OO)C(OO)C	InChI=1S/C3H7O5/c1-2(7-
TQC3H5OHIOQ-P 5)3(4)8-6/h2-6H, 1H2	! C(O)(OO)C(OO)[CH2]	InChI=1S/C3H7O5/c1-2(7-
C2H3COHOH 5/h2-5H, 1H2	! C=CC(O)(OO)	InChI=1S/C3H6O3/c1-2-3(4)6-
COHOHCY(COC) 6-2/h2-5H, 1H2	! OC(C1CO1)OO	InChI=1S/C3H6O4/c4-3(7-5)2-1-
OHCY(COCC)OOH 6-3/h2-5H, 1H2	! OOC1COC1O	InChI=1S/C3H6O4/c4-3-2(7-5)1-
TQC3H5OHTO2 5)3(4)8-6/h2-4, 6H, 1H3	! C(O)(OO)C(O[O])C	InChI=1S/C3H7O5/c1-2(7-
OHCOCOHCH3 6)3(4)5/h2, 6H, 1H3, (H, 4, 5)	! C(O)(=O)C(OO)C	InChI=1S/C3H6O4/c1-2(7-
IQC3H5OHPJ 5/h3-5H, 1-2H2	! C(OO)C(O)[CH2]	InChI=1S/C3H7O3/c1-3(4)2-6-
IQC3H5OHPJO2 8-6/h3-5H, 1-2H2	! C(OO)C(O)C(O[O])	InChI=1S/C3H7O5/c4-3(1-7-5)2-

IQC3H5OTQ-I 8-6/h3,5-6H,1-2H2	! C(OO)C([O])C(OO)	InChI=1S/C3H7O5/c4-3(1-7-5)2-
CHOCH2OOH 4/h1,4H,2H2	! OOC=O ?	InChI=1S/C2H4O3/c3-1-2-5-
IQC3H5OHQ-SJ 8-6/h1,3-6H,2H2	! [CH](OO)C(O)C(OO)	InChI=1S/C3H7O5/c4-3(1-7-5)2-
SC3H5OH 4H,1H3	! CC=CO	InChI=1S/C3H6O/c1-2-3-4/h2-
IC3H5OH 3(2)4/h4H,1H2,2H3	! C=C(C)O	InChI=1S/C3H6O/c1-
C3H5OH 4/h2,4H,1,3H2	! OCC=C	InChI=1S/C3H6O/c1-2-3-
CH2CCH2OH 4/h4H,1,3H2	! C=[C]CO	InChI=1S/C3H5O/c1-2-3-
CHOCOCH2OOH 6/h1,3,5-6H,2H2	! C(=O)C(O)C(OO)	InChI=1S/C3H6O4/c4-1-3(5)2-7-
CHOCHO 2H	! O=CC=O	InChI=1S/C2H2O2/c3-1-2-4/h1-
C3H4-P	! CC#C	InChI=1S/C3H4/c1-3-2/h1H,2H3
C3H4-A	! C=C=C	InChI=1S/C3H4/c1-3-2/h1-2H2
C3H3	! [CH2]C#C	InChI=1S/C3H3/c1-3-2/h1H,2H2
CC3H4 2H,3H2	! C1=CC1	InChI=1S/C3H4/c1-2-3-1/h1-
C3H2	! [CH]=C=[CH]	InChI=1S/C3H2/c1-3-2/h1-2H
H2CCC(S)	! C=C=[C]	InChI=1S/C3H2/c1-3-2/h1H2
C3H2(S) 2/h1-2H	! singlet[CH]=C=[CH]	SINGLELET_InChI=1S/C3H2/c1-3-
C3H2C	! C1=CC=1	InChI=1S/C3H2/c1-2-3-1/h1-2H
PC3H4OH-2 4H,1H3	! C[C]=CO	InChI=1S/C3H5O/c1-2-3-4/h3-
SC3H4OH 3(2)4/h4H,1-2H2	! C=C([CH2])O	InChI=1S/C3H5O/c1-
C3H3O 4/h3H,1H2	! [O]C=C=C	InChI=1S/C3H3O/c1-2-3-
C3H3O2H 4/h3-4H,1H2	! OOC=C=C	InChI=1S/C3H4O2/c1-2-3-5-
C2HCHO	! C#CC=O	InChI=1S/C3H2O/c1-2-3-4/h1,3H
C2H5CHO 4/h3H,2H2,1H3	! CCC=O	InChI=1S/C3H6O/c1-2-3-
C2H5CO 4/h2H2,1H3	! CC[C]=O	InChI=1S/C3H5O/c1-2-3-
CH2CH2CHO 4/h3H,1-2H2	! [CH2]CC=O	InChI=1S/C3H5O/c1-2-3-
C2H3CHO 3H,1H2	! C=CC=O	InChI=1S/C3H4O/c1-2-3-4/h2-
C2H3CO 4/h2H,1H2	! C=C[C]=O	InChI=1S/C3H3O/c1-2-3-
CH3COCH3 2H3	! CC(C)=O	InChI=1S/C3H6O/c1-3(2)4/h1-
CH3COCH2 3(2)4/h1H2,2H3	! [CH2]C(C)=O	InChI=1S/C3H5O/c1-
CH3COCH2O2 5/h2H2,1H3	! CC(=O)CO[O]	InChI=1S/C3H5O3/c1-3(4)2-6-
CH3COCH2O 4/h2H2,1H3	! CC(=O)C[O]	InChI=1S/C3H5O2/c1-3(5)2-
C3KET21 5/h5H,2H2,1H3	! CC(=O)COO	InChI=1S/C3H6O3/c1-3(4)2-6-

!species of Toluene and PAH mechanism from Yuan 2015

!----- C4 species -----		

C4H	! C#CC#[C]	InChI=1S/C4H/c1-3-4-2/h1H
C4H5-2 2/h1H2,2H3	! CC#C[CH2]	InChI=1S/C4H5/c1-3-4-
C4H612 2/h4H,1H2,2H3	! C=C=CC	InChI=1S/C4H6/c1-3-4-
H2C4O 4/h1,3H	! O1C=C1C#C	InChI=1S/C4H2O/c1-2-4-3-5-
C4H6-2	! CC#CC	InChI=1S/C4H6/c1-3-4-2/h1-2H3
C4H6 4H,1-2H2	! C=CC=C	InChI=1S/C4H6/c1-3-4-2/h3-
C4H2	! C#CC#C	InChI=1S/C4H2/c1-3-4-2/h1-2H
nC4H3	! [CH]=CC#C	InChI=1S/C4H3/c1-3-4-2/h1-3H
iC4H3 2/h1H,2H2	! C=[C]C#C	InChI=1S/C4H3/c1-3-4-
C4H4 2/h1,4H,2H2	! C=CC#C	InChI=1S/C4H4/c1-3-4-
C4H5-N 4H,2H2	! C=CC=[CH]	InChI=1S/C4H5/c1-3-4-2/h1,3-
C4H5-I 2H2	! C=[C]C=C	InChI=1S/C4H5/c1-3-4-2/h3H,1-
!----- C5 species -----		

C5H3 2/h1H,2H2	! C=C=C=C=[C]	InChI=1S/C5H3/c1-3-5-4-
cC5H4 1/h1-4H Cyclopentadienylidene	! C1=CC=C[C:]1	InChI=1S/C5H4/c1-2-4-5-3-
C5H4 2H2	! C=C=C=C=C	InChI=1S/C5H4/c1-3-5-4-2/h1-
1C5H5 2/h1,4-5H,2H2	! C#C[C]CC	(pas sur) InChI=1S/C5H5/c1-3-5-4-
C5H5 1/h1-5H Cyclopentadienyl	! C1=CC=C[C]1	InChI=1S/C5H5/c1-2-4-5-3-
C5H6 1/h1-4H,5H2 Cyclopentadiene	! C1=CC=CC1	InChI=1S/C5H6/c1-2-4-5-3-
1C5H7 1/h1-3H,4-5H2	! C1[CH]C=CC1	InChI=1S/C5H7/c1-2-4-5-3-
C5H3O 5/h1-3H	! C1(=O)[C]=CC=C1	InChI=1S/C5H3O/c6-5-3-1-2-4-
C5H5O24 5/h1-5H	! [O]C1C=CC=C1	InChI=1S/C5H5O/c6-5-3-1-2-4-
C5H4O 5/h1-4H	! O=C1C=CC=C1	InChI=1S/C5H4O/c6-5-3-1-2-4-
C5H4OH 5/h1-4,6H	! OC1=CC=C[CH]1	InChI=1S/C5H5O/c6-5-3-1-2-4-
C5H5OH 5/h1-6H	! OC1C=CC=C1	InChI=1S/C5H6O/c6-5-3-1-2-4-
C5H5O13 InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-3H,4H2 and InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1,3-4H,2H2	! C1C([O])=CC=C1 and C1C=C([O])C=C1	
C5H52	!	
C5H2	!	
!----- C6 species -----		

A1	! c1ccccc1	InChI=1S/C6H6/c1-2-4-6-5-3-
1/h1-6H		
A1-	! c1[c]cccc1	InChI=1S/C6H5/c1-2-4-6-5-3-
1/h1-5H		
1-C6H4	! C#CC=CC#C	InChI=1S/C6H4/c1-3-5-6-4-
2/h1-2,5-6H		
o-C6H4	! C1=CC=C=C=C1	InChI=1S/C6H4/c1-2-4-6-5-3-
1/h1-4H		
n-C6H5	! C#CC=CC=[C]	InChI=1S/C6H5/c1-3-5-6-4-
2/h1-3,5-6H		
fulvene	! C=C1C=CC=C1	InChI=1S/C6H6/c1-6-4-2-3-5-
6/h2-5H,1H2		
A1O	! [O]c1ccccc1	InChI=1S/C6H5O/c7-6-4-2-1-3-
5-6/h1-5H		
A1OH	! Oc1ccccc1	InChI=1S/C6H6O/c7-6-4-2-1-3-
5-6/h1-5,7H		
C5H4CH3	! CC1=CC=C[CH]1	InChI=1S/C6H7/c1-6-4-2-3-5-
6/h2-5H,1H3		
O-C6H4O2	! O=C1C=CC=CC1=O	InChI=1S/C6H4O2/c7-5-3-1-2-4-
6(5)8/h1-4H		
P-C6H4O2	! O=C1C=CC(=O)C=C1	InChI=1S/C6H4O2/c7-5-1-2-
6(8)4-3-5/h1-4H		
P-OC6H5OJ	! C1(=O)C=CC([O])C=C1	InChI=1S/C6H5O2/c7-5-1-2-
6(8)4-3-5/h1-5H		
O-OC6H5OJ	! C1(=O)C([O])C=CC=C1	InChI=1S/C6H5O2/c7-5-3-1-2-4-
6(5)8/h1-5H		
P-C6H3O2	! [O]C1=C=CC(=O)C=C1	InChI=1S/C6H3O2/c7-5-1-2-
6(8)4-3-5/h1-3H		
OA1OH	! C1=C([O])C=C(O)C=C1	InChI=1S/C6H5O2/c7-5-2-1-3-
6(8)4-5/h1-4,7H		
C6H4OH	! Oc1c[c]ccc1	InChI=1S/C6H5O/c7-6-4-2-1-3-
5-6/h1-2,4-5,7H		
C6H2	! C#CC#CC#C	InChI=1S/C6H2/c1-3-5-6-4-
2/h1-2H		
C6H3	! C#C[C]=CC#C	InChI=1S/C6H3/c1-3-5-6-4-
2/h1-2,5H		
cC6H7	! [C]1C=CCC=C1	InChI=1S/C6H7/c1-2-4-6-5-3-
1/h1-5H,6H2		
1C6H7	! C=CC=CC=[C]	InChI=1S/C6H7/c1-3-5-6-4-
2/h1,3-6H,2H2		
A1O0	! [O]Oc1ccccc1	InChI=1S/C6H5O2/c7-8-6-4-2-1-
3-5-6/h1-5H		
A1OOH	! OOc1ccccc1	InChI=1S/C6H6O2/c7-8-6-4-2-1-
3-5-6/h1-5,7H		
cC7H7	! [C]1C=CC=CC=C1	InChI=1S/C7H7/c1-2-4-6-7-5-3-
1/h1-7H		
C5H5CH2-2	! C=C1[CH]C=CC1	InChI=1S/C6H7/c1-6-4-2-3-5-
6/h2-4H,1,5H2		
C5H5CH2-3	! C=C1[CH]CC=C1	InChI=1S/C6H7/c1-6-4-2-3-5-
6/h2,4-5H,1,3H2		
C5H5CH2-1	! [CH2]C1C=CC=C1	InChI=1S/C6H7/c1-6-4-2-3-5-
6/h2-6H,1H2		
!-----	C7 species -----	

A1CH3	! Cc1ccccc1	InChI=1S/C7H8/c1-7-5-3-2-4-6-
7/h2-6H,1H3	toluene	
A1CH2	! [C]c1ccccc1	InChI=1S/C7H7/c1-7-5-3-2-4-6-
7/h2-6H,1H2	benzyl	

C7H6	! C=C=C1C=CC=C1	InChI=1S/C7H6/c1-2-7-5-3-4-6-
7/h3-6H, 1H2		
C7H5	! C#CC1=CC=C[CH]1	InChI=1S/C7H5/c1-2-7-5-3-4-6-
7/h1, 3-6H		
A1CO	! O=[C]c1ccccc1	InChI=1S/C7H5O/c8-6-7-4-2-1-
3-5-7/h1-5H		
O-OA1CH3	! Cc1ccccc1[O]	InChI=1S/C7H7O/c1-6-4-2-3-5-
7(6)8/h2-5H, 1H3	o-methyl phenoxy	
P-OA1CH3	! Cc1cc[O]ccc1	InChI=1S/C7H7O/c1-6-2-4-
7(8)5-3-6/h2-5H, 1H3	p-methyl phenoxy	
O-C6H4CH3	! Cc[1]ccccc1	InChI=1S/C7H7/c1-7-5-3-2-4-6-
7/h2-5H, 1H3	o-methyl benzyl	
P-C6H4CH3	! Cc1cc[c]cc1	InChI=1S/C7H7/c1-7-5-3-2-4-6-
7/h3-6H, 1H3	p-methyl benzyl	
A1CH2OH	! OCc1ccccc1	InChI=1S/C7H8O/c8-6-7-4-2-1-
3-5-7/h1-5, 8H, 6H2	benzyl alcohol	
A1CHO	! O=Cc1ccccc1	InChI=1S/C7H6O/c8-6-7-4-2-1-
3-5-7/h1-6H	benzaldehyde	
O-HOA1CH3	! Cc1cccc(c1)O	InChI=1S/C7H8O/c1-6-4-2-3-5-
7(6)8/h2-5, 8H, 1H3	o-cresol	
P-HOA1CH3	! Cc1cc(O)ccc1	InChI=1S/C7H8O/c1-6-2-4-
7(8)5-3-6/h2-5, 8H, 1H3	p-cresol	
A1CH	! [C:]c1ccccc1	InChI=1S/C7H6/c1-7-5-3-2-4-6-
7/h1-6H		
A1CH2O	! [O]Cc1ccccc1	InChI=1S/C7H7O/c8-6-7-4-2-1-
3-5-7/h1-5H, 6H2		
O-OC6H4CH2	! C=C1C=CC=CC1=O	InChI=1S/C7H6O/c1-6-4-2-3-5-
7(6)8/h2-5H, 1H2	o-quinone methide	
C5H5CH3	! CC1C=CC=C1	InChI=1S/C6H8/c1-6-4-2-3-5-
6/h2-6H, 1H3	methyl cyclopentadiene	
A1CH2OO	! [O]OCc1ccccc1	InChI=1S/C7H7O2/c8-9-6-7-4-2-
1-3-5-7/h1-5H, 6H2		
A1CH2OOH	! OOCc1ccccc1	InChI=1S/C7H8O2/c8-9-6-7-4-2-
1-3-5-7/h1-5, 8H, 6H2		
O-HOA1CH2	! [C]c1cccc(c1)O	InChI=1S/C7H7O/c1-6-4-2-3-5-
7(6)8/h2-5, 8H, 1H2	o-hydroxy benzyl	
P-HOA1CH2	! [C]c1cccc(c1)O	InChI=1S/C7H7O/c1-6-2-4-
7(8)5-3-6/h2-5, 8H, 1H2	p-hydroxy benzyl	
eC7H6	! C#CC1C=CC=C1	InChI=1S/C7H6/c1-2-7-5-3-4-6-
7/h1, 3-7H		
HOA1CH2OOH	! OOCc1ccccc1O	InChI=1S/C7H8O3/c8-7-3-1-2-
6(4-7)5-10-9/h1-4, 8-9H, 5H2		
HOA1CH2OO	! [O]OCc1ccccc1O	InChI=1S/C7H7O3/c8-7-3-1-2-
6(4-7)5-10-9/h1-4, 8H, 5H2		
HOA1CH2O	! [O]Cc1ccccc1O	InChI=1S/C7H7O2/c8-5-6-1-3-
7(9)4-2-6/h1-4, 9H, 5H2		
HOA1CHO	! Oc1ccccc1C=O	InChI=1S/C7H6O2/c8-5-6-2-1-3-
7(9)4-6/h1-5, 9H	hydroxybenzaldehyde	
HOA1CO	! Oc1ccccc1[C]=O	InChI=1S/C7H5O2/c8-5-6-2-1-3-
7(9)4-6/h1-4, 9H		
!-----C8 species-----		

A1CC	! c1ccccc1C#[C]	InChI=1S/C8H5/c1-2-8-6-4-3-5-
7-8/h3-7H		
A1C2H-	! c1ccc[c]c1C#C	InChI=1S/C8H5/c1-2-8-6-4-3-5-
7-8/h1, 3-6H		

C6H3C2H ! C1(C#C)=C=C=CC=C1 or C1=C=C=CC=C1(C#C)
InChI=1S/C8H4/c1-2-8-6-4-3-5-7-8/h1,3-4,6H or InChI=1S/C8H4/c1-2-8-6-4-3-5-7-8/h1,4,6-7H
A1C2H ! c1cccc1C#C InChI=1S/C8H6/c1-2-8-6-4-3-5-7-8/h1,3-7H
A1cC2H2 ! InChI=1S/C8H6/c1-2-4-8-6-5-7(8)3-1/h1-6H
A1CCH2 ! InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h3-7H,1H2
styrene radical
A1CHCH ! InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h1-7H
styrene radical
O-C6H4C2H3 ! InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h2-6H,1H2
P-C6H4C2H3 ! InChI=1S/C8H7/c1-2-8-6-4-3-5-7-8/h2,4-7H,1H2
A1C2H5 ! InChI=1S/C8H10/c1-2-8-6-4-3-5-7-8/h3-7H,2H2,1H3
ethylbenzene
A1CH2CH2 ! InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h3-7H,1-2H2
ethylbenzene radical
A1CHCH3 ! InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h2-7H,1H3
ethylbenzene radical
A1C2H3 ! InChI=1S/C8H8/c1-2-8-6-4-3-5-7-8/h2-7H,1H2
styrene
C6H4C2H5 ! InChI=1S/C8H9/c1-2-8-6-4-3-5-7-8/h3-6H,2H2,1H3
ethyl benzyl
A1CHCH3OOH ! InChI=1S/C8H10O2/c1-7(10-9)8-5-3-2-4-6-8/h2-7,9H,1H3
A1CHCH3O ! InChI=1S/C8H9O/c1-7(9)8-5-3-2-4-6-8/h2-7H,1H3
C8H8O ! C1C2OCCC2CCC1 INCHI=1S/C8H8O/C1-2-4-8-7(3-1)5-6-9-8/H1-4H,5-6H2 2,3-dihydrobenzofuran
C8H7O ! INCHI=1S/C8H7O/C1-2-4-8-7(3-1)5-6-9-8/H1-4,6H,5H2
2,3-dihydrobenzofuran radical
C8H7O-1 ! INCHI=1S/C8H7O/C1-2-4-8-7(3-1)5-6-9-8/H1-5H,6H2
2,3-dihydrobenzofuran radical
C8H6O ! C1(C=CO2)=C2C=CC=C1 INCHI=1S/C8H6O/C1-2-4-8-7(3-1)5-6-9-8/H1-6H benzofuran
!-----C9 species-----

C9H7 ! c1ccc2c(c1)C=C[CH]2 InChI=1S/C9H7/c1-2-5-9-7-3-6-8(9)4-1/h1-7H indenyl radical
C9H8 ! c1ccc2c(c1)C=CC2 InChI=1S/C9H8/c1-2-5-9-7-3-6-8(9)4-1/h1-6H,7H2 indene
C9H6O ! O=C1C=Cc2c1cccc2 InChI=1S/C9H6O/c10-9-6-5-7-3-1-2-4-8(7)9/h1-6H indenone
C9H9-1 ! InChI=1S/C9H9/c1-2-5-9-7-3-6-8(9)4-1/h1-2,4-6H,3,7H2 indanyl
C9H10 ! InChI=1S/C9H10/c1-2-5-9-7-3-6-8(9)4-1/h1-2,4-5H,3,6-7H2 indane
O-CH2A1C2H3 ! InChI=1S/C9H9/c1-3-9-7-5-4-6-8(9)2/h3-7H,1-2H2
O-CH3A1C2H3 ! InChI=1S/C9H10/c1-3-9-7-5-4-6-8(9)2/h3-7H,1H2,2H3
methyl styrene
P-CH2A1C2H3 ! InChI=1S/C9H9/c1-3-9-6-4-8(2)5-7-9/h3-7H,1-2H2
P-CH3A1C2H3 ! InChI=1S/C9H10/c1-3-9-6-4-8(2)5-7-9/h3-7H,1H2,2H3
methyl styrene
A1C3H2 ! InChI=1S/C9H7/c1-2-6-9-7-4-3-5-8-9/h3-5,7-8H,1H2
!-----C10 species-----

A2 ! c1ccc2c(c1)cccc2 InChI=1S/C10H8/c1-2-6-10-8-4-3-7-9(10)5-1/h1-8H naphthalene
A2-1 ! InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-7H 1-naphtyl

A2-2 ! InChI=1S/C10H7/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-8H
2-naphtyl
A2T2 ! InChI=1S/C10H6/c1-2-6-10-8-4-3-7-9(10)5-1/h1-2,5-8H
Naphtalyne
A2T1 ! InChI=1S/C10H6/c1-2-6-10-8-4-3-7-9(10)5-1/h1-3,5-7H
Naphtalyne
A1(C2H)2 ! InChI=1S/C10H6/c1-3-9-7-5-6-8-10(9)4-2/h1-2,5-8H
C9H7CH2 ! InChI=1S/C10H9/c1-8-6-7-9-4-2-3-5-10(8)9/h2-6H,1,7H2
1-Methyleneindan-2-yl
C9H6CH2 ! InChI=1S/C10H8/c1-8-6-7-9-4-2-3-5-10(8)9/h2-7H,1H2
methyleneindene
C2H2A1C2H ! InChI=1S/C10H7/c1-3-9-7-5-6-8-10(9)4-2/h1-3,5-8H
A2O-1 ! InChI=1S/C10H7O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
1-Naphthalenoxy
A2O-2 ! InChI=1S/C10H7O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
2-Naphthalenoxy
C9H8CH3 ! InChI=1S/C10H11/c1-8-6-7-9-4-2-3-5-10(8)9/h2-
6,8H,7H2,1H3 1-Methylindan-2-yl
C9H7CH3 ! InChI=1S/C10H10/c1-8-6-7-9-4-2-3-5-10(8)9/h2-8H,1H3
1-Methylindene
CH2A1C3H5 ! InChI=1S/C10H11/c1-3-6-10-8-5-4-7-9(10)2/h3-5,7-8H,1-
2,6H2
C2H4A1C2H3 ! InChI=1S/C10H11/c1-3-9-7-5-6-8-10(9)4-2/h3,5-8H,1-
2,4H2
A1(C2H3)2 ! InChI=1S/C10H10/c1-3-9-7-5-6-8-10(9)4-2/h3-8H,1-2H2
C5H5-C5H5 ! C10H10 InChI=1S/C10H10/c1-2-6-10-8-4-3-7-9(10)5-
1/h1-3,5-7H,4,8H2
C5H5-C5H4 ! C10H9 InChI=1S/C10H9/c1-2-6-10-8-4-3-7-9(10)5-1/h1-
3,5-8H,4H2 Fulvalenyl and Azulyl
A2OH-1 ! InChI=1S/C10H8O/c11-10-7-3-5-8-4-1-2-6-9(8)10/h1-
7,11H 1-Naphthal enol
A2OH-2 ! InChI=1S/C10H8O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-
7,11H 2-Naphthal enol
!-----C11 species-----

A2CH3-1 ! InChI=1S/C11H10/c1-9-5-4-7-10-6-2-3-8-11(9)10/h2-
8H,1H3 1-methyl naphtalene
A2CH2-1 ! InChI=1S/C11H9/c1-9-5-4-7-10-6-2-3-8-11(9)10/h2-
8H,1H2
C11H8 ! InChI=1S/C11H8/c1-2-9-7-8-10-5-3-4-6-11(9)10/h3-
8H,1H2
C11H7 ! InChI=1S/C11H7/c1-2-9-7-8-10-5-3-4-6-11(9)10/h3-
7H,1H2
A2CH3-2 ! InChI=1S/C11H10/c1-9-6-7-10-4-2-3-5-11(10)8-9/h2-
8H,1H3 2-methyl naphtalene
A2CH2-2 ! InChI=1S/C11H9/c1-9-6-7-10-4-2-3-5-11(10)8-9/h2-
8H,1H2
!-----C12 species-----

P2 ! InChI=1S/C12H10/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-
10H Biphenyl
P2- ! InChI=1S/C12H9/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-9H
BIPHEN ! InChI=1S/C12H8/c1-2-6-10-9(5-1)11-7-3-4-8-
12(10)11/h1-8H Biphenylene
A2C2HA ! InChI=1S/C12H8/c1-2-10-7-5-8-11-6-3-4-9-
12(10)11/h1,3-9H
A2C2HA* ! InChI=1S/C12H7/c1-2-10-7-5-8-11-6-3-4-9-
12(10)11/h1,3-6,8-9H

A2C2HB ! InChI=1S/C12H8/c1-2-10-7-8-11-5-3-4-6-12(11)9-
10/h1,3-9H
A2C2HB* ! InChI=1S/C12H7/c1-2-10-7-8-11-5-3-4-6-12(11)9-
10/h1,3-8H
A2R5 ! InChI=1S/C12H8/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-
8H Acenaphthylene
A2R5- ! InChI=1S/C12H7/c1-3-9-4-2-6-11-8-7-10(5-1)12(9)11/h1-
5,7-8H
A2C2H2 ! InChI=1S/C12H9/c1-2-10-7-5-8-11-6-3-4-9-12(10)11/h1-
9H
P2-H ! InChI=1S/C12H11/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-
9H,10H2
C12H9 ! InChI=1S/C12H9/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-9H
BICYCLO ! InChI=1S/C12H10/c1-2-4-12-10-7-5-9(6-8-10)11(12)3-
1/h1-10H benzobicyclo[2,2,2]octatriene
!-----C13 species-----

C13H9 ! InChI=1S/C13H9/c1-3-7-12-10(5-1)9-11-6-2-4-8-
13(11)12/h1-9H Fluorenyl radical
C13H10 ! InChI=1S/C13H10/c1-3-7-12-10(5-1)9-11-6-2-4-8-
13(11)12/h1-8H,9H2 Fluorene
C13H12 ! InChI=1S/C13H12/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-
13/h1-10H,11H2 Diphenylmethane
p-C13H9
C13H11 ! InChI=1S/C13H11/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-
13/h1-11H
p-C13H10
!-----C14 species-----

A3 ! InChI=1S/C14H10/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-
14(12)13/h1-10H phenanthrene
A3-1 ! InChI=1S/C14H9/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-
14(12)13/h1-5,7-10H 1- phenanthrenyl
A3-4 ! InChI=1S/C14H9/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-
14(12)13/h1-7,9-10H 4- phenanthrenyl
A2(C2H)2 ! InChI=1S/C14H8/c1-3-11-9-10-12-7-5-6-8-14(12)13(11)4-
2/h1-2,5-10H
C14H14 ! InChI=1S/C14H14/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-
14/h1-10H,11-12H2 Bibenzyl
C14H13 ! InChI=1S/C14H13/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-
14/h1-11H,12H2 1,2-Diphenylethyl
C14H12 ! InChI=1S/C14H12/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-
14/h1-12H/b12-11+ Stilbene
C14H11 ! InChI=1S/C14H11/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-
14/h1-9,11-12H/b12-11+ b-phenyl-a-styryl
C14H13OO ! InChI=1S/C14H13O2/c15-16-14(13-9-5-2-6-10-13)11-12-7-
3-1-4-8-12/h1-10,14H,11H2
C14H13OOH ! InChI=1S/C14H14O2/c15-16-14(13-9-5-2-6-10-13)11-12-7-
3-1-4-8-12/h1-10,14-15H,11H2
C14H12OOH ! InChI=1S/C14H13O2/c15-16-14(13-9-5-2-6-10-13)11-12-7-
3-1-4-8-12/h1-11,14-15H
C14H12O2H-1O2 ! InChI=1S/C14H13O4/c15-17-13(11-7-3-1-4-8-11)14(18-
16)12-9-5-2-6-10-12/h1-10,13-15H
C14H11O-1O2H ! InChI=1S/C14H12O3/c15-13(11-7-3-1-4-8-11)14(17-
16)12-9-5-2-6-10-12/h1-10,15-16H/b14-13+
C14H13O ! InChI=1S/C14H13O/c15-14(13-9-5-2-6-10-13)11-12-7-3-1-
4-8-12/h1-10,14H,11H2

A3L ! InChI=1S/C14H10/c1-2-6-12-10-14-8-4-3-7-13(14)9-11(12)5-1/h1-10H anthracene
C13H9CH2 ! InChI=1S/C14H11/c1-10-11-6-2-4-8-13(11)14-9-5-3-7-12(10)14/h2-9,13H,1H2 Hydro-methylenefluorene
C13H8CH2 ! InChI=1S/C14H10/c1-10-11-6-2-4-8-13(11)14-9-5-3-7-12(10)14/h2-9H,1H2
A2C2H2A
A2C2H2B
!-----C15 species-----

A3CH3 ! InChI=1S/C15H12/c1-11-5-4-7-13-10-9-12-6-2-3-8-14(12)15(11)13/h2-10H,1H3
A3CH2 ! InChI=1S/C15H11/c1-11-5-4-7-13-10-9-12-6-2-3-8-14(12)15(11)13/h2-10H,1H2
A3C2H ! InChI=1S/C16H10/c1-2-12-7-5-8-14-11-10-13-6-3-4-9-15(13)16(12)14/h1,3-11H
A3C2H-1 ! InChI=1S/C16H10/c1-2-12-7-5-9-16-14-8-4-3-6-13(14)10-11-15(12)16/h1,3-11H
A3C2H-2 ! InChI=1S/C16H10/c1-2-12-7-10-16-14(11-12)9-8-13-5-3-4-6-15(13)16/h1,3-11H
!----->=C16 species-----

A4 ! InChI=1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H Pyrene
A4-1
A4-2
A4-4
A3C2H2 ! InChI=1S/C16H11/c1-2-12-7-5-8-14-11-10-13-6-3-4-9-15(13)16(12)14/h1-11H
FLTHN ! InChI=1S/C16H10/c1-2-8-13-12(7-1)14-9-3-5-11-6-4-10-15(13)16(11)14/h1-10H
A2R5R5 ! InChI=1S/C14H8/c1-2-10-7-8-12-4-3-11-6-5-9(1)13(10)14(11)12/h1-8H
C18H12
CHRYSEN ! InChI=1S/C18H12/c1-3-7-15-13(5-1)9-11-18-16-8-4-2-6-14(16)10-12-17(15)18/h1-12H Chrysene
CHRYSEN-1 !
CHRYSEN-4 !
CHRYSEN-5 !
DIBZFUR ! InChI=1S/C12H8O/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H dibenzofuran

!----- species of xylenes submechanism from Kukkadapu 2018
O-XYL ! InChI=1S/C8H10/c1-7-5-3-4-6-8(7)2/h3-6H,1-2H3
O-CH3A1CH2 ! InChI=1S/C8H9/c1-7-5-3-4-6-8(7)2/h3-6H,1H2,2H3
CH3C6H3CH3 ! InChI=1S/C8H9/c1-7-3-5-8(2)6-4-7/h3-5H,1-2H3
O-XYLYLE ! InChI=1S/C8H8/c1-7-5-3-4-6-8(7)2/h3-6H,1-2H2
P-CHOA1CH2 ! InChI=1S/C8H7O/c1-7-2-4-8(6-9)5-3-7/h2-6H,1H2
O-CHOA1CH2 ! InChI=1S/C8H7O/c1-7-4-2-3-5-8(7)6-9/h2-6H,1H2
BZCYBUT ! InChI=1S/C8H8/c1-2-4-8-6-5-7(8)3-1/h1-4H,5-6H2
OCH3A1CH3 ! InChI=1S/C8H9O/c1-6-3-4-7(2)8(9)5-6/h3-5H,1-2H3
HOCH3A1CH3 ! InChI=1S/C8H10O/c1-6-3-4-7(2)8(9)5-6/h3-5,9H,1-2H3
DMCPD ! InChI=1S/C7H10/c1-6-3-4-7(2)5-6/h3-4H,5H2,1-2H3
O-CH3A1CHO ! InChI=1S/C8H8O/c1-7-4-2-3-5-8(7)6-9/h2-6H,1H3
O-CH3A1CH2OO ! InChI=1S/C8H9O2/c1-7-4-2-3-5-8(7)6-10-9/h2-5H,6H2,1H3
O-CH3A1CH2O ! InChI=1S/C8H9O/c1-7-4-2-3-5-8(7)6-9/h2-5H,6H2,1H3
O-CH3A1CH2OOH ! InChI=1S/C8H10O2/c1-7-4-2-3-5-8(7)6-10-9/h2-5,9H,6H2,1H3

O-XYLDIMER ! InChI=1S/C16H18/c1-13-7-3-5-9-15(13)11-12-16-10-6-4-8-14(16)2/h3-10H,11-12H2,1-2H3
O-XYLDIMERJ ! InChI=1S/C16H17/c1-13-7-3-5-9-15(13)11-12-16-10-6-4-8-14(16)2/h3-11H,12H2,1-2H3
O-XYLQOOH ! InChI=1S/C7H7O2/c1-6-4-2-3-5-7(6)9-8/h2-5,8H,1H2
O-XYLSECO2 ! InChI=1S/C7H7O4/c8-10-5-6-3-1-2-4-7(6)11-9/h1-4,9H,5H2
O-XYLKET ! InChI=1S/C8H8O3/c9-5-7-3-1-2-4-8(7)6-11-10/h1-5,10H,6H2
CHOA1CH2OJ ! InChI=1S/C8H7O2/c9-5-7-3-1-2-4-8(7)6-10/h1-5H,6H2
CHOA1CHO ! InChI=1S/C8H6O2/c9-5-7-3-1-2-4-8(7)6-10/h1-6H
CHOA1CO ! InChI=1S/C8H5O2/c9-5-7-3-1-2-4-8(7)6-10/h1-5H
O-CH3A1C2H5 ! InChI=1S/C9H12/c1-3-9-7-5-4-6-8(9)2/h4-7H,3H2,1-2H3
O-CH3A1CHCH3 ! InChI=1S/C9H11/c1-3-9-7-5-4-6-8(9)2/h3-7H,1-2H3
O-CH3A1CHOOCH3 ! InChI=1S/C9H11O2/c1-7-5-3-4-6-9(7)8(2)11-10/h3-6,8H,1-2H3
O-C2H3A1CH2O ! InChI=1S/C9H9O/c1-2-8-5-3-4-6-9(8)7-10/h2-6H,1,7H2
O-C2H3A1CHO ! InChI=1S/C9H8O/c1-2-8-5-3-4-6-9(8)7-10/h2-7H,1H2
O-C2H3A1CO ! InChI=1S/C9H7O/c1-2-8-5-3-4-6-9(8)7-10/h2-6H,1H2
P-CH3A1C2H5 ! InChI=1S/C9H12/c1-3-9-6-4-8(2)5-7-9/h4-7H,3H2,1-2H3
P-CH3A1CHCH3 ! InChI=1S/C9H11/c1-3-9-6-4-8(2)5-7-9/h3-7H,1-2H3
P-CH3A1CHOOCH3 ! InChI=1S/C9H11O2/c1-7-3-5-9(6-4-7)8(2)11-10/h3-6,8H,1-2H3
P-C2H3A1CH2O ! InChI=1S/C9H9O/c1-2-8-3-5-9(7-10)6-4-8/h2-6H,1,7H2
P-C2H3A1CHO ! InChI=1S/C9H8O/c1-2-8-3-5-9(7-10)6-4-8/h2-7H,1H2
P-C2H3A1CO ! InChI=1S/C9H7O/c1-2-8-3-5-9(7-10)6-4-8/h2-6H,1H2
P-XYL ! InChI=1S/C8H10/c1-7-3-5-8(2)6-4-7/h3-6H,1-2H3
P-CH3A1CH2 ! InChI=1S/C8H9/c1-7-3-5-8(2)6-4-7/h3-6H,1H2,2H3
P-XYLYLE ! InChI=1S/C8H8/c1-7-3-5-8(2)6-4-7/h3-6H,1-2H2
P-CH3A1CHO ! InChI=1S/C8H8O/c1-7-2-4-8(6-9)5-3-7/h2-6H,1H3
P-CH3A1CH2OO ! InChI=1S/C8H9O2/c1-7-2-4-8(5-3-7)6-10-9/h2-5H,6H2,1H3
P-CH3A1CH2OOH ! InChI=1S/C8H10O2/c1-7-2-4-8(5-3-7)6-10-9/h2-5,9H,6H2,1H3
P-XYLDIMER ! InChI=1S/C16H18/c1-13-3-7-15(8-4-13)11-12-16-9-5-14(2)6-10-16/h3-10H,11-12H2,1-2H3
P-XYLDIMERJ ! InChI=1S/C16H17/c1-13-3-7-15(8-4-13)11-12-16-9-5-14(2)6-10-16/h3-11H,12H2,1-2H3
CH3C9H7 ! InChI=1S/C10H10/c1-8-4-2-5-9-6-3-7-10(8)9/h2-6H,7H2,1H3
XYLMETHIDE ! InChI=1S/C8H8O/c1-6-4-3-5-8(9)7(6)2/h3-5H,2H2,1H3
O2CH3A1CH3 ! InChI=1S/C8H9O2/c1-6-3-4-7(2)8(5-6)10-9/h3-5H,1-2H3
O-CH3A1CO ! InChI=1S/C8H7O/c1-7-4-2-3-5-8(7)6-9/h2-5H,1H3
P-CH3A1CO ! InChI=1S/C8H7O/c1-7-2-4-8(6-9)5-3-7/h2-5H,1H3
DMCPDR ! InChI=1S/C7H9/c1-6-3-4-7(2)5-6/h3-5H,1-2H3
O-XYLET ! InChI=1S/C8H8O/c1-2-4-8-6-9-5-7(8)3-1/h1-4H,5-6H2
phthalan

!Species of anisole mechanism (Buttgen 2020 - Wagnon 2018)

A1OCH3 ! COC1CCCCC1 INCHI=1S/C7H8O/C1-8-7-5-3-2-4-6-7/H2-6H,1H3
A1OCH2 ! [CH2]OC1CCCCC1 INCHI=1S/C7H7O/C1-8-7-5-3-2-4-6-7/H2-6H,1H2
C6H4OCH3 ! COC1[C]CCCC1 INCHI=1S/C7H7O/C1-8-7-5-3-2-4-6-7/H2-5H,1H3
A1OCH2O ! InChI=1S/C7H7O2/c8-6-9-7-4-2-1-3-5-7/h1-5H,6H2
A1CYCH2O ! C1=CC2(CO2)C=C[CH]1 INCHI=1S/C7H7O/C1-2-4-7(5-3-1)6-8-7/H1-5H,6H2

PC6H4CHO ! InChI=1S/C7H7O/c8-6-7-4-2-1-3-5-7/h1-7H 2,5-
 cyclohexadien-4-formyl-1-yl
 A1OCH2OO ! [O]OCOC1=CC=CC=C1 INCHI=1S/C7H7O3/C8-10-6-9-7-4-2-1-
 3-5-7/H1-5H,6H2
 OOA1OCH3 ! COC1C(O[O])CCCC1 INCHI=1S/C7H7O3/C1-9-6-4-2-3-5-
 7(6)10-8/H2-5H,1H3
 A1OCH2OOH ! OOCOC1=CC=CC=C1 INCHI=1S/C7H8O3/C8-10-6-9-7-4-2-1-3-
 5-7/H1-5,8H,6H2
 A1OCHO ! InChI=1S/C7H6O2/c8-6-9-7-4-2-1-3-5-7/h1-6H
 A1OCO ! InChI=1S/C7H5O2/c8-6-9-7-4-2-1-3-5-7/h1-5H
 O-HOA1C2H5 ! InChI=1S/C8H10O/c1-2-7-5-3-4-6-8(7)9/h3-6,9H,2H2,1H3
 P-HOA1C2H5 ! InChI=1S/C8H10O/c1-2-7-3-5-8(9)6-4-7/h3-6,9H,2H2,1H3
 O-HOA1C2H4 ! InChI=1S/C8H9O/c1-2-7-5-3-4-6-8(7)9/h3-6,9H,1-2H2
 P-HOA1C2H4 ! InChI=1S/C8H9O/c1-2-7-3-5-8(9)6-4-7/h3-6,9H,1-2H2
 O-HOA1C2H4-S ! InChI=1S/C8H9O/c1-2-7-5-3-4-6-8(7)9/h2-6,9H,1H3
 P-HOA1C2H4-S ! InChI=1S/C8H9O/c1-2-7-3-5-8(9)6-4-7/h2-6,9H,1H3
 O-HOA1C2H3 ! InChI=1S/C8H8O/c1-2-7-5-3-4-6-8(7)9/h2-6,9H,1H2
 P-HOA1C2H3 ! InChI=1S/C8H8O/c1-2-7-3-5-8(9)6-4-7/h2-6,9H,1H2
 O-CH3A1OCH3 ! COC1C(C)CCCC1 INCHI=1S/C8H10O/C1-7-5-3-4-6-8(7)9-
 2/H3-6H,1-2H3
 P-CH3A1OCH3 ! InChI=1S/C8H10O/c1-7-3-5-8(9-2)6-4-7/h3-6H,1-2H3
 O-CH3A1OCH2 ! [CH2]OC1C(C)CCCC1 INCHI=1S/C8H9O/C1-7-5-3-4-6-8(7)9-
 2/H3-6H,2H2,1H3
 P-CH3A1OCH2 ! InChI=1S/C8H9O/c1-7-3-5-8(9-2)6-4-7/h3-6H,2H2,1H3
 O-CH2A1OCH3 ! COC1C([CH2])CCCC1 INCHI=1S/C8H9O/C1-7-5-3-4-6-8(7)9-
 2/H3-6H,1H2,2H3
 P-CH2A1OCH3 ! InChI=1S/C8H9O/c1-7-3-5-8(9-2)6-4-7/h3-6H,1H2,2H3
 O-CH3A1CYCH2O ! InChI=1S/C8H9O/c1-7-4-2-3-5-8(7)6-9-8/h2-5H,6H2,1H3
 P-CH3A1CYCH2O ! InChI=1S/C8H9O/c1-7-2-4-8(5-3-7)6-9-8/h2-5H,6H2,1H3
 O-CH3A1CH2O ! InChI=1S/C8H9O/c1-7-4-2-3-5-8(7)6-9/h2-5H,6H2,1H3
 P-CH3A1CH2O ! InChI=1S/C8H9O/c1-7-2-4-8(6-9)5-3-7/h2-5H,6H2,1H3
 O-CH3A1OCH2OO ! InChI=1S/C8H9O3/c1-7-4-2-3-5-8(7)10-6-11-9/h2-
 5H,6H2,1H3
 P-CH3A1OCH2OO ! InChI=1S/C8H9O3/c1-7-2-4-8(5-3-7)10-6-11-9/h2-
 5H,6H2,1H3
 O-CH3A1OCH2OOH ! InChI=1S/C8H10O3/c1-7-4-2-3-5-8(7)10-6-11-9/h2-
 5,9H,6H2,1H3
 P-CH3A1OCH2OOH ! InChI=1S/C8H10O3/c1-7-2-4-8(5-3-7)10-6-11-9/h2-
 5,9H,6H2,1H3

!Species of o-guaiacol submechanism from Nowakowska 2018

HOA1OCH3 ! COC1C(O)CCCC1 InChI=1S/C7H8O2/c1-9-7-5-3-2-4-
 6(7)8/h2-5,8H,1H3
 HOA1OCH2 ! [CH2]OC1C(O)CCCC1 InChI=1S/C7H7O2/c1-9-7-5-3-2-4-
 6(7)8/h2-5,8H,1H2
 OA1OCH3 ! COC1C([O])CCCC1 InChI=1S/C7H7O2/c1-9-7-5-3-2-4-
 6(7)8/h2-5H,1H3
 HOA1OH ! InChI=1S/C6H6O2/c7-5-3-1-2-4-6(5)8/h1-4,7-8H
 HOA1OHCH3-4 ! InChI=1S/C7H8O2/c1-5-2-3-6(8)7(9)4-5/h2-4,8-9H,1H3
 OA1OHCH3-1 ! InChI=1S/C7H7O2/c1-5-2-3-6(8)7(9)4-5/h2-4,9H,1H3
 OA1OHCH3-2 ! InChI=1S/C7H7O2/c1-5-2-3-6(8)7(9)4-5/h2-4,8H,1H3
 OA1CHO ! InChI=1S/C7H5O2/c8-5-6-3-1-2-4-7(6)9/h1-5H
 C5H4CHO ! InChI=1S/C6H5O/c7-5-6-3-1-2-4-6/h1-3,5-6H
 OC5H3CH3 ! InChI=1S/C6H6O/c1-5-2-3-6(7)4-5/h2-4H,1H3
 HOC5H3CH3 ! InChI=1S/C6H7O/c1-5-2-3-6(7)4-5/h2-3,6-7H,1H3
 OC6H3(O)CH3 ! InChI=1S/C7H6O2/c1-5-2-3-6(8)7(9)4-5/h2-4H,1H3
 OA1OH ! InChI=1S/C6H5O2/c7-5-3-1-2-4-6(5)8/h1-4,7H

C5H5CO ! InChI=1S/C6H5O/c7-5-6-3-1-2-4-6/h1-4,6H
HOA1CYCH2O ! InChI=1S/C7H7O2/c8-6-3-1-2-4-7(6)5-9-7/h1-4,8H,5H2

!Benzodioxole

A1CYOCH2O1-2 ! InChI=1S/C7H6O2/c1-2-4-7-6(3-1)8-5-9-7/h1-4H,5H2
1.3-Benzodioxole
A1CYOCHO1-2 ! InChI=1S/C7H5O2/c1-2-4-7-6(3-1)8-5-9-7/h1-5H

A1CYOCHOO1-2 ! InChI=1S/C7H5O3/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4,7H
A1CYOCOO1-2 ! InChI=1S/C7H4O3/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H

HOA1OCH2O ! InChI=1S/C7H7O3/c8-5-10-7-4-2-1-3-6(7)9/h1-4,9H,5H2
HOA1OCHO ! InChI=1S/C7H6O3/c8-5-10-7-4-2-1-3-6(7)9/h1-5,9H
HOA1OCO ! InChI=1S/C7H5O3/c8-5-10-7-4-2-1-3-6(7)9/h1-4,9H
OA1OCHO ! InChI=1S/C7H5O3/c8-5-10-7-4-2-1-3-6(7)9/h1-5H
A1OCO2 ! InChI=1S/C7H5O3/c8-7(9)10-6-4-2-1-3-5-6/h1-5H
HOA1OCH2OO ! InChI=1S/C7H7O4/c8-6-3-1-2-4-7(6)10-5-11-9/h1-4,8H,5H2

! Cinnamaldehyde

!A1CHCHCHO ! InChI=1S/C9H8O/c10-8-4-7-9-5-2-1-3-6-9/h1-8H/b7-4+
Cinnamaldehyde
!A1CH2CHCHO ! InChI=1S/C9H9O/c10-8-4-7-9-5-2-1-3-6-9/h1-6,8H,7H2
!A1CYOCHCHCH2 ! InChI=1S/C9H9O/c1-2-5-9(6-3-1)7-4-8-10-9/h1-6,8H,7H2
!A1OCH2CHCH2 ! InChI=1S/C9H10O/c1-2-8-10-9-6-4-3-5-7-9/h2-7H,1,8H2
!A1OCHCHCH2 ! InChI=1S/C9H9O/c1-2-8-10-9-6-4-3-5-7-9/h2-8H,1H2
!A1OCHCCH3 ! InChI=1S/C9H9O/c1-2-8-10-9-6-4-3-5-7-9/h3-8H,1H3
!A1OCH2CHCH ! InChI=1S/C9H9O/c1-2-8-10-9-6-4-3-5-7-9/h1-7H,8H2

END

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

REACTIONS

!
++++
! +
+
! + <=== C0-C3 base
model : Curran model <===> +
!
+
!
++++

!\KINETICS_MODULE: C0
!\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) !\COMMENT:
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) !\COMMENT:

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

!

!\ENDSUBMECH: \H2

!

!\SUBMECH: \O2

!\MECHCOMMENTS:

!\MECHWARNINGS:

!

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

!

O+O+M<=>O2+M 6.165E+015 -0.500
0.0 !\AUTHOR: AK !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
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) 309-316 !\COMMENT: 2 PARAMETER FIT

!

!\ENDSUBMECH: \O2

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

!\SUBMECH: \H2O
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
-----
!
-----
!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
-----
H+OH+M<=>H2O+M                        3.500E+022      -2.000
0.0  !\AUTHOR: AK !\REF: LI IJCK 36: 566-575, 2004 !\COMMENT:OPTIMISED TO
FIT H2 AND CH4 FLAMES DATA
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) !\COMMENT:

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

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

!=====
=====
!\ENDSUBSPECIES: \OH*
!=====
=====

!-----
-----
!\ENDSUBMECH: \H2O
!-----
-----

!-----
-----
!\SUBMECH: \H2O2
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
-----
!
-----
!\REACTIONCLASS: \UNIMOL      \A      \N
\EA
!
-----
!H2O2 (+H2O) <=> OH+OH (+H2O)      2.000E+012      0.900
48749.0 !\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601
(2011)! \COMMENT: RATE CONSTANT IS FOR N2
!LOW/      1.865E+025      -2.300
48749.0/
```

!TROE/ 5.100E-001 1.000E-030 1.000E+030/

H2O2 (+M) <=> OH+OH (+M) 2.000E+012 0.900
48749.0 !\AUTHOR: AK !\REF: TROE, COMBUST. FLAME, 158:594-601
(2011)!\COMMENT: RATE CONSTANT IS FOR N2, !\COMMENT: EFFICIENCIES OF H2O
FROM THE SAME REF, SEPERATE REACTION LEAD TO ERROR IN FLAME EXTINCTION
SIMULATION

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) !\COMMENT:

H2O2+H<=>H2+HO2 2.150E+010 1.000
6000.0 !\AUTHOR: AK !\REF: ELLINGSON J. PHYS. CHEM. (2007) 111, (51),
13554-13566 !\COMMENT:

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) !\COMMENT:

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 !\COMMENT:

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: KPS !\REF: NOT A CLUE WHAT REFERENCE IS HERE AS
MECHANISM IS A MESS !\COMMENT: WARNING

HO2+H<=>H2+O2 1.1402E+010 1.0827
553.78 !\AUTHOR: AK !\REF: MICHAEL SUTHERLAND 2000 !\COMMENT:

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 !\COMMENT: WARNING
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 !\COMMENT:
WARNING

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: EFFICIENCIES 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/

!H+O2 (+AR) <=> HO2 (+AR) 4.650E+012 0.440
0.0 !\AUTHOR: AK !\REF: BATES ET AL. PCCP 3 (2001) 2337-2342 !\COMMENT:
WARNING: HAS BEEN REMOVED FROM LATEST VERSION OF KZ MECHANISM
!LOW/ 6.810E+018 -1.200
0.0/
!TROE/ 7.000E-001 1.000E-030 1.000E+030 1.000E+030/

!
!H+O2 (+HE) <=> HO2 (+HE) 4.650E+012 0.440
0.0 !\AUTHOR: AK !\REF: ?? NOT WELL DEFINED IN MECHANISM?! !\COMMENT:
WARNING: LPL OF ABOVE RATE CONSTANT OR THIS ONE HAS BEEN MULTIPLIED BY
1.5
!LOW/ 9.192E+018 -1.200
0.0/
!TROE/ 5.900E-001 1.000E-030 1.000E+030 1.000E+030/

!-----

!\ENDSUBMECH: \H2O2
!-----

!++++
++++
++++
!\END_KINETICS_MODULE: \H2_O2
!++++
++++
++++

!+++++
+++++
+++++
!\KINETICS_MODULE: \C1
!\MODSUBMECHS: CO, CH2O, CH4,
!+++++
+++++
+++++

!-----

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

!

!\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.
!\COMMENT:
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 !\COMMENT:

!

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

CO+O2<=>CO2+O 1.119E+012 0.000
47700.0 !\AUTHOR: ?? !\REF: 86TSA/ HAM * 0.44 !\COMMENT:

!=====
=====

!\SUBSPECIES: \CO2

!=====
=====

!

!\REACTIONCLASS: \RADICAL_ADIDTION\H

!

H+CO2<=>OCHO 7.500E+013 0.000
29000.0 !\AUTHOR: ?? !\REF: CURRAN ESTIMATE !\COMMENT: WARNING

!=====
=====

!\ENDSUBSPECIES: \CO2

!=====
=====

!=====
=====

!\SUBSPECIES: \HOCO

!=====
=====

HOCO<=>CO+OH 6.300E+032 -5.960
32470.0 !\AUTHOR: ?? !\REF: JOHN R. BARKER CALCULATION 7/ 3/ 2013

!\COMMENT: WARNING: RATE CONSTANTS FROM PRIVATE COMMUNICATION WITH JOHN BARKER. IS THERE A LITERATURE REFERENCE?

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

!\COMMENT: WARNING: RATE CONSTANTS FROM PRIVATE COMMUNICATION WITH JOHN BARKER. IS THERE A LITERATURE REFERENCE?

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/

!=====
=====
!\ENDUBSPECIES: \HOCO
!=====
=====

!-----

!\ENDSUBMECH: \CO
!-----

!-----

!\SUBMECH: \CH4
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

!

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

CH3+H(+M)<=>CH4(+M) 1.270E+016 -0.630
383.0 !\AUTHOR: ?? !\REF: GRI MECHANISM !\COMMENT: WARNING: WHAT IS
REFERENCE FOR 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) !\COMMENT:
CH4+O<=>CH3+OH 1.020E+009 1.500
8600.0 !\AUTHOR: !\REF: !REF:GRI 3.0 !\COMMENT: WARNING: WHAT IS
REFERENCE FOR GRI MECHANISM?
CH4+OH<=>CH3+H2O 5.830E+004 2.600
2190.0 !\AUTHOR: !\REF: CURRAN ESTIMATE, FIT TO NIST DATABASE !\COMMENT:
WARNING: WHAT ARE REFERENCES TO RATE CONSTANTS IN NIST?
CH4+HO2<=>CH3+H2O2 1.695E+001 3.740
21010.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
(2008) 112(30): 7047-7054. !\COMMENT:
CH4+CH3O2<=>CH3+CH3O2H 9.600E-001 3.770
17810.0 !\AUTHOR: !\REF: NEW FIT FROM HJC !\COMMENT: WARNING: WHAT IS
SOURCE OF THIS RATE CONSTANT??

CH3+HO2<=>CH4+O2 1.160E+005 2.230
-3022.0 !\AUTHOR: !\REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009)
279-286 !\COMMENT:

!

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

!

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

!

=====

!\SUBSPECIES: \CH2 (S)

!

=====

!

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

!

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

!

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

!

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

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

!=====
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!\ENDSUBSPECIES: \CH2
!=====
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!=====
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!\SUBSPECIES: \CH*
!=====
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!\REACTIONCLASS: \DEACTIVATION \A \N
\EA
!

CH*+AR<=>CH+AR 4.000E+011 0.500
0.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
65-75 (1987) !\COMMENT: CH*+M<=>CH+M

$\text{CH}^* + \text{H}_2\text{O} \rightleftharpoons \text{CH} + \text{H}_2\text{O}$ 5.300E+013 0.000
 0.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
 65-75 (1987) !\COMMENT:
 $\text{CH}^* + \text{CO} \rightleftharpoons \text{CH} + \text{CO}$ 2.440E+012 0.500
 0.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
 65-75 (1987) !\COMMENT:
 $\text{CH}^* + \text{CO}_2 \rightleftharpoons \text{CH} + \text{CO}_2$ 2.410E-001 4.300
 -1694.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
 67, 65-75 (1987) !\COMMENT:
 $\text{CH}^* + \text{O}_2 \rightleftharpoons \text{CH} + \text{O}_2$ 2.480E+006 2.140
 -1720.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
 67, 65-75 (1987) !\COMMENT:
 $\text{CH}^* + \text{H}_2 \rightleftharpoons \text{CH} + \text{H}_2$ 1.470E+014 0.000
 1361.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
 67, 65-75 (1987) !\COMMENT:
 $\text{CH}^* + \text{CH}_4 \rightleftharpoons \text{CH} + \text{CH}_4$ 1.730E+013 0.000
 167.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
 67, 65-75 (1987) !\COMMENT:
 $\text{CH}^* \rightleftharpoons \text{CH}$ 1.860E+006 0.000
 0.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67,
 65-75 (1987) !\COMMENT:
 $\text{CH}^* + \text{N}_2 \rightleftharpoons \text{CH} + \text{N}_2$ 3.030E+002 3.400
 -381.0 !\AUTHOR: ?? !\REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL.
 67, 65-75 (1987) !\COMMENT:
 $\text{C} + \text{H} + \text{M} \rightleftharpoons \text{CH}^* + \text{M}$ 6.000E+014 0.000
 6940.0 !\AUTHOR: ?? !\REF:KATHROTIA ET AL. COMB & FLAME 2010
 !\COMMENT:

!

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

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$\text{CH} + \text{O}_2 \rightleftharpoons \text{CO} + \text{OH}^*$ 4.040E+013 0.000
 0.0 !\AUTHOR: !\REF:KATHROTIA ET AL. COMB & FLAME 2010
 !\COMMENT:
 $\text{CH} + \text{O}_2 \rightleftharpoons \text{HCO} + \text{O}$ 3.300E+013 0.000
 0.0 !\AUTHOR: !\REF: GRI 3.0
 !\COMMENT:
 $\text{CH} + \text{O} \rightleftharpoons \text{CO} + \text{H}$ 5.700E+013 0.000
 0.0 !\AUTHOR: !\REF: MESSING ET AL., J. CHEM. PHYS. 74, 3874 (1981)
 !\COMMENT:
 $\text{CH} + \text{H} \rightleftharpoons \text{C} + \text{H}_2$ 1.100E+014 0.000
 0.0 !\AUTHOR: !\REF: GRI 3.0
 !\COMMENT:
 $\text{CH} + \text{OH} \rightleftharpoons \text{HCO} + \text{H}$ 3.000E+013 0.000
 0.0 !\AUTHOR: !\REF: GLARBORG, MILLER, AND KEE, WESTERN STATES SECTION,
 SAN ANTONIO (1985) !\COMMENT:
 $\text{CH} + \text{H}_2\text{O} \rightleftharpoons \text{H} + \text{CH}_2\text{O}$ 1.774E+016 -1.220
 23.8 !\AUTHOR: !\REF:BERGEAT ET AL., CHEM. PHYS. LETT. 480, 21 (2009)
 !\COMMENT:
 $\text{CH} + \text{CO}_2 \rightleftharpoons \text{HCO} + \text{CO}$ 1.700E+012 0.000
 685.0 !\AUTHOR: !\REF: BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB.
 P. 73, 1982 !\COMMENT: X0.5

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

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

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!\ENDSUBSPECIES: \C
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!=====
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!\SUBSPECIES: \CH3
!=====
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!\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. !\COMMENT:

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) !\COMMENT:

CH3+O2 <=> CH2O+OH 2.641E+000 3.283
8105.0 !\AUTHOR: ?? !\REF: PERSONAL COMMUNICATION, STEVE KLIPPENSTEIN
!\COMMENT: WARNING: HAS THIS BEEN PUBLISHED?

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!\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.
!\COMMENT:

!_____

!\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 !\COMMENT: ONLY INCLUDING TRANS HCOH FOR SIMPLICITY, DO NOT HAVE TO
COMBINE THE K'S. IT'S NOT REALLY SIGNIFICANT ANYWAY
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 !\COMMENT:
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 !\COMMENT: INCREASED BY FACTOR OF 2 TO IMPROVE AGREEMENT WITH CH4
FLAMESPEED. WARNING: ADJUSTING PLOG RATE CONSTANT IN THIS MANNER IS
FUNDAMENTALLY INCORRECT (KPS, 30/07/2015)
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:

!\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) 279-286 !\COMMENT:

!=====
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!\ENDSUBSPECIES: \CH3
!=====
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!=====
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!\SUBSPECIES: \CH3O2
!=====
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!\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. !\COMMENT:
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. !\COMMENT:
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. !\COMMENT:
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) !\COMMENT:
CH3O2+H2O2<=>CH3O2H+HO2 2.410E+012 0.000
9936.0 !\AUTHOR: !\REF:TSANG, W., J. PHYS. CHEM. REF. DATA 15, 1087
(1986) !\COMMENT: ADDED 29/07/2015
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) !\COMMENT:
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. !\COMMENT:
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. !\COMMENT:

!
!\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 !\COMMENT:

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!\REACTIONCLASS: \KHP_DECOMP          \A          \N
\EA
!
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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. !\COMMENT:
CH2O2H<=>CH2O+OH                      9.000E+014    0.000
1500.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
!\COMMENT: KPS: THIS REACTION WAS MOVED FROM THE C4 MECHANISM!!

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!\ENDSUBSPECIES: \CH3O2
!=====
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!\ENDSUBMECH: \CH4
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!\SUBMECH: \CH3OH
!\MECHCOMMENTS: HCOH IS FORMED FROM CH3+OH, IT IS NOT NECESSARY FOR
FORMALDEHYDE OXIDATION, AND MINOR FOR CH4/CH3OH
!\MECHCOMMENTS: MECHANISM FROM MECH_RELEASE "A Detailed Chemical Kinetic
Modeling, Ignition Delay time and Jet-Stirred Reactor Study of Methanol
Oxidation" COMBUSTION AND FLAME, ACCEPTED OCTOBER 2015.
!\MECHWARNINGS:
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!\REACTIONCLASS: \UNIMOL          \A          \N
\EA
!
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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 !\COMMENT: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT
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 !\COMMENT: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT
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 !\COMMENT: NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT

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LOW/ 3.390E+042 -7.244
105230.3/
TROE/ -7.391E+001 3.705E+004 4.150E+004 5.220E+003/

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!\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) !\COMMENT:
WARNING INCOMPLETE REFERENCE
CH3OH+H<=>CH2OH+H2 3.070E+005 2.550
5440.0 !\AUTHOR: !\REF:J. CHEM. PHYS. 134, 094302 (2011)
!\COMMENT: WARNING INCOMPLETE REFERENCE
CH3OH+O<=>CH3O+OH 3.880E+004 2.500
3080.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)!\COMMENT:
REDUCED BY AN ORDER OF MAGNITUDE FROM ABSTRACTION FROM THE METHYL SITE
DUE TO INCREASED BOND STRENGTHS,UB ADDED 21/08/15
CH3OH+O<=>CH2OH+OH 3.880E+005 2.500
3080.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!\COMMENT:
CH3OH+OH<=>CH3O+H2O 1.500E+002 3.030
-763.0 !\AUTHOR: !\REF:XU ET AL. PROC 31 2007 159-166 !\COMMENT:
CH3OH+OH<=>CH2OH+H2O 3.080E+004 2.650
-806.7 !\AUTHOR: !\REF:XU ET AL. PROC 31 2007 159-166
!\COMMENT:
!CH3OH+O2<=>CH2OH+HO2 2.050E+013 0.000
44900.0 !\AUTHOR: !\REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P.
R. CHEMICAL SOCIETY, 1975 !\COMMENT: UB REMOVED 21/08/15
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
!\COMMENT: (ABOVE)REDUCED BY AN ORDER OF MAGNITUDE FROM ABSTRACTION FROM
THE METHYL SITE DUE TO INCREASED BOND STRENGTHS, UB ADDED 21/08/15
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 !\COMMENT: UB ADDED
21/08/15
!CH3OH+HO2<=>CH2OH+H2O2 1.080E+004 2.550
10530.0 !\AUTHOR: !\REF: CURRAN ESTIMATE !\COMMENT: WARNING: UB REMOVED
21/08/15
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 !\COMMENT: UB ADDED 21/08/15
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 !\COMMENT: EA INCREASED BY 500 CAL/MOL
!CH3OH+CH3<=>CH3O+CH4 1.440E+001 3.100
6935.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)!\COMMENT: UB
REMOVED 21/08/15
!CH3OH+CH3<=>CH2OH+CH4 3.190E+001 3.170
7172.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT: UB
REMOVED 21/08/15

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 !\COMMENT: UB ADDED 21/08/15
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 !\COMMENT: UB ADDED 21/08/15

CH3OH+HCO<=>CH2OH+CH2O 9.630E+003 2.900
13110.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!\COMMENT:
CH3OH+CH3O<=>CH2OH+CH3OH 3.000E+011 0.000
4074.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!\COMMENT:
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). !\COMMENT:
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)
!\COMMENT:
CH2OH+HO2<=>CH2O+H2O2 1.200E+013 0.000
0.0 !\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991).
!\COMMENT:
CH2OH+HCO<=>CH2O+CH2O 1.800E+014 0.000
0.0 !\AUTHOR: !\REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998)
!\COMMENT: ULTAN REMOVED 21/08/15
CH2OH+HCO<=>CH3OH+CO 1.000E+013 0.000
0.0 !\AUTHOR: !\REF: !\COMMENT: WARNING, NO REF
CH2OH+CH3O<=>CH2O+CH3OH 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:NORTON, T.S ET AL., IJCK. (1991).
!\COMMENT:
CH2OH+OH<=>H2O+CH2O 2.400E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!\COMMENT:
CH2OH+O<=>OH+CH2O 4.200E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!\COMMENT:
CH2OH+CH2OH<=>CH2O+CH3OH 3.000E+012 0.000
0.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)

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!\REACTIONCLASS: \R+HO2                \A                \N
\EA
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CH2OH+HO2<=>HOCH2O+OH                1.000E+013        0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF
RATE CONSTANT??

!=====
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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) !\COMMENT:
CH3O+H<=>CH2O+H2                        2.000E+013        0.000
0.0 !\AUTHOR: !\REF:HOYERMANN ET AL., 18TH SYMPOSIUM
!\COMMENT:
CH3O+HO2<=>CH2O+H2O2                    3.010E+011        0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986) !\COMMENT:
CH3O+CH3<=>CH2O+CH4                      1.200E+013        0.000
0.0 !\AUTHOR: !\REF: WARNING: NO REFERENCE
!\COMMENT: WARNING: 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) !\COMMENT:

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

!=====
=====
!\SUBSPECIES: \HCOH
!=====
=====
!
-----
!\REACTIONCLASS: \LUMPED_BIMOLECULAR    \A                \N
\EA

```

!

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

!=====

!\ENDSUBSPECIES: \CH3O

!=====

!-----

!\ENDSUBMECH: \CH3OH

!-----

!-----

!\SUBMECH: \CH2O

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

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

!\MECHWARNINGS:

!-----

!-----

!\REACTIONCLASS: \UNIMOL \A \N

\EA

!

HCO+H(+M)<=>CH2O(+M)	1.090E+012	0.480
----------------------	------------	-------

-260.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:

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 !\COMMENT:

WARNING: KPS NOT INDIVIDUALLY REFERENCED IN MECHANISM, ASSUMING IT'S FROM LASKIN ET AL.

LOW/	5.070E+027	-3.420
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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) !\COMMENT:
CH2O+O<=>HCO+OH 6.260E+009 1.150
2260.0 !\AUTHOR: !\REF: CURRAN FIT TO NIST DATABASE
\COMMENT:
CH2O+H<=>HCO+H2 5.740E+007 1.900
2740.0 !\AUTHOR: !\REF: IRDAM ET AL., IJCK 1993, 25, 285
\COMMENT:
CH2O+OH<=>HCO+H2O 7.820E+007 1.630
-1055.0 !\AUTHOR: !\REF: V. VASUDEVAN ET AL. IJCK. 37: 98--109 (2005).
\COMMENT:
CH2O+HO2<=>HCO+H2O2 1.880E+004 2.700
11520.0 !\AUTHOR: !\REF: J. PHYS. CHEM. A 109, 12027-12035, 2005
\COMMENT:
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 !\COMMENT:
CH2O+O2CHO<=>HCO+HO2CHO 1.990E+012 0.000
11660.0 !\AUTHOR: !\REF: ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986
\COMMENT:
CH2O+OCHO<=>HCO+HOCHO 5.600E+012 0.000
13600.0 !\AUTHOR: !\REF: CURRAN ESTIMATE
\COMMENT:
CH2O+CH3O<=>HCO+CH3OH 6.620E+011 0.000
2294.0 !\AUTHOR: !\REF: FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998).
\COMMENT:
CH2O+CH3O2<=>HCO+CH3O2H 1.990E+012 0.000
11660.0 !\AUTHOR: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:

!

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

!

HCO+M<=>H+CO+M 5.700E+011 0.660
14870.0 !\AUTHOR: !\REF: LI ET AL. IJCK 2007 !\COMMENT: X1.2
H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/

!

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

!

HCO+O2<=>CO+HO2	7.580E+012	0.000
410.0 !\AUTHOR: !\REF:TIMONEN ET AL., JPC, 92:651 (1988)		
!\COMMENT:		
HCO+O<=>CO+OH	3.020E+013	0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:		
HCO+H<=>CO+H2	7.340E+013	0.000
0.0 !\AUTHOR: !\REF:TIMONEN ET AL., JPC, 92:651 (1988)		
!\COMMENT:		
HCO+OH<=>CO+H2O	3.011E+013	0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:		
HCO+CH3<=>CH4+CO	2.650E+013	0.000
0.0 !\AUTHOR: !\REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987)		
!\COMMENT:		
HCO+HCO<=>CH2O+CO	1.800E+013	0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:		

!

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

!

HCO+O<=>CO2+H	3.000E+013	0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:		
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) !\COMMENT:		
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) !\COMMENT:		

!

!\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/		

!

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

CH2O+OH<=>HOCH2O 4.500E+015 -1.100
0.0 !\AUTHOR: !\REF:26TH INTL. COMBUSTION SYMP. P 497--504. !\COMMENT:
HOCH2O<=>HOCHO+H 1.000E+014 0.000
14900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF RATE CONSTANT?

!

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

CH2O+HO2<=>OCH2O2H 1.500E+011 0.000
11900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF RATE CONSTANT?
OCH2O2H<=>HOCH2O2 3.000E+011 0.000
8600.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE
OF RATE CONSTANT?
HOCH2O2+HO2<=>HOCH2O2H+O2 3.500E+010 0.000
-3275.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF RATE CONSTANT?
HOCH2O+OH<=>HOCH2O2H 1.000E+013 0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF
RATE CONSTANT?

!

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

HCO+O2<=>O2CHO 1.200E+011 0.000
-1100.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF RATE CONSTANT?

!

=====
!\SUBSPECIES: \HOCHO
=====

!

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

!

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

OCHO+HO2<=>HOCHO+O2 3.500E+010 0.000
-3275.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF RATE CONSTANT?
OCHO+H2O2<=>HOCHO+HO2 2.400E+012 0.000
10000.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:

!

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

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

!

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

OCHO+OH<=>HO2CHO 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:WKM ESTIMATE !\COMMENT: WHAT IS SOURCE OF RATE
CONSTANT?

!=====
=====
!\ENDSUBSPECIES: \HOCHO
!=====
=====

!-----

!\ENDSUBMECH: \CH2O
!-----

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

!\END_KINETICS_MODULE: \C1
!+++++++
+++++++
+++++++

!+++++++
+++++++
+++++++
!\KINETICS_MODULE: \C2
!+++++++
+++++++
+++++++

!-----

!\SUBMECH: \C2H6
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

!

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

CH3+CH3 (+M) <=> C2H6 (+M) 2.277E+015 -0.690
174.9 !\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003) !\COMMENT:
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/

C2H5+H (+M) <=> C2H6 (+M) 5.210E+017 -0.990
1580.0 !\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003) !\COMMENT:
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
!

C2H6+O2 <=> C2H5+HO2 6.030E+013 0.000
51870.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
(1992) !\COMMENT:
C2H6+O <=> C2H5+OH 3.550E+006 2.400
5830.0 !\AUTHOR: !\REF: MIYOSHI, A. ET AL., CHEM. PHYS. LETT. 204, 241-247
(1993) !\COMMENT:
C2H6+H <=> C2H5+H2 1.150E+008 1.900
7530.0 !\AUTHOR: !\REF:WANG ET AL., JPC A 107:11414 (2003) !\COMMENT:
C2H6+OH <=> C2H5+H2O 1.480E+007 1.900
950.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE !\COMMENT: WARNING:
WHAT IS ORIGINAL SOURCE OF NIST DATA?

C2H6+HO2<=>C2H5+H2O2 3.460E+001 3.610
16920.0 !\AUTHOR: !\REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
(2008) 112(30): 7047-7054. !\COMMENT:
C2H6+CH<=>C2H5+CH2 1.100E+014 0.000
-260.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
C2H6+CH2(S)<=>C2H5+CH3 1.200E+014 0.000
0.0 !\AUTHOR: !\REF:MECHANISM AND MODELING OF NITROGEN CHEMISTRY IN
COMBUSTION, WSS/ CI, AUTUMN 1988 !\COMMENT: WARNING: SOURCE SEEMS DATED
C2H6+CH3<=>C2H5+CH4 5.550E-004 4.720
3231.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
C2H6+CH3O<=>C2H5+CH3OH 2.410E+011 0.000
7090.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
C2H6+CH3O2<=>C2H5+CH3O2H 1.940E+001 3.640
17100.0 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
995-1003 !\COMMENT:
C2H6+C2H5O2<=>C2H5+C2H5O2H 8.600E+000 3.760
17200.0 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
995-1003 !\COMMENT:

!

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

!

C2H4+H(+M)<=>C2H5(+M) 9.569E+008 1.463
1355.0 !\AUTHOR: !\REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202
!\COMMENT: :HP AND LP LIMIT*0.7
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
!\COMMENT: WHAT IS SOURCE OF ORIGINAL DATA? EXPERIMENT? THEORY?
C2H4+C2H4<=>C2H5+C2H3 4.820E+014 0.000
71530.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
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) !\COMMENT:

!

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

!

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

!

!\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 !\COMMENT:
 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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?
 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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?
 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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?
 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<=>C2H4+HO2 6.609E+000 3.510
 14160.0 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995-1003 !\COMMENT: RMVD BECAUSE THIS WILL NEVER BE USED BY CHEMKIIN
 !DUP

C2H5+O2<=>C2H4O1-2+OH 1.303E+003 1.930
 -502.7 !\AUTHOR: !\REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)
 995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?
 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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005)				
995-1003 !\COMMENT: WARNING: IS THIS REAL REFERENCE?				
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 !\COMMENT:

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

!

!\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)
995-1003 !\COMMENT:

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

!=====
=====

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

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!\REACTIONCLASS: \UNIMOL                \A                \N
\EA
!
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C2H4O1-2<=>CH3+HCO                      3.630E+013        0.000
57200.0 !\AUTHOR: !\REF:LIFSHITZ ET AL. 1983      !\COMMENT:
C2H4O1-2<=>CH3CHO                          7.407E+012        0.000
53800.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE !\COMMENT: WARNING:
WHAT IS SOURCE OF NIST DATA?

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

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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) !\COMMENT:
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) !\COMMENT:
C2H4O1-2+HO2<=>C2H3O1-2+H2O2             1.130E+013        0.000
30430.0 !\AUTHOR: !\REF:ANALOGY WITH ETHENE
!\COMMENT: WARNING: KPS: WHAT IS JUSTIFICATION FOR THIS ANALOGY??
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) !\COMMENT:
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) !\COMMENT:
C2H4O1-2+CH3O2<=>C2H3O1-2+CH3O2H        1.130E+013        0.000
30430.0 !\AUTHOR: !\REF:ANALOGY WITH ETHENE
!\COMMENT: WARNING: KPS: WHAT IS JUSTIFICATION FOR THIS ANALOGY??
C2H4O1-2+C2H5O2<=>C2H3O1-2+C2H5O2H      1.130E+013        0.000
30430.0 !\AUTHOR: !\REF:ANALOGY WITH ETHENE
!\COMMENT: WARNING: KPS: WHAT IS JUSTIFICATION FOR THIS ANALOGY??

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!\REACTIONCLASS: \RADICAL_ISOMERISATION   \A                \N
\EA
!-----
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C2H3O1-2<=>CH3CO                          8.500E+014        0.000
14000.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984) !\COMMENT:
C2H3O1-2<=>CH2CHO                          1.000E+014        0.000
14000.0 !\AUTHOR: !\REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1,
80, 435 (1984) !\COMMENT:

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!=====
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!\ENDSUBSPECIES: \C2H4O1-2
!=====
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!-----

!\ENDSUBMECH: \C2H6
!-----

!-----

!\SUBMECH: \C2H4
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

!

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

C2H3+H(+M)<=>C2H4(+M) 6.080E+012 0.270
280.0 !\AUTHOR: !\REF:GRI 3.0 !\COMMENT:
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 !\COMMENT: WARNING: IS THIS FROM SAME VERSION
OF GRI AS ABOVE? IF NOT FALL-OFF EFFECTS MAY BE INCORRECT.
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!\!\!\!\!\ !\COMMENT: WARNING: SOURCE
OF REFERENCE IS CONFUSING
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) !\COMMENT:
C2H4+OH<=>C2H3+H2O 2.230E+004 2.745
2215.5 !\AUTHOR: !\REF: FROM STANFORD !\COMMENT: WARNING: SOURCE OF RATE
CONSTANT IS UNCLEAR
C2H4+CH3O<=>C2H3+CH3OH 1.200E+011 0.000
6750.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
C2H4+CH3O2<=>C2H3+CH3O2H 8.590E+000 3.754
27132.0 !\AUTHOR: !\REF:FROM BILL PITZ'S SUGGESTION !\COMMENT: WKM 22/
04/ 2010 WARNING: WHAT IS JUSTIFICATION FOR THIS RATE CONSTANT? WHY WAS
IT SUGGESTED?

C2H4+C2H5O2<=>C2H3+C2H5O2H 8.590E+000 3.754
27132.0 !\AUTHOR: !\REF:FROM BILL PITZ'S SUGGESTION !\COMMENT: WKM 22/
04/ 2010 WARNING: WHAT IS JUSTIFICATION FOR THIS RATE CONSTANT? WHY WAS
IT SUGGESTED?

C2H4+CH3CO3<=>C2H3+CH3CO3H 1.130E+013 0.000
30430.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
(1992) !\COMMENT:

C2H4+CH3<=>C2H3+CH4 9.760E+002 2.947
15148.0 !\AUTHOR: !\REF: WARNING REFERENCE UNCLEAR !\COMMENT: WARNING:
SOURCE OF RATE CONSTANT UNCLEAR IN MECHANISM

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 !\COMMENT: MAKING BRANCHING RATIO
55:45 WARNING:

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 !\COMMENT: MAKING BRANCHING RATIO
55:45 WARNING:

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

CH2(S)+CH3<=>C2H4+H 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:MARINOV ESTIMATE.
!\COMMENT: WARNING: IS RATE CONSTANT MOST UP TO DATE? WHAT IS ESTIMATE
BASED ON?

!

!\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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT: A*1.5"
C2H4+CH3O2<=>C2H4O1-2+CH3O 2.820E+012 0.000
17110.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF ESTIMATE?
C2H4+C2H5O2<=>C2H4O1-2+C2H5O 2.820E+012 0.000
17110.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT: WARNING: WHAT IS
SOURCE OF ESTIMATE?

!

!\SUBSPECIES: \C2H3

!

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

!

C2H2+H(+M)<=>C2H3(+M) 1.710E+010 1.266
2709.0 !\AUTHOR: !\REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202
!\COMMENT:
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<=>C2H3O0 4.07E+27 -4.67 5222 ! !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 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<=>C2H3O0 4.07E+27 -4.67 5222 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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 YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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

C2H300<=>CH2CHO+O 1.22E+29 -4.71 42340 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 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

C2H300<=>CHOCHO+H 4.72E+20 -2.69 32320 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 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

C2H300<=>CHOCHO+H 4.72E+20 -2.69 32320 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 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

C2H300<=>CH2CO+OH 1.55E+24 -3.87 49850 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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 YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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 YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?
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

C2H300<=>CO+CH3O 1.16E-01 3.16 18420 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING WARNING:
Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

PLOG/1.000E-02 5.20E+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

C2H300<=>CO+CH3O 1.16E-01 3.16 18420 !\AUTHOR: !\REF: GOLDSMITH
YEAR JOURNAL ETC !\COMMENT: !REFITTED BY YANG FROM 500K TO 2000K, MAXIMUM
ERROR IS 18.13%

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

!C2H300<=>CO2+CH3 6.03E-03 3.46 17420 !\AUTHOR: !\REF:
GOLDSMITH YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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

!C2H300<=>CO2+CH3 6.03E-03 3.46 17420 !\AUTHOR: !\REF:
GOLDSMITH YEAR JOURNAL ETC !\COMMENT: WARNING: JOURNAL REFERENCE MISSING
WARNING: Y. LI HAS REFITTED SOME RATE CONSTANTS. IS THIS NECESSARY?

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

!

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

C2H3+H<=>C2H2+H2 1.700E+014 0.000
0.0 !\AUTHOR: !\REF:86TSA/ HAM
!\COMMENT:
C2H3+H<=>H2CC+H2 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:USC ESTIMATE
!\COMMENT: WARNING: WHAT IS SOURCE OF USC MECH 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) !\COMMENT:
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) !\COMMENT:
C2H3+C2H3<=>C2H2+C2H4 9.600E+011 0.000
0.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087
(1986) !\COMMENT:

!=====
=====
!\ENDSUBSPECIES: \C2H3
!=====
=====

!-----

!\ENDSUBMECH: \C2H4
!-----

!-----

!\SUBMECH: \C2H2
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

!

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

C2H+H(+M)<=>C2H2(+M) 1.000E+017 0.000
0.0 !\AUTHOR: !\REF: GRI 3.0 !\COMMENT:
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 !\COMMENT:

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
\COMMENT:
C2H2+O<=>HCCO+H 2.958E+009 1.280
2472.0 !\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706
\COMMENT:
C2H2+HO2<=>CH2CO+OH 6.030E+009 0.000
7949.0 !\AUTHOR: !\REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706
\COMMENT:

C2H2+HCO<=>C2H3+CO 1.000E+007 2.000
6000.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H2+CH2<=>C3H3+H 1.200E+013 0.000
6620.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H2+CH2(S)<=>C3H3+H 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?
C2H2+HCCO<=>C3H3+CO 1.000E+011 0.000
3000.0 !\AUTHOR: !\REF:GRI 3.0 AND USC II
\COMMENT: WARNING: WHICH IS FROM GRI AND WHICH IS USC?

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

!

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

!

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

C2H2+OH<=>HCCOH+H 2.800E+005 2.280
12420.0 !\AUTHOR: !\REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055
\COMMENT:
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
!\COMMENT:

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
!\COMMENT:

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
!\COMMENT:

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 !\COMMENT:

!=====
=====

!\SUBSPECIES: \C2H

!=====
=====

C2H+O2<=>CO2+CH* 2.170E+010 0.000
0.0 !\AUTHOR: !\REF:DEVRIENDT, VAN LOOK, CEURSTERS, AND PEETERS, CHEM
PHYS LETT. 261 (1996) 450, C2H+O2 !\COMMENT:

C2H+O2<=>HCO+CO 5.000E+013 0.000
1500.0 !\AUTHOR: !\REF:GRI !\COMMENT:

C2H+O<=>CO+CH* 6.200E+012 0.000
0.0 !\AUTHOR: !\REF:OH* KATHROTIA ET AL. COMB & FLAME 2010 !\COMMENT:
C2H+O<=>CO+CH 5.000E+013 0.000
0.0 !\AUTHOR: !\REF:GRI !\COMMENT:

C2H+H2<=>H+C2H2 4.900E+005 2.500
560.0 !\AUTHOR: !\REF:GRI !\COMMENT:

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C2H+OH<=>H+HCCO                2.000E+013    0.000
0.0 !\AUTHOR: !\REF:GRI !\COMMENT:
!=====
=====
!\SUBSPECIES: \C2H
!=====
=====

!-----
-----
!\ENDSUBMECH: C2H2
!-----
-----

!-----
-----
!\SUBMECH: \CH3CHO
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----
-----
!
!-----
-----
!\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 !\COMMENT:
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 !\COMMENT:
LOW/                                  1.144E+058    -11.300
95912.5/
TROE/  2.490E-003  7.181E+002  6.089E+000  3.780E+003/

!-----
-----
!\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) !\COMMENT:
CH3CHO+O<=>CH3CO+OH                    5.940E+012    0.000
1868.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE !\COMMENT: WARNING:
WHAT IS SOURCE OF NIST DATA?
CH3CHO+H<=>CH3CO+H2                    1.310E+005    2.580
1220.0 !\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010
!\COMMENT:
CH3CHO+OH<=>CH3CO+H2O                  3.370E+012    0.000
-619.0 !\AUTHOR: !\REF:JUAN LI'S PHD THESIS !\COMMENT: WARNING:
UNPUBLISHED RESULTS?

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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) !\COMMENT: !\COMMENT:
 CH3CHO+CH3<=>CH3CO+CH4 7.080E-004 4.580
 1966.0 !\AUTHOR: !\REF: GUPTA ET AL., PROC COMBUST INST 31 (2007) 167-174
 !\COMMENT:
 CH3CHO+CH3O2<=>CH3CO+CH3O2H 3.010E+012 0.000
 11920.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
 (1992) !\COMMENT:
 CH3CHO+CH3CO3<=>CH3CO+CH3CO3H 3.010E+012 0.000
 11920.0 !\AUTHOR: !\REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411
 (1992) !\COMMENT: WARNING: WHY IS THIS RATE CONSTANT SAME AS ABOVE?

 CH3CHO+H<=>CH2CHO+H2 2.720E+003 3.100
 5210.0 !\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010
 !\COMMENT:
 CH3CHO+OH<=>CH2CHO+H2O 1.720E+005 2.400
 815.0 !\AUTHOR: !\REF:TAYLOR ET AL. 1996 !\COMMENT:

!

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

!

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

!

!\SUBSPECIES: \CH3CO

!

!

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

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 !\COMMENT: WARNING: NO SOURCE OF ESTIMATE
CH3CO+O<=>CH2CO+OH 2.000E+013 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE
CH3CO+CH3<=>CH2CO+CH4 5.000E+013 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: NO SOURCE OF ESTIMATE

!

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

CH3CO+O2<=>CH3CO3 1.200E+011 0.000
-1100.0 !\AUTHOR: !\REF: CURRAN ESTIMATE !\COMMENT:

CH3CO3+HO2<=>CH3CO3H+O2 1.750E+010 0.000
-3275.0 !\AUTHOR: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
H2O2+CH3CO3<=>HO2+CH3CO3H 2.410E+012 0.000
9936.0 !\AUTHOR: !\REF: TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA,
15:1087 (1986) !\COMMENT:
CH4+CH3CO3<=>CH3+CH3CO3H 1.810E+011 0.000
18480.0 !\AUTHOR: !\REF:BASED ON CH4+CH3O2 !\COMMENT: WARNING: HAS RATE
CONSTANT BEEN ALTERED? BY OW MUCH?

!=====

!\ENDSUBSPECIES: \CH3CO
!=====

!=====

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

!

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

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

!

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!\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
!\COMMENT: WARNING: WHAT IS SOURCE?
C2H3OH+O<=>CH2CHO+OH                          1.875E+006      1.900
-860.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA
!\COMMENT: WARNING: WHAT IS SOURCE?
C2H3OH+H<=>CH2CHO+H2                          1.480E+003      3.077
7220.0 !\AUTHOR: !\REF:ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-1608,
!\COMMENT: WARNING: EXCEPT FOR SC2H4OH CHANNEL KEPT WKM CALCULATION
C2H3OH+OH<=>CH2CHO+H2O                       3.330E+009      1.100
540.5 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA
!\COMMENT: WARNING: WHAT IS SOURCE?
C2H3OH+CH3<=>CH2CHO+CH4                      2.030E-008      5.900
1052.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA
!\COMMENT: WARNING: WHAT IS SOURCE?
C2H3OH+CH3O2<=>CH2CHO+CH3O2H                 3.400E+003      2.500
8922.0 !\AUTHOR: !\REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA
!\COMMENT: WARNING: WHAT IS SOURCE?

C2H3OH+H<=>C2H2OH+H2                         2.470E+007      2.030
15200.0 !\AUTHOR: !\REF:ENOL+H RAO |J. PHYS. CHEM. A 2011, 115, 1602-
1608, !\COMMENT: WARNING: EXCEPT FOR SC2H4OH CHANNEL KEPT WKM CALCULATION
!
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!\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,
!\COMMENT: WARNING: EXCEPT FOR SC2H4OH CHANNEL KEPT WKM CALCULATION
C2H3OH+HO2<=>CH3CHO+HO2                      1.490E+005      1.670
6810.0 !\AUTHOR: !\REF:DA SILVA BOZZELLI CHEMICAL PHYSICS LETTERS 483
(2009) 25-29 !\COMMENT:
!
=====
!
=====
!\ENDSUBSPECIES: \C2H3OH
!
=====
!
=====
!\SUBSPECIES: CH2CHO
!
=====
!
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!\REACTIONCLASS: \RADICAL_DECOMPOSITION     \A          \N
\EA
!
-----

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CH2CHO (+M) <=> CH2CO+H (+M) 1.430E+015 -0.150
45600.0 !\AUTHOR: !\REF:J. PHYS. CHEM. A 2006, 110, 5772-5781 !\COMMENT:
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 !\COMMENT:
LOW/ 9.520E+033 -5.070
41300.0/
TROE/ 7.130E-017 1.150E+003 4.990E+009 1.790E+009/

!=====
=====
!\ENDSUBSPECIES: \CH2CHO
!=====
=====

!=====
=====
!\SUBSPECIES: \CH3CO3H
!=====
=====

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

CH3CO3H <=> CH3CO2+OH 5.010E+014 0.000
40150.0 !\AUTHOR: !\REF:SAHETCHIAN ET AL. 1992 !\COMMENT:

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

CH3CO3+CH2O <=> CH3CO3H+HCO 1.990E+012 0.000
11660.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH2O !\COMMENT: WARNING: POORLY-
DEFINED IN THIS DIRECTION?
CH3CO3+C2H6 <=> CH3CO3H+C2H5 1.700E+013 0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO CH3O2+CH2O !\COMMENT: WARNING: POORLY-
DEFINED IN THIS DIRECTION?

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

CH3CO2+M <=> CH3+CO2+M 4.400E+015 0.000
10500.0 !\AUTHOR: !\REF:ANALOGY TO CH3CO <=> CH3+CO !\COMMENT:

!\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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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/

!=====
=====
!\ENDSUBSPECIES: \CH3CO3H
!=====
=====

!-----

!\ENDSUBMECH: \CH3CHO
!-----

!-----

!\SUBMECH: \CH2CO
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

CH2+CO (+M) <=> CH2CO (+M) 8.100E+011 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
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 !\COMMENT: WARNING: SEE COMMENTS IN PREVIOUS VERSION OF MECHANISM
CH2CO+O<=>HCCO+OH 1.000E+013 0.000
8000.0 !\AUTHOR: !\REF:WKM ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF
ESTIMATE?
CH2CO+OH<=>HCCO+H2O 1.000E+013 0.000
2000.0 !\AUTHOR: !\REF:WKM ESTIMATE !\COMMENT: WARNING: WHAT IS SOURCE OF
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 !\COMMENT: WARNING: SEE COMMENTS IN PREVIOUS VERSION OF MECHANISM
CH+CH2O<=>H+CH2CO 9.460E+013 0.000
-515.0 !\AUTHOR: !\REF:REG 2.11
!\COMMENT: WARNING: SOURCE OF RATE CONSTANT UNCLEAR
CH2CO+O<=>CH2+CO2 1.750E+012 0.000
1350.0 !\AUTHOR: !\REF:CURRAN ESTIMATE
!\COMMENT:
CH2CO+OH<=>CH2OH+CO 2.000E+012 0.000
-1010.0 !\AUTHOR: !\REF:BROWN ET AL. CHEM. PHYS. LETT. 1989, 161, 491.
!\COMMENT:
CH2CO+CH2(S)<=>C2H4+CO 1.600E+014 0.000
0.0 !\AUTHOR: !\REF:WKM CALCULATION
!\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT
CH2CO+CH3<=>C2H5+CO 4.769E+004 2.312
9468.0 !\AUTHOR: !\REF:WKM CALCULATION
!\COMMENT: CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT

!

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

!

HCCO+OH=>H2+CO+CO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:WKM CALCULATION !\COMMENT: CHEMICALLY ACTIVATED,
APPEARS PRESSURE INDEPENDANT
HCCO+O=>H+CO+CO 8.000E+013 0.000
0.0 !\AUTHOR: !\REF:WKM CALCULATION !\COMMENT: CHEMICALLY ACTIVATED,
APPEARS PRESSURE INDEPENDANT

!

!\SUBSPECIES: \HCCO

!

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

!

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

!

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

!

HCCO+H<=>CH2(S)+CO 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:GRI !\COMMENT:
HCCO+O2=>OH+CO+CO 1.910E+011 -0.020
1020.0 !\AUTHOR: !\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS
JOURNAL/ISSUE?

HCCO+O2=>CO2+CO+H 4.780E+012 -0.142
1150.0 !\AUTHOR: !\REF:KLIPPENSTEIN 2002 !\COMMENT: WARNING: WHAT IS
JOURNAL/ISSUE?
CH+HCCO<=>CO+C2H2 5.000E+013 0.000
0.0 !\AUTHOR: !\REF:REG 2.11 !\COMMENT: WARNING: WHAT IS SOURCE
OF RATE CONSTANT?

!=====
=====
!\ENDSUBSPECIES: \HCCO
!=====
=====

!-----

!\ENDSUBMECH: \CH2CO
!-----

!-----

!\SUBMECH: \C2H5OH
!\MECHCOMMENTS:
!\MECHWARNINGS: KPS, 30/07/2015, LOW TEMPERATURE PATHWAYS FOR ETHANOL
RADICALS+O2 ARE FROM VARYING SOURCES. ARE THERE ANY INCONSISTENCIES IN
HPL/P-DEPENDENT KINETICS
!-----

!

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

C2H5OH<=>C2H4+H2O 3.410E+059 -14.200
83672.6 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO.
35, 2010 !\COMMENT:
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 !\COMMENT:
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 !\COMMENT:
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/

!

!\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		
!\COMMENT:		
C2H5OH+OH<=>C2H5O+H2O	5.810E-003	4.280
-3560.0 !\AUTHOR: !\REF: SMB 04/ 09/ 2013		
!\COMMENT: BRANCHING RATIO CHANGED FOR THE UNDERPREDICIOTN OF C2H4 IN THE JSR AND FLOW REACTOR		
C2H5OH+H<=>C2H5O+H2	9.450E+002	3.140
8701.1 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010 !\COMMENT:		
C2H5OH+HO2<=>C2H5O+H2O2	6.470E-007	5.300
10533.1 !\AUTHOR: !\REF: MITTAL 2013		
!\COMMENT: INCREASED BY 1.75 ZHOU WARNING: WHAT IS SOURCE OF RATE CONSTANT?		
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 !\COMMENT:		
C2H5OH+CH3O2<=>C2H5O+CH3O2H	3.236E-007	5.300
10533.1 !\AUTHOR: !\REF:ANAOLGY WITH C2H5OH+HO2		
!\COMMENT:		
C2H5OH+C2H5<=>PC2H4OH+C2H6	5.000E+010	0.000
13400.0 !\AUTHOR: !\REF:1/ 2 OF C4H10+C2H5		
!\COMMENT: WARNING: POOR ANALOGY?		
C2H5OH+O2<=>SC2H4OH+HO2	1.500E+013	0.000
50150.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010 !\COMMENT:		
C2H5OH+O<=>SC2H4OH+OH	1.450E+005	2.470
876.0 !\AUTHOR: !\REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703		
!\COMMENT:		
C2H5OH+H<=>SC2H4OH+H2	8.790E+004	2.680
2910.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010 !\COMMENT:		
C2H5OH+OH<=>SC2H4OH+H2O	7.520E+004	2.490
-1474.1 !\AUTHOR: !\REF: SMB 04/ 09/ 2013		
!\COMMENT: BRANCHING RATIO CHANGED FOR THE UNDERPREDICIOTN OF C2H4 IN THE JSR AND FLOW REACTOR		
C2H5OH+HO2<=>SC2H4OH+H2O2	2.450E-005	5.260
7475.1 !\AUTHOR: !\REF: MITTAL 2013		
!\COMMENT: INCREASED BY 1.75 ZHOU WARNING: WHAT IS SOURCE OF RATE CONSTANT?		
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 !\COMMENT:		
C2H5OH+CH3O2<=>SC2H4OH+CH3O2H	1.225E-005	5.260
7475.1 !\AUTHOR: !\REF:ANAOLGY WITH C2H5OH+HO2		
!\COMMENT:		

C2H5OH+C2H5<=>SC2H4OH+C2H6 5.000E+010 0.000
 10400.0 !\AUTHOR: !\REF:ESTIMATE
 !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?

 C2H5OH+O2<=>PC2H4OH+HO2 2.000E+013 0.000
 52800.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO.
 35, 2010 !\COMMENT:
 C2H5OH+O<=>PC2H4OH+OH 9.690E+002 3.230
 4658.0 !\AUTHOR: !\REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703
 !\COMMENT:
 C2H5OH+H<=>PC2H4OH+H2 5.310E+004 2.810
 7490.0 !\AUTHOR: !\REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO.
 35, 2010 !\COMMENT:
 C2H5OH+OH<=>PC2H4OH+H2O 3.760E+003 2.780
 -1810.2 !\AUTHOR: !\AUTHOR: !\REF: SMB 04/ 09/ 2013
 !\COMMENT: BRANCHING RATIO CHANGED FOR THE UNDERPREDICIOTN OF C2H4 IN THE
 JSR AND FLOW REACTOR !\COMMENT:
 C2H5OH+HO2<=>PC2H4OH+H2O2 3.986E-002 4.300
 15333.0 !\AUTHOR: !\REF: MITTAL 2013
 !\COMMENT: INCREASED BY 1.75 ZHOU WARNING: WHAT IS SOURCE OF RATE
 CONSTANT?
 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 !\COMMENT:
 C2H5OH+CH3O2<=>PC2H4OH+CH3O2H 1.995E-002 4.300
 15333.0 !\AUTHOR: !\REF:ANAOLGY WITH C2H5OH+HO2
 !\COMMENT:

!

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

SC2H4OH<=>CH3CHO+H 5.690E+052 -13.380
 45049.0 !\AUTHOR: !\REF:WKM CALCULATION. !\COMMENT: WARNING: WHAT IS
 SOURCE OF RATE CONSTANT? THEORY? PAPER?
 PLOG/ 0.0010 5.690E+052 -13.380 45049.0/
 PLOG/ 0.0100 3.290E+056 -14.120 48129.0/
 PLOG/ 0.1000 8.580E+057 -14.160 50743.0/
 PLOG/ 1.0000 5.360E+055 -13.150 51886.0/
 PLOG/ 10.0000 1.660E+048 -10.640 50297.0/
 PLOG/ 20.0000 8.260E+044 -9.590 49218.0/
 PLOG/ 50.0000 1.010E+040 -8.060 47439.0/
 PLOG/ 100.0000 1.100E+036 -6.840 45899.0/
 SC2H4OH<=>C2H3OH+H 5.400E+046 -11.630
 44323.0 !\AUTHOR: !\REF:WKM CALCULATION. !\COMMENT: WARNING: WHAT IS
 SOURCE OF RATE CONSTANT? THEORY? PAPER?
 PLOG/ 0.0010 5.400E+046 -11.630 44323.0/
 PLOG/ 0.0100 1.210E+051 -12.550 47240.0/
 PLOG/ 0.1000 2.870E+054 -13.150 50702.0/
 PLOG/ 1.0000 3.790E+053 -12.510 52560.0/
 PLOG/ 10.0000 6.330E+046 -10.200 51441.0/
 PLOG/ 20.0000 3.870E+043 -9.170 50440.0/
 PLOG/ 50.0000 5.080E+038 -7.650 48713.0/
 PLOG/ 100.0000 5.120E+034 -6.410 47182.0/

SC2H4OH<=>C2H5O 5.480E+045 -11.630
 44328.0 !\AUTHOR: !\REF:WKM CALCULATION. !\COMMENT: WARNING: WHAT IS
 SOURCE OF RATE CONSTANT? THEORY? PAPER?
 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. !\COMMENT: WARNING: WHAT IS
 SOURCE OF RATE CONSTANT? THEORY? PAPER?
 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
 !\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
 CH3CHO+H<=>C2H5O 4.610E+007 1.710
 7090.0 !\AUTHOR: !\REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010
 !\COMMENT:

!

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

C2H5O+O2<=>CH3CHO+HO2 4.280E+010 0.000
 1097.0 !\AUTHOR: !\REF: HARTMANN ET AL. 1990 !\COMMENT:
 O2C2H4OH<=>PC2H4OH+O2 3.900E+016 -1.000
 30000.0 !\AUTHOR: !\REF:BASED ON C3H6OH+O2 REACTION !\COMMENT:
 O2C2H4OH=>OH+CH2O+CH2O 1.250E+011 0.000
 18900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING:
 WHAT IS SOURCE OF RATE CONSTANT?

SC2H4OH+O2<=>CH3CHO+HO2 5.260E+017 -1.638
 869.0 !\AUTHOR: !\REF:DA SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933
 !\COMMENT:
 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
 !\COMMENT:
 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
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

!

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

CH3OCH3 (+M) <=> CH3+CH3O (+M) 2.330E+019 -0.661
84139.0 !\AUTHOR: !\REF:R. SIVARAMAKRISHNAN, J.V. MICHAEL, A.F. WAGNER,
R. DAWES, A.W. JASPER, L.B. HARDING, Y. GEORGIEVSKII, S.J. KLIPPENSTEIN,
COMBUSTION AND FLAME, 158 (2011) 618-632. !\COMMENT:
LOW/ 1.720E+059 -11.400
93295.6/
TROE/ 1.000E+000 1.000E-030 8.80E+002/
H2/ 3.00/ CO/ 2.25/ CO2/ 3.00/ N2/ 1.50/ H2O/ 9.00/ CH3OCH3/ 5.00/ CH4/
3.00/ C2H6/ 4.50/

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

CH3OCH3+OH <=> CH3OCH2+H2O 9.350E+005 2.290
-780.7 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
!\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT? THEORY? EXPERIMENT?
CH3OCH3+H <=> CH3OCH2+H2 7.721E+006 2.090
3384.0 !\AUTHOR: !\REF:CURRAN, FIT TO NIST DATABASE
!\COMMENT: WARNING: WHAT IS SOURCE?
CH3OCH3+O <=> CH3OCH2+OH 7.750E+008 1.360
2250.0 !\AUTHOR: !\REF:CURRAN 08 NIST FIT
!\COMMENT: WARNING: WHAT IS SOURCE OF NIST DATA?
CH3OCH3+HO2 <=> CH3OCH2+H2O2 3.170E-003 4.640
10556.0 !\AUTHOR: !\REF:J. MENDES, C.-W. ZHOU, H.J. CURRAN, THE JOURNAL
OF PHYSICAL CHEMISTRY A, 118 (2014) 1300-1308.
!\COMMENT:
CH3OCH3+CH3O2 <=> CH3OCH2+CH3O2H 1.268E-003 4.640
10556.0 !\AUTHOR: !\REF:J. MENDES, C.-W. ZHOU, H.J. CURRAN, THE JOURNAL
OF PHYSICAL CHEMISTRY A, 118 (2014) 1300-1308.
!\COMMENT: WARNING: IS THIS A DIRECT SOURCE OR ANALOGY?

$\text{CH}_3\text{OCH}_3 + \text{CH}_3 \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{CH}_4$ 7.020E+000 3.780
 9687.1 !\AUTHOR: !\REF:R.S. TRANTER, P.T. LYNCH, C.J. ANNESLEY, THE
 JOURNAL OF PHYSICAL CHEMISTRY A, 116 (2012) 7287-7292.
 !\COMMENT: (A-FACTOR - 3.0)
 $\text{CH}_3\text{OCH}_3 + \text{O}_2 \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{HO}_2$ 4.100E+013 0.000
 44910.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
 !\COMMENT:
 $\text{CH}_3\text{OCH}_3 + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{CH}_3\text{OH}$ 6.020E+011 0.000
 4074.0 !\AUTHOR: !\REF:ESTIMATE, S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. !\COMMENT:
 $\text{CH}_3\text{OCH}_3 + \text{CH}_3\text{OCH}_2\text{O}_2 \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{CH}_3\text{OCH}_2\text{O}_2\text{H}$ 5.000E+012 0.000
 17690.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
 !\COMMENT:
 $\text{CH}_3\text{OCH}_3 + \text{O}_2\text{CHO} \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{HO}_2\text{CHO}$ 4.425E+004 2.600
 13910.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
 !\COMMENT:
 $\text{CH}_3\text{OCH}_3 + \text{OCHO} \rightleftharpoons \text{CH}_3\text{OCH}_2 + \text{HOCHO}$ 1.000E+013 0.000
 17690.0 !\AUTHOR: !\REF:S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
 INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740.
 !\COMMENT:

!

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

!

$\text{CH}_3\text{OCH}_2 + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_3\text{OCH}_3 + \text{CH}_2\text{O}$ 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. !\COMMENT:
 $\text{CH}_3\text{OCH}_2 + \text{CH}_2\text{O} \rightleftharpoons \text{CH}_3\text{OCH}_3 + \text{HCO}$ 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.
 !\COMMENT:
 $\text{CH}_3\text{OCH}_2 + \text{CH}_3\text{CHO} \rightleftharpoons \text{CH}_3\text{OCH}_3 + \text{CH}_3\text{CO}$ 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.
 !\COMMENT:

!

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

!

$\text{CH}_3\text{OCH}_2 \rightleftharpoons \text{CH}_3 + \text{CH}_2\text{O}$ 8.03E+12 0.440284 26490.7
 !\AUTHOR: !\REF:BURKE, CNF 2014 !\COMMENT: KPS: RRKM/ME @ CBS-QB3.
 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 !\COMMENT: BASED ON T. YAMADA, J.W.
BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000)
435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL
OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.
BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000)
435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL
OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.
BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000)
435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL
OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.
BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000)
435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL
OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.

BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.

BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.

BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W.

BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.

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 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR - 55%.
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 !\COMMENT: 3 PARAMETER, A-FACTOR/3

!

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!\SUBSPECIES: \CH3OCH2O2H

!

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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) !\COMMENT: 1/ 2
CH3O2+CH2O<=>CH3O2H+HCO
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. !\COMMENT:
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. !\COMMENT:

!

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!\ENDSUBSPECIES: \CH3OCH2O2H

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!

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!\SUBSPECIES: \HO2CH2OCHO

!

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!

!\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. !\COMMENT: A-FACTOR X5.

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!=====
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!\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
!\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
OCH2OCHO<=>HOCH2OCO                1.000E+011    0.000
14000.0 !\AUTHOR: !\REF: ESTIMATE WKM RECOMMENDATION 8/ 9/ 2010
!\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?
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. !\COMMENT: !\USING NEW THERMODYNAMIC VALUES WARNING: SOURCE OF
RATE CONSTANT POORLY DEFINED
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. !\COMMENT: !\USING NEW THERMODYNAMIC VALUES WARNING: SOURCE OF
RATE CONSTANT POORLY DEFINED
!=====
=====
!\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. !\COMMENT:
CH3OCH2O+O2<=>CH3OCHO+HO2          4.380E-019    9.500
-5501.0 !\AUTHOR: !\REF: WANTUCK, P.J. E AL. J. PHYS. CHEM. 91, 4653
(1987) !\COMMENT: ANALOGY TO CH3O+O2<=>CH2O+HO2
CH3OCH2O<=>CH3OCHO+H                3.300E+013    0.004
26136.3 !\AUTHOR: !\REF: HIPPLER ET AL. PCCP. 3: 3450--2458 (2001).
!\COMMENT: ANALOGY TO CH3O DECOMPOSITION HPL. DECREASED BY A FACTOR OF 2
WARNING: DIFFICULT TO TELL HOW RATE CONSTANT WAS MANIPLUATED?
!=====
=====
!\ENDSUBSPECIES: \CH3OCH2O
!=====
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!\ENDSUBMECH: \CH3OCH3

!

!

!\SUBMECH: \CH3OCHO

!\MECHCOMMENTS:

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

!

!

!\REACTIONCLASS: \UNIMOL

\A

\N

\EA

!

CH3O+HCO<=>CH3OCHO	3.000E+013	0.000
0.0 !\AUTHOR: !\REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000. !\COMMENT: ULTAN REMOVED 21/08/15		
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. !\COMMENT: ULTAN ADDED 21/08/15		
CH3+OCHO<=>CH3OCHO	1.000E+013	0.000
0.0 !\AUTHOR: !\REF:ESTIMATE		
!\COMMENT: WARNING: WHAT IS SOURCE OF RATE CONSTANT?		
CH2OCHO+H<=>CH3OCHO	1.000E+014	0.000
0.0 !\AUTHOR: !\REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000. !\COMMENT:		
CH3OCO+H<=>CH3OCHO	1.000E+014	0.000
0.0 !\AUTHOR: !\REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000. !\COMMENT:		

!

!\REACTIONCLASS: \RH_R_ABSTRACTION

\A

\N

\EA

!

CH3OCHO+O2<=>CH3OCO+HO2	1.000E+013	0.000
49700.0 !\AUTHOR: !\REF:ESTIMATE		
!\COMMENT: WARNING: HOW WERE THESE ESTIMATED?		
CH3OCHO+O2<=>CH2OCHO+HO2	2.050E+013	0.000
52000.0 !\AUTHOR: !\REF:ESTIMATE		
!\COMMENT: WARNING: HOW WERE THESE ESTIMATED?		
CH3OCHO+OH<=>CH3OCO+H2O	1.580E+007	1.800
934.0 !\AUTHOR: !\REF:ANALOGY TO PROPANE		
!\COMMENT: WARNING: POOR ANALOGY?		
CH3OCHO+OH<=>CH2OCHO+H2O	5.270E+009	0.970
1586.0 !\AUTHOR: !\REF:ANALOGY TO PROPANE		
!\COMMENT: WARNING: POOR ANALOGY?		
CH3OCHO+HO2<=>CH3OCO+H2O2	4.820E+003	2.600
13910.0 !\AUTHOR: !\REF:CURRAN ESTIMATE TSANG '88 PRIMARY H		
!\COMMENT: WARNING: POOR ANALOGY?		
CH3OCHO+HO2<=>CH2OCHO+H2O2	2.380E+004	2.550
16490.0 !\AUTHOR: !\REF:CURRAN ESTIMATE TSANG '88 PRIMARY H		
!\COMMENT: WARNING: POOR ANALOGY?		

$\text{CH}_3\text{OCHO} + \text{O} \rightleftharpoons \text{CH}_3\text{OCO} + \text{OH}$ 2.755E+005 2.450
 2830.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT: WARNING:
 $\text{CH}_3\text{OCHO} + \text{O} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{OH}$ 9.800E+005 2.430
 4750.0 !\AUTHOR: !\REF: FIT TO COHEN/ WESTBERG '86
 !\COMMENT: WARNING: IS THIS A DIRECT EXPERIMENT OR ANALOGY?
 $\text{CH}_3\text{OCHO} + \text{H} \rightleftharpoons \text{CH}_3\text{OCO} + \text{H}_2$ 6.500E+005 2.400
 4471.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT: WARNING:
 $\text{CH}_3\text{OCHO} + \text{H} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{H}_2$ 6.650E+005 2.540
 6756.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT: WARNING:
 $\text{CH}_3\text{OCHO} + \text{CH}_3 \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_4$ 7.550E-001 3.460
 5481.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT: WARNING:
 $\text{CH}_3\text{OCHO} + \text{CH}_3 \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_4$ 4.520E-001 3.650
 7154.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT: WARNING:
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_3\text{OH}$ 5.480E+011 0.000
 5000.0 !\AUTHOR: !\REF:ESTIMATE
 !\COMMENT: WARNING: HOW WERE THESE ESTIMATED
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_3\text{OH}$ 2.170E+011 0.000
 6458.0 !\AUTHOR: !\REF:ESTIMATE
 !\COMMENT: WARNING: HOW WERE THESE ESTIMATED
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O}_2 \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_3\text{O}_2\text{H}$ 4.820E+003 2.600
 13910.0 !\AUTHOR: !\REF:ANALOGY WITH HO2
 !\COMMENT: WARNING: IS ANALOGY DATED?
 $\text{CH}_3\text{OCHO} + \text{CH}_3\text{O}_2 \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_3\text{O}_2\text{H}$ 2.380E+004 2.550
 16490.0 !\AUTHOR: !\REF:ANALOGY WITH HO2
 !\COMMENT: WARNING: IS ANALOGY DATED?
 $\text{CH}_3\text{OCHO} + \text{HCO} \rightleftharpoons \text{CH}_3\text{OCO} + \text{CH}_2\text{O}$ 5.400E+006 1.900
 17010.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT:
 $\text{CH}_3\text{OCHO} + \text{HCO} \rightleftharpoons \text{CH}_2\text{OCHO} + \text{CH}_2\text{O}$ 1.025E+005 2.500
 18430.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT: WARNING:

!

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

!

$\text{CH}_3\text{OCO} \rightleftharpoons \text{CH}_2\text{OCHO}$ 1.629E+012 -0.180
 40670.0

$\text{CH}_3\text{OCO} \rightleftharpoons \text{CH}_3 + \text{CO}_2$ 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/

$\text{CH}_3\text{OCO} \rightleftharpoons \text{CH}_3\text{O} + \text{CO}$ 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
!+++++
+++++
+++++

!-----

!\SUBMECH: \C3H8
!\MECHCOMMENTS: THE REACTION NC3H7O2+H2<=>NC3H7O2H+H AND RELATED
ABSTRACTIONS ARE ILL-DEFINED IN THE REVERSE DIRECTION. WE SHOULD HAVE A
RATE RULE FOR ABSTRACTION FROM KHPS DEFINED IN THE OPPOSITE DIRECTION.
!\MECHWARNINGS:
!-----

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

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

NC3H7+H<=>C3H8 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING
IC3H7+H<=>C3H8 1.000E+014 0.000
0.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING

!-----

REACTION CLASS	A	N
!\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. !\COMMENT: WARNING		
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) !\COMMENT:		
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) !\COMMENT:		
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) !\COMMENT:		
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, 1949-1954 !\COMMENT:		
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. !\COMMENT:		
C3H8+CH3<=>IC3H7+CH4	6.400E+004	2.170
7520.0 !\AUTHOR: !\REF: FIT TO NIST DATABASE !\COMMENT:		
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. !\COMMENT: WARNING		
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. !\COMMENT: WARNING		
C3H8+C3H5-A<=>IC3H7+C3H6	7.940E+011	0.000
16200.0 !\AUTHOR: !\REF: DAGAUT ET AL., CST 71, 111(1990) !\COMMENT:		
C3H8+CH3O<=>IC3H7+CH3OH	3.000E+011	0.000
7000.0 !\AUTHOR: !\REF: DRYER ESTIMATE !\COMMENT:		
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. !\COMMENT: SCALED AS PER CARSTENSEN ET AL		
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. !\COMMENT: SCALED AS PER CARSTENSEN ET AL		
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 !\COMMENT:		
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 !\COMMENT:		
C3H8+O2CHO<=>IC3H7+HO2CHO	1.475E+004	2.600
13910.0 !\AUTHOR: !\REF: ANALOGY TO C2H6+HO2 !\COMMENT:		
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 !\COMMENT:		

$C_3H_8 + O_2 \rightleftharpoons NC_3H_7 + HO_2$ 6.000E+013 0.000
 52290.0 !\AUTHOR: !\REF: ANALOGY WITH $C_4H_{10} + O_2 \rightleftharpoons PC_4H_9 + HO_2$
 !\COMMENT:
 $C_3H_8 + H \rightleftharpoons NC_3H_7 + H_2$ 3.490E+005 2.690
 6450.0 !\AUTHOR: !\REF: TSANG, W. CHEMICAL KINETIC DATA BASE FOR
 COMBUSTION CHEMISTRY. PART 3. PROPANE J. PHYS. CHEM. REF. DATA 17, 887
 (1988) !\COMMENT:
 $C_3H_8 + O \rightleftharpoons NC_3H_7 + OH$ 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) !\COMMENT:
 $C_3H_8 + OH \rightleftharpoons NC_3H_7 + H_2O$ 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, 1949-1954
 !\COMMENT:
 $C_3H_8 + HO_2 \rightleftharpoons NC_3H_7 + H_2O_2$ 4.080E+001 3.590
 17160.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054. !\COMMENT:
 $C_3H_8 + CH_3 \rightleftharpoons NC_3H_7 + CH_4$ 9.040E-001 3.650
 7154.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT:
 $C_3H_8 + C_2H_3 \rightleftharpoons NC_3H_7 + C_2H_4$ 1.000E+011 0.000
 10400.0 !\AUTHOR: !\REF: FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F.
 L., AND GLASSMAN, I., TO BE PUBLISHED. !\COMMENT: WARNING
 $C_3H_8 + C_2H_5 \rightleftharpoons NC_3H_7 + C_2H_6$ 1.000E+011 0.000
 10400.0 !\AUTHOR: !\REF: FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F.
 L., AND GLASSMAN, I., TO BE PUBLISHED. !\COMMENT: WARNING
 $C_3H_8 + C_3H_5-A \rightleftharpoons NC_3H_7 + C_3H_6$ 7.940E+011 0.000
 20500.0 !\AUTHOR: !\REF: DAGAUT ET AL., CST 71, 111(1990) !\COMMENT:
 $C_3H_8 + CH_3O \rightleftharpoons NC_3H_7 + CH_3OH$ 3.000E+011 0.000
 7000.0 !\AUTHOR: !\REF: DRYER ESTIMATE !\COMMENT:
 $C_3H_8 + CH_3O_2 \rightleftharpoons NC_3H_7 + CH_3O_2H$ 1.386E+000 3.970
 18280.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054. !\COMMENT: SCALED AS PER CARSTENSEN ET AL
 $C_3H_8 + C_2H_5O_2 \rightleftharpoons NC_3H_7 + C_2H_5O_2H$ 1.386E+000 3.970
 18280.0 !\AUTHOR: !\REF: J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A
 (2008) 112(30): 7047-7054. !\COMMENT: SCALED AS PER CARSTENSEN ET AL
 $C_3H_8 + NC_3H_7O_2 \rightleftharpoons NC_3H_7 + NC_3H_7O_2H$ 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF: ANALOGY TO $C_2H_6 + HO_2$!\COMMENT:
 $C_3H_8 + IC_3H_7O_2 \rightleftharpoons NC_3H_7 + IC_3H_7O_2H$ 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF: ANALOGY TO $C_2H_6 + HO_2$!\COMMENT:
 $C_3H_8 + CH_3CO_3 \rightleftharpoons NC_3H_7 + CH_3CO_3H$ 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF: ANALOGY TO $C_2H_6 + HO_2$!\COMMENT:
 $C_3H_8 + O_2CHO \rightleftharpoons NC_3H_7 + HO_2CHO$ 5.520E+004 2.550
 16480.0 !\AUTHOR: !\REF: ANALOGY TO $C_2H_6 + HO_2$!\COMMENT:

 $C_3H_8 + PC_4H_9O_2 \rightleftharpoons NC_3H_7 + PC_4H_9O_2H$ 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF: ANALOGY TO $C_2H_6 + HO_2$!\COMMENT: MOVED FROM C4
 MECHANISM
 $C_3H_8 + PC_4H_9O_2 \rightleftharpoons IC_3H_7 + PC_4H_9O_2H$ 2.000E+012 0.000
 17000.0 !\AUTHOR: !\REF: WALKER, R. W., REACTION KINETICS, VOL. 1, S. P.
 R. CHEMICAL SOCIETY, 1975 !\COMMENT: !MOVED FROM C4 MECHANISM
 $C_3H_8 + SC_4H_9O_2 \rightleftharpoons NC_3H_7 + SC_4H_9O_2H$ 1.700E+013 0.000
 20460.0 !\AUTHOR: !\REF: ANALOGY TO $C_2H_6 + HO_2$!\COMMENT: MOVED FROM C4
 MECHANISM
 $C_3H_8 + SC_4H_9O_2 \rightleftharpoons IC_3H_7 + SC_4H_9O_2H$ 2.000E+012 0.000
 17000.0 !\AUTHOR: !\REF: WALKER, R. W., REACTION KINETICS, VOL. 1, S. P.
 R. CHEMICAL SOCIETY, 1975 !\COMMENT: !MOVED FROM C4 MECHANISM

!

!\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
!\COMMENT: WARNING: THIS REACTION IS A CHEMICALLY ACTIVATED
RECOMBINATION-DISSOCIATION AND SHOULD BE TREATED AS SUCH
IC3H7+OH<=>C3H6+H2O 2.410E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
!\COMMENT:
IC3H7+O<=>CH3COCH3+H 4.818E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
!\COMMENT:
IC3H7+O<=>CH3CHO+CH3 4.818E+013 0.000
0.0 !\AUTHOR: !\REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
!\COMMENT:

!

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

NC3H7+HO2<=>NC3H7O+OH 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE
NC3H7+CH3O2<=>NC3H7O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE

IC3H7+HO2<=>IC3H7O+OH 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE
IC3H7+CH3O2<=>IC3H7O+CH3O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF: WARNING !\COMMENT: WARNING: NO REFERENCE

!=====
=====
!\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: 250-275. !\COMMENT:
C2H5CHO+H<=>NC3H7O 4.000E+012 0.000
6260.0 !\AUTHOR: !\REF: H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL
KINETICS (2006) 38: 250-275. !\COMMENT:

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

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

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

CH3+CH3CHO<=>IC3H7O 1.000E+011 0.000
9256.0 !\AUTHOR: !\REF: H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL
KINETICS (2006) 38: 250-275. !\COMMENT:
CH3COCH3+H<=>IC3H7O 2.000E+012 0.000
7270.0 !\AUTHOR: !\REF: H.J. CURRAN, INTERNATIONAL JOURNAL OF CHEMICAL
KINETICS (2006) 38: 250-275. !\COMMENT:

!

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

IC3H7O+O2<=>CH3COCH3+HO2 9.090E+009 0.000
390.0 !\AUTHOR: !\REF:BALLA ET AL., CHEM. PHYSICS, 99, 323 (1985)
!\COMMENT: WARNING: INCREDIBLY OLD RATE CONSTANT.

!\ENDSUBSPECIES: \IC3H7O
!=====
=====
!

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

NC3H7+O2<=>C3H6+HO2 3.000E-019 0.000
3000.0 !\AUTHOR: !\REF:REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006
!\COMMENT:

NC3H7+O2<=>NC3H7O2 1.0E11 0.0 0.0 !\AUTHOR: !\COMMENT:
!0512 ADD KWZ
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: !\COMMENT:
!0512 ADD KWZ
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: WARNING NO REFERENCE !\COMMENT: WARNING: CANNOT
TELL WHAT REFERENCE IS
NC3H7O2<=>C3H6+HO2 6.24E+08 1.25
29600 !\AUTHOR: !\REF: \VLN 2011 !\COMMENT: WARNING: CANNOT TELL WHAT
REFERENCE IS

!

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

!

NC3H7O2<=>C3H6OOH1-2 4.090E+008 1.100
30100.0 !\AUTHOR: !\REF:SHARMA !\COMMENT: WARNING: KPS-NO CLUE AS TO
SOURCE
NC3H7O2<=>C3H6OOH1-3 3.566E+006 1.600
21000.0 !\AUTHOR: !\REF !\COMMENT: WARNING: KPS-NO CLUE AS TO
SOURCE
IC3H7O2<=>C3H6OOH2-1 2.917E+009 1.100
33500.0 !\AUTHOR: !\REF !\COMMENT: WARNING: KPS-NO CLUE AS TO
SOURCE

!

!\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 !\COMMENT:
C3H6OOH1-3<=>C3H6O1-3+OH 2.640E+009 0.710
18500.0 !\AUTHOR: !\REF:HIGH PRESSURE RATE RULES FOR ALKYL+O2 REACTIONS 2
VLN2012 !\COMMENT:

C3H6OOH1-2<=>C3H6+HO2 2.340E+010 0.770
15300.0 !\AUTHOR: !\REF:VILLANO !\COMMENT:
C3H6OOH1-3=>OH+CH2O+C2H4 2.890E+009 1.300
26700.0 !\AUTHOR: !\REF:VILLANO !\COMMENT:
C3H6OOH2-1<=>C2H3OOH+CH3 8.560E+010 0.850
30700.0 !\AUTHOR: !\REF:VILLANO !\COMMENT:
C3H6OOH1-2=>C2H4+CH2O+OH 1.310E+033 -7.010
48120.0 !\AUTHOR: !\REF:VILLANO !\COMMENT:

!

!\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 !\COMMENT:
C3H6OOH1-3+O2<=>C3H6OOH1-3O2 3.433E+016 -1.627
198.7 !\AUTHOR: !\REF:MIYOSHI A/2 !\ 080415A !\COMMENT:
C3H6OOH2-1+O2<=>C3H6OOH2-1O2 3.433E+016 -1.627
198.7 !\AUTHOR: !\REF:MIYOSHI A/2 !\ 080415A !\COMMENT:

!

!\REACTIONCLASS: \O2QOOH_ISOMERISATION \A \N
\EA
!

C3H6OOH1-2O2<=>C3H51-2,3OOH 2.917E+009 1.100
33500.0 !\AUTHOR: !\REF: !\ANALOGY TO 1ST ISOMERISATIONS !\COMMENT:
C3H6OOH1-3O2<=>C3H52-1,3OOH 4.009E+008 1.100
30100.0 !\AUTHOR: !\REF: !\ANALOGY TO 1ST ISOMERISATIONS !\COMMENT:
C3H6OOH2-1O2<=>C3H51-2,3OOH 3.566E+006 1.600
21000.0 !\AUTHOR: !\REF: !\ANALOGY TO 1ST ISOMERISATIONS !\COMMENT:

C3H51-2,3OOH<=>AC3H5OOH+HO2 2.560E+013 -0.490
17770.0 !\AUTHOR: !\REF: BOZZELLI AND PITZ, 1993. SINEAD, MOD 0509 KWZ
\COMMENT:
C3H52-1,3OOH<=>AC3H5OOH+HO2 1.150E+014 -0.630
17250.0 !\AUTHOR: !\REF: BOZZELLI AND PITZ, 1993. SINEAD, MOD 0509 KWZ
\COMMENT:
C3H51-2,3OOH<=>C3H5O1-2OOH-3+OH 4.450E+009 0.860
10800.0 !\AUTHOR: !\REF: !\COMMENT:
C3H51-2,3OOH<=>C3H5O1-3OOH-2+OH 2.640E+009 0.710
18500.0 !\AUTHOR: !\REF: !\HYDROPEROXY CYCLIC ETHER FORMATION !\COMMENT:
WARNING: KPS-CANNOT TELL WHAT IS HAPPENING.
C3H52-1,3OOH<=>C3H5O1-2OOH-3+OH 1.210E+009 1.050
11300.0 !\AUTHOR: !\REF: !\HYDROPEROXY CYCLIC ETHER FORMATION !\COMMENT:
WARNING: KPS-CANNOT TELL WHAT IS HAPPENING.
C3H5O1-2OOH-3=>CH2CHO+CH2O+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: !\HYDROPEROXY CYCLIC ETHER FORMATION !\COMMENT:
WARNING: KPS-CANNOT TELL WHAT IS HAPPENING.
C3H5O1-3OOH-2=>CH2CHO+CH2O+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: !\HYDROPEROXY CYCLIC ETHER FORMATION !\COMMENT:
WARNING: KPS-CANNOT TELL WHAT IS HAPPENING.

!

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

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

!

!\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 !\COMMENT:
C3KET13=>CH2O+CH2CHO+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: WARNING !\COMMENT:
C3KET21=>CH2O+CH3CO+OH 1.000E+016 0.000
43000.0 !\AUTHOR: !\REF: WARNING !\COMMENT:
C3KET21=>OH+CH2O+CO+CH3 1.59E+20 -1.5
42879.46 !\AUTHOR: !\REF: WARNING !\COMMENT:
C2H3OOH<=>CH2CHO+OH 8.400E+014 0.000
43000.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT: WARNING
C2H3OOH=>CH2CO+H+OH 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU !REF: ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:

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

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

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

!\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) !\COMMENT:
NC3H7O2+HO2<=>NC3H7O2H+O2 1.750E+010 0.000
-3275.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987)
!\COMMENT:
NC3H7O2+CH2O<=>NC3H7O2H+HCO 5.600E+012 0.000
13600.0 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2
!\COMMENT:
NC3H7O2+CH4<=>NC3H7O2H+CH3 1.120E+013 0.000
24640.0 !\AUTHOR: !\REF:ANALOGY TO CH4+HO2
!\COMMENT:
NC3H7O2+CH3OH<=>NC3H7O2H+CH2OH 6.300E+012 0.000
19360.0 !\AUTHOR: !\REF:ANALOGY TO CH3OH+HO2
!\COMMENT:
NC3H7O2+CH3CHO<=>NC3H7O2H+CH3CO 2.800E+012 0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2
!\COMMENT:

NC3H7O2+C2H4<=>NC3H7O2H+C2H3	1.130E+013	0.000
30430.0 !\AUTHOR: !\REF:ANALOGY TO C2H4+HO2		
!\COMMENT:		
NC3H7O2+C2H6<=>NC3H7O2H+C2H5	1.700E+013	0.000
20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
!\COMMENT:		
NC3H7O2+C2H3CHO<=>NC3H7O2H+C2H3CO	2.800E+012	0.000
13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2		
!\COMMENT:		
NC3H7O2+C2H5CHO<=>NC3H7O2H+C2H5CO	2.000E+011	0.000
9500.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE		
!\COMMENT:		

!=====
 =====
 !\ENDSUBSPECIES: \NC3H7O2H
 !=====
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!\REACTIONCLASS: \RO2_R_PRODUCTS	\A	\N
\EA		

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

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

!

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

IC3H7O+OH<=>IC3H7O2H	1.000E+015	-0.800
0.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT: WARNING: HOW DOES REVERSE		

DECOMPOSITION RATE CONSTANT COMPARE WITH CH3O+OH? ARE THERMODYNAMICS SENSIBLE?

!		
!\REACTIONCLASS: \RH_R_ABSTRACTION	\A	\N
\EA		
!		
IC3H7O2+H2<=>IC3H7O2H+H 26030.0 !\AUTHOR: !\REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) !\COMMENT:	3.010E+013	0.000
IC3H7O2+HO2<=>IC3H7O2H+O2 -3275.0 !\AUTHOR: !\REF:TSANG, JPC REF. DATA, 16:471 (1987) !\COMMENT:	1.750E+010	0.000
IC3H7O2+CH2O<=>IC3H7O2H+HCO 13600.0 !\AUTHOR: !\REF:ANALOGY TO CH2O+HO2 !\COMMENT:	5.600E+012	0.000
IC3H7O2+CH4<=>IC3H7O2H+CH3 24640.0 !\AUTHOR: !\REF:ANALOGY TO CH4+HO2 !\COMMENT:	1.120E+013	0.000
IC3H7O2+CH3CHO<=>IC3H7O2H+CH3CO 13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2 !\COMMENT:	2.800E+012	0.000
IC3H7O2+C2H4<=>IC3H7O2H+C2H3 30430.0 !\AUTHOR: !\REF:ANALOGY TO C2H4+HO2 !\COMMENT:	1.130E+013	0.000
IC3H7O2+CH3OH<=>IC3H7O2H+CH2OH 19360.0 !\AUTHOR: !\REF:ANALOGY TO CH3OH+HO2 !\COMMENT:	6.300E+012	0.000
IC3H7O2+C2H6<=>IC3H7O2H+C2H5 20460.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:	1.700E+013	0.000
IC3H7O2+C2H3CHO<=>IC3H7O2H+C2H3CO 13600.0 !\AUTHOR: !\REF:HALF OF CH2O+HO2 !\COMMENT:	2.800E+012	0.000
IC3H7O2+C2H5CHO<=>IC3H7O2H+C2H5CO 9500.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:	2.000E+011	0.000
!		
!\REACTIONCLASS: \RO2_R_PRODUCTS	\A	\N
\EA		
!		
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2 1860.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:	1.400E+016	-1.610
IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2 1860.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:	1.400E+016	-1.610
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2 1860.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:	1.400E+016	-1.610
IC3H7O2+IC3H7O2=>O2+IC3H7O+IC3H7O 1860.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:	1.400E+016	-1.610
IC3H7O2+NC3H7O2=>IC3H7O+NC3H7O+O2 1860.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:	1.400E+016	-1.610
IC3H7O2+CH3<=>IC3H7O+CH3O -1000.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:	7.000E+012	0.000

IC3H7O2+C2H5<=>IC3H7O+C2H5O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+IC3H7<=>IC3H7O+IC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+NC3H7<=>IC3H7O+NC3H7O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:
IC3H7O2+C3H5-A<=>IC3H7O+C3H5O 7.000E+012 0.000
-1000.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT:

!=====
=====
!\ENDSUBSPECIES: \IC3H7O2H
!=====
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!=====
=====
!\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) !\COMMENT: WARNING: REACTION IN WRONG CLASS
C3H6O1-2+OH=>CH2O+C2H3+H2O 5.000E+012 0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT: WARNING: WHAT ARE
SOURCES OF RATE CONSTANTS?
C3H6O1-2+H=>CH2O+C2H3+H2 2.630E+007 2.000
5000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+O=>CH2O+C2H3+OH 8.430E+013 0.000
5200.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+HO2=>CH2O+C2H3+H2O2 1.000E+013 0.000
15000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H 1.000E+013 0.000
19000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
C3H6O1-2+CH3=>CH2O+C2H3+CH4 2.000E+011 0.000
10000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:

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

C3H6O1-3<=>C2H4+CH2O 6.000E+014 0.000
60000.0 !\AUTHOR: !\REF:WESTBROOK AND PITZ ESTIMATE (1983) !\COMMENT:
WARNING: REACTION IN WRONG CLASS
C3H6O1-3+OH=>CH2O+C2H3+H2O 5.000E+012 0.000
0.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT: WARNING: WHAT ARE SOURCES OF
RATE CONSTANTS?
C3H6O1-3+O=>CH2O+C2H3+OH 8.430E+013 0.000
5200.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT:

C3H6O1-3+H=>CH2O+C2H3+H2 2.630E+007 2.000
5000.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT:
C3H6O1-3+CH3O2=>CH2O+C2H3+CH3O2H 1.000E+013 0.000
19000.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT:
C3H6O1-3+HO2=>CH2O+C2H3+H2O2 1.000E+013 0.000
15000.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT:
C3H6O1-3+CH3=>CH2O+C2H3+CH4 2.000E+011 0.000
10000.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT:

!=====
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!\ENDSUBSPECIES: C3H6O1-2/C3H6O1-3
!=====
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!-----

!\ENDSUBMECH: C3H8
!-----

!-----

!\SUBMECH: \C3H6
!\MECHCOMMENTS:
!\MECHWARNINGS:
!-----

!

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

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

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

CH2(S)+C2H4<=>C3H5-A+H 8.20E+19 -2.06E+00 1.15E+03
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
REFERENCE UNCLEAR IN BASE MECHANISM?

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

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

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

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

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<=>C3H5-A+H 5.73E+15 -7.70E-01 1195.9				
!\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:				
REFERENCE UNCLEAR IN BASE MECHANISM?				
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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:				
REFERENCE UNCLEAR IN BASE MECHANISM?				
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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:				
REFERENCE UNCLEAR IN BASE MECHANISM?				
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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:				
REFERENCE UNCLEAR IN BASE MECHANISM?				
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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:				
REFERENCE UNCLEAR IN BASE MECHANISM?				
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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:				
REFERENCE UNCLEAR IN BASE MECHANISM?				
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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
 REFERENCE UNCLEAR IN BASE MECHANISM?
 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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
 REFERENCE UNCLEAR IN BASE MECHANISM?
 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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
 REFERENCE UNCLEAR IN BASE MECHANISM?
 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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
 REFERENCE UNCLEAR IN BASE MECHANISM?
 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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
 REFERENCE UNCLEAR IN BASE MECHANISM?
 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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
 REFERENCE UNCLEAR IN BASE MECHANISM?
 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: WARNING: WHAT IS REFERENCE? !\COMMENT: WARNING:
REFERENCE UNCLEAR IN BASE MECHANISM?

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

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

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

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

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

!

!\REACTIONCLASS: \RH_R_ABSTRACTION

!

C3H6+H<=>C3H5-A+H2 3.644E+005 2.455
4361.2 !\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE?
!\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?

C3H6+O2<=>C3H5-A+HO2 5.960E+019 -1.670
 46192.1 !\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE
 !\COMMENT:
 C3H6+O<=>C3H5-A+OH 5.240E+011 0.700
 5884.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4
 !\COMMENT: WARNING: HAS CAVALOTTI RELEASED UPDATED RATE CONSTANTS FOR
 THIS?
 C3H6+OH<=>C3H5-A+H2O 4.460E+006 2.072
 1050.8 !\AUTHOR: !\REF: ANALOGY WITH C2H4
 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?
 C3H6+HO2<=>C3H5-A+H2O2 3.070E-002 4.403
 13547.2 !\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE?
 !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
 C3H6+CH3<=>C3H5-A+CH4 2.210E+000 3.500
 5675.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT:
 C3H6+CH3O<=>C3H5-A+CH3OH 8.400E+010 0.000
 2600.0 !\AUTHOR: !\REF: BILL
 !\COMMENT: !\REF: REDUCED EA BY DIFFERENCE BETWEEN BD FOR SECONDARY ALKYL
 AND PRIMARY ALLYLIC WITH F<=>.2: 0.2(98.4-88.2)<=>.2*10.2<=>2.0

 C3H6+CH3O2<=>C3H5-A+CH3O2H 7.680E-002 4.403
 13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM
 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) !\COMMENT:
 C3H6+C2H5O2<=>C3H5-A+C2H5O2H 7.680E-002 4.403
 13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT:
 C3H6+CH3CO3<=>C3H5-A+CH3CO3H 7.680E-002 4.403
 13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM
 C3H6+NC3H7O2<=>C3H5-A+NC3H7O2H 7.680E-002 4.403
 13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM
 C3H6+IC3H7O2<=>C3H5-A+IC3H7O2H 7.680E-002 4.403
 13547.2 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM
 !C3H6+IC4H9O2<=>C3H5-A+IC4H9O2H 5.350E-002 4.207
 13288.1 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM
 !C3H6+TC4H9O2<=>C3H5-A+TC4H9O2H 5.350E-002 4.207
 13288.1 !\AUTHOR: !\REF: ANALOGY TO C3H6+HO2
 !\COMMENT: WARNING: WHERE IS C3H6+HO2 RATE CONSTANT FROM

 C3H6+H<=>C3H5-T+H2 1.498E+002 3.381
 8909.5 !\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE?
 !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
 C3H6+O<=>C3H5-T+OH 6.030E+010 0.700
 7632.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4
 !\COMMENT:
 C3H6+OH<=>C3H5-T+H2O 1.800E+006 1.979
 2235.2 !\AUTHOR: !\REF: ANALOGY WITH C2H4
 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?
 C3H6+HO2<=>C3H5-T+H2O2 1.560E+004 2.820
 24427.9 !\AUTHOR: !\REF: C3 NUIG CALCULATION J.M
 !\COMMENT: WARNING: RESULTS ARE NOW PUBLISHED, UPDATED REFERENCE

C3H6+O2<=>C3H5-T+HO2 1.000E+013 0.000
 58770.0 !\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE
 !\COMMENT: WARNING: HOW WAS THIS ESTIMATED?
 C3H6+CH3<=>C3H5-T+CH4 8.400E-001 3.500
 11660.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887
 (1988) !\COMMENT:

C3H6+H<=>C3H5-S+H2 5.101E+002 3.234
 12357.0 !\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE?
 !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
 DUP
 C3H6+H<=>C3H5-S+H2 3.969E+002 3.252
 12007.0 !\AUTHOR: !\REF: WARNING: WHAT IS REFERENCE?
 !\COMMENT: WARNING: REFERENCE UNCLEAR IN BASE MECHANISM?
 DUP
 C3H6+O2<=>C3H5-S+HO2 2.000E+013 0.000
 62270.0 !\AUTHOR: !\REF: ESTIMATE C3 NUIG S. M. BURKE
 !\COMMENT:
 C3H6+O<=>C3H5-S+OH 1.200E+011 0.700
 8959.1 !\AUTHOR: !\REF: ANALOGY WITH C2H4
 !\COMMENT:
 C3H6+OH<=>C3H5-S+H2O 1.860E+005 2.369
 2502.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4
 !\COMMENT: WARNING: HAS ZADOR NOT COMPUTED THIS REACTION?
 C3H6+HO2<=>C3H5-S+H2O2 9.570E+002 3.059
 20798.6 !\AUTHOR: !\REF: C3 NUIG CALCULATION J.M
 !\COMMENT: WARNING: RESULTS ARE NOW PUBLISHED, UPDATED REFERENCE
 C3H6+CH3<=>C3H5-S+CH4 1.348E+000 3.500
 12850.0 !\AUTHOR: !\REF: TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)
 !\COMMENT:

!

!\REACTIONCLASS: \R_ADDITION\O

!

C3H6+O<=>C2H5+HCO 7.450E+006 1.880
 183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: THE
 PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.
 C3H6+O=>CH2CO+CH3+H 3.050E+006 1.880
 183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: THE
 PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.
 C3H6+O=>CH3CHCO+H+H 3.050E+006 1.880
 183.0 !\AUTHOR: !\REF: ANALOGY WITH C2H4 !\COMMENT: WARNING: THE
 PROBABILITY OF THIS BRANCHING RATIO IS SLIM TO NONE.

!

!\REACTIONCLASS: \R_ADDITION\H

!

C3H6+H<=>NC3H7 1.000E+000 1.000
 0.0 !\AUTHOR: !\REF: CURRAN EST !\COMMENT: WARNING: ARE THESE RATE
 CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
 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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: ARE THESE RATE
CONSTANTS NOT FROM MILLER/KLIPPENSTEIN??
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 !\COMMENT: WARNING: NO REFERENCE IN
BASEMECH2907_C7.INP
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 !\COMMENT: WARNING: NO REFERENCE IN
BASEMECH2907_C7.INP
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 !\COMMENT: WARNING: NO REFERENCE IN
BASEMECH2907_C7.INP
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 !\COMMENT: WARNING: NO REFERENCE IN
BASEMECH2907_C7.INP
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

!

!! WARNING: PART OF PROPYNE/ALLENE+H PES SO HAS BEEN LOCATED THERE TO
KEEP RATE CONSTANTS TOGETHER

!

!\REACTIONCLASS: \R_R_ABSTRACTION

!

C3H5-A+H<=>C3H4-A+H2 1.232E+003 3.035
2582.0 !\AUTHOR: !\REF:KLIPPENSTEIN & HARDING 2007
!\COMMENT:
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.
!\COMMENT:
C3H5-A+CH3<=>C3H4-A+CH4 3.000E+012 -0.320
-131.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!\COMMENT:
C3H5-A+C2H5<=>C3H4-A+C2H6 4.000E+011 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
!\COMMENT:
C3H5-A+C2H3<=>C3H4-A+C2H4 1.000E+012 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
!\COMMENT:
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) !\COMMENT:

C3H5-S+H<=>C3H4-A+H2 3.333E+012 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
!\COMMENT:
C3H5-S+CH3<=>C3H4-A+CH4 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
!\COMMENT:
C3H5-S+H<=>C3H4-P+H2 3.340E+012 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!\COMMENT:
C3H5-S+CH3<=>C3H4-P+CH4 1.000E+011 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!\COMMENT:

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

!

!\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 !\COMMENT:
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). !\COMMENT:

C3H5-A+HCO<=>C3H6+CO 6.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-S+HCO<=>C3H6+CO 9.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:
C3H5-T+HCO<=>C3H6+CO 9.000E+013 0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000 !\COMMENT:

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

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

!

!\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.
!\COMMENT:

!

!\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.
!\COMMENT:
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 !\COMMENT:
WARNING: THIS REFERENCE WAS ABOVE LASKIN, WHICH IS CORRECT? !\AUTHOR:
!\REF:!\WANG, J. PHYS. CHEM. REF. DATA 20, 221-273, (1991) !\COMMENT:
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 !\COMMENT:
WARNING: THIS REFERENCE WAS ABOVE LASKIN, WHICH IS CORRECT? !\AUTHOR:
!\REF:!\WANG, J. PHYS. CHEM. REF. DATA 20, 221-273, (1991) !\COMMENT:
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 !\COMMENT:
WARNING: THIS REFERENCE WAS ABOVE LASKIN, WHICH IS CORRECT? !\AUTHOR:
!\REF:!\WANG, J. PHYS. CHEM. REF. DATA 20, 221-273, (1991) !\COMMENT:
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 !\COMMENT:
C3H5-S+O2<=>CH3CHCHO+O 5.380E+018 -2.140
5142.9 !\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:
C3H5-S+O2<=>C2H3CHO+OH 2.700E+019 -2.140
5142.9 !\AUTHOR: !\REF: ANALOGY C2H3+O2 KLIPPENSTEIN !\COMMENT:

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

!

!\REACTIONCLASS: \R_HO2

!

C3H5-A+HO2<=>C3H5O +OH 1.000E+011 0.000
0.0 !\AUTHOR: !\REF: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.				
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.				
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE				
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN				
ALTERED?				
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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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: LASKIN ET AL IJCK 32 589-614 2000 OR TSANG, W.
J.PHYS.CHEM.REF.DATA 1991, 20, 221. OR FRANKLIN C GOLDSMITH J. PHYS.
CHEM. A, 2012, 116 (13), PP 3325-3346 !\COMMENT: WARNING: WHAT IS THE
SOURCE OF THESE RATE CONSTANTS? ARE THEY GOLDSMITH? HAVE THEY BEEN
ALTERED?

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 !\COMMENT:		
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 !\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	3.400E+029 -5.280 4539.8/

AC4H7OOH<=>C3H5O +CH3O	1.000E+011	0.000
0.0 !\AUTHOR: !\REF: ANOLOGY WITH C3H5-A+HO2 !\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 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, 11040-11053 !\COMMENT:

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, 11040-11053 !\COMMENT:

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, 11040-11053 !\COMMENT:

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, 11040-11053 !\COMMENT: SINEAD, MOD 0509 KWZ

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/

$C_3H_6+OH \rightleftharpoons CH_3CHO+CH_3$ 6.930E+005 1.490
 -536.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-
 11053 !\COMMENT:
 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/

$C_3H_6+OH \rightleftharpoons C_3H_6OH1-2$ 5.100E+054 -20.700
 32402.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-
 11053 !\COMMENT:
 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

$C_3H_6+OH \rightleftharpoons C_3H_6OH1-2$ 1.420E+036 -15.840
 11594.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-
 11053 !\COMMENT:
 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

$C_3H_6+OH \rightleftharpoons C_3H_6OH2-1$ 5.100E+054 -20.700
 32402.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-
 11053 !\COMMENT:
 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

$C_3H_6+OH \rightleftharpoons C_3H_6OH2-1$ 1.420E+036 -15.840
 11594.0 !\AUTHOR: !\REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-
 11053 !\COMMENT:
 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/

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

CH2CCH2OH+O2=>CH2OH+CO+CH2O	4.335E+012	0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:		
C3H5O +O2<=>C2H3CHO+HO2	1.000E+012	0.000
6000.0 !\AUTHOR: !\REF:ACETALDEHYDE ANALOG !\COMMENT:		

!=====
=====
!\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		
!\COMMENT: WARNING: THIS REFERENCE ALSO PRESENT: ANALOGY WITH CH3CHOH -->CH3CHO+H.		
IC3H5OH+H<=>C3H6OH2-1	6.250E+011	0.510
4020.0 !\AUTHOR: !\REF:BASED ON IC4H8+H<=>IC4H9		
!\COMMENT:		
C2H5CHO+H<=>C3H6OH1-2	8.000E+012	0.000
9500.0 !\AUTHOR: !\REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13		
!\COMMENT: WARNING: THIS REFERENCE ALSO PRESENT: ANALOGY WITH CH3CHOH -->CH3CHO+H.		

C3H5-T+OH<=>IC3H5OH	5.000E+013	0.000
0.0 !\AUTHOR: !\REF:REVERSE BY ANALOGY HCO+OH -->PRODUCTS !\COMMENT:		

!

!\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 !\COMMENT:		
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 !\COMMENT:		

!

!\REACTIONCLASS: \R+O2

!

C3H6OH1-2+O2<=>TQJC3H6OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 1.05E+114 -33.81 24741/
PLOG/ 0.01 2.13E+114 -33.44 26448/
PLOG/ 0.1 1.62E+110 -31.75 26612/
PLOG/ 1 6.00E+101 -28.79 25197/
PLOG/ 10 5.36E+89 -24.76 22402/
PLOG/ 40 1.55E+81 -21.95 20197/
PLOG/ 100 1.51E+75 -20 18578/
PLOG/ 200 3.16E+70 -18.48 17287/

C3H6OH1-2+O2<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 1.21E+26 -5.09 5755/
PLOG/ 0.01 1.41E+31 -6.55 8781/
PLOG/ 0.1 5.08E+34 -7.53 11702/
PLOG/ 1 1.67E+34 -7.27 13418/
PLOG/ 10 2.82E+28 -5.41 13318/
PLOG/ 40 2.50E+22 -3.52 12314/
PLOG/ 100 2.82E+17 -1.99 11286/
PLOG/ 200 1.93E+13 -0.71 10340/

DUP

C3H6OH1-2+O2<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 2.45E+21 -4.19 6837/
PLOG/ 0.01 1.40E+30 -6.75 11554/
PLOG/ 0.1 9.11E+39 -9.56 17834/
PLOG/ 1 5.16E+42 -10.17 22412/
PLOG/ 10 6.07E+32 -6.94 22738/
PLOG/ 40 3.88E+20 -3.14 20677/
PLOG/ 100 3.32E+10 -0.03 18552/
PLOG/ 200 1.22E+02 2.57 16623/

DUP

C3H6OH1-2+O2<=>SC3H5OH+HO2 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 1.26E+25 -4.69 5755/
PLOG/ 0.01 1.44E+30 -6.15 8785/
PLOG/ 0.1 4.78E+33 -7.11 11695/
PLOG/ 1 1.40E+33 -6.84 13395/
PLOG/ 10 2.12E+27 -4.96 13277/
PLOG/ 40 1.78E+21 -3.07 12265/
PLOG/ 100 1.97E+16 -1.53 11234/
PLOG/ 200 1.32E+12 -0.25 10285/

DUP

C3H6OH1-2+O2<=>SC3H5OH+HO2 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 3.22E+23 -4.69 5341/
PLOG/ 0.01 4.80E+28 -6.18 8461/
PLOG/ 0.1 1.71E+32 -7.16 11410/
PLOG/ 1 1.53E+32 -7.02 13378/
PLOG/ 10 5.55E+29 -6.14 15100/

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

PLOG/ 200 4.58E+122 -36.86 36374/
 C3H6OH1-2+O2<=>CCY(COC)OH+OH 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:

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

TQJC3H6OH<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:

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

DUP

TQJC3H6OH<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:

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

DUP

TQJC3H6OH<=>TQC3H6OI 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:

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

TQJC3H6OH<=>QC3H5OHP 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:

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

TQJC3H6OH<=>TQC3H5OHI 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:
 PLOG/ 0.001 9.57E+58 -15.99 38293/
 PLOG/ 0.01 7.27E+54 -14.25 38593/
 PLOG/ 0.1 8.30E+49 -12.44 38031/
 PLOG/ 1 1.90E+44 -10.51 36905/
 PLOG/ 10 2.18E+36 -7.9 34865/
 PLOG/ 40 4.10E+31 -6.36 33581/
 PLOG/ 100 3.00E+28 -5.35 32704/
 PLOG/ 200 1.34E+26 -4.59 32035/
 TQC3H6OI<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:
 PLOG/ 0.001 8.09E+38 -9.91 19096/
 PLOG/ 0.01 9.09E+39 -9.93 19135/
 PLOG/ 0.1 1.89E+41 -10.02 19407/
 PLOG/ 1 7.47E+23 -4.1 14658/
 PLOG/ 10 2.95E+33 -6.75 18685/
 PLOG/ 40 4.24E+36 -7.56 20307/
 PLOG/ 100 7.83E+36 -7.54 20747/
 PLOG/ 200 7.63E+35 -7.17 20641/
 QC3H5OHP<=>C3H5OH+HO2 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:
 PLOG/ 0.001 3.29E+57 -15.64 28576/
 PLOG/ 0.01 9.65E+58 -15.75 29927/
 PLOG/ 0.1 2.19E+50 -12.66 28547/
 PLOG/ 1 1.67E+49 -12.05 29204/
 PLOG/ 10 7.08E+40 -9.26 27188/
 PLOG/ 40 1.32E+30 -5.82 24071/
 PLOG/ 100 1.15E+30 -5.8 24053/
 PLOG/ 200 1.12E+30 -5.8 24050/
 QC3H5OHP<=>CY(COC)COH+OH 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:
 PLOG/ 0.001 1.11E+51 -12.97 28497/
 PLOG/ 0.01 5.58E+51 -12.87 29529/
 PLOG/ 0.1 3.03E+44 -10.28 28326/
 PLOG/ 1 1.42E+44 -9.98 28986/
 PLOG/ 10 9.69E+37 -7.93 27491/
 PLOG/ 40 5.90E+29 -5.3 25095/
 PLOG/ 100 5.27E+29 -5.29 25081/
 PLOG/ 200 5.15E+29 -5.28 25078/
 TQC3H5OHI<=>CCY(COC)OH+OH 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:
 PLOG/ 0.001 1.10E+31 -7.21 14640/
 PLOG/ 0.01 1.37E+32 -7.24 14716/
 PLOG/ 0.1 3.34E+33 -7.35 15127/
 PLOG/ 1 1.86E+23 -3.68 12864/
 PLOG/ 10 9.88E+31 -6.23 16040/
 PLOG/ 40 1.25E+34 -6.78 17056/
 PLOG/ 100 7.73E+33 -6.67 17176/
 PLOG/ 200 2.13E+33 -6.45 17170/
 TQC3H5OHI<=>SC3H5OH+HO2 1.420E+036 -15.840 11594.0
 !\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
 !\COMMENT:

PLOG/	0.001	6.01E+27	-7.27	14658/
PLOG/	0.01	7.78E+28	-7.3	14733/
PLOG/	0.1	3.27E+30	-7.48	15191/
PLOG/	1	2.81E+17	-2.82	12336/
PLOG/	10	1.92E+26	-5.22	16146/
PLOG/	40	7.61E+27	-5.49	17483/
PLOG/	100	1.91E+26	-4.86	17429/
PLOG/	200	2.94E+24	-4.18	17285/

C3H6OH2-1+O2<=>IQJC3H6OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:

PLOG/	0.001	3.34E+111	-32.67	25143/
PLOG/	0.01	4.84E+107	-31.05	25460/
PLOG/	0.1	2.41E+100	-28.42	24474/
PLOG/	1	4.55E+89	-24.78	22176/
PLOG/	10	1.14E+76	-20.31	18721/
PLOG/	40	9.25E+66	-17.35	16238/
PLOG/	100	6.20E+60	-15.36	14499/
PLOG/	200	1.30E+56	-13.86	13159/

C3H6OH2-1+O2<=>CHOCOHCH3+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:

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

C3H6OH2-1+O2<=>IQC3H6OT 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:

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

C3H6OH2-1+O2<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:

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

C3H6OH2-1+O2<=>CH3+CHOCH2OOH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 2.91E+40 -9.23 10830/
PLOG/ 0.01 9.66E+43 -10.2 13698/
PLOG/ 0.1 1.34E+44 -10.13 15661/
PLOG/ 1 2.57E+41 -9.18 17047/
PLOG/ 10 1.82E+36 -7.46 18330/
PLOG/ 40 8.82E+29 -5.44 18205/
PLOG/ 100 1.74E+24 -3.65 17600/
PLOG/ 200 2.16E+19 -2.12 16925/

C3H6OH2-1+O2<=>IQC3H5OHPJ 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 1.03E+115 -35.13 25407/
PLOG/ 0.01 1.10E+129 -38.89 32891/
PLOG/ 0.1 5.15E+135 -40.38 38573/
PLOG/ 1 7.27E+129 -38.13 39933/
PLOG/ 10 4.50E+112 -32.49 37045/
PLOG/ 40 7.72E+97 -27.79 33612/
PLOG/ 100 5.17E+86 -24.26 30799/
PLOG/ 200 4.70E+77 -21.41 28440/

C3H6OH2-1+O2<=>C2H3OH+CH2O+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 5.10E+24 -4.31 13009/
PLOG/ 0.01 6.91E+33 -6.97 17935/
PLOG/ 0.1 1.74E+41 -9.03 23613/
PLOG/ 1 2.26E+36 -7.32 25633/
PLOG/ 10 3.15E+17 -1.4 22782/
PLOG/ 40 9.35E+00 3.71 19114/
PLOG/ 100 5.59E-12 7.46 16156/
PLOG/ 200 1.27E-21 10.41 13733/

C3H6OH2-1+O2<=>CY(CCOC)OH+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 3.06E+33 -7.24 11476/
PLOG/ 0.01 6.56E+42 -9.92 17197/
PLOG/ 0.1 8.24E+46 -10.95 22090/
PLOG/ 1 4.48E+38 -8.22 23019/
PLOG/ 10 1.01E+18 -1.77 19496/
PLOG/ 40 1.16E+01 3.44 15637/
PLOG/ 100 4.85E-12 7.23 12599/
PLOG/ 200 8.64E-22 10.21 10126/
!

IQJC3H6OH<=>CHOCOHCH3+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 3.58E+71 -20.62 52656/
PLOG/ 0.01 9.67E+71 -20.08 54935/
PLOG/ 0.1 3.39E+67 -18.18 55330/
PLOG/ 1 7.26E+58 -15.09 54016/
PLOG/ 10 4.57E+46 -11.01 51172/
PLOG/ 40 4.31E+38 -8.38 49054/
PLOG/ 100 2.12E+33 -6.66 47587/

PLOG/ 200 2.72E+29 -5.41 46486/
!
IQJC3H6OH<=>IQC3H6OT 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 1.04E+45 -11.2 31755/
PLOG/ 0.01 2.90E+40 -9.62 30945/
PLOG/ 0.1 4.85E+35 -8.01 29850/
PLOG/ 1 2.62E+30 -6.28 28498/
PLOG/ 10 3.37E+24 -4.37 26873/
PLOG/ 40 9.75E+20 -3.23 25861/
PLOG/ 100 5.61E+18 -2.52 25208/
PLOG/ 200 1.44E+17 -2.01 24740/

IQJC3H6OH<=>IQC3H5OHPJ 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 1.36E+50 -12.93 36743/
PLOG/ 0.01 3.36E+45 -11.27 36143/
PLOG/ 0.1 1.13E+40 -9.41 34990/
PLOG/ 1 5.93E+33 -7.33 33438/
PLOG/ 10 4.24E+26 -5 31502/
PLOG/ 40 1.97E+22 -3.61 30275/
PLOG/ 100 3.43E+19 -2.72 29477/
PLOG/ 200 3.69E+17 -2.09 28900/

IQC3H6OT<=>CH3CHO+CH2O+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 9.82E+39 -9.95 20737/
PLOG/ 0.01 1.19E+41 -9.97 20814/
PLOG/ 0.1 2.60E+42 -10.07 21229/
PLOG/ 1 2.63E+32 -6.47 19139/
PLOG/ 10 1.32E+40 -8.68 22120/
PLOG/ 40 4.04E+41 -9.03 23000/
PLOG/ 100 9.07E+40 -8.77 23008/
PLOG/ 200 6.70E+39 -8.38 22782/

IQC3H6OT<=>CH3+CHOCH2OOH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 2.04E+37 -9.27 20741/
PLOG/ 0.01 2.54E+38 -9.29 20821/
PLOG/ 0.1 7.13E+39 -9.42 21267/
PLOG/ 1 2.95E+28 -5.34 18891/
PLOG/ 10 1.31E+36 -7.46 22106/
PLOG/ 40 2.19E+37 -7.68 23084/
PLOG/ 100 1.39E+36 -7.22 23018/
PLOG/ 200 2.67E+34 -6.63 22672/

IQC3H5OHPJ<=>C2H3OH+CH2O+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.
!\COMMENT:
PLOG/ 0.001 4.25E+16 -3.66 19364/
PLOG/ 0.01 2.98E+33 -8.01 27106/
PLOG/ 0.1 3.46E+38 -8.83 31412/
PLOG/ 1 7.07E+28 -5.46 29633/
PLOG/ 10 2.01E+13 -0.43 25278/

PLOG/ 40 1.43E+13 -0.38 25238/
PLOG/ 100 1.38E+13 -0.38 25234/
PLOG/ 200 1.37E+13 -0.37 25233/

IQC3H5OHPJ<=>CY(CCOC)OH+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

!\COMMENT:

PLOG/ 0.001 1.12E+25 -5.59 19349/
PLOG/ 0.01 7.20E+32 -7.6 23093/
PLOG/ 0.1 2.22E+34 -7.65 25130/
PLOG/ 1 2.40E+27 -5.28 23663/
PLOG/ 10 2.24E+17 -2.04 20810/
PLOG/ 40 1.82E+17 -2.01 20786/
PLOG/ 100 1.78E+17 -2.01 20783/
PLOG/ 200 1.77E+17 -2.01 20782/

IQC3H5OHPJ<=>AC3H5OOH+OH 1.420E+036 -15.840 11594.0
!\AUTHOR: !\ REF: H. SUN, ET AL., J. PHYS. CHEM. A., 2007, 111, 4974.

!\COMMENT:

PLOG/ 0.001 6.07E+13 -4.21 22478/
PLOG/ 0.01 9.74E+39 -10.89 33616/
PLOG/ 0.1 2.18E+49 -12.65 40359/
PLOG/ 1 3.32E+37 -8.42 38539/
PLOG/ 10 2.34E+16 -1.56 32712/
PLOG/ 40 1.44E+16 -1.49 32656/
PLOG/ 100 1.38E+16 -1.48 32651/
PLOG/ 200 1.37E+16 -1.48 32649/

!TQJC3H6OH=>CH3CHO+CH2O+OH 1.250E+011 0.000
18900.0 !\AUTHOR: !\REF:CURRAN ESTIMATE

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

!=====
=====
!\SUBSPECIES: \CY(COC)COH\CCY(COC)OH\CY(CCOC)OH\CHOCOCH3
!=====
=====

CY(COC)COH+OH=>C2H2OH+CH2O+H2O 1.26E3 2.97 -2660.6
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, COMBUST AND FLAME,
2011, 158, 726-731 !\COMMENT:

CY(COC)COH+OH=>C2H3CHO+OH+H2O 5.66E2 2.93 -4039.4
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12,
7221-7233 !\COMMENT:

CY(COC)COH+OH=>CH2CO+CH2OH+H2O 2.26E3 2.73 -4688
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12,
7221-7233 !\COMMENT:

CY(COC)COH+HO2=>C2H2OH+CH2O+H2O2 1.4E-5 5.26 8267.9
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, IJCK, 2012, 44,
155-164 !\COMMENT:

CY(COC)COH+HO2=>C2H3CHO+OH+H2O2 1.81E-1 3.98 9056.7
!\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118,
1300-1308 !\COMMENT:

CY(COC)COH+HO2=>CH2CO+CH2OH+H2O2 8.6 3.46 9732.326
!\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118,
1300-1308 !\COMMENT:

CCY(COC)OH+OH=>CH3CHCO+OH+H2O 2.26E3 2.73 -4688
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12,
7221-7233 !\COMMENT:

CCY(COC)OH+HO2=>CH3CHCO+OH+H2O2 8.6 3.46 9732.326
!\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118,
1300-1308 !\COMMENT:

CY(CCOC)OH+OH=>CH2O+CH2CO+H+H2O 2.26E3 2.73 -4688
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12,
7221-7233 !\COMMENT:

CY(CCOC)OH+OH=>CH2O+C2H2OH+H2O 5.66E2 2.93 -4039.4
!\AUTHOR: !\ C-W ZHOU, J. M. SIMMIE, AND H. J. CURRAN, PCCP, 2010, 12,
7221-7233 !\COMMENT:

CY(CCOC)OH+HO2=>CH2O+CH2CO+H+H2O2 8.6 3.46 9732.326
!\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118,
1300-1308 !\COMMENT:

CY(CCOC)OH+HO2=>CH2O+C2H2OH+H2O2 1.81E-1 3.98 9056.7
!\AUTHOR: !\ J. MENDES, C-W ZHOU, AND H. J. CURRAN, JPCA, 2014, 118,
1300-1308 !\COMMENT:

CHOCOCH3+OH=>CH3CHCO+OH+H2O 61329.9 2.65 -4586.4
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104. !\COMMENT:

!=====
=====
!\ENDSUBSPECIES: \CY(COC)COH\CCY(COC)OH\CY(CCOC)OH\CHOCOCH3
!=====
=====

!=====
=====
!\SUBSPECIES: \SC3H5OH
!=====
=====

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

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

!\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 WARNING: SAUDI ARAMCO MECH 1.3
(NO REFERENCE) !\COMMENT: FOR SC3H5OH, ASSUME THAT THE ALLYL HYDROGEN IS
ABSTRACTED AND THEN C2H3CHO+H ARE FORMED. USE RATE PRIMARY ALLYLIC. USED
RATE OF C3H6+R<=>C2H5-A+RH.

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SC3H5OH+OH=>C2H3CHO+H+H2O          3.100E+006      2.000
-298.0 !\AUTHOR: !\REF: TSANG 1991
!\COMMENT:
SC3H5OH+H=>C2H3CHO+H+H2          1.730E+005      2.500
2492.0 !\AUTHOR: !\REF: TSANG 1991
!\COMMENT:
SC3H5OH+O=>C2H3CHO+H+OH          1.750E+012      0.700
5884.0 !\AUTHOR: !\REF: TSANG 1991
!\COMMENT:
SC3H5OH+HO2=>C2H3CHO+H+H2O2      9.600E+003      2.600
13900.0 !\AUTHOR: !\REF: TSANG 1991
!\COMMENT:
SC3H5OH+CH3=>C2H3CHO+H+CH4        2.210E+000      3.500
5675.0 !\AUTHOR: !\REF: TSANG 1991
!\COMMENT:
SC3H5OH+CH3O2=>C2H3CHO+H+CH3O2H  9.600E+003      2.600
13900.0 !\AUTHOR: !\REF: USE HO2 ABSTRACTION RATE CONSTANT
!\COMMENT:
SC3H5OH+CH3O=>C2H3CHO+H+CH3OH     8.300E+010      0.000
2600.0 !\AUTHOR: !\REF: LITERATURE SOURCE UNKNOWN
!\COMMENT: USED SECONDARY ALKYL H RATE FOR N-ALKANE+CH3O, REDUCED EA BY
DIFFERENCE BETWEEN BD FOR SECONARY ALKYL AND PRIMARY ALLYLIC WITH F<=>.2:
0.2(98.4-88.2)<=>.2*10.2<=>2.0, EST. F IS LARGER THAN OH WHICH IS 0.1.
REDUCED A FACTOR BY 2.6 FOR TYING UP ROTOR (USED SCOTT AND WALKERS,
C&F2002 A-FACTORS TO GET 2.6)
SC3H5OH+HO2<=>C2H5CHO+HO2          1.490E+005      1.670
6810.0 !\AUTHOR: !\REF: DASILVA, BOZZELLI, CHEM. PHYS. LETT. 483 (2009)
25-29.          !\COMMENT: WARNING: THIS REFERENCE ALSO PRESENT--!\REF:
FROM PROPANOL, MAN ET AL. CNF2013:
SC3H5OH+HOCHO<=>C2H5CHO+HOCHO      2.810E-002      3.286
-4509.0 !\AUTHOR: !\REF: DASILVA, ANGEW. CHEM. 122 (2010) 7685-7687
!\COMMENT:

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

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

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

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TQC3H5OHI+O2<=>TQC3H5OHIO2          5.05E+12          -0.1          -695.45
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION          !\COMMENT: !\ ANALOGY TO O2+QOOH_2
TQC3H5OHIO2<=>TQC3H5OHIQ-I          2.56E+12          -0.13         34360
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION          !\COMMENT:
TQC3H5OHIQ-I<=>HO2CHO+CH3CHO+OH     5.819E+05          2.40          22790
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION          !\COMMENT:

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TQC3H5OHIQ-I<=>C3KET12+HO2 1.829E+10 0.790 15100
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
TQC3H5OHIO2<=>TQC3H5OHIQ-P 5.69E+08 7.80E-01 21850
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
TQC3H5OHIQ-P<=>C2H3COHOOH+HO2 1.83E+10 7.90E-01 15100
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
TQC3H5OHIQ-P<=>C2H3OOH+HOCHO+OH 5.38E+11 0.070 24800
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
TQC3H5OHIQ-P<=>COHOOHCY(COC)+OH 2.28E+08 1.29E+00 9890
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
TQC3H5OHIQ-P<=>OHCY(COCC)OOH+OH 4.58E+15 -1.08E+00 18440
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
C2H3COHOOH=>HOCHO+C2H3+OH 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:
COHOOHCY(COC)=>HOCHO+CH2CHO+OH 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:
OHCY(COCC)OOH=>HOCHO+CH2CHO+OH 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:

TQC3H5OHIO2<=>TQC3H5OHTO2 2.956E+09 0.04 16350
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
TQC3H5OHTO2<=>OHCOCOCH3+OH 1.2E+10 0.35 15700
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
OHCOCOCH3=>CO+CH3CHO+2OH 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:

IQC3H5OHPJ+O2<=>IQC3H5OHPJO2 9.35626E+11 0.1 -1072.98
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
IQC3H5OHPJO2<=>IQC3H5OTQ-I 4.13E+07 1.0 21070
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
IQC3H5OTQ-I=>OH+CH2O+CHOCH2OOH 1.20E+10 0.35 15700
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
CHOCH2OOH=>OH+CH2O+HCO 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:

IQC3H5OHPJO2<=>IQC3H5OHQ-SJ 8.204E10 0.13 19470
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:
IQC3H5OHQ-SJ<=>CHOCOCH2OOH+OH 1.2E+10 0.35 15700
!\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F. GOLDSMITH
CALCULATION !\COMMENT:

CHOCOHCH2OOH=>OH+CH2O+H+CHOCHO 1.59E+20 -1.5
42879.46 !\AUTHOR: !\ C ZHOU ESTIMATED SECOND-O2 ADDITION FROM F.
GOLDSMITH CALCULATION !\COMMENT:
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. !\COMMENT:

!=====
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!\ENDSUBSPECIES: \TQC3H5OHI
!=====
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!\REACTIONCLASS: \AROMATIC_GROWTH \A \N
\EA
!

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

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!\ENDSUBMECH: C3H6
!-----

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!\SUBMECH: \C3H4-A\C3H4-P
!\MECHCOMMENTS: KPS, 22/07/2015 REACTION CH3CHCHO+H2<=>C2H5CHO+H MOVED
FROM JOHN BUGLERS C5 MECHANISM TO THIS MECHANISM AS THIS IS FIRST
!\MECHCOMMENTS: INSTANCE OF CH3CHCHO APPEARING IN MASTER MECHANISM. THE
ABOVE CROSS REACTION DOES NOT MEAN THAT A C2H5CHO MECHANISM IS REQUIRED
TO SIMULATE THE
!\MECHCOMMENTS: PYROLYSIS OF C3H4-A/C3H4-P AS CH3CHCHO IS ONLY FORMED IN
THE OXIDATION OF C3H4-A/C3H4-P DUE TO AN OH ADDITION REACTION
!\MECHWARNINGS: THERE APPEAR TO BE SOME POORLY DOCUMENTED RATE CONSTANTS
IN THE C3H2 AND AROMATIC GROWTH SUB-MODULES. THE C3H3 RECOMBINATION RATE
CONSTANTS ARE A MESS. KPS 31/07/2015
!-----

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

C2H+CH3<=>C3H4-P 8.000E+013 0.000
0.0 !\AUTHOR: !\REF:PITZ ESTIMATE !\COMMENT: WARNING: PRESSURE-DEPENDENCE
IS PROBABLY COMPLETELY WRONG, PARTICULARLY AT LOW-PRESSURES, AS THIS
PATHWAY WAS NOT TREATED IN P-DEPENDENT CALC. RATE CONSTANT ONLY VALID AT
INFINITE PRESSURE

C3H4-A<=>C3H4-P 4.786E+048 -10.000
 88685.0 !\AUTHOR: !\REF: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO
 REFERENCE IN BASEMECH2907_C7.INP
 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: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO
 REFERENCE IN BASEMECH2907_C7.INP
 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: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO
 REFERENCE IN BASEMECH2907_C7.INP
 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: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO
 REFERENCE IN BASEMECH2907_C7.INP
 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: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO
 REFERENCE IN BASEMECH2907_C7.INP
 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: WARNING: SOURCE UNKNOWN !\COMMENT: WARNING: NO
 REFERENCE IN BASEMECH2907_C7.INP
 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 !\COMMENT:

!

!\REACTIONCLASS: \RH_R_ABSTRACTION A \N
 \EA

!

C3H4-P+O2<=>C3H3+HO2 3.000E+013 0.000
 42630.0 !\AUTHOR: !\REF: WARNING: SOURCE UNKNOWN !\COMMENT:
 WARNING: NO REFERENCE IN BASEMECH2907_C7.INP
 C3H4-P+O<=>C3H3+OH 7.650E+008 1.500
 8600.0 !\AUTHOR: !\REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST !\COMMENT:
 C3H4-P+H<=>C3H3+H2 3.572E+004 2.825
 4821.0 !\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S !\COMMENT:

C3H4-P+OH<=>C3H3+H2O	4.940E+006	2.027	
1059.6 !\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S			!\COMMENT:
C3H4-P+HO2<=>C3H3+H2O2	9.550E-002	4.170	
9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:
C3H4-P+CH3<=>C3H3+CH4	1.800E+012	0.000	
7700.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000			!\COMMENT:
C3H4-P+CH3O2<=>C3H3+CH3O2H	9.550E-002	4.170	
9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:
C3H4-P+C2H<=>C2H2+C3H3	1.000E+013	0.000	
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000			!\COMMENT:
C3H4-P+C2H3<=>C3H3+C2H4	1.000E+012	0.000	
7700.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:
C3H4-P+C3H5-A<=>C3H3+C3H6	3.000E+012	0.000	
7700.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:
C3H4-A+H<=>C3H3+H2	6.625E+003	3.095	
5522.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP			!\COMMENT:
C3H4-A+O2<=>C3H3+HO2	4.000E+013	0.000	
41320.0 !\AUTHOR: !\REF: ANALOGY WITH CURRAN 2006 ALKYL DECOMP			!\COMMENT:
C3H4-A+OH<=>C3H3+H2O	1.482E+005	2.492	
1807.2 !\AUTHOR: !\REF: ANALOGIES WITH C3H6 A AND S			!\COMMENT:
C3H4-A+CH3<=>C3H3+CH4	1.300E+012	0.000	
7700.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000			!\COMMENT:
C3H4-A+HO2<=>C3H3+H2O2	3.580E-002	4.170	
9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:
C3H4-A+CH3O2<=>C3H3+CH3O2H	7.161E-002	4.170	
9632.8 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:
C3H4-A+C3H5-A<=>C3H3+C3H6	2.000E+011	0.000	
7700.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).			!\COMMENT:

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

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C3H4-A+H<=>C3H4-P+H	2.440E+010	1.040	
2159.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438			!\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN BASEMECH2907_C7.INP
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, 9429-9438			!\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE
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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE
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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE
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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE
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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN BASEMECH2907_C7.INP
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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN BASEMECH2907_C7.INP
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, 9429-9438

!\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN

BASEMECH2907_C7.INP

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-

9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN

BASEMECH2907_C7.INP

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-T 8.850E+051 -13.040

12325.0 !\AUTHOR: !\REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-

9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN

BASEMECH2907_C7.INP

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-

9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN

BASEMECH2907_C7.INP

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-

9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN

BASEMECH2907_C7.INP

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-

9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN

BASEMECH2907_C7.INP

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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-
ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-
ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-
ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-
ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-
ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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 !\COMMENT: WARNING: BASEMECH2907 SUGGESTS DIFFERENT SOURCES FOR H-
ADDITION RATE CONSTANTS. THIS MAY BE A FUNDAMENTALLY WRONG APPROACH
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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN BASEMECH2907_C7.INP

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, 9429-9438 !\COMMENT: WARNING: UNSURE IF CORRECT REFERENCE BASED ON INFO. IN BASEMECH2907_C7.INP

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

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!\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
!\COMMENT:

C3H4-P+O<=>C2H4+CO 1.000E+013 0.000
2250.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!\COMMENT:

C3H4-P+O<=>C2H3+HCO 3.200E+012 0.000
2010.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
!\COMMENT:

C3H4-A+O<=>C2H4+CO 2.000E+007 1.800
1000.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000
!\COMMENT:

C3H4-A+O<=>C2H2+CH2O 3.000E-003 4.610
-4243.0 !\AUTHOR: !\REF:DAGAUT, P. ET AL., CST 71, 111(1990).
!\COMMENT:

!

!\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
!\COMMENT:

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

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
!\COMMENT:
C3H4-P+OH<=>SC3H4OH 2.360E+012 0.000
0.0 !\AUTHOR: !\REF: ESTIMATES C3 NUIG S.M.B FROM ATKINSON 1982 AND 1984
!\COMMENT:
PC3H4OH-2<=>CH3CHCHO 3.560E+010 0.880
23238.0 !\AUTHOR: !\REF: MATHEU ET AL. IJCK, 2003, 35, 95--119
!\COMMENT:
CH3CHCHO<=>C2H3CHO+H 4.164E+012 -0.020
32410.0 !\AUTHOR: !\REF: PELUCCHI ECM 2013
!\COMMENT:
CH3CHCHO<=>CH3CHCO+H 8.328E+012 -0.020
32410.0 !\AUTHOR: !\REF: PELUCCHI ECM 2013
!\COMMENT:

!\MISC
CH3CHCHO+H2<=>C2H5CHO+H 2.160E+005 2.380
18990.0 !\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: THIS
REACTION WAS MOVED FROM C5 MECHANISM WHEN MASTER MECHANISM WAS
CONSTRUCTED. SOURCE MUST BE IDENTIFIED.

!

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

!

!\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 !\COMMENT:

!=====
=====
!\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		
!\COMMENT:		
C3H3+HO2=>OH+CO+C2H3	8.000E+011	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
!\COMMENT:		
C3H3+HCO<=>C3H4-A+CO	2.500E+013	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
!\COMMENT:		
C3H3+HCO<=>C3H4-P+CO	2.500E+013	0.000
0.0 !\AUTHOR: !\REF:LASKIN ET AL. IJCK 32 589-614 2000		
!\COMMENT:		
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) !\COMMENT:		
C3H3+O2<=>CH2CO+HCO	1.700E+005	1.700
1500.0 !\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE		
!\COMMENT: WARNING: UNKNOWN SOURCE		
!C3H3+CH=C4H3-N+H	7.0E13	0.0
0.0 !\AUTHOR: !\REF: JAM		
!\COMMENT: WARNING: PRESUMABLY JAM STANDS FOR JAMES A. MILLER?		

!

!\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 3325-3346 !\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/		
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 3325-3346 !\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 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 3325-3346 !\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/		

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 3325-3346 !\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/
 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: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING:
 UNKNOWN SOURCE
 C2H+HCO<=>C2HCHO 1.000E+013 0.000
 0.0 !\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN
 SOURCE

!

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

!

C3H3+H<=>C3H2+H2 2.140E+005 2.520
 7453.0 !\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING:
 UNKNOWN SOURCE
 C3H3+H<=>C3H2(S)+H2 3.311E+013 0.195
 17579.0 !\AUTHOR: !\REF: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING:
 UNKNOWN SOURCE
 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: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING:
 UNKNOWN SOURCE
 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: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING:
 UNKNOWN SOURCE
 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: WARNING: UNKNOWN SOURCE !\COMMENT: WARNING: UNKNOWN
 SOURCE

!

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

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

!=====
=====

!\SUBSPECIES: \C3H2

!=====
=====

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

!=====
=====

!\ENDSUBSPECIES: \C3H2

!=====
=====

!

!\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 (WARNING: WHAT IS LITERATURE REFERENCE??) !\COMMENT: (WJP: SAME AS
I GOT FROM MILLER 2003). !\BELOW BILL SUGGEST ADD 0718, !\WJP: 10 ATM
RATE SAME AS MILLER AND KLIPPENSTIEN, C6H6 PE SURFACE, JPCA2003 THAT I
GOT
!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) (WARNING:
 WHAT IS LITERATURE REFERENCE??) !\COMMENT: WARNING: ARE THESE RATE
 COSNTANTS FROM A CONSISTENT SOURCE??
 !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) (WARNING:
 WHAT IS LITERATURE REFERENCE??) !\COMMENT: WARNING: ARE THESE RATE
 COSNTANTS FROM A CONSISTENT SOURCE??
 !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 !\COMMENT: WARNING: WHAT IS ORIGINAL
 LITERATURE SOURCE?
 !C3H3+C3H4-A<=> C6H6+H 1.400E+012 0.000
 9990.4 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT: WARNING: THIS IS A
 STRANGE REFERENCE-HAS HENRY WORKED ON AROMATIC CHEMISTRY?

!-----

!\ENDSUBMECH: C3H4-A/C3H4-P

!-----

!=====
 =====

!\SUBSPECIES: \CH3CHCO

!=====
 =====

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

CH3CHCO+OH<=>C2H5+CO2 1.730E+012 0.000
 -1010.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: METHYL KETENE
 CHEMISTRY NOT DETAILED.
 CH3CHCO+OH<=>SC2H4OH+CO 2.000E+012 0.000
 -1010.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: METHYL KETENE
 CHEMISTRY NOT DETAILED.
 CH3CHCO+H<=>C2H5+CO 4.400E+012 0.000
 1459.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: METHYL KETENE
 CHEMISTRY NOT DETAILED.
 CH3CHCO+O<=>CH3CHO+CO 3.200E+012 0.000
 -437.0 !\AUTHOR: !\REF:ESTIMATE !\COMMENT: WARNING: METHYL KETENE
 CHEMISTRY NOT DETAILED.

!=====
 =====

!\SUBSPECIES: \CH3CHCO

CH3COCH3+HO2<=>CH3COCH2+H2O2 1.700E+013 0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO ETHANE
!\COMMENT: WARNING: BAD ANALOGY?
CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H 1.700E+013 0.000
20460.0 !\AUTHOR: !\REF:ANALOGY TO ETHANE
!\COMMENT: WARNING: BAD ANALOGY?
CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21 1.000E+011 0.000
5000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE
!\COMMENT:

!

!\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
!\COMMENT: WARNING: DEFINITELY WRONG REFERENCE
CH3COCH2+CH3O2<=>CH3COCH2O+CH3O 1.205E+013 0.000
0.0 !\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
!\COMMENT: WARNING: DEFINITELY WRONG REFERENCE

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. !\COMMENT:

!

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

!

CH3COCH2+O2<=>CH3COCH2O2 1.200E+011 0.000
-1100.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:
CH2CO+CH3<=>CH3COCH2 1.760E+004 2.480
6130.0 !\AUTHOR: !\REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006
!\COMMENT:

CH2O+CH3COCH2O2<=>HCO+C3KET21 1.288E+011 0.000
9000.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:
HO2+CH3COCH2O2<=>C3KET21+O2 1.000E+012 0.000
0.0 !\AUTHOR: !\REF:WESTBROOK ESTIMATE !\COMMENT:

!

!\ENDSUBMECH: \CH3COCH3

!

!

!\SUBMECH: \C2H3CHO
!\MECHCOMMENTS:
!\MECHWARNINGS:


```

!-----
-----
!
!
! \REACTIONCLASS: \UNIMOL                \A                \N
! \EA
!
-----
C2H5+HCO<=>C2H5CHO                1.810E+013        0.000
0.0 !\AUTHOR: !\REF:CURRAN ESTIMATE !\COMMENT:
!
!
! \REACTIONCLASS: \RH_R_ABSTRACTION      \A                \N
! \EA
!
-----
C2H5CHO+H<=>C2H5CO+H2                4.000E+013        0.000
4200.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+H
!\COMMENT:
C2H5CHO+O<=>C2H5CO+OH                5.000E+012        0.000
1790.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+O
!\COMMENT:
C2H5CHO+OH<=>C2H5CO+H2O              2.690E+010        0.760
-340.0 !\AUTHOR: !\REF:ESTIMATE
!\COMMENT:
C2H5CHO+CH3<=>C2H5CO+CH4              2.608E+006        1.780
5911.0 !\AUTHOR: !\REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17
-2Q98 !\COMMENT:
C2H5CHO+HO2<=>C2H5CO+H2O2            2.800E+012        0.000
13600.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+HO2
!\COMMENT:
C2H5CHO+CH3O<=>C2H5CO+CH3OH           1.000E+012        0.000
3300.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+CH3O
!\COMMENT:
C2H5CHO+CH3O2<=>C2H5CO+CH3O2H        3.010E+012        0.000
11920.0 !\AUTHOR: !\REF:ANALOGY WITH CH3CHO+HO2
!\COMMENT:
C2H5CHO+C2H5<=>C2H5CO+C2H6           1.000E+012        0.000
8000.0 !\AUTHOR: !\REF:ACETALDEHYDE ANALOG
!\COMMENT:
C2H5CHO+C2H5O<=>C2H5CO+C2H5OH        6.026E+011        0.000
3300.0 !\AUTHOR: !\REF:ACETALDEHYDE ANALOG
!\COMMENT:
C2H5CHO+C2H5O2<=>C2H5CO+C2H5O2H      3.010E+012        0.000
11920.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2
!\COMMENT:
C2H5CHO+O2<=>C2H5CO+HO2              1.005E+013        0.000
40700.0 !\AUTHOR: !\REF:ESTIMATE
!\COMMENT:
C2H5CHO+CH3CO3<=>C2H5CO+CH3CO3H      3.010E+012        0.000
11920.0 !\AUTHOR: !\REF:BASED ON CH3CHO+HO2
!\COMMENT:
C2H5CHO+C2H3<=>C2H5CO+C2H4           1.700E+012        0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE
!\COMMENT:

```

C2H5CHO+NC3H7<=>C2H5CO+C3H8 1.700E+012 0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE
!\COMMENT:
C2H5CHO+IC3H7<=>C2H5CO+C3H8 1.700E+012 0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE
!\COMMENT:
C2H5CHO+C3H5-A<=>C2H5CO+C3H6 1.700E+012 0.000
8440.0 !\AUTHOR: !\REF:ANALOGY WITH ACETALDEHYDE
!\COMMENT:

!

!\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) !\COMMENT: WARNING: WOULD THIS BE BETTER DEFINED IN OTHER
DIRECTION?

!

!\ENDSUBMECH: C2H5CHO

!\END_KINETICS_MODULE: \C3

!

#####

#####

!

+++++++
! +
+
! + <=== TOLUENE
MECHANISM FROM YUAN 2015 ==> +
! +
+

!

!

!!!!!!! Submechanism of Toluene
!!!!!!!
!----- Unimolecular dissociation reactions -----

A1CH3(+M) = A1CH2+H(+M) 2.78E+15 0.17 9.1168E+04
! S.J. Klippenstein 2007 PCI

LOW/1.00E+98 -22.855 9.9882E+04/

TROE/6.547194E-02 1.511253E+01
 9.999996E+09 7.596123E+07/
 AlCH3(+M) = Al-+CH3(+M) 1.95E+27 -3.16
 1.07447E+05 ! S.J. Klippenstein 2007 PCI
 LOW/1.00E+98 -22.966
 1.2208E+05/
 TROE/7.054562E-01 9.999989E+09
 4.599180E+02 8.213938E+09/
 P-C6H4CH3+H(+M)=AlCH3(+M) 1.00E+14 0.0
 0.0 !Refer to Al-+H(+M)=Al(+M) 1997 Wang & Frenklach
 LOW / 6.6E+75 -16.30
 7000.0/
 TROE/ 1.0 0.1 584.9
 6113.0/
 H2/2.0/ H2O/6.0/ CH4/2.0/
 CO/1.5/ CO2/2.0/ C2H6/3.0/
 O-C6H4CH3+H(+M)=AlCH3(+M) 1.00E+14 0.0
 0.0 !Refer to Al-+H(+M)=Al(+M) 1997 Wang & Frenklach
 LOW / 6.6E+75 -16.30
 7000.0/
 TROE/ 1.0 0.1 584.9
 6113.0/
 H2/2.0/ H2O/6.0/ CH4/2.0/
 CO/1.5/ CO2/2.0/ C2H6/3.0/
 !----- H-Abstraction reactions-----

 AlCH3+H=AlCH2+H2 6.47E+00 3.98
 3384.0 !2006 Oehlschlaeger et al. J.Phys.Chem A 110,2006 9867-9873
 AlCH3+H=P-C6H4CH3+H2 2.346e+08 1.800
 16352.77 ! A*3/5 on Yuan coeff 3.910e+08 1.800 16352.77
 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898
 AlCH3+H=O-C6H4CH3+H2 1.564e+08 1.800
 16352.77 ! A*2/5 on Yuan coeff 3.910e+08 1.800 16352.77
 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898
 AlCH3+H=Al+CH3 3.90E+08 1.25
 2371 !Vasu, Davidson and Hanson 2010, the data is fitted base on
 the recommendation of Baulch and Ellis
 C3H3+C4H6=AlCH3+H 3.27E+6 1.28 -
 4611.0 !Laskin et al. IJCK 32 589-614 2000 6.53E+5 *5 TO interpret
 the AlCH3 formation in C5H6 flow reactor oxidation
 AlCH3+CH3=AlCH2+CH4 4.220e+14 0.000
 22256.21 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-
 1898
 AlCH3+CH3=P-C6H4CH3+CH4 1.074E-02 4.460
 13637.67 ! A*3/5 on Yuan coeff 1.790E-02 4.460 13637.67
 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898
 AlCH3+CH3=O-C6H4CH3+CH4 0.716E-02 4.460
 13637.67 ! A*2/5 on Yuan coeff 1.790E-02 4.460 13637.67
 !Narayanaswamy et al. Combustion and Flame 157 (2010) 1879-1898
 AlCH3+OH=P-HOAlCH3+H 1.884E+01 3.365
 4719.1 ! A*3/5 on Yuan coeff 3.14E+01 3.365 4719.1 !2006
 Seta et al.J. Phys. Chem. A 110 (2006) 5081-5090
 AlCH3+OH=O-HOAlCH3+H 1.256E+01 3.365
 4719.1 ! A*2/5 on Yuan coeff 3.14E+01 3.365 4719.1 !2006
 Seta et al.J. Phys. Chem. A 110 (2006) 5081-5090
 AlCH3+OH=AlOH+CH3 7.83E+02 2.88
 3221.8 !2006 Seta et al.J. Phys. Chem. A 110 (2006) 5081-5090

A1CH3+OH=A1CH2+H2O		1.77E+05	2.394	-
602.0	!2006 Seta et al.J. Phys. Chem. A 110 (2006) 5081-5090			
A1CH3+OH=P-C6H4CH3+H2O		0.816E+04	2.691	
620.0	! A*3/5 on Yuan coeff 1.36E+04 2.691 620.0 !2006 Seta et al.J. Phys. Chem. A 110 (2006) 5081-5090			
A1CH3+OH=O-C6H4CH3+H2O		0.544E+04	2.691	
620.0	! A*2/5 on Yuan coeff 1.36E+04 2.691 620.0 !2006 Seta et al.J. Phys. Chem. A 110 (2006) 5081-5090			
A1CH3+O=P-OA1CH3+H		0.996E+07	1.8	
3974.0	! A*3/5 on Yuan coeff 1.66E+07 1.8 3974.0			
!Refer to A1+O=A1O+H *5/6 2010, Taatjes et al.J. Phys. Chem. A 114 (2010) 3355-3370				
plog/ 0.1		0.996E+07	1.8	
3974.0/				
plog/ 1.0		0.996E+07	1.8	
3974.0/				
plog/ 10		0.996E+07	1.8	
3974.0/				
plog/ 50		1.776E+10	0.91	
6323.0/				
plog/ 500		0.66E+12	0.47	
8434.8/				
A1CH3+O=O-OA1CH3+H		0.664E+07	1.8	
3974.0	! A*2/5 on Yuan coeff 1.66E+07 1.8 3974.0			
!Refer to A1+O=A1O+H *5/6 2010, Taatjes et al.J. Phys. Chem. A 114 (2010) 3355-3370				
plog/ 0.1		0.664E+07	1.8	
3974.0/				
plog/ 1.0		0.664E+07	1.8	
3974.0/				
plog/ 10		0.664E+07	1.8	
3974.0/				
plog/ 50		1.184E+10	0.91	
6323.0/				
plog/ 500		0.44E+12	0.47	
8434.8/				
A1CH3+O=A1CH2+OH		8.020E+09	1.500	
8600.00	!Refer to CH4+O=CH3+OH GRI			
A1CH3+O=P-C6H4CH3+OH		1.20E+14	0.0	14700.0
!	A*3/5 on Yuan coeff 2.00E+14 0.0 14700.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49			
A1CH3+O=O-C6H4CH3+OH		0.80E+14	0.0	14700.0
!	A*2/5 on Yuan coeff 2.00E+14 0.0 14700.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49			
A1CH3+O=C5H5CH3+CO		6.02E+15	-0.49	
14993.0	!Refer to A1+O=C5H6+CO 2010 Taatjes et al.J. Phys. Chem. A 114 (2010) 3355-3370			
plog/ 0.1		7.22e+13	0.12	
11776.9/				
plog/ 1.0		6.02E+15	-0.49	
14993.0/				
plog/ 10.0		1.38E+38	-6.71	
34631.4/				
PLOG/ 50.0		1.57E+31	-4.73	
33568.4/				
PLOG/ 500		2.23E+56	-11.69	
55598.2/				

A1CH3+O=P-HOAlCH3 1.224E+23 -2.56
 14993.0 ! A*3/5 on Yuan coeff 2.04E+23 -2.56 14993.0 !Refer
 to Al+O=AlOH*5/6 Taatjes et al.J. Phys. Chem. A 114 (2010) 3355-3370
 plog/ 0.1 0.756E+29 -4.72
 13342.7/
 plog/ 1.0 1.224E+23 -2.56
 14993.0/
 plog/ 10.0 1.776E+24 -2.82
 21904.7/
 PLOG/ 50.0 2.922E+35 -5.89
 34534.1/
 PLOG/ 500 2.106E+31 -4.73
 38428.6/
 A1CH3+O=O-HOAlCH3 0.816E+23 -2.56
 14993.0 ! A*2/5 on Yuan coeff 2.04E+23 -2.56 14993.0 !Refer
 to Al+O=AlOH*5/6 Taatjes et al.J. Phys. Chem. A 114 (2010) 3355-3370
 plog/ 0.1 0.504E+29 -4.72
 13342.7/
 plog/ 1.0 0.816E+23 -2.56
 14993.0/
 plog/ 10.0 1.184E+24 -2.82
 21904.7/
 PLOG/ 50.0 1.948E+35 -5.89
 34534.1/
 PLOG/ 500 1.404E+31 -4.73
 38428.6/
 A1CH3+HO2=A1CH2+H2O2 3.97E+10 0.00
 14069.38 !D.L.Baulch et al. J. phys. chem. ref. data 23, 847-1033
 (1994)
 A1CH3+HCO=A1CH2+CH2O 3.77E+13 0.0
 23787.4 !Y. Sakai et al. PCI32 (2009) 411-418
 A1CH3+HO2=P-C6H4CH3+H2O2 2.166E+12 0.0
 30982.0 ! A*3/5 on Yuan coeff 3.61E+12 0.0 30982.0 !M.
 Altarawneh CNF 2010 Al+HO2 /4
 A1CH3+HO2=O-C6H4CH3+H2O2 1.444E+12 0.0
 30982.0 ! A*2/5 on Yuan coeff 3.61E+12 0.0 30982.0 !M.
 Altarawneh CNF 2010 Al+HO2 /4
 A1CH3+O2=A1CH2+HO2 2.18E+07 2.5
 46045.0 !Oehschlager et al.Combustion and Flame (2006)195-208
 A1CH3+O2=>P-OA1CH3+OH 2.4E+13 0.0
 44000.0 ! A*3/5 on Yuan coeff 4.0E+13 0.0 44000.0 !C.
 Saggese et al.Combustion and Flame 160 (2013) 1168-1190 4.00E+13
 A1CH3+O2=>O-OA1CH3+OH 1.6E+13 0.0
 44000.0 ! A*2/5 on Yuan coeff 4.0E+13 0.0 44000.0 !C.
 Saggese et al.Combustion and Flame 160 (2013) 1168-1190 4.00E+13
 A1CH3+O2=>P-C6H4CH3+HO2 1.02E+07 2.0
 51633.86 ! A*3/5 on Yuan coeff 1.704E+07 2.0 51633.86 !C.
 Saggese et al.Combustion and Flame 160 (2013) 1168-1190
 A1CH3+O2=>O-C6H4CH3+HO2 0.68E+07 2.0
 51633.86 ! A*2/5 on Yuan coeff 1.704E+07 2.0 51633.86 !C.
 Saggese et al.Combustion and Flame 160 (2013) 1168-1190
 A1CH3+C2H3=A1CH2+C2H4 3.98E+12 0.0
 8000.0 !1995 Zhang & Mckinnon
 A1CH3+C3H3=A1CH2+C3H4-P 1.6E+12 0.0
 15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49
 A1CH3+C5H5=A1CH2+C5H6 3.2E+12
 0.0 17100.0 !Bounaceur et al. 2005 Int J Chem Kinet
 37: 25-49 1.6E+12

A1CH3+A1-=A1CH2+A1	2.68e-01	3.95
877.06 !W. K. Metcalfe et al. Energy & Fuels 25 (2011) 4915-4936		
A1CH3+C3H5-A=A1CH2+C3H6	1.6E+12	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+C4H5-I=A1CH2+C4H6	1.6E+12	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+C4H5-N=A1CH2+C4H6	1.6E+12	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+A1O=A1CH2+A1OH	5.43E+12	0.00
20923.0 !Y. Sakai et al. PCI32 (2009) 411-418		
A1CH3+O-C6H4CH3=A1CH2+A1CH3	7.9E+13	0.0
12000.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+P-C6H4CH3=A1CH2+A1CH3	7.9E+13	0.0
12000.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+P-OA1CH3=A1CH2+P-HOA1CH3	1.6E+11	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+O-OA1CH3=A1CH2+O-HOA1CH3	1.6E+11	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+A1CH2OO=A1CH2+A1CH2OOH	2.0E+12	0.0
14000.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49*5		
A1CH3+A1CH2O=A1CH2+A1CH2OH	1.6E+11	0.0
11100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+P-HOA1CH2=A1CH2+P-HOA1CH3	1.6E+11	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
A1CH3+O-HOA1CH2=A1CH2+O-HOA1CH3	1.6E+11	0.0
15100.0 !Bounaceur et al. 2005 Int J Chem Kinet 37: 25-49		
nC4H3+C3H4-P=>P-C6H4CH3	2.40E+10	0.0
0.0 !C. Saggese et al. Combustion and Flame 160 (2013) 1168-1190		
P-C6H4CH3=>nC4H3+C3H4-P	4.50E+13	0.0
72500.0 !C. Saggese et al. Combustion and Flame 160 (2013) 1168-1190		
C3H3+O-C6H4CH3=>A2+H+H	5.00E+12	0.0
3000.0 !C. Saggese et al. Combustion and Flame 160 (2013) 1168-1190		
C4H5-N+O-C6H4CH3=>A2CH3-1+H+H	5.00E+13	0.0
1000.0 !C. Saggese et al. Combustion and Flame 160 (2013) 1168-1190		
!***** Decomposition of benzyl(A1CH2), fulvenallene(C7H6) and fulvenallenyl(C7H5) *****		
A1CH2=>C7H6+H	4.47E+129	-32.57
162410.0 !M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011)		
21308-21318		
PLOG / 0.013	4.47E+129	-32.57
162410.0/		
PLOG / 0.130	1.29E+123	-30.34
163830.0/		
PLOG / 1.000	2.95E+97	-22.95
148280.0/ !close to the experimental measured results of Ronald k. hanson at 1.5 bar		
PLOG/ 1.500	8.20E+14	0.00E+00
8.07E+04/		
PLOG / 10.000	1.26E+39	-6.76
99710.0/		
PLOG / 50.000	1.44E+13	0.453
76300/ !HPL		
C7H6+H=>A1CH2	8.80E+8	1.2 -
2020 !C. Cavallotti, M. Derudi, R. Rota, PCI 32 (2009) 115-121.		

A1CH2=O-C6H4+CH3		2.04E+135	-34.08
169130	!M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011) 21308-		
21318			
PLOG/ 0.013		2.04E+135	-34.08
169130/			
PLOG/ 0.130		6.46E+112	-27.50
155360/			
PLOG/ 1.00		5.50E+89	-20.82
141680/			
PLOG/ 10.00		5.13E+55	-11.23
116580/			
A1CH2+H=A1-+CH3		4.50E+58	-11.9
51860	!S. J. Klippenstein, L. B. Harding, Y. Georgievskii, PC31		
(2007) 221-229.			
PLOG/ 0.0395		4.50E+58	-11.9
51860/			
PLOG/ 0.132		2.03E+64	-13.37
59520/			
PLOG/ 1.000		5.83E+67	-14.15
68330/			
PLOG/ 10.00		8.85E+68	-14.23
78410/			
C7H6=cC5H4+C2H2		1.26E+130	-32.19
173970.0	!D. Polino, C. Cavallotti, JPC A 115 (2011) 10281-10289.		
PLOG / 0.100		2.34E+135	-33.58
179460/			
PLOG / 1.000		3.02E+124	-30.18
176460/			
PLOG / 10.000		4.27E+129	-31.11
191020/			
C7H6=C7H5+H		1.02E+116	-28.46
157860.0	!D. Polino, C. Cavallotti, JPC A 115 (2011) 10281-10289.		
PLOG / 0.100		1.02E+116	-28.46
157860.0/			
PLOG / 1.000		4.90E+66	-14.64
119550.0/			
PLOG / 10.000		1.17E+27	-3.54
89150.0/			
C5H5+C2H2=>C7H6+H		1.29E+21	-2.38
32400	!G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114		
(2010) 2275-2283.			
PLOG/ 0.0001		1.29E+21	-2.38
32400/			
PLOG/ 0.001		3.37E+12	0.22
31060/			
PLOG/ 0.01		7.07E+01	3.42
28740/			
PLOG/ 0.1		1.58E-01	4.18
29670/			
PLOG/ 1.0		6.96E-05	5.17
30930/			
PLOG/ 10.0		2.37E-06	5.60
33540/			
PLOG/ 100		1.15E-44	17.07
22460/			
PLOG/ 1000		8.31E-37	14.56
29740/			

C7H6+H=>C5H5+C2H2	6.81E+24	-3.04
14950 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114 (2010) 2275-2283.		
PLOG/ 0.0001	6.81E+24	-3.04
14950/		
PLOG/ 0.001	6.87E+16	-0.62
13700/		
PLOG/ 0.01	5.39E+06	2.41
11550/		
PLOG/ 0.1	3.65E+01	3.93
11460/		
PLOG/ 1.0	1.22E-06	6.15
11040/		
PLOG/ 10.0	2.65E-15	8.75
10810/		
PLOG/ 100	8.55E-21	10.35
12590/		
PLOG/ 1000	2.05E-30	13.09
13020/		
C7H6+H=>eC7H6+H	2.92E+20	-1.70
17550 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114 (2010) 2275-2283.		
PLOG/ 0.0001	2.92E+20	-1.70
17550/		
PLOG/ 0.001	1.16E+14	0.26
16930/		
PLOG/ 0.01	2.28E+11	1.07
17630/		
PLOG/ 0.1	2.26E+01	4.05
15570/		
PLOG/ 1.0	9.40E-04	5.34
16040/		
PLOG/ 10.0	6.73E-07	6.25
17560/		
PLOG/ 100	2.72E-29	12.88
11510/		
PLOG/ 1000	9.14E-39	15.50
10250/		
eC7H6+H=>C7H6+H	3.61E+19	-1.65
14940 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114 (2010) 2275-2283.		
PLOG/ 0.0001	3.61E+19	-1.65
14940/		
PLOG/ 0.001	1.12E+13	0.34
14280/		
PLOG/ 0.01	8.63E+03	3.08
12530/		
PLOG/ 0.1	5.66E-07	6.12
10370/		
PLOG/ 1.0	2.29E-15	8.61
9260/		
PLOG/ 10.0	2.00E-22	10.69
9170/		
PLOG/ 100	8.56E-31	13.10
8670/		
PLOG/ 1000	2.41E-40	15.74
7380/		

C5H5+C2H2=>eC7H6+H	5.58E+11	-0.1
34720 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114		
(2010) 2275-2283.		
PLOG/ 0.0001	5.58E+11	-0.1
34720/		
PLOG/ 0.001	4.55E+07	1.52
24370/		
PLOG/ 0.01	5.75E+06	1.79
24100/		
PLOG/ 0.1	4.52E+07	1.54
24710/		
PLOG/ 1.0	8.17E+11	0.33
27430/		
PLOG/ 10.0	4.40E+15	-0.68
30890/		
PLOG/ 100	7.24E+15	-0.61
34040/		
PLOG/ 1000	1.88E+07	2.07
34340/		
eC7H6+H=>C5H5+C2H2	3.16E+11	0.59
4330 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114		
(2010) 2275-2283.		
PLOG/ 0.0001	3.16E+11	0.59
4330/		
PLOG/ 0.001	3.84E+11	0.57
4460/		
PLOG/ 0.01	1.94E+11	0.66
4410/		
PLOG/ 0.1	2.60E+12	0.34
5110/		
PLOG/ 1.0	5.81E+16	-0.9
7870/		
PLOG/ 10.0	3.09E+20	-1.91
11330/		
PLOG/ 100	4.44E+20	-1.82
14450/		
PLOG/ 1000	1.01E+12	0.89
14730/		
C5H5+C2H2=>cC7H7	8.28E+80	-22.15
31790 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114		
(2010) 2275-2283.		
PLOG/ 0.0001	8.28E+80	-22.15
31790/		
PLOG/ 0.001	3.61E+73	-19.65
30230/		
PLOG/ 0.01	1.31E+64	-16.55
27790/		
PLOG/ 0.1	3.69E+53	-13.14
24810/		
PLOG/ 1.0	1.27E+43	-9.80
21720/		
PLOG/ 10.0	1.07E+34	-6.90
19000/		
PLOG/ 100	1.20E+27	-4.67
16940/		
PLOG/ 1000	1.09E+23	-3.37
15770/		

eC7H6+H=>cC7H7	3.66E+76	-21.98	
17190 !G. da Silva, J. A. Cole, J. W. Bozzelli, J. Phys. Chem. A 114 (2010) 2275-2283.			
PLOG/ 0.0001	3.66E+76	-21.98	
17190/			
PLOG/ 0.001	8.21E+83	-23.57	
21620/			
PLOG/ 0.01	1.67E+81	-22.22	
22630/			
PLOG/ 0.1	4.52E+70	-18.60	
20620/			
PLOG/ 1.0	1.77E+80	-15.06	
18970/			
PLOG/ 10.0	2.17E+50	-11.73	
17880/			
PLOG/ 100	8.74E+38	-8.02	
16230/			
PLOG/ 1000	8.23E+26	-4.22	
14060/			
cC7H7+C2H2=C9H8+H	6.6E+11	0.0	
20031.0 !S. Fascella, C. Cavallotti, R. Rota, S. Carra, J. Phys. Chem. A 109(2005) 7546-7557.			
	REV/ 4.20E+14	0.0	
54218.0/			
cC7H7+H=A1CH2+H	2.20E+63	-13.0	
58627.9 !S. Fascella, C. Cavallotti, R. Rota, S. Carra, J. Phys. Chem. A 109(2005) 7546-7557.			
cC7H7+H=A1-+CH3	1.20E+61	-12.4	
57002.7 !S. Fascella, C. Cavallotti, R. Rota, S. Carra, J. Phys. Chem. A 109(2005) 7546-7557.			
eC7H6+H=C7H5+H2	1.08E+08	1.812	
4491.0 !G. da Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048.			
eC7H6+CH3=C7H5+CH4	6.90E+03	2.730	
5246.0 !G. da Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048.			
C7H6+H=C7H5+H2	1.90E+08	1.847	
4965.0 !G. da Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048.			
C7H6+OH=C7H5+H2O	1.20E+05	2.621	-
515.0 !G. da Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048.			
C7H6+CH3=C7H5+CH4	1.87E+04	2.724	
6008.0 !G. da Silva, J. W. Bozzelli, J. Phys. Chem. A 113 (2009) 12045-12048.			
C7H5=C4H2+C3H3	8.71E+92	-23.08	
117070.0 !M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011) 21308-21318			
PLOG / 0.013	8.71E+92	-23.08	
117070.0/			
PLOG / 0.130	1.82E+102	-25.22	
130330.0/			
PLOG / 1.000	8.51E+82	-19.18	
125340.0/			
PLOG / 10.000	2.40E+56	-11.65	
106750.0/			
nC4H3+C3H3=C7H6	1.00E+13	0.00	
0.0 !Y. Sakai et al. PCI32 (2009) 411-418			

C7H5=C5H3+C2H2		3.16E+83	-20.81	
109410.0	!M. Derudi, D. Polino, C. Cavallotti, PCCP, 13 (2011)			
21308-21318				
PLOG / 0.013		3.16E+83	-20.81	
109410.0/				
PLOG / 0.130		7.59E+102	-25.66	
132390.0/				
PLOG / 1.000		2.82E+90	-21.38	
135620.0/				
PLOG / 10.000		4.37E+90	-21.04	
143990.0/				
O-C6H4CH3=A1CH2		3.09E+73	-18.22	
69670	!Enoch Dames & Hai Wang 2013 PCI34			
PLOG/ 0.1		3.09E+73	-18.22	
69670/				
PLOG/ 1.0		2.91E+59	-13.86	
64518/				
PLOG/ 10.0		6.76E+40	-8.54	
54069/				
PLOG/ 50.0		3.66E+26	-3.98	
49795/				
O-C6H4CH3+H=A1CH2+H		1.0E+13	0.0	
0.0	!Bounaceur et al 2005			
O-C6H4CH3=o-C6H4+CH3		6.11E+45	-8.857	
94350.6	!1997 Madden et al. RRKM A1--o-C6H4+H			
PLOG / 0.500		6.11E+45	-8.857	
94350.6/				
PLOG / 1.000		8.00E+41	-7.72	
92300.3/				
PLOG / 10.000		1.66E+30	-4.318	
85756.9/				
O-C6H4CH3=P-C6H4CH3		1.42e14	0.0	65042
	! Nicolas Delort from Enoch Dames & Hai Wang 2013 PCI34			
A1CH2=C5H5+C2H2		4.08E+134	-34.08	
169130	!EST this work 5 times slower than the reaction A1CH2=o-C6H4+ch3			
PLOG/ 0.013		4.08E+134	-34.08	
169130/				
PLOG/ 0.130		1.29E+112	-27.50	
155360/				
PLOG/ 1.00		1.10E+89	-20.82	
141680/				
PLOG/ 10.00		1.03E+55	-11.23	
116580/				
PLOG/ 50.000		1.44E+13	0.453	
76300/				
A1CH2=cC7H7		1.12E+128	-32.57	
162410.0	!Est this work			
PLOG / 0.013		1.12E+128	-32.57	
162410.0/				
PLOG / 0.130		3.23E+121	-30.34	
163830.0/				
PLOG / 1.000		7.38E+95	-22.95	
148280.0/				
PLOG/ 1.500		2.05E+13	0.00E+00	
8.07E+04/				
PLOG / 10.000		3.15E+37	-6.76	
99710.0 /				

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PLOG / 50.000          3.60E+11    0.453  76300
/
!-----
A1CH2+OH( +M)=A1CH2OH(+M)          6.300E+13    0.000
0.0      !refer to GRI CH3+OH( +M)=CH3OH(+M)
          LOW / 2.700E+38  -6.300
3100.0/
          TROE/ 0.2105 83.5 5398.00
8370.0/
          H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/
CO2/2.0/ C2H6/3.0/
A1CH2+O=A1CH2O          2.280e+14    0.000
0.0      !K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
A1CH2+HO2=A1CH2O+OH          1.19E+09    1.03    -
2250.0    !800-2000 K da Silva et al. PCI32(2009)! 1.19E+9
A1CH2OO(+M)=A1CH2+O2(+M)          4.17E+36    -7.07
3.22E+04    !Murakami et al. 2007 J. Phys. Chem. A 2007, 111, 13200-
13208
          LOW / 1.797E-06  5.40  -
7.63E+03/
          TROE /6.114198E-01  9.999806E+09
1.037924E+00  1.786062E+09/

!Nicolas Delort - ranges of TCHEB and PCHEB from Yuan anisole (2019)
A1CH2+O2(+M)=A1CHO+OH( +M)          1.00E+00    0.00
0.0      !Murakami2007
          TCHEB/ 290 4000/  PCHEB/ 0.0132 132./
          CHEB/ 8 4 /
          CHEB/3.3275E+00 -2.0397E-02 -7.4256E-03
-1.6060E-03  4.6378E+00/
          CHEB/ 3.0525E-02  1.2498E-02  1.5728E-
03 -5.7846E-01 -1.9992E-02 -4.8833E-03/
          CHEB/-6.9279E-04 -4.6568E-01  4.2674E-
03  2.3797E-03  8.6549E-05 -3.0958E-01/
          CHEB/ 1.0799E-03  8.5564E-04  9.5221E-
04 -1.5915E-01 -4.2760E-04 -4.5489E-04/
          CHEB/-1.4374E-04 -6.6780E-02 -7.0974E-
04 -3.7832E-04 -1.1982E-04 -3.5604E-03/
          CHEB/ 8.9127E-04  4.8533E-04  2.0474E-
04/
A1CH2+O2(+M)=A1O+CH2O( +M)          1.00E+00    0.00    0.0
!Murakami2007
          TCHEB/ 290 4000/  PCHEB/ 0.0132 132./
          CHEB/ 8 4 /
          CHEB/3.0394E+00 -2.0427E-02 -7.4206E-03
-1.5642E-03  4.6629E+00/
          CHEB/ 3.0663E-02  1.2467E-02  1.5536E-
03 -5.7691E-01 -2.0237E-02 -4.9039E-03/
          CHEB/-6.9407E-04 -4.7028E-01  4.4329E-
03  2.3943E-03  8.6199E-05 -3.1107E-01/
          CHEB/ 1.0074E-03  9.0046E-04  9.9645E-
04 -1.5780E-01 -4.6735E-04 -4.8802E-04/
          CHEB/-1.2891E-04 -6.7900E-02 -4.9726E-
04 -3.2486E-04 -1.8352E-04 -2.0165E-03/
          CHEB/ 7.1428E-04  4.2833E-04  2.5845E-
04/

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A1CH2+O2=A1CH2O+O          6.3E12      0.0      40.0E3
!Brezynsky84
A1CH2OO=A1CHO+OH          1.4E+10      1.0
37.5E3          !Herbinet et al. 2013 PCI
                Plog/1.0          1.4E+09      1.0      37.5E3/
!
                Plog/10.0         1.6E+10      1.0      37.5E3/
!
                Plog/50.0         3.2E+10      1.0      37.5E3/
!
!4.20 test mais pas influence sur guaiacol -> benzaldehyde
!A1CH2OO=A1O+CH2O          +1.0000000E+000 +0.0000000E+000 +0.0000000E+000
!\AUTHOR: !\REF: !\COMMENT:
!PLOG /          +1.0000000E-001 +9.8190000E+059 -1.6131000E+001
+4.2369180E+004 /
!PLOG /          +1.0000000E+000 +2.8250000E+053 -1.3630000E+001
+4.1916640E+004 /
!PLOG /          +1.0000000E+001 +1.4940000E+042 -9.7850000E+000
+3.9545940E+004 /
!PLOG /          +1.0000000E+002 +3.5470000E+032 -6.5880000E+000
+3.7139520E+004 /

A1CH2OO+H=A1CH2O+OH          3.80E14
-0.19  1.89E3          !da silva J Chem Theory Comput 2009
A1CH2OO+H=A1CH2OOH          4.35e60          -15.92
11.40E3          !da silva J Chem Theory Comput 2009
A1CH2OO+H=A1CH2+HO2          1.96E4          2.47
1.43E3          !da silva J Chem Theory Comput 2009
A1CH2OO+HO2=A1CH2OOH+O2          2.0E11      0.0      -
1.3E3          !Herbinet et al. 2013 PCI
2A1CH2OO=A1CH2OH+A1CHO+O2          1.4E10      0.0      -725.0
!Herbinet et al. 2013 PCI
A1CH2OO+A1CH2OO=2A1CH2O+O2          6.3E10      0.0      -725.0
!Herbinet et al. 2013 PCI
A1CH2OOH=A1CH2O+OH          1.50E+16      0.00      42000.0
!Bounaceur et al.IJCK 37, 25-49, 2005
A1CH2O+H(+M) = A1CH2OH(+M)          2.430e+12      0.520      50.19
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
                LOW / 4.660e+41      -7.440      14079.83
/
                TROE/ 0.7  100.00  90000.00
10000.00 /
                H2/2.00/ H2O/12.00/ CO2/3.60/ CO/1.75/ AR/0.70/
CH4/2.00/ C2H6/3.00/
A1CH2OH+H=A1CH2O+H2          4.200E+06      2.100      4870.94
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
A1CH2OH+O=A1CH2O+OH          1.300E+05      2.500      5000.00
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
A1CH2OH+OH=A1CH2O+H2O          6.300E+06      2.000      1500.96
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
A1CH2OH+CH3=A1CH2O+CH4          1.000E+07      1.500      9940.25
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
A1-+CH2O=A1+HCO          8.550E+04      2.190      38.24
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157
!Nicolas Delort - in anisole mech!A1CH2O=A1CHO+H
3.04E+32      -6.665      21880          !G. da silva and J W. Bozzelli 2009 jpc
113
! PLOG/ 0.01          3.04E+32      -6.665      21880/

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! PLOG/ 0.1	6.13E+31	-6.261	22360/
! PLOG/ 1.0	5.26E+28	-5.081	22250/
! PLOG/ 10.0	1.68E+22	-2.901	20760/
! PLOG/ 100	2.44E+17	-1.307	19540/
!Nicolas Delort -in anisole mech!A1CH2O=A1-+CH2O			
4.59E+43	-9.513	39050	!G. da silva and J W. bozzelli 2009 jpc
113			
! PLOG/ 0.01	4.59E+43	-9.513	39050/
! PLOG/ 0.1	2.88E+38	-7.786	37770/
! PLOG/ 1.0	7.21E+33	-6.210	36850/
! PLOG/ 10.0	1.32E+27	-4.009	35070/
! PLOG/ 100	1.08E+21	-2.057	33310/
A1CH2O=A1+HCO	2.57E+31	-6.215	25760
!G. da silva and J W. bozzelli 2009 jpc 113			
PLOG/ 0.01	2.57E+31	-6.215	25760/
PLOG/ 0.1	5.27E+31	-6.153	26880/
PLOG/ 1.0	2.37E+32	-6.095	28810/
PLOG/ 10.0	3.82E+31	-5.663	29840/
PLOG/ 100	2.04E+28	-4.576	29200/
A1CH2O+H=A1CHO+H2	1.330E+13	0.000	0.00
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157			
A1CH2O+O=A1CHO+OH	6.670E+12	0.000	0.00
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157			
A1CH2O+OH=A1CHO+H2O	3.330E+12	0.000	0.00
!K. Narayanaswamy, G. Blanquart, H. Pitsch 2010 cnf 157			
A1CH2O+O2=A1CHO+HO2	6.0E+10	0.0	1600.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO=A1CO+H	4.0E+15	0.0	83700.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1-+HCO=A1CHO	5.00E+12	0.00	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+O2=A1CO+HO2	7.0E+11	0.0	39500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+H=A1+HCO	5.8E+13	0.0	8100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+H=A1CO+H2	4.0E+13	0.0	3200.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+O=A1CO+OH	6.0E+12	0.0	1800.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+OH=A1CO+H2O	7.8E+12	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+HO2=A1CO+H2O2	3.0E+12	0.0	11000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+CH3=A1CO+CH4	2.0E-6	5.6	1500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+C2H5=A1CO+C2H6	1.3E+12	0.0	7500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+C3H5-A=A1CO+C3H6	1.3E+12	0.0	
11500.0	!Bounaceur et al.IJCK 37, 25-49, 2005		
A1CHO+C4H5-I=A1CO+C4H6	1.3E+12	0.0	
11500.0	!Bounaceur et al.IJCK 37, 25-49, 2005		
A1CHO+C4H5-N=A1CO+C4H6	1.3E+12	0.0	7500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+C5H5=A1CO+C5H6	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+A1-=A1CO+A1	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			

A1CHO+A1CH2=A1CO+A1CH3	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+A1O=A1CO+A1OH	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+P-OA1CH3=A1CO+P-HOA1CH3	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+O-OA1CH3=A1CO+O-HOA1CH3	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+P-HOA1CH2=A1CO+P-HOA1CH3	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CHO+O-HOA1CH2=A1CO+O-HOA1CH3	1.3E+11	0.0	11500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CO=A1+CO	4.0E+14	0.0	29500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			

!----- Reactions of cresoxyl radical(oc6h4ch3) and cresol (hoc6h4ch3) -----

!C6H4CH3+O2=OA1CH3+O	2.44E+18	-1.60	5040.0
!da Silva2007			
! PLOG / 0.0001	2.44E+18	-1.60	
5040.0/			
! PLOG / 0.001	2.45E+18	-1.60	
5040.0/			
! PLOG / 0.01	2.62E+18	-1.61	
5060.0/			
! PLOG / 0.1	4.99E+18	-1.68	
5320.0/			
! PLOG / 1.0	9.18E+20	-2.30	
7370.0/			
! PLOG / 10.0	7.27E+29	-4.72	
15600.0/			
! PLOG / 100.0	1.52E+43	-8.30	
29100.0/			
! PLOG /1000.0	2.03E+48	-9.55	
38300.0/			

P-C6H4CH3+O2=P-OA1CH3+O			
+9.1800000E+020 -2.3000000E+000 +7.3700000E+003 ! Nicolas Delort - from			
Kukkadapu model - AUTHORS: SILVA ET AL. JPC, 2007, 111:8663-8676			
PLOG / 1.00E-02	1.05E+18	-1.61E+00	5.06E+03 /
PLOG / 1.00E-01	2.00E+18	-1.68E+00	5.32E+03 /
PLOG / 1.00E+00	3.67E+20	-2.30E+00	7.37E+03 /
PLOG / 1.00E+01	2.91E+29	-4.72E+00	1.56E+04 /
PLOG / 1.00E+02	6.08E+42	-8.30E+00	2.91E+04 /

O-C6H4CH3+O2=O-OA1CH3+O			
+9.1800000E+020 -2.3000000E+000 +7.3700000E+003 ! Nicolas Delort - from			
Kukkadapu model - AUTHORS: SILVA ET AL. JPC, 2007, 111:8663-8676			
PLOG / 1.00E-02	1.05E+18	-1.61E+00	5.06E+03 /
PLOG / 1.00E-01	2.00E+18	-1.68E+00	5.32E+03 /
PLOG / 1.00E+00	3.67E+20	-2.30E+00	7.37E+03 /
PLOG / 1.00E+01	2.91E+29	-4.72E+00	1.56E+04 /
PLOG / 1.00E+02	6.08E+42	-8.30E+00	2.91E+04 /

O-C6H4CH3+O2=O-OC6H4CH2+OH	8.725E+08	0.64	-
4200.0			
!da Silva2007,*4			
PLOG / 0.0001	8.725E+08	0.64	-4200.0/
PLOG / 0.001	8.70E+08	0.65	-4200.0/
PLOG / 0.01	8.70E+08	0.65	-4200.0/

PLOG / 0.1	1.245E+09	0.60	-4060.0/
PLOG / 1.0	9.25E+11	-0.18	-1520.0/
PLOG / 10.0	4.35E+23	-3.36	8980.0/
PLOG / 100.0	9.30E+39	-7.77	24940.0/
PLOG /1000.0	1.435E+47	-9.58	35890.0/
O-OC6H4CH2=A1+CO 67160.0 !Dorrestijn1997	6.31E+14	0.0	
P-C6H4CH3+O=P-OA1CH3 !Bounaceur et alf-IJCK 37, 25-49, 2005	1.0E+14	0.0	0.0
O-C6H4CH3+O=O-OA1CH3 !Bounaceur et alf-IJCK 37, 25-49, 2005	1.0E+14	0.0	0.0
P-C6H4CH3+OH=P-HOA1CH3 !Bounaceur et alf-IJCK 37, 25-49, 2005	1.0E+13	0.0	0.0
O-C6H4CH3+OH=O-HOA1CH3 !Bounaceur et alf-IJCK 37, 25-49, 2005	1.0E+13	0.0	0.0
P-C6H4CH3+HO2=P-OA1CH3+OH !Bounaceur et alf-IJCK 37, 25-49, 2005	5.0E+12	0.0	0.0
O-C6H4CH3+HO2=O-OA1CH3+OH !Bounaceur et alf-IJCK 37, 25-49, 2005	5.0E+12	0.0	0.0
P-C6H4CH3+O2=O-C6H4O2+CH3 9000.0 !reference? 3.0E+13 20131028	2.0E+14	0.0	
O-C6H4CH3+O2=O-C6H4O2+CH3 9000.0 !reference? 3.0E+13 20131028	2.0E+14	0.0	
P-OA1CH3=CO+C5H4CH3 68564 !refer to A1O=CO+C5H5,2011 You et al. J. Phys. Chem. A 2011, 115, 14184-14190	5.71E+59	-14.4	
PLOG / 0.0100 68564/ !The rate of You is similar to that of Carstensen	5.71E+59	-14.4	
PLOG / 0.1000 81843/	1.65E+71	-17.2	
PLOG / 1.0000 88985/	1.32E+74	-17.6	
PLOG / 10.000 89456/	4.41E+68	-15.8	
PLOG /100.0000 98611/	3.77E+71	-16.18	
!HPL	1.25E+06	2.25	50194
O-OA1CH3=CO+C5H4CH3 68564 !refer to A1O=CO+C5H5,2011 You et al. J. Phys. Chem. A 2011, 115, 14184-14190	5.71E+59	-14.4	
PLOG / 0.0100 68564/ !The rate of You is similar to that of Carstensen	5.71E+59	-14.4	
PLOG / 0.1000 81843/	1.65E+71	-17.2	
PLOG / 1.0000 88985/	1.32E+74	-17.6	
PLOG / 10.000 89456/	4.41E+68	-15.8	
PLOG /100.0000 98611/	3.77E+71	-16.18	
!HPL	1.25E+06	2.25	50194
!---para---			
!P-OA1CH3+H(+M)=P-HOA1CH3(+M) !refer to A1O+H(+M)=A1OH(+M) 1996 Davis et al 20140221	0.50E+14	0.0	0.0
	2.5 to 0.5	1.0 to 0.2	

!	LOW / 0.20E+94	-21.84	13880.0/
!	TROE/ 0.043	340.0	60000.0 5900.0/
!	H2/2.0/	H2O/6.0/	CH4/2.0/ CO/1.5/
CO2/2.0/			
P-HOAlCH3+O2=P-OAlCH3+HO2	1.0E+12	0.0	38900.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+O2=P-HOAlCH2+HO2	2.1E+12	0.0	39700.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+H=A1OH+CH3	5.8E+13	0.0	8100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+H=P-OAlCH3+H2	1.2E+14	0.0	12400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+O=P-OAlCH3+OH	1.3E+13	0.0	2900.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+OH=P-OAlCH3+H2O	1.4E+8	1.4	-960.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+HO2=P-OAlCH3+H2O2	1.0E+12	0.0	10000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+CH3=P-OAlCH3+CH4	1.8E+11	0.0	7700.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+A1==P-OAlCH3+A1	4.9E+12	0.0	4400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C5H5=P-OAlCH3+C5H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C3H5-A=P-OAlCH3+C3H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C4H5-I=P-OAlCH3+C4H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C4H5-N=P-OAlCH3+C4H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+A1O=P-OAlCH3+A1OH	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+H=P-HOAlCH2+H2	1.2E+14	0.0	8400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+O=P-HOAlCH2+OH	6.3E+11	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+OH=P-HOAlCH2+H2O	5.2E+9	1.0	870.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+HO2=P-HOAlCH2+H2O2	4.0E+11	0.0	14000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+CH3=P-HOAlCH2+CH4	1.6E+12	0.0	11100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C3H5-A=P-HOAlCH2+C3H6	1.6E+12	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C3H3=P-HOAlCH2+C3H4-P	1.6E+12	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C4H5-I=P-HOAlCH2+C4H6	1.6E+12	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C4H5-N=P-HOAlCH2+C4H6	1.6E+12	0.0	11100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+C5H5=P-HOAlCH2+C5H6	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+A1==P-HOAlCH2+A1	7.9E+13	0.0	12000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+A1O=P-HOAlCH2+A1OH	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+P-C6H4CH3=P-OAlCH3+A1CH3	7.9E+13	0.0	
12000.0 !Bounaceur et al.IJCK 37, 25-49, 2005			

P-HOAlCH3+O-C6H4CH3=P-OAlCH3+A1CH3	7.9E+13	0.0	
12000.0 !Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+P-OAlCH3=P-HOAlCH2+P-HOAlCH3	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+O-OAlCH3=P-HOAlCH2+O-HOAlCH3	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+A1CH2OO=P-HOAlCH2+A1CH2OOH	4.0E+11	0.0	14000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH3+A1CH2O=P-HOAlCH2+A1CH2OH	1.6E+11	0.0	11100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH2+O2=HOAlCH2OO	4.6E+11	0.0	-380.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH2+O2=HOAlCH2O+O	6.3E+12	0.0	40000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH2+H=P-HOAlCH3	1.0E+14	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH2+HO2=HOAlCH2OOH	5.0E+12	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
P-HOAlCH2+CH3=A1OH+C2H4	5.0E+12	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
!---ortho---			
O-OAlCH3+H(+M)=O-HOAlCH3(+M)	0.50E+14	0.0	0.0
!refer to A1O+H(+M)=A1OH(+M) 1996 Davis et al	2.5 to 0.5	1.0 to 0.2	
20140221			
	LOW / 0.20E+94	-21.84	13880.0/
	TROE/ 0.043	340.0	60000.0
	H2/2.0/	H2O/6.0/	CH4/2.0/
		CO/1.5/	
CO2/2.0/			
O-HOAlCH3+O2=O-OAlCH3+HO2	1.0E+12	0.0	38900.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+O2=O-HOAlCH2+HO2	2.1E+12	0.0	39700.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+H=A1OH+CH3	5.8E+13	0.0	8100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+H=O-OAlCH3+H2	1.2E+14	0.0	12400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+O=O-OAlCH3+OH	1.3E+13	0.0	2900.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+OH=O-OAlCH3+H2O	1.4E+8	1.4	-960.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+HO2=O-OAlCH3+H2O2	1.0E+12	0.0	10000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+CH3=O-OAlCH3+CH4	1.8E+11	0.0	7700.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+A1-=O-OAlCH3+A1	4.9E+12	0.0	4400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C5H5=O-OAlCH3+C5H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C3H5-A=O-OAlCH3+C3H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C4H5-I=O-OAlCH3+C4H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C4H5-N=O-OAlCH3+C4H6	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			

O-HOAlCH3+A1O=O-OAlCH3+A1OH	4.9E+11	0.0	9400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+H=O-HOAlCH2+H2	1.2E+14	0.0	8400.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+O=O-HOAlCH2+OH	6.3E+11	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+OH=O-HOAlCH2+H2O	5.2E+9	1.0	870.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+HO2=O-HOAlCH2+H2O2	4.0E+11	0.0	14000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+CH3=O-HOAlCH2+CH4	1.6E+12	0.0	11100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C3H5-A=O-HOAlCH2+C3H6	1.6E+12	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C3H3=O-HOAlCH2+C3H4-P	1.6E+12	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C4H5-I=O-HOAlCH2+C4H6	1.6E+12	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C4H5-N=O-HOAlCH2+C4H6	1.6E+12	0.0	11100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+C5H5=O-HOAlCH2+C5H6	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+A1-=O-HOAlCH2+A1	7.9E+13	0.0	12000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+A1O=O-HOAlCH2+A1OH	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+P-C6H4CH3=O-OAlCH3+A1CH3	7.9E+13	0.0	
12000.0	!Bounaceur et al.IJCK 37, 25-49, 2005		
O-HOAlCH3+O-C6H4CH3=O-OAlCH3+A1CH3	7.9E+13	0.0	
12000.0	!Bounaceur et al.IJCK 37, 25-49, 2005		
O-HOAlCH3+P-OAlCH3=O-HOAlCH2+P-HOAlCH3	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+O-OAlCH3=O-HOAlCH2+O-HOAlCH3	1.6E+11	0.0	15100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+A1CH2OO=O-HOAlCH2+A1CH2OOH	4.0E+11	0.0	14000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH3+A1CH2O=O-HOAlCH2+A1CH2OH	1.6E+11	0.0	11100.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH2+O2=HOAlCH2OO	4.6E+11	0.0	-380.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH2+O2=HOAlCH2O+O	6.3E+12	0.0	40000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH2+H=O-HOAlCH3	1.0E+14	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH2+HO2=HOAlCH2OOH	5.0E+12	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
O-HOAlCH2+CH3=A1OH+C2H4	5.0E+12	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
HOAlCH2OO=HOAlCHO+OH	3.4E+9	1.0	37500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
!Nicolas Delort - rather coeff from Nowakowska 2018!			
!HOAlCH2O=HOAlCHO+H	2.0E+13	0.0	27500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			

HOA1CH2O+O2=HOA1CHO+HO2	6.0E+10	0.0	1600.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
HOA1CHO+O=HOA1CO+OH	6.0E+12	0.0	1800.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
HOA1CHO+OH=HOA1CO+H2O	7.8E+12	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
HOA1CHO+HO2=HOA1CO+H2O2	3.0E+12	0.0	11000.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
! Nicolas Delort			
!HOA1CHO+CH3=HOA1CO+CH4	2.0E-6	5.6	1500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
!HOA1CHO+H=HOA1CO+H2	4.0E+13	0.0	3200.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
HOA1CHO+CH3=HOA1CO+CH4	0.5E-6	5.6	1500.0
! A/4			
HOA1CHO+H=HOA1CO+H2	1.0E+13	0.0	3200.0
! A/4			
!Nicolas Delort - delumping of the pathway			
!HOA1CO=A1O+CO	4.0E+14	0.0	29500.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
HOA1CO=C6H4OH+CO	4.0E+14	0.0	29500.0
! as A1CO=A1-+CO			
!Nicolas Delort!C6H4OH=A1O			1.65E07
1.83	33290	! Nowakowska 2018 - CBS-QB3+tunneling PAG	
HOA1CH2O+OH=HOA1CH2OOH	2.0E+13	0.0	0.0
!Bounaceur et al.IJCK 37, 25-49, 2005			
A1CH+O=A1+CO	1.00E+13	0.0	0.0
!2002 Howard&richter est.			
A1CH+OH=A1+HCO	1.00E+13	0.0	0.0
!2002 Howard&richter est.			
P-OA1CH3+H(+M)=P-HOA1CH3(+M)	4.00E+14	0.0	0.0
!refer to A1O+H(+M)=A1OH(+M) 1996 Davis et al			
	LOW /	1.00E+94	-21.84
13880.0/			
	TROE/	0.043	340.0 60000.0
5900.0/			
	H2/2.0/	H2O/6.0/	CH4/2.0/ CO/1.5/
CO2/2.0/			
CH3+A1O=>P-OA1CH3+H	1.998E+39	-7.80	31670
! A*3/5 on Yuan coeff 3.33E+39 -7.80 31670 !Polimi V2012			
CH3+A1O=>O-OA1CH3+H	1.332E+39	-7.80	31670
! A*2/5 on Yuan coeff 3.33E+39 -7.80 31670 !Polimi V2012			
! Nicolas Delort! OH+PC6H4CH3=>A1CH2OH+0.5O2			1.600E+14
0.0	0.0	!Polimi V2012	
OH+O-HOA1CH2=>A1CH2OH+0.5O2	.600E+14	0.0	0.0
! Nicolas Delort from Polimi V2012 OH+RCRESOLC=>C6H5CH2OH+.5O2			
!A1O+CH3<=>HOA1CH3	2.31e73	-17.37	38.78e3 !
Nicolas Delort from Pecullan_1997			
! Nicolas Delort as in Buttgen mech			

A1O+CH3<=>P-HOA1CH3 +0.6900000E+073 -
 1.7370000E+001 +3.8800000E+004 ! coeff Buttgen with A*3/5
 A1O+CH3<=>O-HOA1CH3 +0.4600000E+073 -
 1.7370000E+001 +3.8800000E+004 ! coeff Buttgen with A*2/5
 A1O+CH3=C5H5CH3+CO 2.05e75 -18.29 38.88e3
 !Pecullan_1997!

!Nicolas Delort - cresols -> benzaldehyde from CRECK
 O+O-HOA1CH2=>OH+A1CHO 5.0000e+14
 0.000 0.00 ! O+RCRESOLC=>OH+C6H5CHO in CRECK
 O+P-HOA1CH2=>OH+A1CHO 5.0000e+14
 0.000 0.00
 OH+O-HOA1CH2=>H2O+A1CHO 6.0000e+13
 0.000 0.00 ! OH+RCRESOLC=>H2O+C6H5CHO in CRECK
 OH+P-HOA1CH2=>H2O+A1CHO 6.0000e+13
 0.000 0.00
 OH+O-OA1CH3=>H2O+A1CHO 6.0000e+13
 0.000 0.00 ! OH+RCRESOLO=>H2O+C6H5CHO in CRECK
 OH+P-OA1CH3=>H2O+A1CHO 6.0000e+13
 0.000 0.00

!***** Reactions of benzene(A1) and
 fulvene *****

A1-H(+M)=A1(+M) 1.00E+14 0.0 0.0
 !1997 Wang&Frenklach RRKM
 LOW / 6.6E+75 -16.30 7000.0/
 TROE/ 1.0 0.1 584.9 6113.0/
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/
 CO2/2.0/ C2H6/3.0/
 A1+H=1C6H7 1.22E+22 -1.87 31200.0
 !Pitz2001
 A1+H=cC6H7 1.20E+125 -33.66 55212.0
 !Pitz2001
 PLOG / 1.0 1.20E+125 -33.66
 55212.0/
 PLOG / 3.0 4.98E+128 -34.47
 59329.0/
 PLOG / 10.0 3.27E+130 -34.75
 62718.0/
 PLOG / 30.0 2.40E+129 -34.20
 64174.0/
 PLOG / 100.0 3.33E+124 -32.58
 63531.0/
 cC6H7+O2=A1+HO2 7.90E+11 0.00 9900.0
 !Bounaceur2005
 cC6H7+H=A1+H2 3.30E+12 0.00 0.0
 !Bounaceur2005
 cC6H7+OH=A1+H2O 1.00E+13 0.00 0.0
 !Bounaceur2005
 cC6H7+H=C4H6+C2H2 6.50E+13 0.0 0.0
 !Pitz2001
 cC6H7=1C6H7 3.00E+13 0.0 46400.0
 !Pitz2001
 1C6H7=C4H5-N+C2H2 5.50E+14 0.0 41000.0
 !Pitz2001

!-----

A1+H=A1-+H2	2.50E+14	0.0	16000.0
!Emdee et al.J. Phys. Chem. 1992, 96, 2151-2161			
A1+OH=A1-+H2O	2.34E+04	2.68	733.2
!2006 Seta and Nakajima and Miyoshi			
A1+OH=A1OH+H	4.99E+08	1.31	6543.0
!PITZ2001			
PLOG / 1.0	4.99E+08	1.31	6543.0/
!same as seta et al.			
PLOG / 10.0	8.21E+13	-0.13	10673.0/
PLOG / 100.0	6.68E+20	-2.02	16758.0/
A1-+CH4=A1+CH3	3.89E-03	4.6	5256.0
!1999 Tokmakov et al.			
A1-+C2H6=A1+C2H5	2.10E+11	0.0	4443.0
!2001 Park et al.			
C5H6+A1-=C5H5+A1	3.10E+11	0.0	5500.0
!2001 Bacskay&Mackie			
A1+O=C5H6+CO	6.02E+15	-0.49	14993.0
!2010 Taatjes et al. 1atm			
plog/ 0.1	7.22e+13	0.12	
11776.9/			
plog/ 1.0	6.02E+15	-0.49	
14993.0/			
plog/ 10.0	1.38E+38	-6.71	
34631.4/			
PLOG/ 50.0	1.57E+31	-4.73	
33568.4/			
PLOG/ 500	2.23E+56	-11.69	
55598.2/			
A1+O2=A1-+HO2	6.30E+13	0.0	60000.0
!Emdee et al.1992			
A1+O2=>OH+A1O	4.00E+13	0.00	44000.0
!Polimi V2012			
A1+O=A1O+H	1.99E+07	1.8	3974.0
!2010 Taatjes et al 20131028			
plog/ 0.1	1.99E+07	1.8	3974.0/
plog/ 10	1.99E+07	1.8	3974.0/
plog/ 50	3.55e+10	0.91	6323.0/
plog/ 500	1.32e+12	0.47	8434.8/
A1+O=A1OH	7.22E+22	-2.56	14993.0
!A1+O=A1OH 2010 Taatjes et al.			
plog/ 0.1	1.51E+29	-4.72	
13342.7/			
plog/ 1.0	7.22E+22	-2.56	
14993.0/			
plog/ 10.0	3.55E+24	-2.82	
21904.7/			
PLOG/ 50.0	5.84E+35	-5.89	
34534.1/			
PLOG/ 500	4.21E+31	-4.73	
38428.6/			
A1+O=A1-+OH	2.0E13	0.0	14700.0
!Alzueta et al.2000			
A1+HO2=A1-+H2O2	1.44E+13	0.0	
30982.0			!M. Altarawneh CNF 2010
A1-+HCO=A1+CO	8.55E+4	2.19	38.0
!Chaos 2007			
A1-+HO2=A1O+OH	5.0E+12	0.0	0.0
!da costa et al.2003			

A1-+O2=A1O+O	2.6E13	0.0	6.1E3
!Frank,P. Herzler,J. Just,Th. Wahl,C. Symp. Int. Combust. Proc. 25, 833-840 (1994)			
A1-+O2=O-C6H4O2+H	3.0E13	0.0	9.0E3
!Frank,P. Herzler,J. Just,Th. Wahl,C. Symp. Int. Combust. Proc. 25, 833-840 (1994)			
A1-+O2=C5H5+CO2	1.70E+33	-5.96	18648.0
!Pitz2001			
PLOG / 1.0	1.70E+33	-5.96	18648.0
/			
PLOG / 8.5	2.41E+40	-7.86	26448.0
/			
A1-+O2=A1O0	6.91E+132	-36.41	49920.0
!PITZ2001			
PLOG / 1.0	6.91E+132	-36.41	49920.0
/			
PLOG / 8.5	5.67E+132	-35.91	53659.0
/			
A1O0=A1O+O	9.59E+80	-19.82	79043.0
!PITZ2001			
PLOG / 1.0	9.59E+80	-19.82	79043.0
/			
PLOG / 8.5	7.51E+67	-15.72	73699.0
/			
A1-+CH2O=A1CHO+H	2.91E+4	2.09	-411.0
A1O0+A1CH3=A1OOH+A1CH2	4.0E+11	0.0	14000.0
A1O+OH=A1OOH	2.0E+13	0.0	0.0
A1O0+A1OH=A1OOH+A1O	1.33E+11	0.0	14000.0
nC4H3+C2H3=A1	2.87E+14	0.0	817.0
!1988 Duran et al. Fit data in 2005 Sivaramakrishnan et al.			
C3H3+C3H5-A=fulvene+2H	3.26E+29	-5.4	3390.0
!Miller&Klippenstein 2003.			
C3H4-A+C3H2=A1	7.40E+12	-0.7	920.0
!2002 D'Anna et al.			
C3H4-P+C3H2=A1	1.40E+13	-0.8	1030.0
!2002 D'Anna et al.			
C3H4-A+C3H3=A1+H	2.20E+11	0.0	2000.0
!2002 D'Anna et al.			
C4H4+C2H3=A1+H	1.90E+12	0.0	2510.0
!1997 Lindstedt&Skevis			
C3H4-P+C3H3=A1+H	2.20E+11	0.0	2000.0
!1987 Wu&Kern			
C4H4+C2H2=A1	4.47E+11	0.0	30010.0
!1986 Chanmugathas&Heicklen			
C2H2+C4H5-N=H+A1	1.37E16	-1.00	8896
!Miller&Klippenstein 2003			
PLOG /0.01	1.37E16	-1.00	8896./
PLOG /0.025	2.94E16	-1.09	9259./
PLOG /0.1	1.37E16	-1.00	8898./
PLOG /1.	1.385E16	-1.00	8900./
PLOG /10.	1.69E16	-1.03	8967./
PLOG /100.	1.65E16	-1.01	9480./
C2H2+C4H5-N=H+fulvene	1.52E15	-0.76	8767
!Miller&Klippenstein 2003			
PLOG /0.01	1.52E15	-0.76	8767./
PLOG /0.025	1.52E15	-0.76	8767./
PLOG /0.1	1.52E15	-0.76	8769./
PLOG /1.	4.63E15	-0.89	9142./

PLOG /10.	1.74E19	-1.86	12383./
PLOG /100.	1.23E20	-2.00	16152./
!Miller&Klippenstein 2003			
C2H2+C4H5-I=H+A1	1.47E+23	-3.28	24907
!Miller&Klippenstein 2003			
PLOG /0.01	1.47E+23	-3.28	24907./
PLOG /0.025	1.47E+23	-3.28	24907./
PLOG /0.1	1.47E+23	-3.28	24907./
PLOG /1.	1.67E+23	-3.30	24959./
PLOG /10.	8.25E+24	-3.76	24562./
PLOG /100.	5.37E+32	-5.84	35023./
C2H2+C4H5-I=H+fulvene	6.50E+24	-3.44	20319.
!Miller&Klippenstein 2003			
PLOG /0.01	6.50E+24	-3.44	20319./
PLOG /0.025	1.01E+34	-5.94	28786./
PLOG /0.1	6.50E+24	-3.44	20319./
PLOG /1.	6.80E+24	-3.45	20337./
PLOG /10.	9.70E+25	-3.76	21326./
PLOG /100.	5.22E+41	-7.94	39597./
C4H5-N+C2H3=A1+H2	1.84E-13	7.1	-3611.0
!1989 Westmoreland et al.			
C3H3+C3H3=fulvene	6.3069E+76	-19.07	31542.
!Miller&Klippenstein 2003			
PLOG /0.03947	6.3069E+76	-19.07	31542./
PLOG /1.	1.3798E+66	-15.66	28260./
PLOG /10.	1.2584E+56	-12.61	23515./
C3H3+C3H3=A1	1.8189E+74	-18.14	31896.
!Miller&Klippenstein 2003			
PLOG /0.03947	1.8189E+74	-18.14	31896./
PLOG /1.	3.1609E+55	-12.55	22264./
PLOG /10.	3.8888E+50	-11.01	20320./
fulvene=A1	5.62E+81	-19.36	121500.0
!2003 Miller&Klippenstein 2003			
PLOG / 0.0395	5.62E+81	-19.36	
121500.0/			
PLOG / 1.0000	1.45E+45	-8.90	96999.0/
PLOG / 10.0000	2.95E+31	-4.97	88465.0/
C3H3+C3H3=A1-+H	1.0467E+54	-11.88	28757.
!2003 Miller&Klippenstein 2003			
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./
fulvene+H=A1+H	4.94E+18	-1.28	5411
!Ahren W. Jasper 2013			
PLOG/ 0.00132	4.94E+18	-1.28	
5411/			
PLOG/ 0.0132	2.15E+22	-2.28	
8429/			
PLOG/ 0.132	5.60E+26	-3.47	
12818/			
PLOG/ 1.000	1.66E+25	-2.99	
13691/			
PLOG/ 1.312	5.06E+25	-3.12	
14226/			
PLOG/ 13.12	2.20E+27	-3.48	
19199/			
fulvene+H=C5H4CH3	1.72E+51	-11.47	
16731			
!Ahren W. Jasper 2013			

PLOG/ 0.00132	1.72E+51	-11.47	
16731 /			
PLOG/ 0.0132	5.32E+44	-9.34	
15127 /			
PLOG/ 0.132	6.59E+35	-6.56	
11939 /			
PLOG/ 1.000	1.06E+27	-3.88	
8299/			
PLOG/ 1.312	7.07E+25	-3.53	
7786/			
PLOG/ 13.12	2.14E+21	-2.09	
7022/			
fulvene=A1-+H	2.57E+97	-23.2	153470.0
!2003 Miller&Klippenstein 2003			
PLOG / 0.0395	2.57E+97	-23.2	153470.0/
PLOG / 1.0000	2.24E+68	-14.7	142570.0/
PLOG / 10.0000	8.51E+24	-2.5	113330.0/
!***** Reactions of A1-			
!*****			
!*****			
A1- (+M)=o-C6H4+H (+M)	4.300E+12	0.616	77313.
! RRKM 00-HAI-FRE			
	LOW/ 1.000E+84	-18.866	
90064 / ! 20130218			
	TROE/ 0.902 696. 358. 3856.		/
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/			
C4H2+A1-=>A2-1	5.000E+12	0.000	3000.0
C4H2+A1-=>A2-2	5.000E+12	0.000	3000.0
C4H2+A1=>A2	1.500E+11	0.000	22500.0
!Est			
n-C6H5 = A1-	3.70E+63	-16.49	36100.
!1997Wang&Frenklach RRKM			
PLOG/ 0.013	3.70E+63	-16.49	36100./
PLOG/ 0.026	1.30E+62	-15.94	35800./
PLOG/ 0.118	1.30E+59	-14.78	35600./
PLOG/ 1.00	5.10E+54	-13.11	35700./
PLOG/ 10.00	3.50E+46	-10.44	33600./
n-C6H5=o-C6H4+H	1.60E+65	-16.00	58400.
!1997Wang&Frenklach RRKM			
PLOG/ 0.013	1.60E+65	-16.00	58400./
PLOG/ 0.026	2.70E+65	-15.93	59700./
PLOG/ 0.118	1.50E+64	-15.32	61500./
PLOG/ 1.00	1.30E+59	-13.56	62000./
PLOG/ 10.00	1.10E+50	-10.69	60900./
n-C6H5+H = C4H4+C2H2	1.60E+19	-1.60	2220.0
!1997Wang&Frenklach RRKM			
PLOG/ 0.026	1.60E+19	-1.60	2220.0/
PLOG/ 0.118	1.30E+20	-1.85	2960.0/
PLOG/ 1.00	6.30E+25	-3.34	10014.0/
A1- = nC4H3+C2H2	3.55E+78	-17.787	137467.2
!1997 Madden et al. RRKM			
PLOG / 0.500	3.55E+78	-17.787	137467.2/
PLOG / 1.000	3.92E+74	-16.6	135581.1/
PLOG / 10.000	1.79E+61	-12.663	128678.3/
nC4H3+C2H2=o-C6H4+H	1.90E+36	-7.21	17900.0
!1994 Wang&Frenklach RRKM			

PLOG / 0.0132	9.20E+33	-6.57	15900.0/
PLOG / 0.0263	1.90E+36	-7.21	17900.0/
PLOG / 0.1184	3.50E+41	-8.63	23000.0/
PLOG / 1.0000	6.90E+46	-10.01	30100.0/
PLOG / 10.0000	3.10E+49	-10.59	37700.0/
A1-H=O-C6H4+H2	2.36E-06	5.80	
11714 !2001 A. M. Mebel and M.C.Lin			
PLOG/ 0.132	2.36E-06	5.80	
11714/			
PLOG/ 1.000	1.16E-14	8.13	
8766/			
PLOG/ 10.00	2.58E-22	10.22	
5350/			
1-C6H4+H=A1-	4.00E+77	-19.99	28100.0
!1994 Wang&Frenklach RRKM			
plog / 0.0132	4.40E+74	-19.09	25800.0/
plog / 0.0263	4.00E+77	-19.99	28100.0/
plog / 0.1184	4.70E+78	-20.10	29500.0/
plog / 1.0000	1.70E+78	-19.72	31400.0/
plog / 10.0000	3.90E+69	-16.63	34100.0/
A1OH+C3H5-A=A1O+C3H6	4.9E+11	0.0	9400.0
A1OH+C4H5-I=A1O+C4H6	4.9E+11	0.0	9400.0
!Nicolas Delort - in guaiacol bloc !OA1OH=C5H4OH+CO			
7.4E+11 0.0 43800.0			
A1O+O=C5H5+CO2	1.0E+13	0.0	0.0
A1O+O=OA1OH	2.6E+10	0.47	800.0
!----- Reactions of benzoquinone -----			
!A1O+HO2=O-OC6H5OJ+OH	5.00E+10	0.0	0.0
!Est Metcalfe et al.			
A1O+HO2=O-OC6H5OJ+OH	+1.2000000E+016		
+0.0000000E+000 2.0000000E+004 ! 4.20 from Buttgen mech			
P-C6H4O2+H=P-OC6H5OJ	4.0E+12	0.0	9740.0
O-C6H4O2+H=O-OC6H5OJ	4.0E+12	0.0	6960.0
A1O+O=P-C6H4O2+H	4.25E+13	0.0	0.0
A1O+O=O-C6H4O2+H	8.5E+13	0.0	0.0
P-C6H4O2+H=C5H5O24+CO	2.5E+13	0.0	4700.0
P-C6H4O2+H=P-C6H3O2+H2	2.0E+12	0.0	8100.0
P-C6H4O2+O=P-C6H3O2+OH	1.4E+13	0.0	14700.0
P-C6H4O2+OH=P-C6H3O2+H2O	1.0E+6	2.0	4000.0
P-C6H3O2+H=P-C6H4O2	1.0E+14	0.0	0.0
P-C6H3O2+H=2C2H2+2CO	1.0E+14	0.0	0.0
P-C6H3O2+O=C2H2+HCCO+2CO	1.0E+14	0.0	0.0
P-C6H4O2+O=2CO+C2H2+CH2CO	3.000E+13	0.0	5000.0
!***** reactions of A1O and A1OH			

O+A1O=>HCO+C2H2+C2H2+CO	6.0E+12	0.00	0.000E+00
!			
O-C6H4O2=C5H4O+CO	1.0E+12	0.0	40000.0
!Alzueta et al.1998			
P-C6H4O2=C5H4O+CO	3.7E+11	0.0	59000.0
!Alzueta et al.1998			
A1O=CO+C5H5	5.71E+59	-14.4	
68564 !2011 You et al. J. Phys. Chem. A 2011, 115, 14184-14190			
PLOG / 0.0100	5.71E+59	-14.4	
68564/ !The rate of You is similar to that of Carstensen et al.			

PLOG / 0.1000	1.65E+71	-17.2	
81843/			
PLOG / 1.0000	1.32E+74	-17.6	
88985/			
PLOG / 10.000	4.41E+68	-15.8	
89456/			
PLOG /100.0000	3.77E+71	-16.18	
98611/			
!HPL	1.25E+06	2.25	50194
A1O+H(+M)=A1OH(+M)	0.50E+14	0.0	0.0
!1996 Davis et al (Reduced from 2.5 to 1.0 by F.L. Dryer to 0.5 by ywh)			
	LOW / 1.00E+94	-21.84	13880.0/
	TROE/ 0.043	340.0	60000.0 5900.0/
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/			
A1O+H=C5H5+HCO	1.000E+13	0.000	
12000.00			
A1O+H=C5H6+CO	5.000E+13	0.000	
0.00 !			
A1OH+OH=A1O+H2O	1.4E+08	1.4	-960.0
!da costa et al 2003			
A1OH+H=A1O+H2	1.15E+14	0.0	12398.0
!1988 He et al.			
A1OH+O=A1O+OH	2.81E+13	0.0	7352.0
!USC Mech II			
A1OH+O2=A1O+HO2	0.5E+13	0.0	38800.0
!da costa et al 2003/3			
A1OH+O=OA1OH+H	1.6E+13	0.0	3400.0
!da costa et al 2003			
A1OH+HO2=A1O+H2O2	1.0E+12	0.0	10000.0
!da costa et al 2003			
A1OH+CH3=A1O+CH4	1.8E+11	0.0	7700.0
!da costa et al 2003			
A1OH+A1-=A1O+A1	4.910E+12	0.000	4400.00
!USC Mech V2.0			
A1OH=C5H6+CO	5.02E+15	-0.61	74115.0
!2006 Xu&Lin 8.62E+15/2			
A1OH+C2H3=A1O+C2H4	6.000E+12	0.000	0.00
!1992 Emdee et al., est. from phenol + OH			
A1OH+C4H5-N=A1O+C4H6	6.000E+12	0.000	0.00
!1992 Emdee et al., est. from phenol + OH			
C6H4OH+H=A1OH	1.0E+14	0.0	0.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200			
A1OH+H=C6H4OH+H2	1.7E+14	0.0	16000.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200			
A1OH+O=C6H4OH+OH	2.0e+13	0.0	14700.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200			
A1OH+OH=C6H4OH+H2O	1.4e+13	0.0	4600.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200			
A1OH+HO2=C6H4OH+H2O2	4.0e+11	0.0	28900.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200			

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A1OH+CH3=C6H4OH+CH4          2.0e+12    0.0    15000.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200
C6H4OH+O2=OAlOH+O            2.1E+13    0.0    6100.0
!da costa et al.Int J Chem Kinet 35: 503-524, 200
OH+A1OH=>OH+C5H6+CO          4.00E+12    0.0    0.0
!
!***** Reactions of
C5H5CH3 (Methylcyclopentadiene)*****
*****
C5H5+CH3=>C5H5CH3            9.10E+109   -29.19
  41906      !Sandeep Sharma and William H. Green J. Phys. Chem. A
2009, 113, 8871-8882
  PLOG/ 0.01            9.10E+109   -29.19
  41906/
  PLOG/ 1.00            3.06E+105 -27.05
  47952/
  PLOG/ 10.0           2.38E+94 -23.52
  45184/
  PLOG/ 100            1.09E+70 -16.33
  32296/
C5H5+CH3=>fulvene+H2          9.25E+01  2.19
8815      !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009,
113, 8871-8882
  PLOG/ 0.01            9.25E+01  2.19
8815 /
  PLOG/ 1.00            1.14E+15 -1.40
20266 /
  PLOG/ 10.0           3.62E+31 -5.90
35631 /
  PLOG/ 100            3.38E+43 -9.05
49742 /
C5H5CH3=>C5H5+CH3            4.49E+77 -19.26      89496
!Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-
8882
  PLOG/ 0.01            4.49E+77 -19.26
  89496/
  PLOG/ 1.00            2.01E+89 -21.78
  105380/
  PLOG/ 10.0           6.89E+84 -20.17
  106554/
  PLOG/ 100            4.46E+71 -16.16
  100961/
C5H5CH3=>fulvene+H2          3.38E+77 -21.53
96791      !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009,
113, 8871-8882
  PLOG/ 0.01            3.38E+77 -21.53
96791/
  PLOG/ 1.00            2.04E+94 -25.05
118602/
  PLOG/ 10.0           1.05E+97 -25.23
126838/
  PLOG/ 100            3.85E+84 -21.21
124346/
C5H5+CH3=>C5H4CH3+H          3.03E+15 -0.58      10871
!Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-
8882
  PLOG/ 0.01            3.03E+15 -0.58      10871/
! /4

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PLOG/ 1.00	1.23E+31-4.85	24769/
! /4		
PLOG/ 10.0	3.23E+46-9.02	39791/
! /4		
PLOG/ 100	1.49E+56-11.53	
52592/ ! /4		
C5H5CH3=>C5H4CH3+H	2.35E+80-20.72	
95019 !Sandeep Sharma and William H. Green	J. Phys. Chem. A 2009,	
113, 8871-8882		
PLOG/ 0.01	2.35E+80-20.72	
95019/		
PLOG/ 1.00	1.74E+97-24.38	
116128/		
PLOG/ 10.0	5.77E+97-24.00	
122296/		
PLOG/ 100	1.75E+87-20.60	
120401/		
C5H5+CH3=>C5H5CH2-2+H	7.49E+13-0.30	11640
!Sandeep Sharma and William H. Green	J. Phys. Chem. A 2009, 113, 8871-	
8882		
PLOG/ 0.01	7.49E+13-0.30	11640/
PLOG/ 1.00	7.93E+27-4.14	24060/
PLOG/ 10.0	7.18E+44-8.75	40084/
PLOG/ 100	1.31E+53-10.86	
51760/		
C5H5+CH3=>C5H5CH2-3+H	2.18E+14-0.40	17024
!Sandeep Sharma and William H. Green	J. Phys. Chem. A 2009, 113, 8871-	
8882		
PLOG/ 0.01	2.18E+14-0.40	17024/
PLOG/ 1.00	1.31E+23-2.81	24726/
PLOG/ 10.0	6.08E+38-7.08	39076/
PLOG/ 100	1.81E+52-10.67	
54105/		
C5H5+CH3=>C5H5CH2-1+H	8.13E+25-3.51	41018
!Sandeep Sharma and William H. Green	J. Phys. Chem. A 2009, 113, 8871-	
8882		
PLOG/ 0.01	8.13E+25-3.51	41018/
PLOG/ 1.00	3.83E+26-3.69	41579/
PLOG/ 10.0	1.16E+33-5.47	47110/
PLOG/ 100	1.03E+48-9.54	61181/
C5H5CH3=>C5H5CH2-2+H	1.38E+96-24.49	
116744 !Sandeep Sharma and William H. Green	J. Phys. Chem. A 2009,	
113, 8871-8882		
PLOG/ 1.00	1.38E+96-24.49	
116744/		
PLOG/ 10.0	1.54E+98-24.53	
124128/		
PLOG/ 100	3.13E+86-20.76	
121667/		
C5H5CH3=>C5H5CH2-3+H	1.61E+100 -25.89	
121934 !Sandeep Sharma and William H. Green	J. Phys. Chem. A 2009,	
113, 8871-8882		
PLOG/ 1.00	1.61E+100 -25.89	
121934/		
PLOG/ 10.0	2.05E+103 -26.14	
130620/		
PLOG/ 100	7.82E+93-22.94	
130454/		

C5H5CH3=>C5H5CH2-1+H	9.33E+109	-29.66	
135070 !Sandeep Sharma and William H. Green J. Phys. Chem. A 2009, 113, 8871-8882			
PLOG/ 1.00	9.33E+109	-29.66	
135070/			
PLOG/ 10.0	1.07E+116	-30.36	
147389/			
PLOG/ 100	1.21E+114	-28.95	
154902/			
C5H5CH2-2=fulvene+H	1.35e+58	-13.11	73890
!Polimi V2012			
C5H5CH2-2=A1+H	9.25e+43	-9.19115	
55756.8 !Polimi V2012			
C5H5CH3+H=C5H5CH2-2+H2	1.30e+06	2.38	
2800.00 !Polimi V2012			
C5H5CH2-1=C5H5CH2-2	1.69e+30	-5.9432	
21537.5 !Polimi V2012			
C5H5CH2-2=C5H5CH2-3	1.08e+41	-8.73397	44399
!Polimi V2012			
C5H5CH2-3=fulvene+H	3.67e+43	-9.19	57330
!Polimi V2012			
C5H5CH2-1=C5H5CH2-3	9.23e+27	-5.12362	
28314.7 !Polimi V2012			
C5H5CH2-3=A1+H	1.38e+46	-9.72349	57338
!Polimi V2012			
C5H5CH2-1=fulvene+H	1.07e+29	-5.32	32810
!Polimi V2012			
C5H5CH2-1=A1+H	1.98e+31	-6.06562	
20629.6 !Polimi V2012			
C5H4CH3+O2=HO2+fulvene	4.82E+11	0.0	0.0
!Polimi V2012			
C5H5CH3+H=C5H4CH3+H2	7.2E+13	0	
3500.0 !EST			
C5H5CH3+OH=C5H4CH3+H2O	3.08E+06	2.0	
0.0 !EST			
H+C5H5CH3=>CH3+C5H6	1.500E+13	0.0	2000.0
!Polimi V2012			
O2+C5H5CH3=>HO2+A1+H	1.704E+07	2.0	
38570.96 !Polimi V2012			
H+C5H5CH3=>H2+A1+H	2.407E+07	2.0	
2663.07 !Polimi V2012			
OH+C5H5CH3=>H2O+A1+H	3.994E+06	2.0	-
3152.53 !Polimi V2012			
O+C5H5CH3=>OH+A1+H	1.353E+07	2.0	
1356.53 !Polimi V2012			
HO2+C5H5CH3=>H2O2+A1+H	5.388E+05	2.0	
10318.80 !Polimi V2012			
HCO+C5H5CH3=>CH2O+A1+H	1.263E+06	2.0	
10777.87 !Polimi V2012			
CH3+C5H5CH3=>CH4+A1+H	3.903E+05	2.0	
3544.16 !Polimi V2012			
C2H5+C5H5CH3=>C2H6+A1+H	2.298E+05	2.0	
6224.33 !Polimi V2012			

!***** Reactions of C5H5(1,3-Cyclopentadienyl) and C5H6(1,3-cyclopentadiene)

C3H3+C2H2=>C5H5	6.17E+66	-15.7	47729
!L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	6.17E+66	-15.7	
47729/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	6.87E+55	-12.5	
42000/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	1.13E+43	-8.80	
34983/ !L. V. Moskaleva, M. C. Lin 1999			
C5H5=>C3H3+C2H2	2.79E+79	-18.3	
130768 !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	2.79E+79	-18.3	
130768/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	1.98E+68	-15.0	
124824/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	5.70E+54	-11.10	
116874/ !L. V. Moskaleva, M. C. Lin 1999			
C5H5=1C5H5	2.25E+108	-28.2	
127755 !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	2.25E+108	-28.2	
127755/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	1.21E+109	-28.1	
130355/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	2.08E+112	-28.6	
136922/ !L. V. Moskaleva, M. C. Lin 1999			
C5H5=C5H52	5.17E+80	-20.4	96136
!L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	5.17E+80	-20.4	
96136/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	5.92E+78	-19.5	
96640/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	1.32E+78	-19.0	
99133/ !L. V. Moskaleva, M. C. Lin 1999			
C3H3+C2H2=>1C5H5	6.87E+71	-18.2	45334
!L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	6.87E+71	-18.2	
45334/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	4.11E+72	-18.2	
45411/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	1.55E+77	-19.1	
49598/ !L. V. Moskaleva, M. C. Lin 1999			
1C5H5=>C3H3+C2H2	3.12E+82	-20.6	68862
!L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	3.12E+82	-20.6	
68862/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	1.95E+83	-20.6	
68951/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	5.61E+87	-21.5	
73148/ !L. V. Moskaleva, M. C. Lin 1999			
C3H3+C2H2=>C5H52	1.34E+68	-16.9	51542
!L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 0.132	1.34E+68	-16.9	
51542/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 1.000	2.70E+53	-12.6	
41445/ !L. V. Moskaleva, M. C. Lin 1999			
PLOG/ 10.00	1.81E+35	-7.6	
76409/ !L. V. Moskaleva, M. C. Lin 1999			
C5H52=>C3H3+C2H2	3.40E+80	-19.2	
102213 !L. V. Moskaleva, M. C. Lin 1999			

PLOG/ 0.132		3.40E+80	-19.2
102213/	!L. V. Moskaleva, M. C. Lin 1999		
PLOG/ 1.000		7.48E+65	-15.0
92200/	!L. V. Moskaleva, M. C. Lin 1999		
PLOG/ 10.00		4.57E+47	-9.9
51542/	!L. V. Moskaleva, M. C. Lin 1999		
C5H5+H(+M)=C5H6(+M)		1.000E+14	0.000
0.00	!92-EMD-BRE, est., 94-FRA-HER		
	LOW /	4.400E+80	-18.280
12994.0/	!96-DAV-WAN, 97-WAN-FRE		
	TROE /	0.068 400.7 4135.8 5501.9	
/			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/			
C5H6(+M)= C3H4-A+C2H2(+M)		3.8E+17	0.0
1.04E+05	!Mackie et al. 2001 PCCP		
	LOW /	1.00E+98	-22.25
126321.5/			
	TROE /	1.440547E-01 5.357622E+00	
3.283766E+03 6.710101E+09/			
	CO /1.5/ CO2 /2.0/ H2O /6.0/ H2 /2.0/		
CH4 /2.0/			
!Nicolas Delort!C5H6+H=C5H5+H2			7.2E+13
0	3500.0 !Better for C5H6 flow reactor pyrolysis		
C5H6+H=C5H5+H2	6.67E+07 1.874 4259.0		
!Nicolas Delort!	from Biopox <CBSQB3> !		
C5H6+H=C2H2+C3H5-A		7.74E+36	-6.2
32890.0	!zhong & bozzeli j phys chem a 102 ! sensitive reaction		
better for C5H6 flow reactor pyrolysis			
C5H6+C2H3=C5H5+C2H4		6.00E+12	0.0
0.0	!2001 Bacskay&Mackie 6.00E+12		
C5H6+CH3=C5H5+CH4		0.18	4.0 0.0
!zhong & bozzeli j phys chem a 102: 3537 1998			
C3H5-A+C2H2=1C5H7		3.0e+11	0.0
6883.4	!ziegler et al. j. anal.apply.pyrolysis 73 212-230 (2005)		
C5H6+H=1C5H7		2.4e+73	-17.85
31500.0	!1998 Zhong&Bozzelli		
C5H6+O=C5H5+OH		4.77E+04	2.7
1106.0	!1998 Zhong&Bozzelli Est.		
C5H6+OH=C5H5+H2O		3.08E+06	2.0
0.0	!1998 Zhong&Bozzelli Est.		
C5H6+HO2=C5H5+H2O2		1.1E+4	2.6
12900.0	!Zhong & Bozzeli J PHYS CHEM A 102: 3537 1998		
C5H6+O2=C5H5+HO2		4.0E+13	0
37150.0	!Zhong & Bozzeli J PHYS CHEM A 102: 3537 1998		
C5H6+O=C4H5-N+CO+H		8.70E+51	-11.1
33240.0	!1998 Zhong&Bozzelli		
C5H6+HCO=C5H5+CH2O		1.08E+8	1.9
16000.0	!Zhong & Bozzeli J PHYS CHEM A 102: 3537 1998		
OH+C5H6=>HCO+C4H6		3.00E+12	0.0
0.0	!Polimi 8.00E+12 sensitive		
C5H6+O=>CO+C4H6		1.00E+13	0.0
0.0	!Polimi		

C5H6+O=>C2H4+C2H2+CO	3.890e+08	1.360
886.71 !Banquant 2012 20130423 night		
C5H6+OH=>C2H4+C2H2+HCO	3.750e+36	-7.800
7060.23 !Banquant 2012 20130423 night		
C5H6+O=>CH2CO+C3H4-A	3.00E+12	0.00
0.0 !EST 20131022		
C5H6+O=>CH2CO+C3H4-P	3.00E+12	0.00
0.0 !EST 20131022		
1C5H5+H=C5H4+H2	1.81E+12	0.0
0.0 !1986 Tsang&Hampson C2H5+H in 2002 Richter&Howard		
1C5H5+OH=C5H4+H2O	2.41E+13	0.0
0.0 !1986 Tsang&Hampson C2H5+OH in 2002 Richter&Howard		
1C5H5+CH3=C5H4+CH4	1.95E+13	-0.50
0.0 !1986 Tsang&Hampson C2H5+CH3 in 2002 Richter&Howard		
C3H5-A+C2H3=1C5H7+H	1.00E+13	0.0
0.0 !USC Mech II Est.		
1C5H7+O=C2H3CHO+C2H3	5.00E+13	0.0
0.0 !USC Mech II Est.		
C5H5+C3H4-A=A1+C2H3	2E+10	0
0 !EST		
C5H5+C3H4-P=A1+C2H3	2E+10	0
0 !EST		

!***** Reactions of C5H5O and C5H4O

C5H5+O2=C5H5O24+O	7.78E+15	-0.7
48740.0 !1998 Zhong&Bozzelli		
C5H5+O2=C5H4O+OH	1.80E+12	0.080
18000.0 !USC Mech II RRKM 1atm		
C5H5+HO2=C5H5O24+OH	6.86E+10	2.52E-01
5088.57 !R.K. Robinson, R.P. Lindstedt 2011		
C5H5+HO2=C5H4O+H2O	1.19E+33	-6.52
13400 !1998 Zhong&Bozzelli JPCA 102		
HO2+C5H5=>C2H4+C2H+CO+OH	6.00E+12	0.00
0.0 !Polimi V2012		
HO2+C5H5=>C4H5-I+CO+OH	6.300E+12	0.00
0.0 !Polimi V2012		
HO2+C5H5=>CH4+CO2+C3H2	9.00E+12	0.00
0.0 !Polimi V2012		
C5H5+OH=C5H5OH	6.49E+14	-0.85 -
2730.0 !1998 Zhong&Bozzelli JPCA 102		
DUPLICATE		
C5H5+OH=C5H5OH	1.15E+43	-8.76
18730.0 !1998 Zhong&Bozzelli JPCA 102		
DUPLICATE		
C5H5+OH=C5H5OH	1.06E+59	-13.08
33450.0 !1998 Zhong&Bozzelli JPCA 102		
DUPLICATE		
C5H5+OH=C5H4OH+H	3.51E+57	-12.2
48350.0 !1998 Zhong&Bozzelli JPCA 102		
C5H5+OH=C5H5O24+H	1.36E+51	-10.5
57100.0 !1998 Zhong&Bozzelli JPCA 102		
C5H5+OH=cC5H4+H2O	2.11E+14	0.0
4571.0 !1998 Zhong&Bozzelli JPCA 102		
C5H5+O=cC5H4+OH	2.00E+13	0.0
14694.0 !1994 Lindstedt&Skevis		

C5H5+O=C5H5O24	1.12E-12	5.9	-
17310.0 !1998 Zhong&Bozzelli JPCA 102			
C5H5+O=C5H4O+H	5.81E+13	0.0	
20.0 !1998 Zhong&Bozzelli JPCA 102			
C5H5+O=C4H5-N+CO	3.20E+13	-0.2	
440.0 !1998 Zhong&Bozzelli JPCA 102 Est.			
OH+C5H5=>CO+C4H6	1.250E+13	.250	
4350.0 !Polimi V2012			
C5H5OH=C5H4OH+H	8.506E+70	-16.413	
94532.7 !R.K. Robinson, R.P. Lindstedt 2011			
PLOG/ 1	8.506E+70	-16.413	
94532.7/			
PLOG/ 10	1.180E+62	-13.596	
91737.6/			
PLOG/ 100	2.047E+18	-0.337	
72792.8/			
C5H5OH=C5H5O24+H	6.539E+48	-9.478	
122484 !R.K. Robinson, R.P. Lindstedt 2011			
PLOG/ 1	6.539E+48	-9.478	
122484/			
PLOG/ 10	9.714E+37	-6.213	
117730/			
PLOG/ 100	1.933E+18	-0.318	
108532/ !HPL			
C5H5OH+H=C5H5O24+H2	1.15E+14	0.0	
15400.0 !1998 Zhong&Bozzelli JPCA 102			
C5H5OH+H=C5H4OH+H2	1.20E+05	2.5	
1492.0 !1998 Zhong&Bozzelli JPCA 102			
C5H5OH+OH=C5H4OH+H2O	5.5E12	0.0	
1731.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H5OH+OH=C5H5O24+H2O	1.0E+13	0.0	
1697.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H5OH+O=C5H4OH+OH	4.7E+11	0.0	
0.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H5OH+O=C5H5O24+OH	1.0E+13	0.0	
4683.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H5OH+HO2=C5H4OH+H2O2	3.6E+3	2.55	
10531.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H5OH+HO2=C5H5O24+H2O2	1.0E+13	0.0	
15800.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H4OH=C5H4O+H	2.10E+13	0.0	
48000.0 !H Wang est			
C5H4OH+H=C5H4O+H2	2.1E+13	0.0	
54000.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H4OH+O2=C5H4O+HO2	3.0E+13	0.0	
5000.0 !Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H5O24=C5H4O+H	8.183E+16	-2.319	
8719.9 !R.K. Robinson, R.P. Lindstedt			
PLOG/ 1	8.183E+16	-2.319	
8719.9/			
PLOG/ 10	5.064E+18	-2.543	
9508.2/			
PLOG/ 100	9.101E+19	-0.957	
18443.1/ !HPL			
C5H5O24+O2=C5H4O+HO2	1.00E+11	0.0	
0.0 !USC Mech II			
C5H6+O=C5H5O13+H	8.91E+12	-0.150	
590.0 !1998 Zhong&Bozzelli C5H5O1_1			

DUPLICATE			
C5H6+O=C5H5O13+H	5.60E+12	-0.060	
200.0	!1998 Zhong&Bozzelli C5H5O1_2		
DUPLICATE			
C5H5O13+O2=C5H4O+HO2	1.00E+11	0.0	
0.0	!USC Mech II		
C5H4O+H=C4H5-N+CO	2.1E+61	-13.27	
40810.0	!1998 Zhong&Bozzelli		
C5H4O+H=C5H5O13	2.00E+13	0.0	
2000.0	!USC Mech II		
C5H4O=CO+C2H2+C2H2	7.0E+31	-6.88	
66900	!Wang and Brezinsky J PHYS CHEM A 102: 1530 1998		
PLOG/ 0.1	7.0E+31	-6.88	
66900/			
PLOG/ 0.1	1.1E+47	-9.63	
99500/			
PLOG/ 1.0	5.7E+32	-6.76	
68500/			
PLOG/ 1.0	6.2E+41	-7.87	
98700/			
PLOG/ 10.0	4.4E+31	-6.06	
69500/			
PLOG/ 10.0	1.8E+33	-5.22	
95800/			
PLOG/ 100	2.9E+37	-4.50	
69100/			
PLOG/ 100	7.3E+30	-4.39	
96300/			
C5H4O=C4H4+CO	1.0E+12	0.00	
52988	!Dagaut 2001		
C5H4O+O=C4H4+CO2	1.0E13	0.0	
2000.0	!Alzueta & Glarborg IJCK 32: 498-522, 2000.		
C5H4O+H=C5H3O+H2	2.0E+12	0.0	
8100.0	!Alzueta & Glarborg IJCK 32: 498-522, 2000.		
C5H4O+O=C5H3O+OH	1.4E+13	0.0	
1470.0	!Alzueta & Glarborg IJCK 32: 498-522, 2000.		
C5H3O+H=C5H4O	1.0E14	0.0	0.0
!Alzueta & Glarborg IJCK 32: 498-522, 2000.			
C5H3O+O2=>CO2+C2H2+HCCO	9.7E+58	-13.47	
38180.0	!Alzueta & Glarborg IJCK 32: 498-522, 2000.		
C5H3O=>C2H2+CO+C2H	2.0E13	0.0	
51000.0	!Alzueta & Glarborg IJCK 32: 498-522, 2000.		
C5H4O+OH=C5H3O+H2O	1.1E+8	1.42	
1450.0	!Alzueta & Glarborg IJCK 32: 498-522, 2000.		
C5H4O+O=CO+HCO+C3H3	1.20E+08	1.4	-
858.0	!USC Mech II		
!***** Reactions of C6H4			

o-C6H4=C4H2+C2H2	6.50E+13	0.0	
83000.0	!1999 Moskaleva et al. RRKM		
PLOG / 0.1315	1.95E+90	-21.3	
139396.2/			
PLOG / 1.0000	2.07E+85	-19.6	
138901.4/			
PLOG/ 5.000	7.89E+75	-16.8	
134903.4/			
PLOG / 10.0000	7.89E+75	-16.8	
134903.4/			

1-C6H4+H=O-C6H4+H	8.70E+45	-9.61	22300.
!1997 Wang&Frenklach			
PLOG/ 0.013	8.70E+45	-9.61	
22300./			
PLOG/ 0.026	2.20E+47	-9.98	
24000./			
PLOG/ 0.118	9.70E+48	-10.37	
27000./			
PLOG/ 1.000	1.40E+54	-11.70	
34500./			
PLOG/ 10.00	5.70E+55	-11.98	
41900./			
1-C6H4+H=C6H3+H2	1.33E+06	2.5	
9240.0	!USC Mech II		
C3H2+C3H2=1-C6H4	3.00E+11	0.0	
0.0	!1987 Wu&Kern C3H3+C3H3=A1		
C4H2+C2H2=1-C6H4	4.47E+11	0.0	
30010.0	!1986 Chanmugathas&Heicklen C4H4+C2H2=A1 in 2002		
Richter&Howard			
nC4H3+C2H2=1-C6H4+H	3.70E+16	-1.2	
11100.0	!1997 Wang&Frenklach RRKM 20Torr		
C4H4+C2H=1-C6H4+H	1.20E+13	0.0	
0.0	!USC Mech II		
C6H3+H=1-C6H4	4.20E+44	-10.27	
7890.0	!1Wang&Frenklach RRKM iC4H3+H=C4H4 in 1997 Wang&Frenklach		
PLOG / 0.0263	4.20E+44	-10.27	
7890.0/			
PLOG / 0.1184	5.30E+46	-10.68	
9270.0/			
PLOG / 1.0000	3.40E+43	-9.01	
12120.0/			
C4H2+C2H=C6H3	1.10E+30	-6.30	
2790.0	!1997 Wang&Frenklach RRKM		
PLOG / 0.0263	1.10E+30	-6.30	
2790.0/			
PLOG / 0.1184	1.30E+30	-6.12	
2510.0/			
PLOG / 1.0000	4.50E+37	-7.68	
7100.0/			
C6H2+H=C6H3	4.30E+45	-10.15	
13250.0	!1997 Wang&Frenklach RRKM C4H2+H=iC4H3 in 1997 Wang&Frenklach		
PLOG / 0.0263	4.30E+45	-10.15	
13250.0/			
PLOG / 0.1184	2.60E+46	-10.15	
15500.0/			
PLOG / 1.0000	1.10E+30	-4.92	
10800.0/			
C6H3+H=C4H2+C2H2	2.40E+19	-1.6	
2800.0	!1997 Wang&Frenklach RRKM 20Torr iC4H3+H=C2H2+C2H2 in 1997		
Wang&Frenklach			
O-C6H4+C3H3=>C7H5+C2H2	6.93E+59	-12.732	
53252	!Akira Matsugi and Akira Niyoshi 2012 PCCP,14.		
PLOG/ 0.0132	6.93E+59	-12.732	
53252/			
PLOG/ 0.132	4.36E+61	-13.054	
61485/			
PLOG/ 1.000	9.61E+54	-11.098	
61937/			

PLOG/ 10.00		2.58E+38	-6.427	
55219/				
PLOG/ 100.0		3.29E+15	-0.001	
45393/				
C7H5+C2H2=>o-C6H4+C3H3		4.68E+61	-13.236	
79195	!Akira Matsugi and Akira Niyoshi 2012 PCCP,14.			
PLOG/ 0.0132		4.68E+61	-13.236	
79195/				
PLOG/ 0.132		2.76E+63	-13.551	
87406/				
PLOG/ 1.000		5.74E+56	-11.587	
87838/				
PLOG/ 10.00		1.44E+40	-6.908	
81096/				
PLOG/ 100.0		1.81E+17	-0.480	
71271/				
o-C6H4+C3H3=>C9H7		7.46E+100	-25.035	
61535.403	!Akira Matsugi and Akira Niyoshi 2012 PCCP,14.			
20130823				
PLOG/ 0.0132		1.49E+100	-25.035	
61535.403/	!/5			
PLOG/ 0.132		1.12E+79	-18.907	
49031.8081	/ !/5			
PLOG/ 1.000		7.14E+57	-12.867	
34883.772	/ !/5			
PLOG/ 10.00		1.12E+37	-6.994	
20138.245	/ !/5			
PLOG/ 100.0		6.12E+24	-3.553	
11067.3913	/ !/5			
C9H7=>o-C6H4+C3H3		5.46E+121	-29.395	
199434.5939				
PLOG/ 0.0132		8.44E+108	-29.395	
199434.5939	/			
PLOG/ 0.132		4.77E+92	-25.566	
193628.3812	/			
PLOG/ 1.000		9.17E+71	-20.893	
183479.1826	/			
PLOG/ 10.00		3.91E+54	-15.042	
168832.8069	/			
PLOG/ 100.0		2.35E+78	-10.189	
155667.9384	/			
!***** reactions of C5H2 C5H3				
cC5H4 (cyclopentadienylidene)C5H4				

C4H2+CH2 (S)=C5H3+H		1.30E+13	0.0	
0.0	!1992 Miller&Melius			
C4H2+CH2=C5H3+H		3.00E+13	0.0	
0.0	!1992 Miller&Melius			
C4H2+CH=C5H2+H		1.00E+14	0.0	
0.0	!1992 Miller&Melius			
C5H3+H=C5H2+H2		6.03E+13	0.0	
15103.0	!1992 Baulch et al. CH3+H=CH2+H2 in 2002 Richter&Howard			
C5H3+CH3=A1		4.3E+12	0.0	
0.0	!Estimated			
C5H3+OH=C5H2+H2O		1.00E+13	0.0	0.0
!	Estimated			
C5H3+CH=C6H2+H+H		5.00E+13	0.0	0.0
!	Estimated			

C5H3+CH2=1-C6H4+H	5.00E+13	0.0	0.0
! = C3H3+CH2			
C5H2+OH=>C4H2+H+CO	2.00E+13	0.0	0.0
! Estimated			
C5H2+CH=C6H2+H	5.00E+13	0.0	0.0
! Estimated			
C5H2+O2=H2C4O+CO	1.00E+12	0.0	0.0
! Estimated			
cC5H4=C5H4	1.98E+12	0.56	
42240.0			
PLOG / 0.1	2.30E+39	-8.81	
47800.0 / != CC3H4 = C3H4-A 99DAV/LAW RRKM			
PLOG / 0.4	7.59E+40	-9.07	
48831.0 /			
PLOG / 1	4.89E+41	-9.17	
49594.0 /			
PLOG / 2	8.81E+41	-9.15	
50073.0 /			
PLOG / 5	4.33E+41	-8.93	
50475.0 /			
PLOG / 10	7.20E+40	-8.60	
50600.0 /			
PLOG / 100	1.60E+35	-6.64	
49500.0 /			
cC5H4+H=>C5H5	6.61E+12	0.3	770
! Marco Derudi, Daniela Polino and Carlo Cavallotti PCCP 2011,13			
C5H5=>cC5H4+H	5.37E+17	-0.55	
115500 ! Marco Derudi, Daniela Polino and Carlo Cavallotti PCCP			
2011,13			
cC5H4+A1CH3=C5H5+A1CH2	4.47E+03	2.37	3300
! Marco Derudi, Daniela Polino and Carlo Cavallotti PCCP 2011,13			
C4H2+CH3=C5H4+H	2.40E+09	0.91	
20700.0 !1999 Davis et al. C2H2+CH3=C3H4-A+H in 2010 Li(Ph.D. Thesis)			
C4H+CH4=C5H4+H	2.40E+09	0.91	
20700.0 !1999 Davis et al. C2H2+CH3=C3H4-A+H in 2010 Li(Ph.D. Thesis)			
C3H4-A+C2H=C5H4+H	9.60E+13	0.0	
0.0 !2000 Appel et al. C2H2+C2H=C4H2+H in 2010 Li(Ph.D. Thesis)			
C5H3+H=C5H4	3.6308E+36	-7.36	
6039. !2008 Miller & Senosiain & Klippenstein C3H3+H=C3H4-P			
20130821			
PLOG /0.03947	7.26E+36	-7.36	
6039./ !*2			
PLOG /1.	1.59E+30	-5.06	
4861./ !*2			
PLOG /10.	2.14E+24	-3.15	
3261./ !*2			
C5H4+H=C5H3+H2	1.00E+06	2.50	
5000.0 !Alzqueta et al. 1998			
!***** Reactions of			
CnH2*****			

C4H+H(+M) = C4H2(+M)	1.000E+17	-1.000	
0.00 != C2H +H			
	LOW /	3.750E+33	-4.800
1900.00 /			
	TROE/	0.6464	132.00 1315.00
5566.0 /			

```

C4H+H2=H+C4H2          4.90E+05    2.500
560.00
C4H2+C2H=C6H2+H        9.60E+13    0.0
0.      != C2H2 + C2H HACA
C2H2+C4H=C6H2+H        7.80E+13    0.0
0.      != C2H2 + C2H
C4H+C2H=C6H2           5.00E+13    0.0
0.0     != C2H+C2H
C3H2+C3H2=C6H2+H2      1.00E+13    0.0
0.0     !MODIF
!C6H2+C2H=C8H2+H        9.60E+13    0.0
0.      != C2H2 + C2H HACA
!#####
#####
!##### C4 pour la formation des
aromatiques#####

!***** reactions of C4H6
*****
C2H3+C2H3<=>C4H6        7.00E+57    -13.82
17629.
      PLOG / 2.63e-2          7.00E+57    -13.82
17629. / !USC Mech
      PLOG / 0.12           1.50E+52    -11.97
16056. /
      PLOG / 1.0            1.50E+42    -8.84
12483. /
IC3H7+C2H2=C4H6+CH3     2.770E+10    0.0
6504.0 ! (88TSA)
C4H6 = C4H4+H2           2.50E+15    0.0
94700. !USC Mech II (96HID/HIG)
C4H6 = H2CC+C2H4         1.00E+13    0.0
85000.0 !Est
C4H612+H = C4H6+H        2.00E+13    0.0
4000.   !Estimated
C4H6+H=C4H5-N+H2        5.000E+15    0.0
22800.0 ! (93hiD/hiG)
C4H6+H=C4H5-I+H2        2.500E+15    0.0
22800.0 ! (93hiD/hiG)
C2H4+C2H3=C4H6+H        5.00E+11    0.0    7304
!Tsang 1996
C4H6+H = C3H4-P+CH3      2.00E+12    0.0
7000.   !Estimated USC
C4H6+H = C3H4-A+CH3      2.00E+12    0.0
7000.   !Estimated USC
C4H6+CH3 = C4H5-N+CH4    2.00E+14    0.0
22800.   !96HID/HIG
C4H6+CH3 = C4H5-I+CH4    1.00E+14    0.0
19800.   !96HID/HIG
C4H6+C3H3 = C4H5-N+C3H4-A 1.00E+13    0.0
22500.   !96HID/HIG
C4H6+C3H3 = C4H5-I+C3H4-A 0.50E+13    0.0
19500.   !96HID/HIG
C4H5-I+H=C4H6           1.00E+12    0.0
0.0     !EST
C4H5-N+H=C4H6           1.00E+12    0.0
0.0     !EST
C4H5-N+H(+m)=C4H612(+m) 1.0E0 0.0 0.0

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TCHEB / 300.0 4000.0 / PCHEB / 0.01 100.0 /
CHEB / 7 4 /
CHEB / 0.12963091E+02 0.68936216E+00 -0.14635237E+00
0.25287469E-01/
CHEB / -0.10469090E+01 0.78094522E+00 -0.28031755E-01 -
0.32168604E-01/
CHEB / -0.61132158E+00 0.32224229E+00 0.51871850E-01 -
0.17874012E-01/
CHEB / -0.30035559E+00 0.82704668E-01 0.42510265E-01
0.95307506E-03/
CHEB / -0.12374636E+00 -0.11538350E-02 0.16128529E-01
0.56036263E-02/
CHEB / -0.38226593E-01 -0.16183721E-01 0.12500383E-02
0.30951442E-02/
CHEB / -0.32128918E-02 -0.11586030E-01 -0.26470124E-02
0.58929137E-03/
C4H5-N+H(+m)=C4H6(+m) 1.0E0 0.0 0.0
TCHEB / 300.0 4000.0 / PCHEB / 0.01 100.0 /
CHEB / 7 4 /
CHEB / 0.93415345E+01 -0.10692347E+01 -0.16291075E+00
0.24437127E-01/
CHEB / 0.69292521E+00 0.10598192E+01 -0.23660041E-01 -
0.29908641E-01/
CHEB / -0.36185347E-01 0.38987240E+00 0.50524154E-01 -
0.31823050E-02/
CHEB / -0.13334020E+00 0.81364911E-01 0.17118281E-01
0.13670746E-01/
CHEB / -0.83328821E-01 0.39418106E-02 -0.13086532E-01
0.84330942E-02/
CHEB / -0.33360186E-01 0.19010024E-02 -0.16058069E-01
0.19777740E-03/
CHEB / -0.82554374E-02 0.68296075E-02 -0.80215779E-02 -
0.26272400E-02/
C4H6+OH=C4H5-N+H2O 1.000E+07 2.0
7253.0 !(88LiU/MUL E>*RTi/2.29)
C4H6+OH=C4H5-I+H2O 8.000E+06 2.0
3744.0 !(88LiU/MUL E>*RTi/2.17)
O+C4H6=>CO+C3H6 1.500E+12 0.000
0.0 !ranzi 20131016
C4H6=C2H4+C2H2 1.000E+87 -20.85
132930 !2000 Tsang C4H6 mechanism /30 for pressure falloff
C4H6=C4H612 8.190E+74 -17.56
115782 !2000 Tsang C4H6 mechanism
C4H6-2 = C4H6 0.600E+13 0.000
65000. !96HID/HIG 3.00E+13
C4H6-2 = C4H612 0.600E+13 0.000
67000. !96HID/HIG 3.00E+13
C4H6-2+H = C4H612+H 2.000E+13 0.0
4000. !USC Mech II (Estimated)
C4H6-2+H =CH3+C3H4-P 2.600E+05 2.500
1000. !96HID/HIG 2.60E+5
C4H6-2 =H+C4H5-2 2.000E+14 0.000
87300. !96HID/HIG 5.00E+15
C4H6-2+CH3 = C4H5-2+CH4 1.400E+14 0.0
18500. !USC Mech II (Estimated)
C4H6-2+H = C4H5-2+H2 3.400E+05 2.5
2490. !USC Mech II (= C3H6+H )

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!***** reactions of C4H612
*****
C4H612+H=C3H3+CH4          1.00E+13      0.0
0.0
C4H612+H=C2H3+C2H4          4.00E+11      0.0
0.0
C3H3+CH3 (+M) = C4H612 (+M)  1.50E+12      0.0
0.0      !97WAN/FRE
                                LOW / 2.60E+57      -11.94
9770.0 /
                                TROE /0.175 1340.6 60000.0
9769.8 /
                                H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/
C2H6/3.0/ AR/0.7/
C4H612+H = C3H4-A+CH3          2.00E+13      0.0
2000.      !97WAN/FRE
C4H612+H = C3H4-P+CH3          2.00E+13      0.0
2000.      !97WAN/FRE
C4H612+CH3=C4H5-I+CH4          2.20E+00      3.5
5700
C4H612+H = C4H5-I+H2          3.16E+06      2.5
6756      !Ref C6H12+H=SAXC6H11+H2 in 2009 Kiefer et al.
C4H612+H = C4H5-N+H2          1.16E+06      2.5
6756      !Ref C6H12+H=SAXC6H11+H2 in 2009 Kiefer et al.
C4H5-I+H =C4H612              5.00E+13      0.0
5000.0    !USC Mech II
C4H612+O = CH2CO+C2H4          1.20E+08      1.65
327.      != C3H6+O
C4H612+O = C4H5-I+OH          1.80E+11      0.70
5880.      != C3H6+O
C4H612+OH = C4H5-I+H2O          3.10E+06      2.00      -
298.      != C3H6+OH
!***** reactions of
C4H5*****
C4H5-N = C4H5-I                2.40E+60      -16.08
47500.    !USC Mech II
          PLOG/ 0.013          2.40E+60      -16.08
47500./  !USC Mech II
          PLOG/ 0.026          1.30E+62      -16.38
49600./  !USC Mech II
          PLOG/ 0.118          4.90E+66      -17.26
55400./  !USC Mech II
          PLOG/ 1.000          1.50E+67      -16.89
59100./  !USC Mech II
          PLOG/ 10.00          2.00E+60      -14.46
58600./  !USC Mech II
C4H5-N +H = C4H5-I +H          1.00E+36      -6.26
17486.    !RRKMWAN/FRE
          PLOG/ 0.026          1.00E+36      -6.26
17486./  !RRKMWAN/FRE
          PLOG/ 0.118          1.00E+34      -5.61
18476./  !RRKM WAN/FRE
          PLOG/ 1.000          3.10E+26      -3.35
17423./  !RRKM WAN/FRE
C2H3+C2H2 = C4H5-N            1.320e+12      0.160
8312.62   !Pitsch 20131205
C2H3+C2H2 = C4H4+H            7.20E+13      -0.48
6100.     !RRKM WAN/FRE

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PLOG/ 0.013	7.20E+13	-0.48	
6100./			
PLOG/ 0.026	5.00E+14	-0.71	
6700./			
PLOG/ 0.118	4.60E+16	-1.25	
8400./			
PLOG/ 1.000	2.00E+18	-1.68	
10600./			
PLOG/ 10.00	4.90E+16	-1.13	
11800./			
C2H2+C2H3+M=C4H5-I+M	7.630E+40	-7.760	
12000.0			
C4H4+H=C4H5-I	6.10E+53	-13.19	
14200. !RRKM WAN/FRE			
PLOG/ 0.013	6.10E+53	-13.19	
14200./			
PLOG/ 0.026	9.60E+52	-12.85	
14300./			
PLOG/ 0.118	2.10E+52	-12.44	
15500./			
PLOG/ 1.000	4.90E+51	-11.92	
17700./			
PLOG/ 10.00	1.50E+48	-10.58	
18800./			
OH+C4H4=>CO+C3H5-A	3.00E+13	0.00	0.0
!			
C4H4+H = C4H5-N	1.20E+51	-12.57	
12300. !RRKM WAN/FRE			
PLOG/ 0.013	1.20E+51	-12.57	
12300./			
PLOG/ 0.026	4.20E+50	-12.34	
12500./			
PLOG/ 0.118	1.10E+50	-11.94	
13400./			
PLOG/ 1.000	1.30E+51	-11.92	
16500./			
PLOG/ 10.00	6.20E+45	-10.08	
15800./			
C2H3+C2H3<=>C4H5-I+H	1.50E+30	-4.95	
12958.			
PLOG / 2.63E-2	1.50E+30	-4.95	12958.
/			
PLOG / 0.12	7.20E+28	-4.49	14273.
/			
PLOG / 1.0	1.20E+22	-2.44	13654.
/			
C2H3+C2H3<=>C4H5-N+H	1.10E+24	-3.28	
12395.			
PLOG / 2.63E-2	1.10E+24	-3.28	12395.
/			
PLOG / 0.12	4.60E+24	-3.38	14650.
/			
PLOG / 1.0	2.40E+20	-2.04	15361.
/			
C4H5-I+H = C4H4+H2	3.0E+13	0.00	
0. !USC Mech II (97WAN/FRE)			

C4H5-I+H = C3H3+CH3	2.00E+13	0.0	
2000. !USC Mech II (Estimated)			
C4H5-2=C4H4+H	3.33E+20	-3.125	
47560 !EST			
C4H5-N+OH = C4H4+H2O	2.00E+12	0.00	
0. !97WAN/FRE			
C4H5-N+HCO = C4H6+CO	5.00E+12	0.0	
0. !97WAN/FRE			
C4H5-N+HO2 = C2H3+CH2CO+OH	6.60E+12	0.0	
0. !97WAN/FRE			
C4H5-N+H2O2 = C4H6+HO2	1.21E+10	0.0	-
596. !97WAN/FRE			
C4H5-N+HO2 = C4H6+O2	6.00E+11	0.0	
0. !Estimated			
C4H5-N+O2 = HCO+C2H3CHO	9.20E+16	-1.39	
1010. != C2H3+O2=>HCO+CH2O			
C4H5-I+OH<=>C4H4+H2O	4.0E+12	0.00	
0.			
C4H5-I+HCO<=>C4H6+CO	5.00E+12	0.0	
0.			
C4H5-I+HO2<=>C4H6+O2	6.000E+11	0.00	
0.			
C4H5-I+HO2=>C2H3+CH2CO+OH	6.60E+12	0.0	
0.			
C4H5-I+H2O2<=>C4H6+HO2	1.21E+10	0.000	
-596.			
C4H5-I+O2<=>CH2CO+CH2CHO	2.16E+10	0.00	
2500.			
O2+C4H5-I=>C2H3CHO+HCO	2.500E+13	0.000	
15000.0 !ranzi			
C4H5-I+O2=C3H4-A+CO+OH	5.000E+12	0.0	
15000.0			
C4H5-I+O2=C3H4-P+CO+OH	5.000E+12	0.0	
15000.0			
C4H5-N+C4H4 =A1C2H3+H	3.16E+11	0.0	
600. !84COL/BIT			
OH+P-C6H4O2=>H2O+C2H2+C2H+CO+CO	.1398E+08	2.0	
2076.14 !20131021			
!***** Reaction of C4H4 *****			
H2CC+C2H2 (+M) = C4H4 (+M)	3.50E+05	2.055	-
2400. !USC Mech II (99LAS/WAN)			
	LOW /1.40E+60	-12.599	
7417. /			
	TROE /0.98 560.	580.	4164.
/			
H2/2.0/ CH4/2.0/ H2O/6.0/ C2H2/3.0/ CO/1.5/			
C2H4/3.0/ C2H6/3.0/ CO2/2.0/			
C2H3+C2H = C4H4	1.00E+14	0.00	0.
!1988 Duran			
C3H5-A+CH = C4H4+H2	1.00E+13	0.0	
0.0			
C3H3+CH2 (S) = C4H4+H	4.00E+13	0.0	
0.0 !2007 Gueniche & Glaude & Fournet & Battin			
C4H4+H = nC4H3+H2	6.65E+05	2.53	
12240. !USC Mech II (97WAN/FRE)			

C4H4+H = iC4H3+H2	3.33E+05	2.53	
9240. !USC Mech II (97WAN/FRE)			
C3H3+CH2=C4H4+H	5.00E+13	0.00	0.
!2007 Gueniche & Glaude & Fournet & Battin(1992 Miller)			
C3H2+CH3=C4H4+H	5.00E+12	0.00	0.
!USC Mech II			
C4H4+OH = nC4H3+H2O	3.10E+07	2.0	
3430. !97WAN/FRE			
C4H4+OH = iC4H3+H2O	1.55E+07	2.0	
430. !97WAN/FRE			
C4H4+O2=nC4H3+HO2	1.000E+13	0.00	
63200.0 !(Est Walker95)			
C4H4+O2=iC4H3+HO2	1.000E+13	0.00	
44640.0 !(Est Walker95)			
!Nicolas Delort ! C4H4+HO2=nC4H3+H2O2			
2.000E+11 0.00 12600.0 !(Estc4h6)			
C4H4+HO2=iC4H3+H2O2	1.000E+11	0.00	
9920.0 !(Estc4h6)			
C4H4+HO2=C3H3+HCO+OH	4.000E+11	0.00	
8000.0 !(=C2H4+HO2*2)			
C4H4+O = C3H3+HCO	6.000E+08	1.450	-
860 ! = C4H6+O			
!***** reactions of C4H3			

C2H2+C2H(+M) = nC4H3(+M)	8.30E+10	0.899	-
363.00 !USC Mech II (92WAN)			
	LOW /1.240E+31	-4.718	
1871.00 /			
	TROE /1.0 100.	5613.	
13387. /			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/ C2H6/3.0/			
		C2H2/2.5/	
C2H4/2.5/			
C2H2+C2H(+M) = iC4H3(+M)	8.30E+10	0.899	-
363.00 !USC Mech II (92WAN)			
	LOW /1.240E+31	-4.718	
1871.00 /			
	TROE /1.0 100.	5613.	
13387. /			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/ C2H6/3.0/			
C2H2/2.5/ C2H4/2.5/			
C3H3+CH = nC4H3+H	5.00E+13	0.0	
0.0 !USC Mech II (Estimated)			
C3H3+CH = iC4H3 +H	5.00E+13	0.0	
0.0			
C2H2+C2H = C4H2+H	9.60E+13	0.00	
0.00 !USC Mech II (91SHI/MIC, 92KOS/FUK, 93FAR/MOR)			
C2H2+C2H2=C4H4	1.89E58	-13.60	
62790.0 !MIT W.H. Green 1.89E58			
C3H2+CH2 = nC4H3+H	5.00E+13	0.0	0.
!USC Mech II (92MIL/MEL)			

```

C2H2+C2H2 = C4H2+H2                1.50E+13    0.0
42700    !2007 Gueniche & Glaude & Fournet & Battin(Leung 95) 13

!***** reactions of C4H2
*****
C4H2 +H = nC4H3                1.70E+49   -11.67
12804.0    !RRKM WAN/FRE
           plog/0.026                1.70E+49   -11.67
12804.0/    !0.026 atm RRKM WAN/FRE
           plog/0.118                3.30E+50   -11.80
15010.0/    !0.118 atm RRKM WAN/FRE
           plog/1.00                 1.10E+42    -8.72
15300.0/    !1 atm RRKM WAN/FRE
C4H2 +H = iC4H3                4.30E+45   -10.15
13250.0    !RRKM WAN/FRE
           plog/0.026                4.30E+45   -10.15
13250.0/    !0.026 atm RRKM WAN/FRE
           plog/0.118                2.60E+46   -10.15
15500.0/    !0.118 atm RRKM WAN/FRE
           plog/1.00                 1.10E+30    -4.92
10800.0/    !1 atm RRKM WAN/FRE
C4H2 +OH=CO + C3H3            2.11E+23   -3.47      3820
!J.P. Senosiain and S.J. Klippenstein and J.A. Miller 2007
C4H2 +OH=H2C4O+H              8.19E+16   -1.59      2116
!J.P. Senosiain and S.J. Klippenstein and J.A. Miller 2007 8.19E+16
H2C4O+H<=>C2H2+HCCO           5.00E+13    0.0
3000.0    !J.A. MILLER 92
H2C4O+OH<=>CH2CO+HCCO         1.00E+07    2.0
2000.0!    !J.A. MILLER 92
C4H2+O=C3H2+CO                1.200E+12   0.0      0.0
!J.A. MILLER 89
iC4H3+H<=>C2H2+H2CC           2.80E+23   -2.55
10780.0    !J.A. MILLER 92
iC4H3+OH = C4H2+H2O           4.00E+12   0.00      0.
!= C2H3+OH
iC4H3+O2 = HCCO+CH2CO         7.86E+16   -1.80      0.
!89SLA/BER
iC4H3+CH2<=>C3H4-A+C2H        2.0E+13    0.0
0.0    !ziegler et al. j. anal.apply.pyrolysis 73 212-230 (2005)
!*****reactions des blocs C3 de Cai impliquant des C4
d'interet*****

C3H6+C2H3 = C4H6+CH3          7.23E+11    0.0
5000.0    !91TSA
C3H5-A+CH2=C4H6+H             3.000E+13   0.00
0.0    ! (91TSA)
O+A1O=>2CO+C4H5-I             .1000E+15   .000
.0
C3H3+HCCO = C4H4+CO           2.50E+13    0.0
0.0    !Estimated
C3H2+CH=C4H2+H                5.00E+13    0.0
0.0
C3H2+HCCO=nC4H3+CO            1.00E+13    0.0
0.0

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#####
#####
##### Submechanism of PAH
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!*****
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A1C2H-=C6H3C2H+H          6.11E+45   -8.857
94350.6      !1997 Madden et al. RRKM A1-=o-C6H4+H
  plog /    0.500          6.11E+45   -8.857
94350.6/
  plog /    1.000          8.00E+41   -7.72
92300.3/
  plog /   10.000          1.66E+30   -4.318
85756.9/
A1C2H-=C6H3+C2H2          3.55E+78  -17.787
137467.2     !1997 Madden et al. RRKM A1-=nC4H3+C2H2
  plog /    0.500          3.55E+78  -17.787
137467.2/
  plog /    1.000          3.92E+74  -16.6
135581.1/
  plog /   10.000          1.79E+61  -12.663
128678.3/
A1C2H-+H=C6H3C2H+H2      4.40E-13    7.831
9261.0       !2001 Mebel et al. A1-+H=o-C6H4+H2
A1C2H-=nC4H3+C4H2        3.55E+78  -17.787
137467.2     !1997 Madden et al. RRKM A1-=nC4H3+C2H2
  plog /    0.500          3.55E+78  -17.787
137467.2/
  plog /    1.000          3.92E+74  -16.6
135581.1/
  plog /   10.000          1.79E+61  -12.663
128678.3/
C6H3C2H=C4H2+C4H2        1.95E+90  -21.3
139396.2     !refer to 1999 Moskaleva et al. o-C6H4=C4H2+C2H2
  PLOG /   0.1315          1.95E+90  -21.3
139396.2/
  PLOG /   1.0000          2.07E+85  -19.6
138901.4/
  PLOG /   5.000          7.89E+75  -16.8
134903.4/
  PLOG /  10.0000          7.89E+75  -16.8
134903.4/

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!***** Reactions of A1C2H (Phenylacetylene)
*****

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A1C2H-+H(+M)=A1C2H(+M)          1.00E+14    0.0
0.0      !1997 Wang&Frenklach A1-+H(+M)=A1(+M) in 1997 Wang&Frenklach
          LOW / 6.60E+75  -16.30
7000.0/
          TROE/ 1.0    0.1    584.9
6113.0/
          H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/
C2H6/3.0/
!Nicolas Delort!

```

!A1C2H(+m)=A1-+C2H(+m) 7.80e+27 -3.16
1.07447e+05 !estimated from Klippenstein 2007
!
! LOW/4.00E+98 -22.966
1.2208E+05/
!
! TROE/7.054562E-01 9.999989E+09
4.599180E+02 8.213938E+09/

A1-+C2H=A1C2H 1.20E+27 -4.22 7200.0
!Nicolas Delort from Yuan 2019 on anisole - Refer to A1-+C2H3=A1C2H3
1997 Wang&Frenklach RRKM
plog / 0.0263 1.90E+48 -10.52
17489.0/
plog / 0.1184 3.90E+38 -7.63
12900.0/
plog / 1.0000 1.20E+27 -4.22
7200.0/

A1C2H(+M)=A1CC+H(+M) 2.78E+15 0.17 9.1168E+04
!estimated from 2007 Klippenstein et al. A1CH3(+M) = A1CH2+H(+M)
LOW/1.00E+98 -22.855
9.9882E+04/
TROE/6.547194E-02 1.511253E+01
9.999996E+09 7.596123E+07/

A1C2H+H=A1cC2H2+H 2.30E+15 -0.26
7600.0 !1999 Davis et al. C3H4-P+H=C3H4-A+H 0.1atm
A1C2H+OH=CH2CO+A1- 1.10E+13 0.0
7170.0 !refer to 2007 Coppens et al. C2H2+OH=CH2CO+H
A1C2H+OH=A1+HCCO 1.000e+13 0.000
0.00
A1C2H+O=HCCO+A1- 1.63E+07 2.0
1900.0 !GRI C2H2+O=HCCO+H in 2011 Li et al.(Toluene)

A1+C2H=A1C2H+H 5.00E+13 0.0
0.0 !1997 Wang&Frenklach
A1C2H+H=A1CC+H2 2.50E+14 0.0
16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in 1997 Wang&Frenklach

A1C2H+H=A1C2H-+H2 1.084e17 -0.70
20011.2 !ref A1+H=A1-+H2 *5/6
A1C2H+OH=A1C2H-+H2O 2.11E+13 0.0
4571.0 !1985 Madronich&Felder A1+OH=A1-+H2O in 2002 Richter&Howard

A1C2H+O=A1CH+CO 3.60E+12 0.0
633.0 !1994 Eichholtz et al.
A1-+C2H2=A1C2H+H 2.66E+32 -5.3
23786.9 !I.V. Tokmakov, M.C. Lin, J. Am. Chem. Soc. 125(2003) 11397-
11408.
A1-+C4H4=A1C2H+C2H3 3.20E+11 0.0
1350.0 !1988 Harris et al.
C4H5-N+C4H2=A1C2H+H 3.16E+11 0.0
1800.0 !1984 Cole et al.

!***** Reactions of A1C2H2

A1-+C2H3=A1CCH2+H		1.80E+31	-4.63
31652.	!1997 Wang&Frenklach RRKM		
PLOG/ 0.026		1.80E+31	-4.63
31652./			
PLOG/ 0.118		5.80E+18	-1.00
26852./			
PLOG/ 1.000		8.50E-02	4.71
18424./			
A1-+C2H3=A1CHCH+H		1.50E+32	-4.91
35504.	!1997 Wang&Frenklach RRKM		
PLOG/ 0.026		1.50E+32	-4.91
35504./			
PLOG/ 0.118		5.10E+20	-1.56
31412./			
PLOG/ 1.000		9.40E+00	4.14
23234./			
A1CHCH+H=A1CCH2+H		2.30E+37	-6.00
35164.	!1997 Wang&Frenklach RRKM		
PLOG/ 0.026		2.30E+37	-6.00
35164./			
PLOG/ 0.118		1.20E+25	-2.42
30530./			
PLOG/ 1.000		9.90E+04	3.37
22040./			
A1-+C2H2=A1CHCH		7.70E+40	-9.19
13400.0	!1994 Wang&Frenklach RRKM		
plog / 0.0132		4.00E+39	-8.94
12000.0/			
plog / 0.0263		7.70E+40	-9.19
13400.0/			
plog / 0.1184		9.90E+41	-9.26
15700.0/			
plog / 1.0000		7.00E+38	-8.02
16400.0/			
plog / 10.0000		7.90E+29	-5.15
13700.0/			
A1CHCH+O2=A1CHO+HCO		4.60E+16	-1.39
1010.0	!1996 Mebel et al. C2H3+O2=HCO+CH2O		
A1CCH2+O2=A1CO+CH2O		4.60E+16	-1.39
1010.0	!1996 Mebel et al. C2H3+O2=HCO+CH2O		
A1CCH2+OH=A1CHO+CH2		4.00E+07	1.83
220.0	!1994 Wang&Frenklach		
A1C2H+H=A1CHCH		1.00E+54	-12.76
17185.0	!1997 Wang&Frenklach RRKM		
plog / 0.0263		1.00E+54	-12.76
17185.0/			
plog / 0.1184		1.20E+51	-11.69
17300.0/			
plog / 1.0000		3.00E+43	-9.22
15300.0/			
A1C2H+H=A1CCH2		1.00E+54	-12.76
17185.0	!1997 Wang&Frenklach RRKM A1C2H+H=A1CCH2 in 1997		
Wang&Frenklach			
plog / 0.0263		1.00E+54	-12.76
17185.0/			
plog / 0.1184		1.20E+51	-11.69
17300.0/			


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plog / 1.0000          3.00E+43   -9.22
15300.0/
A1CHCH+H=A1C2H+H2          3.00E+13    0.0
0.0      !GRI C2H3+H=C2H2+H2in 1997 Wang&Frenklach
A1CCH2+H=A1C2H+H2          3.00E+13    0.0
0.0      !GRI C2H3+H=C2H2+H2 in 1997 Wang&Frenklach
A1CHCH+OH=A1C2H+H2O        5.00E+12    0.0
0.0      !GRI C2H3+OH=C2H2+H2O in 1997 Wang&Frenklach
A1CCH2+OH=A1C2H+H2O        5.00E+12    0.0
0.0      !GRI C2H3+OH=C2H2+H2O in 1997 Wang&Frenklach
A1CCH2+O=CH2CO+A1-          4.80E+13    0.0
0.0      !1986 Tsang&Hampson C2H3+O=CH2CO+H
A1CHCH=O-C6H4C2H3          6.40E+61   -14.59
88200.0      !1999 Davis et al. C3H4-P=C3H4-A
plog / 0.100          6.40E+61   -14.59
88200.0/
plog / 0.400          5.81E+62   -14.63
91211.0/
plog / 1.000          5.15E+60   -13.93
91117.0/
plog / 2.000          7.64E+59   -13.59
91817.0/
plog / 5.000          3.12E+58   -13.07
92680.0/
plog / 10.000         1.90E+57   -12.62
93300.0/
plog /100.000         1.40E+52   -10.86
95400.0/
A1CHCH+H=O-C6H4C2H3+H      2.30E+37    -6.00
35164.0      !1997 Wang&Frenklach A1CHCH+H=A1CCH2+H
O-C6H4C2H3=o-C6H4+C2H3      6.11E+45    -8.857
94350.6      !1997 Madden et al. RRKM A1-==o-C6H4+H
plog / 0.500          6.11E+45    -8.857
94350.6/
plog / 1.000          8.00E+41    -7.72
92300.3/
plog / 10.000         1.66E+30    -4.318
85756.9/
O-C6H4C2H3=P-C6H4C2H3      1.42e14     0.0
65042      ! Nicolas Delort from Enoch Dames & Hai Wang 2013 PCI34
!***** Reactions of A1C2H3
*****
O-C6H4C2H3+H(+M)=A1C2H3(+M) 1.00E+14     0.0
0.0      !1997 Wang&Frenklach A1-+H(+M)=A1(+M)
LOW / 6.60E+75   -16.30
7000.0/
TROE/ 1.0    0.1    584.9
6113.0/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/
C2H6/3.0/
P-C6H4C2H3+H(+M)=A1C2H3(+M) 1.00E+14     0.0
0.0      !1997 Wang&Frenklach A1-+H(+M)=A1(+M)
LOW / 6.60E+75   -16.30
7000.0/
TROE/ 1.0    0.1    584.9
6113.0/

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H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/		
C2H6/3.0/		
A1+C2H3=A1C2H3+H	7.90E+11	0.0
6400.0 !1989 Fahr&Stein		
A1+C2H4=A1C2H3+H	2.51E+12	0.0
6190.0 !1989 Fahr&Stein in 1997 Wang&Frenklach		
A1+C2H3=A1C2H3	1.90E+48	-10.52
17489.0 !1997 Wang&Frenklach RRKM		
plog / 0.0263	1.90E+48	-10.52
17489.0/		
plog / 0.1184	3.90E+38	-7.63
12900.0/		
plog / 1.0000	1.20E+27	-4.22
7200.0/		
C5H5+C3H3=A1C2H3	9.92E+66	-15.9
27529.0 !2009 Hansen et al. C3H3+C3H3=A1 1.64E+66*3		
DUPLICATE		
C5H5+C3H3=A1C2H3	1.20E+35	-7.4
5058.0 !2009 Hansen et al. C3H3+C3H3=A1		
DUPLICATE		
C4H4+C4H4=A1C2H3	1.50E+14	0.0
38000.0 !1984 Lundgard&Heicklen		
A1C2H3=A1CCH2+H	1.20E+46	-9.07
118323.0 !1997 Wang&Frenklach RRKM		
plog / 0.0263	1.20E+46	-9.07
118323.0/		
plog / 0.1184	3.80E+37	-6.55
114200.0/		
plog / 1.0000	5.30E+27	-3.63
109300.0/		
A1C2H3+H=A1CCH2+H2	3.33E+05	2.53
9240.0 !HACA		
A1C2H3+OH=A1CCH2+H2O	1.55E+06	2.0
430.0 !HACA		
A1C2H3=A1CHCH+H	1.90E+54	-11.39
130224.0 !1997 Wang&Frenklach RRKM		
plog / 0.0263	1.90E+54	-11.39
130224.0/		
plog / 0.1184	1.30E+44	-8.36
125400.0/		
plog / 1.0000	1.10E+32	-4.77
119500.0/		
A1C2H3+H=A1CHCH+H2	6.65E+05	2.53
12240.0 !GRI C2H4+H=C2H3+H2 in 1997 Wang&Frenklach		
A1C2H3+OH=A1CHCH+H2O	6.20E+06	2.0
3430.0 !1997 Wang&Frenklach C4H6+OH=C4H5-N+H2O in 1997 Wang&Frenklach		
A1C2H3+O=A1CHCH+OH	1.51E+07	1.90
3740.0 !1987 Mahmud et al. C2H4+O=C2H3+OH		
A1C2H3+O=A1CCH2+OH	1.51E+07	1.90
3740.0 !1987 Mahmud et al. C2H4+O=C2H3+OH		
A1C2H3+O=A1CH2+HCO	1.92E+07	1.83
220.0 !1987 Mahmud et al. C2H4+O=CH3+HCO		
A1C2H3+O=A1CO+CH3	1.92E+07	1.83
220.0 !1987 Mahmud et al. C2H4+O=CH3+HCO		
A1C2H3+O=A1CHO+CH2	3.84E+05	1.83
220.0 !1987 Mahmud et al. C2H4+O=CH2+CH2O		

!***** Reactions of AlC2H4

*
 AlC2H3+H(+M)=AlCHCH3(+M) 1.367E+09 1.463
 1355.0 !2004 Miller&Klippenstein C2H4+H(+M)=C2H5(+M)
 LOW / 2.027E+39 -6.642
 5769.0/
 TROE/-0.569 299.0 9147.0 -
 152.4/
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
 AR/0.7/
 AlC2H3+H(+M)=AlCH2CH2(+M) 1.367E+09 1.463
 1355.0 !2004 Miller&Klippenstein C2H4+H(+M)=C2H5(+M)
 LOW / 2.027E+39 -6.642
 5769.0/
 TROE/-0.569 299.0 9147.0 -
 152.4/
 H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/
 AR/0.7/
 AlCH2CH2=C2H4+Al- 7.1E+14 0.0
 43500.0 !bounaceur et al Int J Chem Kinet 37: 25-49, 2005
 AlCHCH3=AlCH2CH2 6.40E+61 -14.59
 88200.0 !1999 Davis et al. C3H4-P=C3H4-A
 plog / 0.100 6.40E+61 -14.59
 88200.0/
 plog / 0.400 5.81E+62 -14.63
 91211.0/
 plog / 1.000 5.15E+60 -13.93
 91117.0/
 plog / 2.000 7.64E+59 -13.59
 91817.0/
 plog / 5.000 3.12E+58 -13.07
 92680.0/
 plog / 10.000 1.90E+57 -12.62
 93300.0/
 plog /100.000 1.40E+52 -10.86
 95400.0/
 Al-+C4H6=AlC2H3+C2H3 3.20E+11 0.0
 1900.0 !1988 Harris et al.
 AlCHCH3+O2=AlC2H3+HO2 7.0E+11 0.0
 15000.0 !Bounaceur et al 2005
 AlCH2CH2+O2=AlC2H3+HO2 1.5E+12 0.0
 5000.0 !Bounaceur et al 2005
 AlCHCH3+HO2=AlCHO+CH3+OH 5.0E+12 0.0 0.0
 !Bounaceur et al 2005
 AlCH2CH2+HO2=AlCH2+CH2O+OH 5.0E+12 0.0 0.0
 !Bounaceur et al 2005
 AlCHCH3+HO2=AlCHCH3OOH 0.72E12 0.0 0.0
 !MF KINGAS 3.60E12
 AlCHCH3OOH=OH+AlCHCH3O 5.00E15 0.0 42500
 !MF
 AlCHCH3O=Al-+CH3CHO 1.74E14 0.0 20458

!***** Reactions of AlC2H5

A1C2H5 (+m) = A1CHCH3+H (+m)	2.78e+15	0.17
9.1168e+04 !		
	LOW/	1.00E+98 -22.855
9.9882E+04/		
	TROE/	6.547194E-02 1.511253E+01
9.999996E+09 7.596123E+07/		
A1C2H5 (+m) = A1-+C2H5 (+m)	1.95E+27	-3.16
1.07447E+05		
	LOW/	1.00E+98 -22.966
1.2208E+05/		
	TROE/	7.054562E-01 9.999989E+09
4.599180E+02 8.213938E+09/		
A1CH2CH2+H (+M)=A1C2H5 (+M)	5.21E+17	-0.990
1580.0 !GRI3.0 C2H5+H (+M)=C2H6 (+M)		
	LOW /	1.99E+41 -7.080
6685.0/		
	TROE/	0.8422 125.0 2219.00
6882.0/		
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/	
CO2/2.0/ C2H6/3.0/ AR/0.7/		
A1CH2+CH3 (+M)=A1C2H5 (+M)	6.120E+16	-0.970
620.00 != CH3+CH3 (+M)=C2H6 (+M)		
	LOW /	1.770E+50 -9.670
6220.0/ !		
	TROE/	0.5325 151.0 1038.00
4970.0/		
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/ C2H6/3.0/	
AR/0.7/		
A1CH2+CH3=A1CHCH3+H	1.730e+039	-7.2310
35366.0 ! Miyoshi 2012		
	rev /	2.210e+039 -6.8522
24335.7 /		
A1CH2+CH3=A1CH2CH2+H	6.348e+032	-5.1046
40697.1 ! Miyoshi 2012		
	rev /	1.169e+031 -4.6094
14826.4 /		
A1CH2+CH3=A1-+C2H5	2.028e+033	-5.2232
40498.3 ! Miyoshi 2012		
	rev /	3.313e+032 -5.4269
14897.5 /		
A1CHCH3+H=A1CH2CH2+H	1.614e+024	-2.5623
29906.1 ! Miyoshi 2012		
	rev /	2.325e+022 -2.4459
15065.6 /		
A1CHCH3+H=A1-+C2H5	5.150e+024	-2.6808
29738.4 ! Miyoshi 2012		
	rev /	6.584e+023 -3.2634
15168.0 /		
A1CH2CH2+H=A1-+C2H5	6.974e+014	0.0003
17190.1 ! Miyoshi 2012		
	rev /	6.181e+015 -0.6985
17459.8 /		
A1C2H5+OH=A1OH+C2H5	7.83E+02	2.880
3221.8 !2006 Seta et al. A1CH3+OH=A1OH+CH3		
A1C2H5+H=A1CHCH3+H2	3.31E+07	2.0
5345.3 !2005 Baulch et al.		
A1C2H5+H=A1CH2CH2+H2	7.22E+08	1.50
7412.0 !2005 Baulch et al.		

A1C2H5+CH3=A1CHCH3+CH4		1.1E+12	0.0	
9100.0	!Bounaceur et al 2005	Int J Chem Kinet 37: 25-49		
A1C2H5+CH3=A1CH2CH2+CH4		0.3	4.0	
8200.0	!Bounaceur et al 2005	Int J Chem Kinet 37: 25-49		
A1C2H5+OH=A1CHCH3+H2O		3.5E9	1.0	-1.13E3
	!battin 2013			
A1C2H5+OH=A1CH2CH2+H2O		3.6E6	2.0	
4.82E2	!MF correlation	Dean-Bozzelli 2000		
A1C2H5+O=A1CHCH3+OH		3.9E+9	1.0	-
1100.0	!Bounaceur et al 2005			
A1C2H5+O=A1CH2CH2+OH		5.1E+13	0.0	
7800.0	!Bounaceur et al 2005			
A1C2H5+H=A1+C2H5		1.20E+13	0.0	
5100.0	!Ergut et al 2006	Combustion and Flame 144 (2006)	757-772	
A1C2H5+H=C6H4C2H5+H2		1.93E+07	2.00	
9697.0	!2005 Baulch et al.			
A1C2H5+HO2=A1CHCH3+H2O2		6.80E+03	2.50	
10114.0	!2005 Baulch et al.			
A1C2H5+HO2=A1CH2CH2+H2O2		3.55E+04	2.50	
16851.0	!2005 Baulch et al.			
A1C2H5+HO2=C6H4C2H5+H2O2		1.81E+04	2.50	
27621.0	!2005 Baulch et al.			
A1C2H5+O2=A1CHCH3+HO2		1.81E+12	0.0	
39740.0	!Ergut et al 2006			
A1C2H5+O2=A1CH2CH2+HO2		1.2E+13	0.0	
49000.0	!Bounaceur et al 2005			
!***** Reactions of benzofuran				

A1O+C2H2=>C8H6O+H		0.4E+10	0.0	460
	!est			
C8H8O+H=A1O+C2H4		5.67E+8	1.43	
5650	!as A1CH3+H			
H+C8H7O=C8H8O		1.0E+14	0.0	0
C8H8O+H=C8H7O+H2			9.6E+6	
2.0	5000	!AS EB		
C8H8O+O=C8H7O+OH			1.6E+13	
0.0	5200	!AS EB		
C8H8O+OH=C8H7O+H2O			2.6E+6	
2.0	-770	!AS EB		
C8H8O+CH3=C8H7O+CH4		2.0E+11	0.0	
	9600	!AS EB		
C8H8O+H=C8H7O-1+H2			8.0E+13	
0.0	6400	!AS EB		
C8H8O+O=C8H7O-1+OH			4.2E+11	
0.0	-2.0	!AS EB		
C8H8O+OH=C8H7O-1+H2O			3.5E+9	
1.0	-1130	!AS EB		
C8H8O+CH3=C8H7O-1+CH4		1.1E+12	0.0	
	9100	!AS EB		
C8H7O=C8H6O+H		3.30E+10	0.885	
35770	!as indanyl=indene+H			
H+C8H7O-1=C8H8O		1.0E+14	0.0	0
C8H7O-1=C8H6O+H		1.21E+11	0.985	
42200	!as indanyl=indene+H			

C8H7O+O2=C8H6O+HO2	1.58E+12	0.0	
5000 !as indanyl			
C8H7O-1+O2=C8H6O+HO2	1.58E+12	0.0	
15200 !as indanyl			
C8H6O+OH=>O-C6H4CH3+CO2	1.37E+12	0.0	-
1040 !add on double bond!			
C8H6O+OH=>A1CO+CH2O	1.37E+12	0.0	-
1040			
C8H6O+O=>A1CO+CO+H	6.00E+4	2.56	-
1130			

!***** Reactions of C9H7(indenyl) and C9H8(indene)

!Nicolas Delort!A1-+C3H3=C9H7+H			2.0e13
0.0 0.0 ! est.			

C5H5+C4H2=C9H7	2.0e13	0.0	
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10000.0 ! est.

C9H7+H(+M)=C9H8(+M)	1.00E+14	0.0	
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0.0 !USC Mech II C5H5+H(+M)=C5H6(+M)

LOW / 4.40E+80 -18.280

12994.0/

TROE/ 0.068 400.7 4135.8

5501.9/

H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/

CO2/2.0/			
C9H7+H2=>C9H8+H	1.000E+12	.000	

13000.0 !E.ranzi

H+C9H8=>H2+C9H7	1.444E+07	2.0	
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4212.94 !Ranzi

C9H8+O=C9H7+OH	4.77E+04	2.7	
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2105.6 !2009 Blanquart et al.

C9H8+OH=C9H7+H2O	3.08E+06	1.6	-
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35.9 !2009 Blanquart et al.

C9H8+HCO=C9H7+CH2O	1.08E+08	1.9	
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15999.0 !2009 Blanquart et al.

C9H8+CH3=C9H7+CH4	1.80E-01	4.0	
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456.5 !2009 Blanquart et al.

C9H8+HO2<=>C9H7+H2O2	1.100e+04	2.600	
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12899.14

C9H8+O2<=>C9H7+HO2	4.000e+13	0.000	
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49639.10

C9H8+O=>C9H6O+2H	6.65E+12	-0.1	
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360.9 !2009 Blanquart et al.

C9H7+O<=>C9H6O+H	2.80E+13	0.0	
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0.0 !2009 Blanquart et al.

C9H7+HO2=>C9H6O+H+OH	1.31E+29	-4.7	
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11649.1 !2009 Blanquart et al.

C9H7+O=A1CHCH+CO	1.00E+14	0.0	
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0.0 !1996 Marinov et al.

C9H7+O2=>C9H6O+H+O	3.090e+15	-0.730	
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48740.44

C9H7+HO2<=>C9H6O+H2O	4.760e+32	-6.520	
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13401.05

C9H7+O2=C9H6O+OH	1.740e+07	1.300	
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17667.30 !Henzi Pitsch 2011

C9H7+OH=>C9H6O+2H	4.080e+13	0.000
0.00 !Henzi Pitsch 2011		
C9H6O=>o-C6H4+C2H2+CO	3.370e+44	-8.000
108675.91 !Henzi Pitsch 2011		
C7H5+C2H2=>C9H7	1.10E+86	-21.259
65862 !Akira Matsugi and Akira Niyoshi 2012 PCCP,14.		
PLOG/ 0.0132	1.10E+86	-21.259
65862/		
PLOG/ 0.132	2.29E+65	-15.332
52600/		
PLOG/ 1.000	2.58E+46	-9.963
39426/		
PLOG/ 10.00	5.47E+28	-4.989
26622/		
PLOG/ 100.0	2.50E+18	-2.092
18906/		
C9H7=>C7H5+C2H2	1.526E+108	-25.979
180259 !Akira Matsugi and Akira Niyoshi 2012 PCCP,14.		
PLOG/ 0.0132	1.526E+108	-25.979
180259/		
PLOG/ 0.132	4.288E+94	-22.023
172714/		
PLOG/ 1.000	1.476E+79	-17.617
162389/		
PLOG/ 10.00	1.894E+60	-12.304
148632/		
PLOG/ 100.0	1.412E+44	-7.806
136273/		
C7H6+C2H2=C9H8	1.44E+292	-78.17
245010.0 !2009 da Silva&Bozzelli		
C7H6+C2H2=C9H7+H	9.70E-42	16.72
37520.0 !2009 da Silva&Bozzelli		
A1CH2+C2H2=C9H8+H	3.124E-6	4.712
1417.5 !Luc Vereecken and Jozef Peeters Phys. Chem. Chem. Phys.,		
2003, 5, 2807-2817		
A1-+C3H4-A=C9H8+H	7.695e1	3.192
2787.8 !Luc Vereecken and Jozef Peeters PCCP 2003, 5, 2807-2817 *0.15		
A1-+C3H4-A=A1+C3H3	2.565e2	3.192
2787.8 !Luc Vereecken and Jozef Peeters PCCP 2003, 5, 2807-2817 *0.50		
A1-+C3H4-A=A1CH2+C2H2	5.130e1	3.192
2787.8 !Luc Vereecken and Jozef Peeters PCCP 2003, 5, 2807-2817 *0.10		
A1-+C3H4-A=A1C2H+CH3	2.565e1	3.192
2787.8 !Luc Vereecken and Jozef Peeters PCCP 2003, 5, 2807-2817 *0.05		
A1-+C3H4-P=A1+C3H3	1.794e4	2.546
2759.1 !Luc Vereecken and Jozef Peeters PCCP 2003, 5, 2807-2817 *0.50		
A1-+C3H4-P=A1C2H+CH3	7.175e3	2.546
2759.1 !Luc Vereecken and Jozef Peeters PCCP 2003, 5, 2807-2817 *0.20		
A1+C3H3=C9H8+H	6.26E+09	2.61
56500.0 !Est		
C7H5+C2H4=C9H8+H	3.124E-6	4.712
1417.5 !		
o-C6H4+C3H5-A=C9H8+H	1.52e9	1.028
-1035.5 ! est. ref: HPL of o-C6H4+C3H3		
o-C6H4+C3H4-A=C9H8	1.00e13	0.0
10000.0 ! est.		
o-C6H4+C3H4-P=C9H8	1.00e13	0.0
10000.0 ! est.		

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nC4H3+C5H6=>C9H8+H          5.00E+11    0.0
5000.0      ! est.
CH3+A1C2H=>C9H8+H          3.00E+11    0.0
7600.0      ! est.
O-C6H4CH3+C2H2=C9H8+H      1.00E+12    0.0
5000.0      ! est.

!***** Reactions of C9H9-1(indanyl) and
C9H10(indane)*****
A1CH2+C2H4= C9H10+H          3.16E+04    2.5
11061.2     !2009 Blanquart et al. A1CH2+C2H2=C9H8+H
C9H9-1+H(+M)=C9H10(+M)      2.40E+13    0.0
0.0         !(JetSurf v2.0 /2
                                LOW / 8.50E+57 -12.08
11263.7/
                                TROE/ 0.649 1213.1 1213.1
13369.7/
                                H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/
AR/0.7/
!Nicolas Delort!
!C9H9-1(+M)=C9H8+H(+M)      1.17E+11    0.69
33947.9     !JetSurF v2.0 cC6H11(+M)=cC6H10+H(+M) in 2013 Li et
al.(Tetralin) /2
!
                                LOW / 1.50E-40 17.33 -
602.7/
!
                                TROE / -19.22 230.0 28.0
50000.0/
!
                                H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/
AR/0.7/

H+C9H8=C9H9-1              1e+12    0.0    0.0 ! Nicolas
Delort

C9H9-1(+M)=O-CH2A1C2H3(+M)  3.02E+12    0.07
27982.9     !JetSurF v2.0 cC6H11(+M)=PXC6H11(+M) in 2013 Li et
al.(Tetralin) /2
!
                                LOW / 2.55E-33 15.29 -
602.6/
!
                                TROE/-25.11 225.0 28.0
50000.0/
!
                                H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/
AR/0.7/
C9H10+H=C9H9-1+H2          .3851E+08    2.0
3950.57     !P.Dagaut et al. Tetralin+H
C9H10+CH3=C9H9-1+CH4        .6245E+06    2.0
4871.29     !P.Dagaut et al. Tetralin+CH3
C9H10+OH=C9H9-1+H2O        .6390E+07    2.0 -
2259.83     !P.Dagaut et al. Tetralin+OH
C9H10+O=C9H9-1+OH          .2165E+08    2.0
2579.54     !P.Dagaut et al. Tetralin+O
C9H10+O2=C9H9-1+HO2        .2726E+08    2.0
40722.49    !P.Dagaut et al. Tetralin+O2
O-CH3A1C2H3=O-CH2A1C2H3+H  2.83E+64   -13.99
120613.0    !2010 Zhang et al.(Toluene) A1CH3=A1CH2+H
O-CH3A1C2H3+H=O-CH2A1C2H3+H2  6.47E+00    3.98
3394.0      !2006 Oehlschlaeger A1CH3+H=A1CH2+H2
O-CH3A1C2H3=O-C6H4C2H3+CH3  3.60E+86   -20.61
144292.0    !2013 Li et al.(Tetralin) Est.

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P-CH3A1C2H3=P-CH2A1C2H3+H 2.83E+64 -13.99
 120613.0 !2010 Zhang et al.(Toluene) A1CH3=A1CH2+H
 P-CH3A1C2H3+H=P-CH2A1C2H3+H2 6.47E+00 3.98
 3394.0 !2006 Oehlschlaeger A1CH3+H=A1CH2+H2
 P-CH3A1C2H3=P-C6H4C2H3+CH3 3.60E+86 -20.61
 144292.0 !2013 Li et al.(Tetralin) Est.
 C9H10=O-C6H4C2H3+CH3 5.40E+86 -20.61
 144292.0 !2013 Li et al.(Tetralin) Est.
 O-CH2A1C2H3+H=O-C6H4C2H3+CH3 4.50E+58 -11.9
 51860.0 !2007 Klippenstein et al. A1CH2+H=A1-+CH3
 O-CH3A1C2H3+H=A1C2H3+CH3 1.56E+13 0.0
 5796.0 !2005 Baulch et al. A1CH3+H=A1+CH3
 P-CH2A1C2H3+H=P-C6H4C2H3+CH3 4.50E+58 -11.9
 51860.0 !2007 Klippenstein et al. A1CH2+H=A1-+CH3
 P-CH3A1C2H3+H=A1C2H3+CH3 1.56E+13 0.0
 5796.0 !2005 Baulch et al. A1CH3+H=A1+CH3
 A1CH3+C2H3=O-CH3A1C2H3+H 2.872E+11 0.0
 6400.0 ! A*2/5 on Yuan coeff 7.18E+11 0.0 6400.0 !1997
 Wang&Frenklach A1+C2H3=A1C2H3+H
 A1CH3+C2H3=P-CH3A1C2H3+H 4.308E+11 0.0
 6400.0 ! A*3/5 on Yuan coeff 7.18E+11 0.0 6400.0 !1997
 Wang&Frenklach A1+C2H3=A1C2H3+H
 O-C6H4CH3+C2H4=O-CH3A1C2H3+H 2.51E+12 0.0
 6190.0 !1997 Wang&Frenklach A1-+C2H4=A1C2H3+H
 O-C6H4CH3+C2H3=O-CH3A1C2H3 1.90E+48 -10.52
 17489.0 !1997 Wang&Frenklach A1-+C2H3=A1C2H3
 P-C6H4CH3+C2H4=P-CH3A1C2H3+H 2.51E+12 0.0
 6190.0 !1997 Wang&Frenklach A1-+C2H4=A1C2H3+H
 P-C6H4CH3+C2H3=P-CH3A1C2H3 1.90E+48 -10.52
 17489.0 !1997 Wang&Frenklach A1-+C2H3=A1C2H3

!***** Reactions of
 C10H6(naphthalyne)*****

!Nicolas Delort
 !A2T2+H=A1-+C4H2 2.06E+08 1.4 -
 3410.0 !2009 Cavallotti et al. C7H6+H=C5H5+C2H2
 !A2T1+H=A1-+C4H2 2.06E+08 1.4 -
 3410.0 !2009 Cavallotti et al. C7H6+H=C5H5+C2H2

A1-+C4H2<=>A2T2+H +1.15000000E-044
 +1.70700000E+001 +2.24600000E+004 !!Nicolas Delort: analogy with
 C5H5+C2H2<=>C7H6+H from NUIG1.1
 PLOG / +1.00000000E-002 +7.07000000E+001
 +3.42000000E+000 +2.87400000E+004 /
 PLOG / +1.00000000E-001 +1.58000000E-001
 +4.18000000E+000 +2.96700000E+004 /
 PLOG / +1.00000000E+000 +6.96000000E-005
 +5.17000000E+000 +3.09300000E+004 /
 PLOG / +1.00000000E+001 +2.37000000E-006
 +5.60000000E+000 +3.35400000E+004 /
 PLOG / +1.00000000E+002 +1.15000000E-044
 +1.70700000E+001 +2.24600000E+004 /
 A1-+C4H2<=>A2T1+H +1.15000000E-044
 +1.70700000E+001 +2.24600000E+004 !!Nicolas Delort: analogy with
 C5H5+C2H2<=>C7H6+H from NUIG1.1
 PLOG / +1.00000000E-002 +7.07000000E+001
 +3.42000000E+000 +2.87400000E+004 /

PLOG / +1.00000000E-001 +1.58000000E-001
+4.18000000E+000 +2.96700000E+004 /
PLOG / +1.00000000E+000 +6.96000000E-005
+5.17000000E+000 +3.09300000E+004 /
PLOG / +1.00000000E+001 +2.37000000E-006
+5.60000000E+000 +3.35400000E+004 /
PLOG / +1.00000000E+002 +1.15000000E-044
+1.70700000E+001 +2.24600000E+004 /

A1CC+C2H=A2T2 1.00E+13 0.0
0.0 !2010 Li(Ph.D. Thesis) Est.
A1C2H-+C2H=A2T2 1.00E+13 0.0
0.0 !2010 Li(Ph.D. Thesis) Est.
A1CC+C2H=A1(C2H)2 5.00E+13 0.0
0.0 !2010 Zhang et al.(Toluene) Est.
A1CC+C2H2=A2T2+H 2.30E+58 -12.9
44600.0 !1994 Wang&Frenklach RRKM 20Torr
A1(C2H)2+H=A2T2+H 3.90E+74 -16.9
53700.0 !1994 Wang&Frenklach RRKM 20Torr
A2-1(+M)=A2T2+H(+M) 4.300E+12 0.616
77313. !A1-(+M)=o-C6H4+H(+M) RRKM 00-HAI-FRE
LOW/ 1.000E+84 -18.866
90064 / ! 20130218

TROE/ 0.902 696. 358. 3856.

/

H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/

CO2/2.0/
A2-2(+M)=A2T2+H(+M) 4.300E+12 0.616
77313. !A1-(+M)=o-C6H4+H(+M) RRKM 00-HAI-FRE
LOW/ 1.000E+84 -18.866

90064 / ! 20130218

TROE/ 0.902 696. 358. 3856.

/

H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/

CO2/2.0/

A1C2H+C2H=A1(C2H)2+H 5.00E+13 0.0
0.0 !1997 Wang&Frenklach
A1C2H-+C2H=A1(C2H)2 5.00E+13 0.0
0.0 !1997 Wang&Frenklach A1C2H+C2H=A1(C2H)2+H in 2010 Li(Ph.D.
Thesis)
A1C2H-+C2H2=A1(C2H)2+H 4.00E+13 0.0
0.0 !EST

!***** Reactions of A2(naphthalene) A2-(naphthalenyl) A2O *****

A2-1+H(+M)=A2(+M) 1.00E+14 0.0

0.0 !1997 Wang&Frenklach

LOW / 3.80E+127 -31.434

18676.0/

TROE/ 0.200 122.8 478.4

5411.9/

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

C2H6/3.0/

A2-2+H(+M)=A2(+M) 1.00E+14 0.0

0.0 !1997 Wang&Frenklach

LOW / 9.50E+129 -32.132

18782.0/

TROE/ 0.870 492.7 117.9

5652.0/
H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/
C2H6/3.0/
C5H5+C5H5=>C5H5-C5H5 3.14E+174 -49.43
62602 !Miyoshi 2013
PLOG/ 0.0132 3.14E+174 -49.43
62602/
PLOG/ 1 1.80E+188 -52.62
76380/
PLOG/ 100 4.28E+174 -47.91
75125/
C5H5-C5H5=>C5H5+C5H5 4.15E+70 -17.55 62254
PLOG/ 0.0132 4.15E+70 -17.55
62254/
PLOG/ 1 2.95E+77 -18.71
73651/
PLOG/ 100 2.49E+64 -14.25
72842/
C5H5-C5H5=C5H5-C5H4+H 7.59E+07 -2.63 27409
!Miyoshi 2013
PLOG/ 0.0132 7.59E+07 -2.63
27409/
PLOG/ 1 5.08E+77 -20.36
92326/
PLOG/ 100 6.25E+86 -21.39
111744/
C5H5-C5H5+H=C5H5-C5H4+H2 1.718E+08 1.847 3335.0
!ref C5H6+H=C5H5+H2 *2 R.K. Robinson, R.P. Lindstedt 2011
C5H5-C5H5+CH3=C5H5-C5H4+CH4 1.00E+12 0.0 5000.0
!ref C5H6+CH3=C5H5+CH4 *2 2001 Bacskay&Mackie

C5H5-C5H5+OH=C5H5-C5H4+H2O 6.16E+06 2.0 0.0
!ref C5H6+OH=C5H5+H2O *2 1998 Zhong&Bozzelli Est.
C5H5-C5H5+HO2=C5H5-C5H4+H2O2 2.2E+4 2.6 12900.0
!ref C5H6+HO2=C5H5+H2O2 *2 Zhong & Bozzeli J PHYS CHEM A 102: 3537 1998
C5H5-C5H5+O2=C5H5-C5H4+HO2 8.0E+13 0 37150.0
!ref C5H6+O2=C5H5+HO2 *2 Zhong & Bozzeli J PHYS CHEM A 102: 3537 1998

C5H5+C5H5=>C5H5-C5H4+H 5.24807E+14 -0.853 7254
!Carlo Cavallotti and Daniela Polino 2013 PCI to 9H-fulvalenyl radical
duplicate
C5H5+C5H5=>C5H5-C5H4+H 2.00E+10 0.951
15793 !Carlo Cavallotti and Daniela Polino 2013 PCI to azulyl
radical
duplicate

C5H5-C5H4=A2+H 3.08e12 0.0 43334.0
!A.M. Mebel, J. Phys. Chem. A 113(2009) 9825-33.
duplicate
C5H5-C5H4=A2+H 1.28e15 0.0 54534.0
!A.M. Mebel, J. Phys. Chem. A 113(2009) 9825-33.
duplicate

A1-+nC4H3=A2 1.51E+75 -17.9 39600.0
!2002 Richter&Howard QRRK-HR
PLOG/ 0.0263 1.51E+75 -17.9
39600.0/

PLOG/ 1.00	6.62E35	-6.485	
15420.0/			
A1-+nC4H3=A2-2+H	1.84E+72	-16.1	57630.0
!2002 Richter&Howard QRRK-HR			
PLOG/ 0.0263	1.84E+72	-16.1	
57630.0/			
PLOG/ 1.00	2.43E31	-4.541	
36700.0/			
A1-+nC4H3=A2-1+H	1.84E+72	-16.1	57630.0
!2002 Richter&Howard QRRK-HR			
PLOG/ 0.0263	1.84E+72	-16.1	
57630.0/			
PLOG/ 1.00	2.43E31	-4.541	
36700.0/			
A1-+C4H4=A2+H	1.26E+04	2.61	1434.0
!2009 Blanquart et al.			
A1+nC4H3=A2+H	4.00E+13	0.0	
15976.0			
!2011 Li et al.(Toluene) Est.			
A1CH2+C3H3=C9H7CH2+H	1.56E+13	-0.967	-
3266.5			
!A. Matsugi, A. Miyoshi, Int. J. Chem. Kinet 20130907			
C9H7+CH3=>C9H7CH3	9.10E+109	-29.19	
41906			
!refer to C5H5+CH3=>C5H5CH3 Sandeep Sharma and William			
H. Green J. Phys. Chem. A 2009, 113, 8871`C8882			
PLOG/ 0.01	9.10E+109	-29.19	
41906/			
PLOG/ 1.00	3.06E+105	-27.05	
47952/			
PLOG/ 10.0	2.38E+94	-23.52	
45184/			
PLOG/ 100	1.09E+70	-16.33	
32296/			
C9H7CH3=>C9H7+CH3	4.49E+77	-19.26	89496
!refer to C5H5CH3=>C5H5+CH3 Sandeep Sharma and William H. Green J. Phys.			
Chem. A 2009, 113, 8871`C8882			
PLOG/ 0.01	4.49E+77	-19.26	
89496/			
PLOG/ 1.00	2.01E+89	-21.78	
105380/			
PLOG/ 10.0	6.89E+84	-20.17	
106554/			
PLOG/ 100	4.46E+71	-16.16	
100961/			
C9H7+CH3=>C9H7CH2+H	7.49E+13	-0.30	11640
!refer to C5H5+CH3=>C5H5CH2-2+H			
PLOG/ 0.01	7.49E+13	-0.30	11640/
PLOG/ 1.00	7.93E+27	-4.14	24060/
PLOG/ 10.0	7.18E+44	-8.75	40084/
PLOG/ 100	1.31E+53	-10.86	
51760/			
C9H7CH3=>C9H7CH2+H	2.35E+80	-20.72	
95019			
!20131115			
PLOG/ 0.01	2.35E+80	-20.72	
95019/			
PLOG/ 1.00	1.74E+97	-24.38	
116128/			
PLOG/ 10.0	5.77E+97	-24.00	
122296/			

PLOG/ 100	1.75E+87	-20.60	
120401/			
C9H7CH3+H=C9H7CH2+H2	7.2E+13	0	
3500.0 !EST C5H5CH3+H=C5H4CH3+H2			
C9H7CH3+OH=C9H7CH2+H2O	3.08E+06	2.0	
0.0 !EST C5H5CH3+OH=C5H4CH3+H2O			
O2+C9H7CH3=>HO2+A2+H	1.704E+07	2.0	
38570.96 !Polimi V2012 O2+C5H5CH3=>HO2+A1+H			
H+C9H7CH3=>H2+A2+H	2.407E+07	2.0	
2663.07 !Polimi V2012 H+C5H5CH3=>H2+A1+H			
OH+C9H7CH3=>H2O+A2+H	3.994E+06	2.0	-
3152.53 !Polimi V2012 OH+C5H5CH3=>H2O+A1+H			
O+C9H7CH3=>OH+A2+H	1.353E+07	2.0	
1356.53 !Polimi V2012 O+C5H5CH3=>OH+A1+H			
HO2+C9H7CH3=>H2O2+A2+H	5.388E+05	2.0	
10318.80 !Polimi V2012 HO2+C5H5CH3=>H2O2+A1+H			
HCO+C9H7CH3=>CH2O+A2+H	1.263E+06	2.0	
10777.87 !Polimi V2012 HCO+C5H5CH3=>CH2O+A1+H			
CH3+C9H7CH3=>CH4+A2+H	3.903E+05	2.0	
3544.16 !Polimi V2012 CH3+C5H5CH3=>CH4+A1+H			
C2H5+C9H7CH3=>C2H6+A2+H	2.298E+05	2.0	
6224.33 !Polimi V2012 C2H5+C5H5CH3=>C2H6+A1+H			
C9H7CH2=C9H6CH2+H	6.28E+71	-18.204	
65710.8 !2012 Matsugi&Miyoshi			
plog / 0.0013	6.28E+71	-18.204	
65710.8/			
plog / 0.0132	2.82E+61	-14.813	
62789.9/			
plog / 0.1316	3.77E+47	-10.443	
58071.8/			
plog / 1.0000	7.54E+33	-6.226	
52769.3/			
plog / 10.0000	4.44E+21	-2.491	
47796.0/			
plog /100.0000	2.86E+13	0.015	
44394.9/			
C9H7CH2=A2+H	3.68E+63	-15.806	
57409.9 !2012 Matsugi&Miyoshi			
plog / 0.0013	3.68E+63	-15.806	
57409.9/			
plog / 0.0132	6.88E+51	-12.098	
53279.3/			
plog / 0.1316	2.37E+38	-7.917	
48317.2/			
plog / 1.0000	9.04E+25	-4.123	
43307.9/			
plog / 10.0000	4.13E+16	-1.278	
39451.4/			
plog /100.0000	5.55E+12	-0.065	
38027.7/			
C9H6CH2+H=A2+H	5.35E+11	0.627	
2422.4 !2012 Matsugi&Miyoshi			
C7H5+C3H3=A2-1+H	1.0467E+54	-11.88	
28757. !2003 Miller&Klippenstein 2003			
PLOG /0.03947	2.09E+53	-11.88	28757./
!1.0467E+54/5			
PLOG /1.	3.40E+47	-9.977	36755./
!1.6975E+48/5			

PLOG /10.	7.34E+25	-3.879	28963./
!3.6712E+26/5			
C7H5+C3H3=A2	1.8189E+74	-18.14	
31896. !refer to Miller&Klippenstein 2003	C3H3+C3H3=A1		
PLOG /0.03947	3.64E+73	-18.14	
31896./ !1.8189E+74/5			
PLOG /1.	6.32E+54	-12.55	
22264./ !3.1609E+55			
PLOG /10.	7.78E+49	-11.01	
20320./ !3.8888E+50			
C7H5+C5H5=P2	1.8189E+74	-18.14	
31896. !refer to Miller&Klippenstein 2003			
PLOG /0.03947	3.64E+73	-18.14	
31896./ !1.8189E+74/5			
PLOG /1.	6.32E+54	-12.55	
22264./ !3.1609E+55			
PLOG /10.	7.78E+49	-11.01	
20320./ !3.8888E+50			
C9H6CH2=A2	5.62E+81	-19.36	
121500.0 !2003 Miller&Klippenstein fulvene=A1			
plog / 0.0395	5.62E+81	-19.36	
121500.0/ !			
plog / 1.0000	1.45E+45	-8.90	
96999.0/ !			
plog / 10.0000	2.95E+31	-4.97	
88465.0/ !			
C9H6CH2=A2-1+H	2.57E+97	-23.2	
153470.0 !2009 Hansen et al. fulvene=A1-+H			
plog / 0.0395	2.57E+97	-23.2	
153470.0/			
plog / 1.0000	2.24E+68	-14.7	
142570.0/			
plog / 10.0000	8.51E+24	-2.5	
113330.0/			
C9H6CH2=A2-2+H	2.57E+97	-23.2	
153470.0 !2009 Hansen et al. fulvene=A1-+H			
plog / 0.0395	2.57E+97	-23.2	
153470.0/			
plog / 1.0000	2.24E+68	-14.7	
142570.0/			
plog / 10.0000	8.51E+24	-2.5	
113330.0/			
O-C6H4C2H3+C2H2=A2+H	2.10E+15	-1.1	
6000.0 !1997 Wang&Frenklach RRKM 20Torr			
A1CHCH+C2H2=A2+H	2.10E+15	-1.1	
4800.0 !1994 Wang&Frenklach n-C4H5+C2H2=A1+H in 1997 Wang&Frenklach			
A1CCH2+C2H2=A2+H	3.02E+03	2.55	
3181.17 !2009 Blanquart et al.			
A1C2H+C2H3=A2+H	3.60E+17	-1.44	
15757.65 !2009 Blanquart et al.			
A1C2H3+C2H=A2+H	1.00E+13	0.0	
0.0 !2010 Li(Ph.D. Thesis) Est.			
A1CHCH+C2H=A2	1.00E+13	0.0	
0.0 !2010 Li(Ph.D. Thesis) Est.			
A1CC+C2H2=A2-1	5.20E+72	-18.11	
33900.0 !1994 Wang&Frenklach RRKM			
plog / 0.0132	7.50E+74	-18.83	
34200.0/			

plog / 0.0263	5.20E+72	-18.11
33900.0/		
plog / 0.1184	2.00E+72	-17.74
36600.0/		
plog / 1.0000	1.10E+62	-14.56
33100.0/		
plog / 10.0000	5.10E+48	-10.53
28000.0/		
A1CC+C2H2=A1 (C2H) 2+H	5.50E+32	-5.5
27600.0 !1994 Wang&Frenklach RRKM 20Torr		
A1CC+C2H2=C2H2A1C2H	3.90E+48	-11.30
27200.0 !1994 Wang&Frenklach RRKM		
plog / 0.0132	1.00E+51	-12.06
28900.0/		
plog / 0.0263	3.90E+48	-11.30
27200.0/		
plog / 0.1184	1.10E+43	-9.57
23100.0/		
plog / 1.0000	1.40E+32	-6.28
14800.0/		
plog / 10.0000	1.90E+21	-2.93
8100.0/		
A1 (C2H) 2+H=C2H2A1C2H	3.00E+48	-10.87
20500.0 !1994 Wang&Frenklach RRKM		
plog / 0.0132	2.70E+51	-11.78
22700.0/		
plog / 0.0263	3.00E+48	-10.87
20500.0/		
plog / 0.1184	7.10E+42	-9.13
16300.0/		
plog / 1.0000	2.00E+27	-4.55
4800.0/		
plog / 10.0000	1.60E+26	-3.92
5400.0/		
A1 (C2H) 2+H=A2-1	2.00E+82	-20.23
36900.0 !1994 Wang&Frenklach RRKM		
plog / 0.0132	9.50E+84	-21.09
37600.0/		
plog / 0.0263	2.00E+82	-20.23
36900.0/		
plog / 0.1184	2.00E+75	-18.06
34500.0/		
plog / 1.0000	6.90E+63	-14.57
29900.0/		
plog / 10.0000	1.50E+51	-10.77
25500.0/		
A2+H=A2-1+H2	2.50E+14	0.0
16000.0 !=A1+H=A1-+H2 Emdee et al.J. Phys. Chem. 1992, 96, 2151-2161		
A2+H=A2-2+H2	2.50E+14	0.0
16000.0 !=A1+H=A1-+H2 Emdee et al.J. Phys. Chem. 1992, 96, 2151-2161		
A2-1+CH4=A2+CH3	3.89E-03	4.6
5256.0 !1999 Tokmakov et al. A1-+CH4=A1+CH3		
A2-2+CH4=A2+CH3	3.89E-03	4.6
5256.0 !1999 Tokmakov et al. A1-+CH4=A1+CH3		
A2-1+H=A2-2+H	8.80E+58	-11.68
60974.0 !1997 Wang&Frenklach RRKM		
PLOG/ 0.026	8.80E+58	-11.68
60974.0/		

PLOG/ 0.118		6.50E+45	-7.90
55488.0/			
PLOG/ 1.000		2.40E+24	-1.81
45281.0/			
A2+OH=A2-1+H2O		2.34E+04	2.68
733.2	!2006 Seta and Nakajima and Miyoshi		
A2+OH=A2-2+H2O		2.34E+04	2.68
733.2	!2006 Seta and Nakajima and Miyoshi		
A2+OH=A2OH-1+H		4.99E+08	1.31
6543.0	!PITZ2001		
PLOG / 1.0		4.99E+08	1.31
6543.0/	!same as seta et al.		
PLOG / 10.0		8.21E+13	-0.13
10673.0/	!		
PLOG / 100.0		6.68E+20	-2.02
16758.0/	!		
A2+OH=A2OH-2+H		4.99E+08	1.31
6543.0	!PITZ2001		
PLOG / 1.0		4.99E+08	1.31
6543.0/	!same as seta et al.		
PLOG / 10.0		8.21E+13	-0.13
10673.0/	!		
PLOG / 100.0		6.68E+20	-2.02
16758.0/	!		
A2+O2=A2-1+HO2		6.30E+13	0.0
60000.0	!Emdee et al.1992 A1+O2=A1-+HO2		
A2+O2=A2-2+HO2		6.30E+13	0.0
60000.0	!Emdee et al.1992 A1+O2=A1-+HO2		
A2+O=A2-1+OH		2.0E13	0.0
14700.0	!Alzueta et al.2000 A1+O=A1-+OH		
A2+O=A2-2+OH		2.0E13	0.0
14700.0	!Alzueta et al.2000 A1+O=A1-+OH		
A2+O=A2O-1+H		1.99E+07	1.8
3974.0	!2010 Taatjes et al 20131028		
plog/ 0.1		1.99E+07	1.8
3974.0/			
plog/ 10		1.99E+07	1.8
3974.0/			
plog/ 50		3.55e+10	0.91
6323.0/			
plog/ 500		1.32e+12	0.47
8434.8/			
A2+O=A2O-2+H		1.99E+07	1.8
3974.0	!2010 Taatjes et al 20131028		
plog/ 0.1		1.99E+07	1.8
3974.0/			
plog/ 10		1.99E+07	1.8
3974.0/			
plog/ 50		3.55e+10	0.91
6323.0/			
plog/ 500		1.32e+12	0.47
8434.8/			
A2+O=C9H8+CO		6.02E+15	-0.49
14993.0	!A1+O=C5H6+CO2010 Taatjes et al. 1atm		
plog/ 0.1		7.22e+13	0.12
11776.9/			
plog/ 1.0		6.02E+15	-0.49
14993.0/			

plog/ 10.0	1.38E+38	-6.71	
34631.4/			
PLOG/ 50.0	1.57E+31	-4.73	
33568.4/			
PLOG/ 500	2.23E+56	-11.69	
55598.2/			
A2+HO2=A2-1+H2O2	5.5E+12	0.0	
28900.0 !F.L.Dryer 2010 A1+HO2=A1-+H2O2			
A2+HO2=A2-2+H2O2	5.5E+12	0.0	
28900.0 !F.L.Dryer 2010 A1+HO2=A1-+H2O2			
A2-1+OH=A2O-1+H	5.00E+13	0.0	
0.0 !2002 Richter&Howard			
A2-2+OH=A2O-2+H	5.00E+13	0.0	
0.0 !2002 Richter&Howard			
A2-1+O2=A2O-1+O	2.6E+13	0.0	
6120.0 !A1-+O2=A1O+O Frank, P.Herzler, J.Just, Th.Wahl, C. Symp. Int. Combust. Proc. 25, 833-840 (1994)			
A2-1+O2=>C9H6O+CO+H	3.0E+13	0.0	
8981.0 !Frank, P.Herzler, J.Just, Th.Wahl, C. Symp. Int. Combust. Proc. 25, 833-840 (1994)			
A2-2+O2=A2O-1+O	2.6E+13	0.0	
6120.0 !A1-+O2=A1O+O Frank, P.Herzler, J.Just, Th.Wahl, C. Symp. Int. Combust. Proc. 25, 833-840 (1994)			
A2-2+O2=>C9H6O+CO+H	3.0E+13	0.0	
8981.0 !Frank, P.Herzler, J.Just, Th.Wahl, C. Symp. Int. Combust. Proc. 25, 833-840 (1994)			
A2O-1=C9H7+CO	5.71E+59-14.4		
68564 !refer to A1O=CO+C5H5, 2011 You et al. J. Phys. Chem. A 2011, 115, 14184-14190			
PLOG / 0.0100	5.71E+59-14.4		
68564/ !The rate of You is similar to that of Carstensen			
PLOG / 0.1000	1.65E+71-17.2		
81843/			
PLOG / 1.0000	1.32E+74-17.6		
88985/			
PLOG / 10.000	4.41E+68-15.8		
89456/			
PLOG /100.0000	3.77E+71-16.18		
98611/			
!HPL	1.25E+062.25		50194
A2O-2=C9H7+CO	5.71E+59-14.4		
68564 !refer to A1O=CO+C5H5, 2011 You et al. J. Phys. Chem. A 2011, 115, 14184-14190			
PLOG / 0.0100	5.71E+59-14.4		
68564/ !The rate of You is similar to that of Carstensen			
PLOG / 0.1000	1.65E+71-17.2		
81843/			
PLOG / 1.0000	1.32E+74-17.6		
88985/			
PLOG / 10.000	4.41E+68-15.8		
89456/			
PLOG /100.0000	3.77E+71-16.18		
98611/			
!HPL	1.25E+062.25		50194
C3H3+A2=>C13H10+H	3.00E+12	0.00	23000.0
!Polimi V2012			
C5H5+A2=>A3+CH3	3.00E+12	0.00	23000.0
!Polimi V2012			

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A1-+A2=>A4+H+H2          3.00E+12  0.00    10000.0
!Polimi V2012
A2O-1+H(+M)=A2OH-1(+M)    0.50E+14   0.0
0.0      !1996 Davis et al
                                LOW / 1.00E+94  -21.84
13880.0/      !
                                TROE/ 0.043 340.0 60000.0
5900.0/
                                H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/
CO2/2.0/
A2O-2+H(+M)=A2OH-2(+M)    0.50E+14   0.0
0.0      !1996 Davis et al
                                LOW / 1.00E+94  -21.84
13880.0/      !
                                TROE/ 0.043 340.0 60000.0
5900.0/
                                H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/
CO2/2.0/
A2OH-1+H = A2O-1+H2          6.830e+01   3.400
7232.31      !Blanquant
A2OH-2+H = A2O-2+H2          6.830e+01   3.400
7232.31      !Blanquant
A2OH-1+OH = A2O-1+H2O        1.730e+01   3.400  -
1142.45      !Blanquant
A2OH-2+OH = A2O-2+H2O        1.730e+01   3.400  -
1142.45      !Blanquant
A2OH-1+CH3 = A2O-1+CH4        3.700e-04   4.700
4827.92      !Blanquant
A2OH-2+CH3 = A2O-2+CH4        3.700e-04   4.700
4827.92      !Blanquant
A2OH-1=C9H8+CO                8.620e+15  -0.610
74118.07     !Blanquant
A2OH-2=C9H8+CO                8.620e+15  -0.610
74118.07     !Blanquant
A2+O = A2OH-1                 1.830e+13   0.000
4529.16      !Blanquant
A2+O = A2OH-2                 1.830e+13   0.000
4529.16      !Blanquant

!***** Reactions of C9H8CH3 and C9H7CH3
*****
**
C9H8CH3=CH2A1C3H5            6.35E+12   0.15
58710.0      !2013 Li et al.(Tetralin) Est.
C9H8+CH3(+M)=C9H8CH3(+M)     9.60E+10   0.00
8003.6      !JetSurF v2.0 C3H6+CH3(+M)=iC4H9(+M) /2 in 2013 Li et
al.(Tetralin)
                                LOW / 1.30E+28  -4.27
2431.1/
                                TROE/ 0.565 60000.0 534.2
3007.2/
                                H2/2/ H2O/6/ CH4/2/ CO/1.5/ CO2/2/ C2H6/3/
AR/0.7/
C9H8CH3+H=C9H7CH3+H2         1.00E+13   0.00
0.0      !2013 Li et al.(Tetralin) Est.
C9H8CH3=C9H7CH3+H            2.72E+26  -5.579
24712.2      !2013 Li et al.(Tetralin) Est.

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C9H7CH3+H=C9H8+CH3	1.56E+13	0.0
5796.0 !2005 Baulch et al. A1CH3+H=A1+CH3		
O-C6H4C2H3+C2H5=C2H4A1C2H3+H	1.50E+32	-4.91
35504.0 !1997 Wang&Frenklach A1-+C2H3=A1CHCH+H		
P-C6H4C2H3+C2H5=C2H4A1C2H3+H	1.50E+32	-4.91
35504.0 !1997 Wang&Frenklach A1-+C2H3=A1CHCH+H		
O-C6H4C2H3+C2H4=C2H4A1C2H3	7.70E+40	-9.2
13400.0 !1994 Wang&Frenklach A1-+C2H2=A1CHCH		
P-C6H4C2H3+C2H4=C2H4A1C2H3	7.70E+40	-9.2
13400.0 !1994 Wang&Frenklach A1-+C2H2=A1CHCH		
C2H4A1C2H3=A1(C2H3)2+H	3.16E+13	0.0
50669.0 !1988 Mueller-Markgraf&Troe A1C2H4=A1C2H3+H		
C2H4A1C2H3+H=A1(C2H3)2+H2	2.00E+12	0.0
0.0 !GRI3.0 C2H5+H=C2H4+H2		
A1C2H3+C2H3=A1(C2H3)2+H	7.20E+11	0.0
6400.0 !1997 Wang&Frenklach A1+C2H3=A1C2H3+H		
O-C6H4C2H3+C2H4=A1(C2H3)2+H	2.55E+11	0.0
6190.0 !1997 Wang&Frenklach A1-+C2H4=A1C2H3+H		
P-C6H4C2H3+C2H4=A1(C2H3)2+H	2.55E+11	0.0
6190.0 !1997 Wang&Frenklach A1-+C2H4=A1C2H3+H		
O-C6H4C2H3+C2H3=A1(C2H3)2	1.90E+48	-10.52
17489.0 !1997 Wang&Frenklach A1-+C2H3=A1C2H3		
P-C6H4C2H3+C2H3=A1(C2H3)2	1.90E+48	-10.52
17489.0 !1997 Wang&Frenklach A1-+C2H3=A1C2H3		
!H2A2 pas consommé - puit de C dans l'oxidation de l'anisole!		
!Nicolas Delort ! A1O+A1O=>2CO+H2A2		
.2500E+13 .000 6000.0 !		

!***** Reactions of C11 species

A2CH3-1=A2-1+CH3	4.23E+121-30.1	
168551 !Benoite Lefort and Wing Tsang 2011		
PLOG/ 0.1	4.23E+121-30.1	
168551/		
PLOG/ 1.0	6.51E+90	-21.2
150039/		
PLOG/ 10.0	1.03E+59	-12.1
129282/		
PLOG/ 100.0	8.15E+36	-5.8
114347/		
A2CH3-2=A2-2+CH3	4.23E+121-30.1	
168551 !!Benoite Lefort and Wing Tsang 2011		
PLOG/ 0.1	4.23E+121-30.1	
168551/		
PLOG/ 1.0	6.51E+90	-21.2
150039/		
PLOG/ 10.0	1.03E+59	-12.1
129282/		
PLOG/ 100.0	8.15E+36	-5.8
114347/		
A2CH3-1=A2CH2-1+H	4.23E+121-30.1	
168551 !Benoite Lefort and Wing Tsang 2011		
PLOG/ 0.1	4.23E+121-30.1	
168551/		
PLOG/ 1.0	6.51E+90	-21.2
150039/		

PLOG/ 10.0		1.03E+59	-12.1	
129282/				
PLOG/ 100.0		8.15E+36	-5.8	
114347/				
A2CH3-2=A2CH2-2+H		4.23E+121	-30.1	
168551	!Benoite Lefort and Wing Tsang 2011			
PLOG/ 0.1		4.23E+121	-30.1	
168551/				
PLOG/ 1.0		6.51E+90	-21.2	
150039/				
PLOG/ 10.0		1.03E+59	-12.1	
129282/				
PLOG/ 100.0		8.15E+36	-5.8	
114347/				
A2CH2-1+H=A2-1+CH3		4.50E+58	-11.9	
51860	!refer to A1CH2+H=A1-+CH3 2007 Klippenstein et al.			
PLOG/ 0.0395		4.50E+58	-11.9	
51860/	!700-2500 K			
PLOG/ 0.132		2.03E+64	-13.37	
59520/	!1000-2500 K			
PLOG/ 1.000		5.83E+67	-14.15	
68330/	!1000-2500 K			
PLOG/ 10.00		8.85E+68	-14.23	
78410/	!1200-2500 K			
A2CH2-2+H=A2-2+CH3		4.50E+58	-11.9	
51860	!refer to A1CH2+H=A1-+CH3 2007 Klippenstein et al.			
PLOG/ 0.0395		4.50E+58	-11.9	
51860/	!700-2500 K			
PLOG/ 0.132		2.03E+64	-13.37	
59520/	!1000-2500 K			
PLOG/ 1.000		5.83E+67	-14.15	
68330/	!1000-2500 K			
PLOG/ 10.00		8.85E+68	-14.23	
78410/	!1200-2500 K			
A2CH3-1+H=A2CH2-1+H2		6.47E+00	3.98	
3394.0	!2006 Oehlschlaeger et al. A1CH3+H=A1CH2+H			
A2CH3-1+H=A2+CH3		5.78E+13	0.0	
8095.0	!A1CH3+H=A1+CH3 1994 Baulch et al. J. Phys. Chem. Ref. Data			
A2CH3-2+H=A2CH2-2+H2		6.47E+00	3.98	
3394.0	!2006 Oehlschlaeger et al. A1CH3+H=A1CH2+H			
A2CH3-2+H=A2+CH3		5.78E+13	0.0	
8095.0	!A1CH3+H=A1+CH3 1994 Baulch et al. J. Phys. Chem. Ref. Data			
A2CH3-1+CH3=A2CH2-1+CH4		3.16E+11	0.0	
9500.0	!A1CH3+CH3=A1CH2+CH4 J.L.Emdee et al. J. Phys. Chem. 96 (1992)			
2151°C2161				
A2CH3-2+CH3=A2CH2-2+CH4		3.16E+11	0.0	
9500.0	!A1CH3+CH3=A1CH2+CH4 J.L.Emdee et al. J. Phys. Chem. 96 (1992)			
2151°C2161				
A2CH3-1+OH=A2CH2-1+H2O		1.77E+05	2.394	-
602.0	!A1CH3+OH=A1CH2+H2O 2006 Seta et al.			
A2CH3-2+OH=A2CH2-2+H2O		1.77E+05	2.394	-
602.0	!A1CH3+OH=A1CH2+H2O 2006 Seta et al.			
A2CH3-1+OH=A2OH-1+CH3		7.83E+02	2.88	
3221.8	!A1CH3+OH=A1OH+CH3 2006 Seta et al.			
A2CH3-2+OH=A2OH-2+CH3		7.83E+02	2.88	
3221.8	!A1CH3+OH=A1OH+CH3 2006 Seta et al.			
A2CH2-1=>C11H8+H		4.47E+129	-32.57	
162410.0	!2011 Derudi et al. RRKM A1CH2=>C7H6+H			

PLOG / 0.013	4.47E+129	-32.57	
162410.0/			
PLOG / 0.130	1.29E+123	-30.34	
163830.0/			
PLOG / 1.000	2.95E+97	-22.95	
148280.0/			
PLOG/ 1.500	8.20E+14	0.00E+00	
8.07E+04/			
PLOG / 10.000	1.26E+39	-6.76	
99710.0/			
PLOG / 50.000	1.44E13	0.453	76300/
C9H7+C2H2=>C11H8+H	1.29E+21	-2.38	
32400 !Gabriel da silva et al. 2010 JPCA 114	C5H5+C2H2=C7H6+H		
PLOG/ 0.0001	1.29E+21	-2.38	
32400/ !Gabriel da silva et al. 2010 JPCA 114			
PLOG/ 0.001	3.37E+12	0.22	
31060/ !Gabriel da silva et al. 2010 JPCA 114			
PLOG/ 0.01	7.07E+01	3.42	
28740/ !Gabriel da silva et al. 2010 JPCA 114			
PLOG/ 0.1	1.58E-01	4.18	
29670/ !Gabriel da silva et al. 2010 JPCA 114			
PLOG/ 1.0	6.96E-05	5.17	
30930/ !Gabriel da silva et al. 2010 JPCA 114			
PLOG/ 10.0	2.37E-06	5.60	
33540/ !Gabriel da silva et al. 2010 JPCA 114			
PLOG/ 100	1.15E-44	17.07	
22460/ !Gabriel da silva et al. 2010 JPCA 114			
C9H8+C2H=C11H8+H	5.00E+13	0.0	
0.0 !A1+C2H=A1C2H+H2011 1997 Wang&Frenklach			
C7H5+nC4H3=C11H8	5.00E+13	0.0	
0.0 !est			
C7H5+iC4H3=C11H8	5.00E+13	0.0	
0.0 !est			

!***** Reactions of C12H8

A2C2HB*+H(+M)=A2C2HB(+M)	1.00E+14	0.0	
0.0 !1997 Wang&Frenklach A2-1+H(+M)=A2(+M) in 1997 Wang&Frenklach			
	LOW / 3.80E+127	-31.434	
18676.0/			
	TROE/ 0.200	122.8	478.4
5411.9/			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/		
C2H6/3.0/			
A2C2HA*+H(+M)=A2C2HA(+M)	1.00E+14	0.0	
0.0 !1997 Wang&Frenklach A2-2+H(+M)=A2(+M) in 1997 Wang&Frenklach			
	LOW / 9.50E+129	-32.132	
18782.0/			
	TROE/ 0.870	492.7	117.9
5652.0/			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/		
C2H6/3.0/			
A2R5-+H(+M)=A2R5(+M)	1.00E+14	0.0	
0.0 !1997 Wang&Frenklach A1-+H(+M)=A1(+M) in 2000 Appel et al.			
	LOW / 6.60E+75	-16.30	
7000.0/			

	TROE/	1.0	0.1	584.9
6113.0/				
	H2/2.0/	H2O/6.0/	CH4/2.0/	CO/1.5/
	CO2/2.0/			
C2H6/3.0/				
C9H7+C3H3=A2R5+H2		4.10E+43	-9.2	
15153.0	!2009	Blanquart et al.		
A2+C2H=A2C2HA+H		5.00E+13	0.0	
0.0	!1997	Wang&Frenklach		
A2+C2H=A2C2HB+H		5.00E+13	0.0	
0.0	!1997	Wang&Frenklach		
A2-1+C2H2=A2C2H2		4.50E+39	-8.71	
14300.0	!1997	Wang&Frenklach		
plog /	0.0132	3.80E+37	-8.23	
12600.0/				
plog /	0.0263	4.50E+39	-8.71	
14300.0/				
plog /	0.1184	3.40E+43	-9.56	
18200.0/				
plog /	1.0000	1.70E+43	-9.12	
21100.0/				
plog /	10.0000	2.00E+28	-4.59	
14400.0/				
A2-1+C2H2=A2C2HA+H		1.40E+22	-2.6	
17400.0	!1997	Wang&Frenklach		
plog /	0.0132	1.20E+21	-2.35	
16300./				
plog /	0.0263	1.40E+22	-2.64	
17400./				
plog /	0.1184	9.10E+24	-3.39	
20400./				
plog /	1.0000	1.30E+24	-3.06	
22600./				
plog /	10.0000	1.60E+14	-0.19	
20000./				
A2-1+C2H2=A2R5+H		2.691e6	2.05	3720.0
!ref HPL of A1-+C2H2=A1C2H+H				
A2C2HA+H=A2C2H2		1.90E+50	-11.63	
16200.0	!1997	Wang&Frenklach RRKM		
plog /	0.0132	1.80E+48	-11.17	
14200.0/				
plog /	0.0263	1.90E+50	-11.63	
16200.0/				
plog /	0.1184	3.30E+51	-11.72	
18900.0/				
plog /	1.0000	5.90E+46	-10.03	
19100.0/				
plog /	10.0000	1.70E+30	-5.07	
11200.0/				
A2C2HA+H=A2R5+H		3.520e+12	0.000	
13360.42				
A2C2H2=A2R5+H		2.10E+50	-12.05	
37800.0	!1997	Wang & Frenklach RRKM		
PLOG /	0.0132	4.40E+50	-12.26	
37100.0/				
PLOG /	0.0263	2.10E+50	-12.05	
37800.0/				

PLOG / 0.1184	2.20E+50	-11.80	
40100.0/			
PLOG / 1.0000	1.50E+46	-10.27	
41300.0/			
PLOG / 10.0000	6.60E+40	-8.42	
42500.0/			
A2C2H2+H=A2C2HA+H2	1.50E+13	0.0	
0.0 !1997 Wang&Frenklach			
A2C2HA+H=A2C2HA*+H2	2.50E+14	0.0	
16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in	1997 Wang&Frenklach		
A2C2HB+H=A2C2HB*+H2	2.50E+14	0.0	
16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in	1997 Wang&Frenklach		
A2C2HA*+C2H3 = A3	6.000e+12	0.000	
0.00			
A2C2HB*+C2H3 = A3	6.000e+12	0.000	
0.00			
A2C2HA+C2H3 = A3+H	1.800e+17	-1.440	
15757.65			
A2C2HB+C2H3 = A3+H	1.800e+17	-1.440	
15757.65			
A2C2HA*+C2H4 = A3+H	3.620e+28	-4.240	
23864.72			
A2C2HB*+C2H4 = A3+H	3.620e+28	-4.240	
23864.72			
A2R5+H=A2R5-+H2	2.50E+14	0.0	
16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in	2000 Appel et al.		
A2R5+O=C11H8+CO	3.20E+13	-0.2	
440.0 !1998 Zhong&Bozzelli C5H5+O=C4H5-N+CO in	2011 Li et		
al.(Toluene) Est.			
A2R5-+O=C11H7+CO	3.20E+13	-0.2	
440.0 !1998 Zhong&Bozzelli C5H5+O=C4H5-N+CO in	2011 Li et		
al.(Toluene) Est.			
A2R5-+OH=C11H8+CO	3.00E+12	0.0	
0.0 !2011 Li et al.(Toluene) Est.			
A2R5+OH=A2CH2-1+CO	1.00E+13	0.0	
0.0 !2011 Li et al.(Toluene) Est.			
A2R5+OH=A2R5- +H2O	3.00E+13	0.0	
0.0 !2011 Li et al.(Toluene) Est.			
!***** Reactions of C12H10			

P2-+H=BIPHEN+H2	6.02E+12	0.0	
0.0 !1997 Mebel et al. C6H7+H=C6H6+H2			
A1-+C3H3=A1C3H2+H	3.00E+12	0.0	
0.0 !1998 D'Anna&Violi			
A1C3H2+C3H3=P2-+H	3.00E+12	0.0	
0.0 !1998 D'Anna&Violi			
A1-+A1-=P2	1.66E+64	-14.68	33262
!R.S. Tranter, S.J. Klippenstein and L.B. Harding 2010			
PLOG/ 0.01	1.66E+64	-14.68	
33262/			
PLOG/ 0.1	6.14E+37	-7.14	
15703/			
PLOG/ 1.0	7.34E+20	-2.335	4125/
PLOG/ 10.0	1.11E+14	-0.405	-610/
PLOG/ 100.0	3.09E+12	0.036	-
1702/			

A1-+A1-=A1+o-C6H4	4.26e-3	4.57	-5739.1
!R.S. Tranter, S.J. Klippenstein and L.B. Harding 2010 O,M,P			
P2-=BIPHEN+H	2.794e+013	0.0	53019.8
!B. Shukla, K. Tsuchiya, M. Koshi, J. Phys. Chem. A 115(2011) 5284-5293.			
P2-=A2R5+H	7.421e+012	0.0	46757.7
!B. Shukla, K. Tsuchiya, M. Koshi, J. Phys. Chem. A 115(2011) 5284-5293.			
C12H9=BIPHEN+H	1.30E16	0.0	33203.0
! Mebel et al. 1997 for A1H=A1+H			
C12H9+H=BIPHEN+H2	6.02E12	0.0	0.0
! Mebel et al. 1997 for A1H+H=A1+H2			
C12H9=A2R5+H	1.00E13	0.0	20000.0
! estimate			
A1+A1-=P2-H	8.10E+36	-8.62	
9125.0	!1997 Wang&Frenklach RRKM	20130319	note for flame speed
simulation converge			
plog / 0.0263	8.10E+36	-8.62	
9125.0/			
plog / 0.1184	2.20E+36	-8.21	
9920.0/			
plog / 1.0000	3.70E+32	-6.74	
9870.0/			
A1+A1-=P2+H	5.600E+12	-0.074	
7550.00	!97-WAN-FRE		
plog / 0.0263	5.600E+12	-0.074	
7550.00/	!by ywh 20130507		
plog / 0.1184	1.500E+14	-0.450	
8915.00/	!		
plog / 1.0000	1.100E+23	-2.920	
15890.00/	!		
plog / 5.0000	1.100E+23	-2.920	
15890.00/	!		
P2+H=P2-H	1.16E+41	-9.51	
10830.0	!1997 Wang&Frenklach RRKM		
plog / 0.0263	1.16E+41	-9.51	
10830.0/			
plog / 0.1184	2.40E+40	-9.06	
11570.0/			
plog / 1.0000	6.82E+35	-7.37	
11230.0/			
A1-+A1-=P2-+H	7.00E+23	-2.3	
38540.0	!1997 Wang&Frenklach RRKM		
plog / 0.0263	7.00E+23	-2.33	
38540.0/			
plog / 0.1184	8.60E+13	0.50	
34820.0/			
plog / 1.0000	2.30E-01	4.62	
28950.0/			
P2=P2-+H	9.00E+37	-6.63	
119580.0	!1997 Wang&Frenklach RRKM		
plog / 0.0263	9.00E+37	-6.63	
119580.0/			
plog / 0.1184	8.10E+31	-4.79	
117120.0/			
plog / 1.0000	1.10E+25	-2.72	
114270.0/			

P2+H=P2-+H2 1.294E+01 3.98 3384.0
!A1CH3+H=A1CH2+H2 *2 2006 Oehlschlaeger et al. J.Phys.Chem A 110,2006
9867-9873

P2+CH3=P2-+CH4 3.16E+11 0.0
9500.0 !A1CH3+CH3=A1CH2+CH4 J.L.Emdee et al. J. Phys. Chem. 96 (1992)
2151`C2161
P2+OH=P2-+H2O 1.77E+05 2.394 -
602.0 !A1CH3+OH=A1CH2+H2O 2006 Seta et al.

!***** Reactions of C13 species

A1-+A1CH2=C13H12 1.66E+64 -14.68 33262
!R.S. Tranter, S.J. Klippenstein and L.B. Harding 2010 A1-+A1-=P2
PLOG/ 0.01 1.66E+64 -14.68
33262/ !
PLOG/ 0.1 6.14E+37 -7.14
15703/ !
PLOG/ 1.0 7.34E+20 -2.335 4125/
!
PLOG/ 10.0 1.11E+14 -0.405 -610/
!
PLOG/ 100.0 3.09E+12 0.036 -
1702/ !
C13H12+H=A1CH2+A1 5.78E+13 0.0
8090.0 !A1CH3+H=A1+CH3 D.L.Baulch et al. J. Phys.Chem.Ref.Data 34
2005 757-1397
C13H11+H=A1-+A1CH2 4.50E+58 -11.9
51860 ! A1CH2+H=A1-+CH3 2007 Klippenstein et al.
PLOG/ 0.0395 4.50E+58 -11.9
51860/ !700-2500 K
PLOG/ 0.132 2.03E+64 -13.37
59520/ !1000-2500 K
PLOG/ 1.000 5.83E+67 -14.15
68330/ !1000-2500 K
PLOG/ 10.00 8.85E+68 -14.23
78410/ !1200-2500 K
C13H12+H=C13H11+H2 6.47E+00 3.98
3384.0 !A1CH3+H=A1CH2+H2 2006 Oehlschlaeger et al. J.Phys.Chem A
110,2006 9867-9873
C13H12+CH3=C13H11+CH4 3.16E+11 0.0
9500.0 !A1CH3+CH3=A1CH2+CH4 J.L.Emdee et al. J. Phys. Chem. 96 (1992)
2151`C2161
C13H12+A1-=C13H11+A1 2.68e-01 3.95
877.06 !A1CH3+A1-=A1CH2+A1 2011 Dryer
C13H12(+M)=C13H11+H(+M) 2.78E+16 0.17
9.1168E+04 !refer A1CH3(+M)=A1CH2+H(+M) S.J. Klippenstein 2007 PCI
2.78E+15 1.00E+98
LOW/1.00E+99 -22.855
9.9882E+04/
TROE/6.547194E-02 1.511253E+01
9.999996E+09 7.596123E+07/
C13H11=C13H10+H 7.649E+107 -26.919
126052 ! Miyoshi 2012 pccp
PLOG/ 0.0132 7.649E+107 -26.919
126052/ ! Miyoshi 2012 pccp

PLOG/ 0.132	2.716E+97	-23.642	
123613/ ! Miyoshi 2012 pccp			
PLOG/ 1.000	1.685E+78	-18.074	
112260/ ! Miyoshi 2012 pccp			
PLOG/ 10.00	9.204E+49	-10.084	
92354/ ! Miyoshi 2012 pccp			
PLOG/ 100.0	1.919E+32	-5.117	
79423/ ! Miyoshi 2012 pccp			
C13H11=o-C6H4+A1CH2	1.650E+130	-33.457	
166047			
PLOG/ 0.0132	1.650E+130	-33.457	
166047/ ! Miyoshi 2012 pccp			
PLOG/ 0.132	9.434E+128	-32.360	
175686/			
PLOG/ 1.000	5.046E+111	-27.042	
170080/			
PLOG/ 10.00	3.143E+77	-17.161	
149543/			
PLOG/ 100.0	7.839E+54	-10.616	
137664/			
C13H11+H=C13H10+H2	1.00E+13	0.0	
0.0 !2010 Zhang et al.(Toluene) Est.			
C13H9+H(+M)=C13H10(+M)	2.60E+14	0.0	
0.0 !USC Mech II C5H5+H(+M)=C5H6(+M)			
	LOW / 4.40E+80	-18.280	
12994.0/			
	TROE/ 0.068 400.7	4135.8	
5501.9/			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/			
C13H10+H=C13H9+H2	7.2E+13	0	
3500.0 !C5H6+H=C5H5+H2			
!!C9H7+C4H4=C13H10+H	3.00E+11	0.0	
0.0 !2001 D'Anna et al. A1CH2+C3H3=A2+2H	shielded 20131118		
!!C9H7+iC4H3=C13H10	4.00E+13	0.0	
7500.0 !2013 Li et al.			
A2-1+C3H3=p-C13H10	1.50E+75	-17.8	
39600.0 !2002 Richter&Howard A1-+C4H3=A2			
A2+C3H3=p-C13H10+H	6.26E+09	2.61	
56500.0 !2010 Zhang et al.(Toluene) A1+C3H3=C9H8+H			
p-C13H9+H(+M)=p-C13H10(+M)	2.60E+14	0.0	
0.0 !USC Mech II C5H5+H(+M)=C5H6(+M)			
	LOW / 4.40E+80	-18.280	
12994.0/			
	TROE/ 0.068 400.7	4135.8	
5501.9/			
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/		
CO2/2.0/			
p-C13H10+H=p-C13H9+H2	7.2E+13	0	3500.0
!C5H6+H=C5H5+H2			
A2-1+C3H2=p-C13H9	1.50E+75	-17.8	39600.0
!2002 Richter&Howard A1-+C4H3=A2			
!***** Reactions of C14 species			

A3-1+H(+M)=A3(+M)	1.00E+14	0.0	
0.0 !2000 Appel et al. RRKM			

	LOW / 4.00E+148	-37.505
20551.0/		
	TROE/ 1.000	536.3 144.9
5632.8/		
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/	
C2H6/3.0/		
A3-4+H(+M)=A3(+M)	1.00E+14	0.0
0.0 !2000 Appel et al. RRKM		
	LOW / 2.10E+139	-34.803
18378.0/		
	TROE/ 0.001	171.4 171.4
4992.8/		
	H2/2.0/ H2O/6.0/ CH4/2.0/ CO/1.5/ CO2/2.0/	
C2H6/3.0/		
A2C2HB*+C2H2=A3-1	5.20E+72	-18.11
33900.0 !1997 Wang&Frenklach		
plog / 0.0132	7.50E+74	-18.83
34200.0/		
plog / 0.0263	5.20E+72	-18.11
33900.0/		
plog / 0.1184	2.00E+72	-17.74
36600.0/		
plog / 1.0000	1.10E+62	-14.56
33100.0/		
plog / 10.0000	5.10E+48	-10.53
28000.0/		
A2C2HB*+C2H2=A2 (C2H) 2+H	5.50E+32	-5.5
27600.0 !1997 Wang&Frenklach		
A2 (C2H) 2+H=A3-1	2.00E+82	-20.23
36900.0 !1997 Wang&Frenklach		
plog / 0.0132	9.50E+84	-21.09
37600.0/		
plog / 0.0263	2.00E+82	-20.23
36900.0/		
plog / 0.1184	2.00E+75	-18.06
34500.0/		
plog / 1.0000	6.90E+63	-14.57
29900.0/		
plog / 10.0000	1.50E+51	-10.77
25500.0/		
A2C2HA*+C2H2=A3-4	5.20E+72	-18.11
33900.0 !1997 Wang&Frenklach		
plog / 0.0132	7.50E+74	-18.83
34200.0/		
plog / 0.0263	5.20E+72	-18.11
33900.0/		
plog / 0.1184	2.00E+72	-17.74
36600.0/		
plog / 1.0000	1.10E+62	-14.56
33100.0/		
plog / 10.0000	5.10E+48	-10.53
28000.0/		
A2C2HA*+C2H2=A2 (C2H) 2+H	5.50E+32	-5.5
27600.0 !1997 Wang&Frenklach		
A2 (C2H) 2+H=A3-4	2.00E+82	-20.23
36900.0 !1997 Wang&Frenklach		

plog / 0.0132	9.50E+84	-21.09	
37600.0/			
plog / 0.0263	2.00E+82	-20.23	
36900.0/			
plog / 0.1184	2.00E+75	-18.06	
34500.0/			
plog / 1.0000	6.90E+63	-14.57	
29900.0/			
plog / 10.0000	1.50E+51	-10.77	
25500.0/			
A2C2HA+C2H=A2 (C2H) 2+H	5.00E+13	0.0	
0.0 !1997 Wang&Frenklach			
A2C2HB+C2H=A2 (C2H) 2+H	5.00E+13	0.0	
0.0 !1997 Wang&Frenklach			
A3+H=A3-1+H2	2.50E+14	0.0	
16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in	1997 Wang&Frenklach		
A3+H=A3-4+H2	2.50E+14	0.0	
16000.0 !1985 Kiefer et al. A1+H=A1-+H2 in	1997 Wang&Frenklach		
A3-1+H=A3-4+H	1.70E+72	-15.2	
77175.0 !1997 Wang&Frenklach RRKM 20Torr			
C9H7+C5H5=>A3+2H	2.560e+29	-4.030	
35205.54 !2009 Banquant			
A2+nC4H3=>A3+H	4.00E+13	0.0	
15976.0 !2011 Li et al A1+nC4H3=A2+H			
A2-1+nC4H3=>A3	1.50E+75	-17.8	
39600.0 !2002 Richter&Howard A1-+C4H3=A2			
A2-2+nC4H3=>A3	1.50E+75	-17.8	
39600.0 !2002 Richter&Howard A1-+C4H3=A2			
A2-1+C4H4=A3+H	3.30E+33	-5.7	
25500.0 !1997 Wang&Frenklach A1-+C2H2=A1C2H+H 1atm			
A2-2+C4H4=A3+H	3.30E+33	-5.7	
25500.0 !1997 Wang&Frenklach A1-+C2H2=A1C2H+H 1atm			
A2R5-+C2H2=A3-4	2.00E+13	0.0	
55000.0 !2010 Zhang et al.			
A1CC+A1=A3+H	5.60E+12	-0.074	
7550.0 !1997 Wang&Frenklach A1-+A1=P2+H			
A1-+A1C2H=A3+H	1.00E+13	0.0	
2430.0 !2007 Nam et al.			
A2-2+C4H4=A3L+H	1.26E+04	2.61	
1434.03 !2009 Blanquant et al. A1-+C4H4=A2+H			
A2+nC4H3=A3L+H	1.00E+13	0.0	
0.0 !			
A3L=A3	7.94E+12	0.0	
65000.0 !1994 Colket&Seery			
A1CH2+C7H5=C13H9CH2+H	1.56E+13	-0.967	-
3266.5 !refer to A1CH2+C3H3=C9H7CH2+H A. Matsugi, A. Miyoshi, Int. J. Chem. Kinet 20130907			
C13H9CH2=C13H8CH2+H	6.28E+71	-18.204	
65710.8 !2012 Matsugi&Miyoshi C9H7CH2=C9H6CH2+H			
plog / 0.0013	6.28E+71	-18.204	
65710.8/			
plog / 0.0132	2.82E+61	-14.813	
62789.9/			
plog / 0.1316	3.77E+47	-10.443	
58071.8/			

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plog / 1.0000          7.54E+33   -6.226
52769.3/
plog / 10.0000        4.44E+21   -2.491
47796.0/
plog /100.0000       2.86E+13    0.015
44394.9/
C13H9CH2=A3+H        3.68E+63  -15.806
57409.9      !2012 Matsugi&Miyoshi C9H7CH2=A2+H
plog / 0.0013        3.68E+63  -15.806
57409.9/
plog / 0.0132        6.88E+51  -12.098
53279.3/
plog / 0.1316        2.37E+38   -7.917
48317.2/
plog / 1.0000        9.04E+25   -4.123
43307.9/
plog / 10.0000       4.13E+16   -1.278
39451.4/
plog /100.0000       5.55E+12   -0.065
38027.7/
C13H8CH2+H=A3+H      5.35E+11    0.627
2422.4      !2012 Matsugi&Miyoshi C9H6CH2+H=A2+H
C13H9+CH3=>C13H9CH2+H  7.49E+13  -0.30    11640
!refer to C5H5+CH3=>C5H5CH2-2+H
PLOG/ 0.01          7.49E+14  -0.30    11640/
!7.49E+13*10
PLOG/ 1.00          7.93E+28  -4.14    24060/
!7.93E+27
PLOG/ 10.0          7.18E+45  -8.75    40084/
!7.18E+44
PLOG/ 100           1.31E+54 -10.86
51760/      !1.31E+53

!***** mechanism of C14H14
*****
C14H14=A1CH2+A1CH2    4.6321E+115  -29.7848293
120099.9107      ! est
PLOG/ 0.006578947    4.6321E+115  -29.7848293
120099.9107/
PLOG/ 0.039473684    4.2051E+101  -25.53235006
114021.0263/
PLOG/ 0.092105263    1.38414E+93  -23.01400394
109754.8055/
PLOG/ 0.197368421    7.41807E+84  -20.57728425
105373.9016/
PLOG/ 0.263157895    4.48855E+81  -19.63256747
103627.1964/
PLOG/ 1              8.69779E+66  -15.33470231
95390.18985/
PLOG/ 10             5.49778E+55   -
11.7831324288414.3428 /
PLOG/ 100            1.16051E+53   -
11.2950575287459.88495/
H+C14H14=C13H12+CH3  6.000E+12    0.000    5000.0
!PolimiV12
H+C14H14=A1CH3+O-C6H4CH3
15000.0              2.500E+12    0.000
H+C14H14=>A1+H+A1C2H3  2.500E+12    0.000    5000.0

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C14H13+H(+M)=C14H14(+M)	5.210E+17	-0.990	1580.0
!GRI C2H5+H(+M)=C2H6(+M)			
	LOW /	1.990E+41	-7.080
6685.0/			
	TROE/	0.8422	125.0 2219.0
6882.0/			
	H2/2.0/	H2O/6.0/	CH4/2.0/ CO/1.5/ CO2/2.0/
C2H6/3.0/ AR/0.7/			
C14H14+H=C14H13+H2	3.16E+12	0.0	0.0
!OEHLSCHLAEGER2005			
C14H14+O2=C14H13+HO2	2.80E+12	0.0	
35000.0 !OEHLSCHLAEGER2005			
C14H14+O=C14H13+OH	8.40E+11	0.0	-
2000.0 !OEHLSCHLAEGER2005			
C14H14+OH=C14H13+H2O	7.00E+09	1.0	-
1100.0 !OEHLSCHLAEGER2005			
C14H14+HO2=C14H13+H2O2	5.40E+11	0.0	
12000.0 !OEHLSCHLAEGER2005			
C14H14+CH3=C14H13+CH4	2.20E+12	0.0	9100.0
!OEHLSCHLAEGER2005			
C14H14+C3H5-A=C14H13+C3H6	2.2E+12	0.0	
9100.0 !			
C14H14+A1-=C14H13+A1	1.06E+14	0.0	9949.0
!BOUNACEUR2005, TABLEV ESTIMATED AA			
C14H14+A1O=C14H13+A1OH	5.43E+12	0.0	
20923.0 !EQUAL TO A1CH3+A1O			
C14H13+O2=A1CHO+A1CH2O	3.94E+50	-11.5	
4.225E+04 !C2H5+O2, A-FACTOR*(4/5)			
C14H13+HO2=A1CH2+A1CHO+OH	1.920E+13	0.0	0.0
!EQUAL TO C2H5+HO2			
C14H12+O2=HO2+C14H11	4.00E+13	0.0	
58200.0 !EQUAL TO C2H4+O2=C2H3+HO2			
C14H12+H=C14H11+H2	8.42E-03	4.62	2583.0
!EQUAL TO C2H4+H=C2H3+H2			
C14H12+OH=C14H11+H2O	2.02E+13	0.0	5955.0
!EQUAL TO C2H4+OH=C2H3+H2O			
C14H12+O=A1CO+A1CH2	7.95E+03	1.66	657.4
!			
C14H11=>A1-+C2H+A1-	1.074E+25	-2.217	
88474.6 !			
C14H11+O2=A1CO+A1CHO	1.70E+29	-5.31	6500.0
!EQUAL TO C2H3+O2=CH2O+HCO			
C14H12+O=C14H11+OH	4.2E+11	0.0	-
1940.0			
C14H12+HO2=C14H11+H2O2	2.7E+11	0.0	
11640.0			
C14H12+CH3=C14H11+CH4	1.1E+12	0.0	8827.0
C14H12+C3H5-A=C14H11+C3H6	1.1E+12	0.0	
8827.0			
C14H12+A1O=C14H11+A1OH	5.43E+12	0.0	
20923.0			
C14H12+A1CH2=C14H11+A1CH3	1.1E+11	0.0	8827.0
A1CH2+A1CH2=C14H13+H	3.360E+38	-6.889	
47618.9 !A.Miyoshi			
A1C2H3+A1-=C14H12+H	1.864e13	-0.385	4163.4
!A.Miyoshi			
C14H13=C14H12+H	1.11E+88	-23.18	
69248 !A.Miyoshi			

PLOG/ 0.0132	1.11E+88	-23.18	
69248/			
PLOG/ 1.00	1.41E+86	-21.83	
74937/			
PLOG/ 100.0	7.80E+55	-12.39	
63902/			
C14H12=C14H11+H	6.22E+129	-31.84	
188442 !A.Miyoshi			
PLOG/ 0.0132	6.22E+129	-31.84	
188442/			
PLOG/ 1.00	6.45E+80	-17.87	
155434 /			
PLOG/ 100.0	5.81E+23	-2.07	
108357/			
C14H11=A3+H	1.06E+72	-18.34	
56760 !A.Miyoshi			
PLOG/ 0.0132	1.06E+72	-18.34	
56760/			
PLOG/ 1.00	5.88E+58	-13.89	
54671/			
PLOG/ 100.0	6.51E+29	-5.13	
41588/			
!Nicolas Delort!			
!C14H11=A1C2H+A1-	1.48E+86	-22.28	
71855 !A.Miyoshi			
! PLOG/ 0.0132	1.48E+86	-22.28	
71855/			
! PLOG/ 1.00	1.16E+74	-17.92	
71936/			
! PLOG/ 100.0	1.67E+41	-7.81	
59061/			
A1-+A1C2H=C14H11	1.10E+41	-8.61	18152.0
!Nicolas Delort: analogy with C6H5+C2H2 = C6H5CCH2 from Marco Mehl PCI 35 (2015) 341-348			
C7H5+C7H5=A3	6.39E+29	-4.03	
35205.54 !2009 Blanquart et al. C5H5+C5H5=A2			
A1CC+A1-=A3	5.00E+12	0.0	6000.0
!2011 Li et al.(Toluene) Est.			
A1C2H-+A1-=A3	5.00E+12	0.0	6000.0
!2011 Li et al.(Toluene) Est.			
A1C2H-+A1=A3+H	1.00E+13	0.0	6000.0
!2013 Li et al.(Tetralin) Est.			
P2-+C2H2=A3+H	4.60E+06	2.0	7300.0
!1997 Wang&Frenklach			
P2+C2H=A3+H	1.00E+13	0.0	0.0
!2011 Li et al.(Toluene) Est.			
A3+OH=A3-1+H2O	2.34E+04	2.68	733.2
!refer to A1+OH			
A3+OH=A3-4+H2O	2.34E+04	2.68	733.2
!refer to A1+OH			
A3+O=A2C2HA+CH2CO	2.20E+13	0.0	4530
!refer to A1+O			
A3+O=A2C2HB+CH2CO	2.20E+13	0.0	4530
!reder to A1+O			
A3+OH => A2C2HA+CH3+CO	1.100e+02	3.250	
5590.34 !Henzi Pitsch 2011			

A3+OH => A2C2HB+CH3+CO	1.100e+02	3.250	
5590.34 !Henzi Pitsch 2011			
A3-1+O2 => A2C2H2B+2CO	8.570e+20	-2.270	
7189.29 !Henzi Pitsch 2011			
A3-4+O2 => A2C2H2A+2CO	8.570e+20	-2.270	
7189.29 !Henzi Pitsch 2011			
C14H13+O2=C14H13OO	8.0E+12	0.0	0.0
!Y. Sakai et al. PCI32 (2009) 411-418			
C14H13+HO2=C14H13OOH	7.0E+12	0.0	-
1000.0 !Y. Sakai et al. PCI32 (2009) 411-418			
A1CH2+A1CHO=C14H13O	1.0E+11	0.0	
12900.0 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H13OOH+A1CH2=C14H13OO+A1CH3	1.44E+10	0.0	
17700.0 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H13OO+HO2=C14H13OOH+O2	1.750E+10	0.0	-
3.275E+03 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H13OO+H2O2=C14H13OOH+HO2	2.400E+12	0.0	
1.000E+04 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H13O+OH=C14H13OOH	2.0E+13	0.0	0.0
!Y. Sakai et al. PCI32 (2009) 411-418			
C14H13OO=C14H12OOH	2.59E+12	0.0	
21374.0 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H12+HO2=C14H12OOH	1.0E+11	0.0	
10530.0 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H12OOH+O2=C14H12O2H-1O2	8.0E+12	0.0	0.0
!Y. Sakai et al. PCI32 (2009) 411-418			
C14H12O2H-1O2=C14H11O-1O2H+OH	1.295E+12	0.0	
18374.0 !Y. Sakai et al. PCI32 (2009) 411-418			
C14H11O-1O2H=A1CHO+A1CO+OH	1.0E+16	0.0	
43000.0 !Y. Sakai et al. PCI32 (2009) 411-418			
o-C6H4+A1=>BICYCLO		1.1618E+04	
2.526 5915.9 !A. Comandini, T. Malewicki, and K. Brezinsky			
J. Phys. Chem. A 2012, 116, 2409-2434			
BICYCLO=>o-C6H4+A1		4.910E+16	
0.00 66811 !A. Comandini, T. Malewicki, and K. Brezinsky J.			
Phys. Chem. A 2012, 116, 2409-2434			
BICYCLO=A2+C2H2		7.458E+14	
0.0956 54780.1 !A. Comandini, T. Malewicki, and K. Brezinsky J. Phys.			
Chem. A 2012, 116, 2409-2434			
!Nicolas Delort			
!A1O+A1O=>DIBZFUR+H2O	4.000E+13	0.00	
11000.0 !Polimi			
!OH+DIBZFUR=>HCO+CO+A2	2.000E+13	0.00	0.0
!Polimi			
A1O+A1O=>DIBZFUR+H2O			
15000.0 !current Polimi coeff - Nicolas Delort	1.500E+13	0.00	
OH+DIBZFUR=>HCO+CO+A2	5.000E+12	0.00	0.0
!current Polimi coeff - Nicolas Delort			
!***** Reactions of C15 and C16 species			

P2+C3H3=A3CH3+H	3.00E+13	0.0	
16000.0 !2011 Li et al.			
A3CH3=A3-1+CH3	3.15E+116	-28.4	
167981 !Benoite Lefort and Wing Tsang 2011 CNF 158			

PLOG/ 0.1		3.15E+116	-28.4
167981/			
PLOG/ 1.0		1.13E+84	-19.1
147456/			
PLOG/ 10.0		1.59E+52	-10.0
126155/			
PLOG/ 100.0		1.12E+33	-4.6
113054/			
A3CH3=A3-4+CH3		3.15E+116	-28.4
167981	!Benoite Lefort and Wing Tsang 2011 CNF 158		
PLOG/ 0.1		3.15E+116	-28.4
167981/			
PLOG/ 1.0		1.13E+84	-19.1
147456/			
PLOG/ 10.0		1.59E+52	-10.0
126155/			
PLOG/ 100.0		1.12E+33	-4.6
113054/			
A3CH3=A3CH2+H		1.72E+95	-22.6
142804			
PLOG/ 0.1		1.72E+95	-22.6
142804/	!Benoite Lefort and Wing Tsang 2011 CNF 158		
PLOG/ 1.0		1.13E+84	-19.1
147456/			
PLOG/ 10.0		1.73E+38	-6.3
105175/			
PLOG/ 100.0		4.46E+22	-1.9
94482/			
A3CH3+H=A3CH2+H2		3.98E+02	3.44
3120.0	!2002 Richter&Howard		
A3CH3+H=A3+CH3		5.78E+13	0.0
8090.0	!2002 Richter&Howard		
A2T2+A1-=FLTHN+H		5.00E+12	0.0
0.0	!2011 Li (Toluene) Est.		
A2-1+A1-=FLTHN+H+H		1.39E+13	0.0
111.0	!1997 Park&Lin A1-+A1-=P2 in 2002 Richter&Howard		
A2-1+A1=FLTHN+H+H2		8.51E+11	0.0
3986.0	!1999 Park et al. A1-+A1=P2+H in 2002 Richter&Howard		
A2T2+o-C6H4=FLTHN		6.50E+39	-7.56
27260.0	!2002 Richter&Howard QRRK-HR 20Torr		
A2T1+o-C6H4=FLTHN		6.50E+39	-7.56
27260.0	!2002 Richter&Howard QRRK-HR 20Torr		
A3+C2H=A3C2H+H		5.00E+13	0.0
0.0	!1997 Wang&Frenklach		
A3-4+C2H2=A3C2H2		6.70E+45	-10.55
21200.0	!1994 Wang&Frenklach RRKM		
plog / 0.0132		8.10E+44	-10.38
20600.0/			
plog / 0.0263		6.70E+45	-10.55
21200.0/			
plog / 0.1184		6.50E+53	-12.59
26900.0/			
plog / 1.0000		8.00E+61	-14.50
34800.0/			
plog / 10.0000		5.60E+50	-10.96
31300.0/			
A3-4+C2H2=A3C2H+H		8.00E+17	-1.2
22600.0	!1994 Wang&Frenklach RRKM		

```

!***** Formation and consumption of A4
*****
*****
A3-4+C2H2=A4+H          1.87E+07   1.787   3262
!O. Mazyar, HP-limit
C13H9+C3H3=A4+H2       1.50E+75  -17.8
39600.0 !2002 Richter&Howard A1-+C4H3=A2
C13H9+C3H2=A4+H        1.50E+75  -17.8
39600.0 !2002 Richter&Howard A1-+C4H3=A2
C13H10+C3H2=A4+H2      1.50E+12   1.8
56500.0 !2010 Zhang et al.(Toluene) A1+C3H3=C9H8+H
p-C13H9+C3H3=A4+H2     1.50E+75  -17.8
39600.0 !2002 Richter&Howard A1-+C4H3=A2
p-C13H9+C3H2=A4+H      1.50E+75  -17.8
39600.0 !2002 Richter&Howard A1-+C4H3=A2
p-C13H10+C3H2=A4+H2    1.50E+12   1.8
56500.0 !2010 Zhang et al.(Toluene) A1+C3H3=C9H8+H
A1C2H-+A1C2H=A4+H      1.10E+23  -2.9
15890.0 !1994 Wang&Frenklach A1-+A1=P2+H 1atm
A1CC+A1CC=A4           5.00E+12   0.0
6000.0 ! A1C2H-+A1-=A3
A1C2H-+A1C2H-=A4      5.00E+12   0.0
6000.0 ! A1C2H-+A1-=A3
A1CC+A1C2H-=A4        5.00E+12   0.0
6000.0 ! A1C2H-+A1-=A3
A3C2H+H=A3C2H2        5.20E+47 -11.05
14700.0 !1994 Wang&Frenklach RRKM
  PLOG / 0.0132         4.90E+37  -8.29
8400.0/
  PLOG / 0.0263         5.20E+47 -11.05
14700.0/
  PLOG / 0.1184         1.40E+56 -13.21
21000.0/
  PLOG / 1.0000         1.90E+64 -15.12
29300.0/
  PLOG / 10.0000        4.50E+51 -11.16
24900.0/
A3C2H+H=A4+H           3.18e09   1.175
4580. !rate updated from Raj et al, Combust Flame, 2009
A3C2H2=A4+H            7.30E+48 -11.86
28100.0 !1994 Wang&Frenklach RRKM
  PLOG / 0.0132         7.90E+46 -11.42
26400.0/
  PLOG / 0.0263         7.30E+48 -11.86
28100.0/
  PLOG / 0.1184         6.30E+59 -14.70
36900.0/
  PLOG / 1.0000         2.00E+63 -15.28
43200.0/
  PLOG / 10.0000        2.50E+33  -6.48
26800.0/
A4+H=A4-1+H2           2.50E+14   0.0
16000.0 ! ref A1+H=A1-+H2 *4/6
A4+H=A4-2+H2           2.50E+14   0.0
16000.0 ! ref A1+H=A1-+H2 *2/6
A4+H=A4-4+H2           2.50E+14   0.0
16000.0 ! ref A1+H=A1-+H2 *4/6

```

A4+CH3=>A4-1+CH4	7.98E-01	3.933	11771
! DFT calculation, KAUST	7.98E-01		
A4-1+CH4=>A4+CH3	4.48E-02	4.248	4277
! DFT calculation, KAUST	4.48E-02		
A4+CH3=>A4-2+CH4	7.98E-01	3.933	11771
! DFT calculation, KAUST	7.98E-01		
A4-2+CH4=>A4+CH3	4.48E-02	4.248	4277
! DFT calculation, KAUST	4.48E-02		
A4+CH3=>A4-4+CH4	7.98E-01	3.933	11771
! DFT calculation, KAUST	7.98E-01		
A4-4+CH4=>A4+CH3	4.48E-02	4.248	4277
! DFT calculation, KAUST	4.48E-02		
A4-1+H(+M)=A4(+M)	1.0e14	0.0	0.0
! ref A1-+H(+M)=A1(+M)			
	LOW /	6.6e75	-16.3 7000.
/			
	TROE/	1.0	0.1 585.
6113. /			
A4-2+H(+M)=A4(+M)	1.0e14	0.0	0.0
! ref A1-+H(+M)=A1(+M)			
	LOW /	6.6e75	-16.3 7000.
/			
	TROE/	1.0	0.1 585.
6113. /			
A4-4+H(+M)=A4(+M)	1.0e14	0.0	0.0
! ref A1-+H(+M)=A1(+M)			
	LOW /	6.6e75	-16.3 7000.
/			
	TROE/	1.0	0.1 585.
6113. /			
A3+C2H=A4+H	1.00E+13	0.0	
0.0 !1997 Wang&Frenklach			
A2R5-+C2H2=A2R5R5+H	8.20E+30	-5.4	
16900.0 !1994 Wang&Frenklach	A2-1+C2H2=A2R5+H		in 2010 Zhang et al. (Toluene)
A2R5+C2H=A2R5R5+H	8.20E+30	-5.4	
16900.0 !1994 Wang&Frenklach	A2-1+C2H2=A2R5+H		in 2010 Zhang et al. (Toluene)
A4+OH=A4-1+H2O	2.34E+04	2.68	
733.2 !refer to A1+OH			
A4+OH=A4-2+H2O	2.34E+04	2.68	
733.2 !refer to A1+OH			
A4+OH=A4-4+H2O	2.34E+04	2.68	
733.2 !refer to A1+OH			
A4+OH=>A3-4+CH2CO	1.30E+13	0.0	
10600.0 ! CEC			
A4+OH=>A3+HCCO	5.500e+02	3.250	
5590.34 !			
A4+O=>A3-4+HCCO	2.20E+13	0.0	
4530.0 !=A1 + O			
A4-1+O2=>A3-4+CO+CO	2.10E+12	0.0	
7470.0 ! = A1- + O2			
A4-2+O2=>A3-4+CO+CO	2.10E+12	0.0	
7470.0 ! = A1- + O2			
A4-4+O2=>A3-4+CO+CO	2.10E+12	0.0	
7470.0 ! = A1- + O2			

!!***** Reactions of C18 species

A3C2H-2+C2H2=CHRYSEN-1 5.60E05 2.282 3261
 !QRRK,Oleg, HP-limit
 A3C2H-1+C2H2=CHRYSEN-4 1.87E07 1.787 3262
 !O. Mazyar, HP-limit

!Nicolas Delort!
 !A2-2+A1C2H=CHRYSEN+H 8.51E11 0.0
 3986 !Park et al. 99 HP limit
 !A2+A1C2H-=CHRYSEN+H 8.51E11 0.0
 3986 !Park et al. 99 HP limit
 A2-2+A1C2H=CHRYSEN+H 2.51E+12 0.0
 6200.0 !Nicolas Delort :as A1-+C2H4=A1C2H3+H in NUIG 1.1
 A2+A1C2H-=CHRYSEN+H 2.51E+12 0.0
 6200.0 !Nicolas Delort : as A1-+C2H4=A1C2H3+H in NUIG 1.1

CHRYSEN+H=CHRYSEN-1+H2 1.301e17 -0.70
 20011.2 !ref A1+H=A1-+H2 *6/6 (J1,J2,J3 are lumped)
 CHRYSEN+H=CHRYSEN-4+H2 6.667e11 -0.70
 20011.2 !ref A1+H=A1-+H2 *2/6
 CHRYSEN+H=CHRYSEN-5+H2 6.667e11 -0.70
 20011.2 !ref A1+H=A1-+H2 *2/6
 CHRYSEN-1+H(+M)=CHRYSEN(+M) 1.0e14 0.0
 0.0 !ref A1-+H(+M)=A1(+M)

7000. / LOW/ 6.6e75 -16.3
 TROE/ 1.0 0.1 585.

6113. /
 CHRYSEN-4+H(+M)=CHRYSEN(+M) 1.0e14 0.0 0.0
 !ref A1-+H(+M)=A1(+M)

7000. / LOW/ 6.6e75 -16.3
 TROE/ 1.0 0.1 585.

6113. /
 CHRYSEN-5+H(+M)=CHRYSEN(+M) 1.0e14 0.0 0.0
 ! ref A1-+H(+M)=A1(+M)

7000. / LOW/ 6.6e75 -16.3
 TROE/ 1.0 0.1 585.

6113. /
 P2-+A1-=C18H12+H2 1.00E+13 0.0 0.0
 !2011 Li(Toluene) Est.
 C9H7+C9H7=CHRYSEN+2H 1.00E+12 0.0 6000
 !2009 Blanquart et al. C5H5+C5H5=A2+2H

End of PAH gas phase
 mechanism #####

 #####
 #####

!
 ++++++
 ! +
 +
 ! + <=== XYLENES

MECHANISMS FROM KUKKADAPU 2018 ==> +

!
+
!
++++
!

!P-XYLENE

!***** INITIATION *****

P-XYL (+M) <=> P-CH3A1CH2+H (+M) 5.56E+15 1.70E-01 9.12E+04
LOW/ 2.00E+98 -2.29E+01 9.99E+04 /
TROE/ 6.55E-02 1.51E+01 1.00E+10 7.60E+07 /

P-XYL (+M) <=> P-C6H4CH3+CH3 (+M) 3.90E+27 -3.16E+00 1.07E+05
LOW/ 1.00E+98 -2.30E+01 1.22E+05 /
TROE/ 7.05E-01 1.00E+10 4.60E+02 8.21E+09 /

CH3C6H3CH3+H (+M) = P-XYL (+M) 1.00E+14 0.00E+00 0.00E+00
LOW / 6.60E+75 -1.63E+01 7.00E+03 /
TROE / 1.00E+00 1.00E-01 5.85E+02 6.11E+03 /
H2/2.000/ H2O/6.000/ CH4/2.000/ CO/1.500/ CO2/2.000/ C2H6/3.000/

!SUBSTITUTIONS

P-XYL+H=A1CH3+CH3 1.90E+06 2 943

P-XYL+OH=P-HOA1CH3+CH3 1.57E+03 2.88E+00 3.22E+03

!***** ABSTRACTIONS *****

P-XYL+H<=>P-CH3A1CH2+H2 12.94 3.98E+00 3.38E+03
P-XYL+O<=>P-CH3A1CH2+OH 15.08E+04 2.57 3.15E+03 !! LI ET AL., J.
PHYS. CHEM. A 2016, 120, 3424 3432
P-XYL+OH<=>P-CH3A1CH2+H2O 3.54E+05 2.39 -602 !!! !! A/1.35 !!
1.77E+05 2.39 -602 !!A/1.35 !!! !! A/1.35 !! !! A*2 FOR DEGENERACY
354000 2.39E+00 -6.02E+02 !!
P-XYL+O2<=>P-CH3A1CH2+HO2 8720000 2.50E+00 4.60E+04
P-XYL+HO2<=>P-CH3A1CH2+H2O2 4.201E+13 0 1.89E+04
P-XYL+CH3<=>P-CH3A1CH2+CH4 5.12E+00 3.80E+00 7.40E+03 !! LI ET
AL., J. PHYS. CHEM. A 2016, 120, 3424 3432
P-XYL+CH3O2=P-CH3A1CH2+CH3O2H 0.146 4.12E+00 1.28E+04
P-XYL+HCO<=>P-CH3A1CH2+CH2O 7.54E+13 0.00E+00 2.38E+04
P-XYL+C2H3<=>P-CH3A1CH2+C2H4 8.00E+03
P-XYL+C3H5-A<=>P-CH3A1CH2+C3H6 7.94E+11 0.00E+00 2.05E+04
P-XYL+C3H3<=>P-CH3A1CH2+C3H4-P 7.94E+11 0.00E+00 2.05E+04
P-XYL+C4H5-I<=>P-CH3A1CH2+C4H6 7.94E+11 0.00E+00 2.05E+04
P-XYL+C4H5-N<=>P-CH3A1CH2+C4H6 7.94E+11 0.00E+00 2.05E+04
!P-XYL+C5H5<=>P-CH3A1CH2+C5H6 3.2E+12 0 11100
P-XYL+C5H5<=>P-CH3A1CH2+C5H6 1.086E+13 0.00E+00 2.09E+04
P-XYL+A1-<=>P-CH3A1CH2+A1 0.536 3.95 877.06
P-XYL+A1O<=>P-CH3A1CH2+A1OH 1.086E+13 0.00E+00 2.09E+04

P-XYL+P-C6H4CH3<=>P-CH3A1CH2+A1CH3 1.58E+14 0.00E+00 1.20E+04
P-XYL+O-C6H4CH3<=>P-CH3A1CH2+A1CH3 1.58E+14 0.00E+00 1.20E+04
P-XYL+A1OO=P-CH3A1CH2+A1OOH 20400 2.50E+00 1.23E+04
P-XYL+P-OA1CH3<=>P-CH3A1CH2+P-HOA1CH3 1.6E+11 0.00E+00 1.51E+04
P-XYL+O-OA1CH3<=>P-CH3A1CH2+O-HOA1CH3 1.6E+11 0.00E+00 1.51E+04
P-XYL+A1CH2OO<=>P-CH3A1CH2+A1CH2OOH 8E+11 0.00E+00 1.40E+04
P-XYL+A1CH2O<=>P-CH3A1CH2+A1CH2OH 1.086E+13 0.00E+00 2.09E+04
P-XYL+P-HOA1CH2<=>P-CH3A1CH2+P-HOA1CH3 3.2E+11 0.00E+00 1.51E+04
P-XYL+O-HOA1CH2<=>P-CH3A1CH2+O-HOA1CH3 3.2E+11 0.00E+00 1.51E+04

P-XYL+H=CH3C6H3CH3+H2 1.60E+08 1.83E+00 1.44E+04! LI ET AL., J.
PHYS. CHEM. A 2016, 120, 3424 3432!
P-XYL+O<=>CH3C6H3CH3+OH 24.12E+010 0.700 7632.0 !! 0.90E+11
0.7 8960 !! 2.08E+13 0.00E+00 1.47E+04
P-XYL+OH<=>CH3C6H3CH3+H2O 1.09E+04 2.69E+00 6.20E+02
P-XYL+HO2<=>CH3C6H3CH3+H2O2 2.20E+12 0.00E+00 28811.5
P-XYL+CH3<=>CH3C6H3CH3+CH4 1.75E-04 5.00E+00 1.23E+04
!
! ***** BENZYL+O *****

P-XYL+O<=>OCH3A1CH3+H 1.66E+07 1.8 3974
!
P-XYL+O=HOCH3A1CH3 3.86E+22 -2.56 14993
DUP
P-XYL+O=HOCH3A1CH3 8.00E+20 -2.6 6684
DUP
P-XYL+O=DMCPD+CO 4.82E+15 -4.90E-01 1.50E+04
CH3C6H3CH3+O<=>OCH3A1CH3 1.00E+14 0.00E+00 0.00E+00
P-XYL+OH<=>HOCH3A1CH3+H 2.51E+01 3.37E+00 4.72E+03

CH3C6H3CH3+OH<=>HOCH3A1CH3 3.00E+13 0.00E+00 0.00E+00
!
P-CH3A1CH2+O<=>A1CH3+HCO 10.50E+12 0.329 686 !!A*1.5 DA
SILVA&BOZZELLI, PHYS. CHEM. CHEM. PHYS., 2012, 14, 16143 16154
P-CH3A1CH2+O=P-CH3A1CHO+H 4.25E+13 0.0723 732 !! DA SILVA&BOZZELLI,
PHYS. CHEM. CHEM. PHYS., 2012, 14, 16143 16154
!
!
P-CH3A1CH2=P-XYLYLE+H 2.50E+15 0.00E+00 7.05E+04 !! LP RATE, J.
PHYS. CHEM. A, VOL. 113, NO. 38, 2009
P-XYLYLE+O=>P-CHOA1CH2+H 9.00E+008 1.450 -860.0 !!
!Nicolas Delort! P-CH3A1CH2+C2H2=CH3C9H7+H 3.20E+12 0.00 1.38E+04 !! SAME
AS A1CH2+C2H2...GOK ADDITION,, NEED MORE INFO ABOUT THIS PATH..
!PLOG/3.947E-02 1.54E+31 -5.60 22640.0/
!PLOG/3.947E-02 1.40E+08 0.91 10080.0/ ! fit btw. 500 and 2500 K with MAE
of 0.6%, 1.6%
!PLOG/1.000E+00 2.24E+36 -6.98 27250.0/
!PLOG/1.000E+00 1.08E+55 -11.29 72720.0/ ! fit btw. 500 and 2500 K with
MAE of 1.0%, 3.7%
!PLOG/1.000E+01 6.32E+194 -47.77 254800.0/
!PLOG/1.000E+01 1.85E+42 -8.50 34890.0/ ! fit btw. 500 and 2500 K with
MAE of 4.9%, 14.6%
!PLOG/1.000E+02 5.70E+44 -8.96 43510.0/
!PLOG/1.000E+02 7.19E+175 -52.00 76360.0/ ! fit btw. 500 and 2500 K with
MAE of 5.6%, 15.5%
!
P-CH3A1CH2=C7H6+CH3 0.500E+15 0.00 7.62E+04 !! LP RATE,, J. PHYS.
CHEM. A, VOL. 113, NO. 38, 2009

P-CH3A1CH2+O2=P-CH3A1CH2OO 1.382E+41 -9.44 9020.0
PLOG / 0.1 3.28E+46 -11.59 9.00E+03 /!! MURAKAMI_BENZYL
PLOG / 1 2.82E+45 -10.974 9.730E+03 /!! MURAKAMI_BENZYL
PLOG / 10 9.56E+38 -8.765 8.43E+03 /!! MURAKAMI_BENZYL!
PLOG / 100 4.60E+31 -6.36 6.51E+03 /!! MURAKAMI_BENZYL
!
P-CH3A1CH2OO=P-CH3A1CHO+OH 1.00E+00 0.00E+00 0.00E+00 !! /!!
MURAKAMI_BENZYL +O2 RATES
PLOG/ 0.1 1.54E+47 -13.01 4.12E+04/ !! REFIT BY GOUTHAM,
PLOG/ 1 6.65E+45 -11.77 4.36E+04/ !! REFIT BY GOUTHAM,
PLOG/ 10 7.17E+45 -11.03 4.77E+04/ !! REFIT BY GOUTHAM,
PLOG/ 100 5.46E+46 -10.43 5.35E+04/ !! REFIT BY GOUTHAM,
!
P-CH3A1CH2OO=P-OA1CH3+CH2O 1.00E+00 0.00E+00 0.00E+00 !!
/!! MURAKAMI_BENZYL +O2 RATES
PLOG/ 0.1 3.59333E+47 -13.01 4.12E+04/ !! REFIT BY GOUTHAM,
PLOG/ 1 1.55167E+46 -11.77 4.36E+04/ !! REFIT BY GOUTHAM,
PLOG/ 10 1.673E+46 -11.03 4.77E+04/ !! REFIT BY GOUTHAM,
PLOG/ 100 1.274E+47 -10.43 5.35E+04/ !! REFIT BY GOUTHAM,
!
!
!
P-CH3A1CH2+O2=P-CH3A1CH2O+O 6.30E+12 0.00E+00 4.00E+04
P-CH3A1CH2OO+H=P-CH3A1CH2O+OH 3.80E+14 -0.19 1.89E+03
P-CH3A1CH2OO+H=P-CH3A1CH2OOH 4.35E+60 -15.92 1.14E+04
P-CH3A1CH2OO+H=P-CH3A1CH2+HO2 1.96E+04 2.47 1.43E+03
P-CH3A1CH2OO+P-CH3A1CH2OO=>2P-CH3A1CH2O+O2 6.30E+10 0.00E+00 -
7.25E+02
!
!! !NEW BLOCK ADDED BY GOUTHAM
!
P-CH3A1CH2+P-CH3A1CH2=P-XYLDIMER 1.550E+024 -3.784 2.03E+03 !! XYLENE
RATE_RATE FROM MATSUGI AND MYOSHI_DOI:10.1016/J.CPLETT.2011.11.043!!!
!
!
P-XYLDIMER+OH=P-XYLDIMERJ+H2O 39.0E+005 2.200 -
437.18
P-XYLDIMER+O2=P-XYLDIMERJ+HO2 2.80E+12 0.00 35000.0
P-XYLDIMERJ+HO2=P-CH3A1CH2+P-CH3A1CHO+OH 5.00E+12 0.00 0.000E+00
!
!
!***** PHENYL+O2 *****
!
!CH3C6H3CH3+O2=XYLMETHIDE+OH
+3.7000000E+012 -1.8000000E-001 -1.5200000E+003 !AUTHORS: SILVA ET AL.
JPC, 2007, 111:8663-8676
!PLOG / +1.0000000E-002
+3.4800000E+009 +6.5000000E-001 -4.2000000E+003 /
!PLOG / +1.0000000E-001
+4.9800000E+009 +6.0000000E-001 -4.0600000E+003 /
!PLOG / +1.0000000E+000
+3.7000000E+012 -1.8000000E-001 -1.5200000E+003 /
!PLOG / +1.0000000E+001
+1.7400000E+024 -3.3600000E+000 +8.9800000E+003 /
!PLOG / +1.0000000E+002
+3.7200000E+040 -7.7700000E+000 +2.4940000E+004 /

CH3C6H3CH3+O2=XYLMETHIDE+OH
 +11.1000000E+012 -1.8000000E-001 -1.5200000E+003 ! Nicolas Delort A*3
 PLOG / +1.0000000E-002
 +10.4400000E+009 +6.5000000E-001 -4.2000000E+003 /
 PLOG / +1.0000000E-001
 +14.9400000E+009 +6.0000000E-001 -4.0600000E+003 /
 PLOG / +1.0000000E+000
 +11.1000000E+012 -1.8000000E-001 -1.5200000E+003 /
 PLOG / +1.0000000E+001
 +5.2200000E+024 -3.3600000E+000 +8.9800000E+003 /
 PLOG / +1.0000000E+002
 +11.1600000E+040 -7.7700000E+000 +2.4940000E+004 /

O2CH3A1CH3=XYLMETHIDE+OH
 +2.0300000E+045 -1.0170000E+001 +4.0220000E+004 !AUTHORS: SILVA ET AL.
 JPC, 2007, 111:8663-8676
 PLOG/ 1.00E-01 3.91E+38 -8.69E+00 32140 /
 PLOG/ 1.00E+00 2.03E+45 -1.02E+01 40220 /
 PLOG/ 1.00E+01 2.14E+44 -9.50E+00 43440 /
 PLOG/ 1.00E+02 6.02E+33 -6.25E+00 39470 /
 !
 !
 XYLMETHIDE=A1CH3+CO
 +6.3100000E+014 +0.0000000E+000 +6.7160000E+004 !DORRESTIJN1997
 !
 !
 !CH3C6H3CH3+O2=OCH3A1CH3+O 8.570E+20 -2.270 7190.0
 !WAGNON1@LLNL.GOV! AS P-C6H4CH3+O2=P-OA1CH3+O DA SILVA JPCA 117 (2007)
 8663-8676
 !PLOG/ 1.00E-01 4.99E+18 -1.68 5320 /
 !PLOG/ 1.00E+00 9.18E+20 -2.3 7370 /
 !PLOG/ 1.00E+01 7.27E+29 -4.72 15600 /
 !PLOG/ 1.00E+02 1.52E+43 -8.3 29100 /
 CH3C6H3CH3+O2=OCH3A1CH3+O 2.860E+20 -2.270 7190.0
 ! Nicolas Delort A/3
 PLOG/ 1.00E-01 1.663E+18 -1.68 5320 /
 PLOG/ 1.00E+00 3.06E+20 -2.3 7370 /
 PLOG/ 1.00E+01 2.423E+29 -4.72 15600 /
 PLOG/ 1.00E+02 0.507E+43 -8.3 29100 /
 !
 CH3C6H3CH3+O2=>O2CH3A1CH3 1.950E+11 0.420 -631.1
 !WAGNON1@LLNL.GOV! AS P-C6H4CH3+O2=>P-O2C6H4CH3 DA SILVA JPCA 117 (2007)
 8663-8676
 PLOG/ 1.00E-01 6.51+107 -32.05 12220 /
 PLOG/ 1.00E+00 3.21+132 -38.08 33960 /
 PLOG/ 1.00E+01 2.35+160 -45.03 60240 /
 PLOG/ 1.00E+02 6.57+179 -49.68 81660 /
 !
 O2CH3A1CH3=>CH3C6H3CH3+O2 3.240E+36 -7.200 50220.0
 !WAGNON1@LLNL.GOV! AS P-O2C6H4CH3=>P-C6H4CH3+O2 DA SILVA JPCA 117 (2007)
 8663-8676
 PLOG/ 1.00E-01 2.78E+29 -5.55E+00 45160 /
 PLOG/ 1.00E+00 1.52E+34 -6.56E+00 48790 /
 PLOG/ 1.00E+01 3.27E+41 -8.25E+00 56050 /
 PLOG/ 1.00E+02 9.47E+41 -8.01E+00 59770 /
 !

O2CH3A1CH3=>OCH3A1CH3+O 3.700E+40 -8.440 45870.0
!WAGNON1@LLNL.GOV! AS P-O2C6H4CH3=P-OA1CH3+O DA SILVA JPCA 117 (2007)
8663-8676

PLOG/ 1.00E-01 2.28E+29 -5.69 36320 /
PLOG/ 1.00E+00 3.05E+37 -7.61 43660 /
PLOG/ 1.00E+01 1.64E+43 -8.82 50880 /
PLOG/ 1.00E+02 3.00E+38 -7.15 51140 /

!
!
!
!

!Nicolas Delort ! CH3C6H3CH3+O2=>C3H4-P+C3H4-P+HCO+CO
10.200E+13 -0.440 -1650.0 !WAGNON1@LLNL.GOV! A*2 AS P-
C6H4CH3+O2=METHYLDIOXOHEXADIENYL DA SILVA JPCA 117 (2007) 8663-8676

!PLOG/ 1.00E-01 1.39E+10 5.20E-01 -4500 /
!PLOG/ 1.00E+00 1.12E+13 -2.80E-01 -1940 /
!PLOG/ 1.00E+01 1.03E+25 -3.54E+00 8780 /
!PLOG/ 1.00E+02 7.58E+41 -8.10E+00 25180 /

!
!

O2CH3A1CH3=>C5H4CH3+CH2O+CO 3.580E+50 -11.550 43310.0
!WAGNON1@LLNL.GOV! AS P-O2C6H4CH3=>METHYLDIOXOHEXADIENYL DA SILVA JPCA
117 (2007) 8663-8676

PLOG/ 1.00E-01 0.95E+42 -9.68E+00 33810 /
PLOG/ 1.00E+00 0.95E+48 -1.10E+01 41370 /
PLOG/ 1.00E+01 3.32E+46 -1.02E+01 44320 /
PLOG/ 1.00E+02 2.82E+37 -7.30E+00 42030 /

!

O2CH3A1CH3=>C5H4O+C2H5CO 3.580E+50 -11.550 43310.0 !WAGNON1@LLNL.GOV!
AS P-O2C6H4CH3=>METHYLDIOXOHEXADIENYL DA SILVA JPCA 117 (2007) 8663-8676

PLOG/ 1.00E-01 1.90E+42 -9.68E+00 33810 /
PLOG/ 1.00E+00 1.89E+48 -1.10E+01 41370 /
PLOG/ 1.00E+01 6.64E+46 -1.02E+01 44320 /
PLOG/ 1.00E+02 5.64E+37 -7.30E+00 42030 /

!

!***** BENZYL+HO2

P-CH3A1CH2OOH<=>P-CH3A1CH2O+OH 1.00E+00 1.00E+00
1.00E+00

PLOG / 1.00E-03 9.39E+69 -1.77E+01 5.80E+04 /
PLOG / 1.00E-03 9.93E+35 -8.71E+00 5.69E+04 /
PLOG / 1.00E-02 3.42E+67 -1.66E+01 5.92E+04 /
PLOG / 1.00E-02 5.84E+40 -9.72E+00 6.07E+04 /
PLOG / 1.00E-01 9.00E+60 -1.43E+01 5.84E+04 /
PLOG / 1.00E-01 9.54E+41 -9.67E+00 6.35E+04 /
PLOG / 1.00E+00 1.48E+50 -1.08E+01 5.53E+04 /
PLOG / 1.00E+00 3.94E+36 -7.71E+00 6.33E+04 /
PLOG / 1.00E+01 1.20E+38 -6.99E+00 5.10E+04 /
PLOG / 1.00E+01 1.04E+26 -4.31E+00 6.01E+04 /
PLOG / 1.00E+02 1.88E+29 -4.28E+00 4.75E+04 /
PLOG / 1.00E+02 1.80E+16 -1.27E+00 5.66E+04 /

P-CH3A1CH2OOH<=>P-CH3A1CHO+H2O 1.00E+00 1.00E+00
1.00E+00

PLOG / 1.00E-03 5.23E+53 -1.36E+01 5.78E+04 /
PLOG / 1.00E-02 2.81E+52 -1.28E+01 5.95E+04 /
PLOG / 1.00E-01 7.04E+46 -1.08E+01 5.92E+04 /

PLOG / 1.00E+00 3.91E+36 -7.41E+00 5.64E+04 /
PLOG / 1.00E+01 3.68E+24 -3.64E+00 5.22E+04 /
PLOG / 1.00E+02 3.87E+15 -8.70E-01 4.87E+04 /

P-CH3A1CH2+CH3=P-CH3A1C2H5 0.600E+013 +0.0000000E+000 +2.2100000E+002!

!
!

P-CH3A1CH2+HO2<=>P-CH3A1CH2OOH 3.750E+30 -6.00 2.50E+03 !! MARCO FIT,
A

!
!!

P-CH3A1CH2+HO2<=>P-CH3A1CH2O+OH 1.00E+97 -2.50E+01 4.40E+04 !!

DUP

P-CH3A1CH2+HO2<=>P-CH3A1CH2O+OH 1.00E+35 -6.00E+00 2.00E+04 !! C

DUP

P-CH3A1CH2+HO2<=>P-CH3A1CHO+H2O 1.00E+00 1.00E+00

1.00E+00

PLOG / 1.00E-03 5.06E-03 3.88E+00 4.11E+02 /

PLOG / 1.00E-02 2.02E-01 3.43E+00 1.46E+03 /

PLOG / 1.00E-01 7.38E+03 2.13E+00 4.66E+03 /

PLOG / 1.00E+00 2.51E+09 6.10E-01 9.47E+03 /

PLOG / 1.00E+01 2.66E+09 7.30E-01 1.25E+04 /

PLOG / 1.00E+02 1.24E+02 2.93E+00 1.17E+04 /

P-CH3A1CH2OO+HO2<=>P-CH3A1CH2OOH+O2 2.00E+11 0.00E+00
-1.30E+03

P-CH3A1CH2OOH+H=>P-CH3A1CHO+H2+OH 6.47E+00 3.98E+00

3.38E+03

P-CH3A1CH2OOH+OH=>P-CH3A1CHO+H2O+OH 3.00E+05 2.39E+00

-6.02E+02

P-CH3A1CH2OOH+O2=>P-CH3A1CHO+HO2+OH 2.18E+07 2.50E+00

4.60E+04

P-CH3A1CH2OOH+HO2=>P-CH3A1CHO+H2O2+OH 2.45E-05 5.26E+00

7.48E+03

P-CH3A1CH2OOH+CH3=>P-CH3A1CHO+CH4+OH 2.94E+11 0.00E+00

9.25E+03

P-CH3A1CH2+CH3O2=P-CH3A1CH2O+CH3O 1.00E+97 -2.50E+01 4.40E+04

DUP

P-CH3A1CH2+CH3O2=P-CH3A1CH2O+CH3O 1.00E+35 -6.00E+00 2.00E+04

DUP

P-CH3A1CH2+C2H5O2=P-CH3A1CH2O+C2H5O 1.00E+97 -2.50E+01 4.40E+04

DUP

P-CH3A1CH2+C2H5O2=P-CH3A1CH2O+C2H5O 1.00E+35 -6.00E+00 2.00E+04

DUP

CH3C6H3CH3+HO2<=>OCH3A1CH3+OH 2.00E+12 0.00E+00

0.00E+00

!

P-CH3A1CH2O=P-CH3A1CHO+H 3.04E+32 -6.67E+00 2.19E+04

PLOG/ 1.00E-02 2.43E+32 -6.67E+00 2.19E+04 / !!

PLOG/ 1.00E-01 4.90E+31 -6.26E+00 2.24E+04 / !!

PLOG/ 1.00E+00 4.21E+28 -5.08E+00 2.23E+04 / !!

PLOG/ 1.00E+01 1.34E+22 -2.90E+00 2.08E+04 / !!
 PLOG/ 1.00E+02 1.95E+17 -1.31E+00 1.95E+04 / !!
 ! !
 P-CH3A1CH2O=P-C6H4CH3+CH2O 4.59E+43 -9.51E+00 3.91E+04
 PLOG/ 1.00E-02 3.67E+43 -9.51E+00 3.91E+04/ !!
 PLOG/ 1.00E-01 2.30E+38 -7.79E+00 3.78E+04/ !!
 PLOG/ 1.00E+00 5.77E+33 -6.21E+00 3.69E+04/ !!
 PLOG/ 1.00E+01 1.06E+27 -4.01E+00 3.51E+04/ !!
 PLOG/ 1.00E+02 8.64E+20 -2.06E+00 3.33E+04/ !!
 P-CH3A1CH2O=A1CH3+HCO 2.57E+31 -6.22E+00 2.58E+04
 PLOG/ 1.00E-02 3.21E+31 -6.22E+00 2.58E+04/ !!
 PLOG/ 1.00E-01 6.59E+31 -6.15E+00 2.69E+04/ !!
 PLOG/ 1.00E+00 2.96E+32 -6.10E+00 2.88E+04/ !!
 PLOG/ 1.00E+01 4.78E+31 -5.66E+00 2.98E+04/ !!
 PLOG/ 1.00E+02 2.55E+28 -4.58E+00 2.92E+04/ !!
 !
 P-CH3A1CH2O+H=P-CH3A1CHO+H2 1.33E+13 0.00E+00 0.00E+00
 P-CH3A1CH2O+O=P-CH3A1CHO+OH 6.67E+12 0.00E+00 0.00E+00
 P-CH3A1CH2O+OH=P-CH3A1CHO+H2O 3.33E+12 0.00E+00
 0.00E+00
 P-CH3A1CH2O+O2<=>P-CH3A1CHO+HO2 6.00E+10 0.00E+00
 1.60E+03

O-CH3A1CH2O=O-CH3A1CHO+H 3.04E+32 -6.67E+00 2.19E+04
 PLOG/ 1.00E-02 2.43E+32 -6.67E+00 2.19E+04 / !!
 PLOG/ 1.00E-01 4.90E+31 -6.26E+00 2.24E+04 / !!
 PLOG/ 1.00E+00 4.21E+28 -5.08E+00 2.23E+04 / !!
 PLOG/ 1.00E+01 1.34E+22 -2.90E+00 2.08E+04 / !!
 PLOG/ 1.00E+02 1.95E+17 -1.31E+00 1.95E+04 / !!
 ! !
 O-CH3A1CH2O=O-C6H4CH3+CH2O 4.59E+43 -9.51E+00 3.91E+04
 PLOG/ 1.00E-02 3.67E+43 -9.51E+00 3.91E+04/ !!
 PLOG/ 1.00E-01 2.30E+38 -7.79E+00 3.78E+04/ !!
 PLOG/ 1.00E+00 5.77E+33 -6.21E+00 3.69E+04/ !!
 PLOG/ 1.00E+01 1.06E+27 -4.01E+00 3.51E+04/ !!
 PLOG/ 1.00E+02 8.64E+20 -2.06E+00 3.33E+04/ !!
 O-CH3A1CH2O=A1CH3+HCO 2.57E+31 -6.22E+00 2.58E+04
 PLOG/ 1.00E-02 3.21E+31 -6.22E+00 2.58E+04/ !!
 PLOG/ 1.00E-01 6.59E+31 -6.15E+00 2.69E+04/ !!
 PLOG/ 1.00E+00 2.96E+32 -6.10E+00 2.88E+04/ !!
 PLOG/ 1.00E+01 4.78E+31 -5.66E+00 2.98E+04/ !!
 PLOG/ 1.00E+02 2.55E+28 -4.58E+00 2.92E+04/ !!
 !
 O-CH3A1CH2O+H=O-CH3A1CHO+H2 1.33E+13 0.00E+00 0.00E+00
 O-CH3A1CH2O+O=O-CH3A1CHO+OH 6.67E+12 0.00E+00 0.00E+00
 O-CH3A1CH2O+OH=O-CH3A1CHO+H2O 3.33E+12 0.00E+00
 0.00E+00
 O-CH3A1CH2O+O2<=>O-CH3A1CHO+HO2 6.00E+10 0.00E+00
 1.60E+03

!***** A1CHO *****

P-CH3A1CHO<=>P-CH3A1CO+H 4.00E+15 0.00E+00 8.37E+04
 P-C6H4CH3+HCO=P-CH3A1CHO 5.00E+12 0.00E+00 0.00E+00

P-CH3A1CHO+O2=>P-CH3A1CO+HO2 2.000E+013 0.000 40700.0 !\AUTHOR:
!\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:
P-CH3A1CHO+H=>P-CH3A1CO+H2 1.31E+05 2.58E+00 1.22E+03!
P-CH3A1CHO+O=>P-CH3A1CO+OH 5.94E+12 0.00E+00 1.87E+03!!
!
P-CH3A1CHO+OH=>P-CH3A1CO+H2O 3.10E+13 0.00 2760 !! !! RATE FROM
STANFORD, WANG ET AL., 36 (2017),151-160!!! KUKKADAPU1@LLNL.GOV!! !! GOK
REFIT TO RATE !! 7.80E+12 0 0.00E+00 !!
P-CH3A1CHO+HO2 =>P-CH3A1CO+H2O2 1.1773E-4 4.91966 3684.27444
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104. !!!
!
P-CH3A1CHO+OH=>P-CHOA1CH2+H2O 1.77E+05 2.39 -602 !!A/1.35 !!! !!
A/1.35 !! 1.77E+05 2.39 -602 !!A/1.35 !! !! !!
P-CH3A1CHO+HO2<=>P-CHOA1CH2+H2O2 1.05E+13 0 1.89E+04

P-CH3A1CHO+O2=P-CHOA1CH2+HO2 4.36E+07 2.50E+00 4.60E+04 !!
KUKKDAPU : A*2 A1CH3+O2=A1CH2+HO2

!
P-CH3A1CHO+CH3<=>P-CH3A1CO+CH4 2.00E-06 5.60E+00 1.50E+03
P-CH3A1CHO+C2H5<=>P-CH3A1CO+C2H6 1.30E+12 0.00E+00 7.50E+03
P-CH3A1CHO+C3H5-A<=>P-CH3A1CO+C3H6 1.30E+12 0.00E+00 1.15E+04
P-CH3A1CHO+C4H5-I<=>P-CH3A1CO+C4H6 1.30E+12 0.00E+00 1.15E+04
P-CH3A1CHO+C4H5-N<=>P-CH3A1CO+C4H6 1.30E+12 0.00E+00 7.50E+03
P-CH3A1CHO+C5H5<=>P-CH3A1CO+C5H6 1.30E+11 0.00E+00 1.15E+04
P-CH3A1CHO+A1<=>P-CH3A1CO+A1 1.30E+11 0.00E+00 1.15E+04
P-CH3A1CHO+A1O<=>P-CH3A1CO+A1OH 1.30E+11 0.00E+00 1.15E+04
P-CH3A1CHO+P-OA1CH3<=>P-CH3A1CO+P-HOA1CH3 1.30E+11 0.00E+00
1.15E+04
P-CH3A1CHO+O-HOA1CH2<=>P-CH3A1CO+O-HOA1CH3 1.30E+11 0.00E+00
1.15E+04
P-C6H4CH3+CH2O<=>P-CH3A1CHO+H 2.91E+04 2.09E+00 -4.11E+02
P-CH3A1CO=P-C6H4CH3+CO 1.370E+21 -2.179 3.941E+04

O-CH3A1CHO<=>O-CH3A1CO+H 4.00E+15 0.00E+00 8.37E+04
O-C6H4CH3+HCO=O-CH3A1CHO 5.00E+12 0.00E+00 0.00E+00
O-CH3A1CHO+O2=>O-CH3A1CO+HO2 2.000E+013 0.000 40700.0 !\AUTHOR:
!\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS) !\COMMENT:
O-CH3A1CHO+H=>O-CH3A1CO+H2 1.31E+05 2.58E+00 1.22E+03!
O-CH3A1CHO+O=>O-CH3A1CO+OH 5.94E+12 0.00E+00 1.87E+03!!
!
O-CH3A1CHO+OH=>O-CH3A1CO+H2O 3.10E+13 0.00 2760 !! !! RATE FROM
STANFORD, WANG ET AL., 36 (2017),151-160!!! KUKKADAPU1@LLNL.GOV!! !! GOK
REFIT TO RATE !! 7.80E+12 0 0.00E+00 !!
O-CH3A1CHO+HO2 =>O-CH3A1CO+H2O2 1.1773E-4 4.91966 3684.27444
!\AUTHOR: !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118,
12089-12104. !!!
!
O-CH3A1CHO+OH=>O-CHOA1CH2+H2O 1.77E+05 2.39 -602 !!A/1.35 !!! !!
A/1.35 !! 1.77E+05 2.39 -602 !!A/1.35 !! !! !!
O-CH3A1CHO+HO2<=>O-CHOA1CH2+H2O2 1.05E+13 0 1.89E+04

O-CH3A1CHO+O2=O-CHOA1CH2+HO2 4.36E+07 2.50E+00 4.60E+04 !!
KUKKDAPU : A*2 A1CH3+O2=A1CH2+HO2
!
O-CH3A1CHO+CH3<=>O-CH3A1CO+CH4 2.00E-06 5.60E+00 1.50E+03

O-CH3A1CHO+C2H5<=>O-CH3A1CO+C2H6 1.30E+12 0.00E+00 7.50E+03
O-CH3A1CHO+C3H5-A<=>O-CH3A1CO+C3H6 1.30E+12 0.00E+00 1.15E+04
O-CH3A1CHO+C4H5-I<=>O-CH3A1CO+C4H6 1.30E+12 0.00E+00 1.15E+04
O-CH3A1CHO+C4H5-N<=>O-CH3A1CO+C4H6 1.30E+12 0.00E+00 7.50E+03
O-CH3A1CHO+C5H5<=>O-CH3A1CO+C5H6 1.30E+11 0.00E+00 1.15E+04
O-CH3A1CHO+A1-<=>O-CH3A1CO+A1 1.30E+11 0.00E+00 1.15E+04
O-CH3A1CHO+A1O<=>O-CH3A1CO+A1OH 1.30E+11 0.00E+00 1.15E+04
O-CH3A1CHO+O-OA1CH3<=>O-CH3A1CO+O-HOA1CH3 1.30E+11 0.00E+00
1.15E+04
O-CH3A1CHO+P-OA1CH3<=>O-CH3A1CO+P-HOA1CH3 1.30E+11 0.00E+00
1.15E+04
O-CH3A1CHO+O-HOA1CH2<=>O-CH3A1CO+O-HOA1CH3 1.30E+11 0.00E+00
1.15E+04
O-CH3A1CHO+P-HOA1CH2<=>O-CH3A1CO+P-HOA1CH3 1.30E+11 0.00E+00
1.15E+04
O-C6H4CH3+CH2O<=>O-CH3A1CHO+H 2.91E+04 2.09E+00 -4.11E+02
O-CH3A1CO=O-C6H4CH3+CO 1.370E+21 -2.179 3.941E+04

!

!***** HOA1CH3 *****
HOCH3A1CH3=OCH3A1CH3+H 8.0E+14 0.0 87000 !MM NIST
2003ZHU/BOZ3696-3703

!

HOCH3A1CH3+O2<=>OCH3A1CH3+HO2 1.00E+13 0.00E+00 3.89E+04
HOCH3A1CH3+H<=>OCH3A1CH3+H2 1.20E+14 0.00E+00 1.24E+04
HOCH3A1CH3+O<=>OCH3A1CH3+OH 1.30E+13 0.00E+00 2.90E+03
HOCH3A1CH3+OH<=>OCH3A1CH3+H2O 1.40E+08 1.40E+00 -9.60E+02
HOCH3A1CH3+HO2<=>OCH3A1CH3+H2O2 1.00E+12 0.00E+00 1.00E+04
HOCH3A1CH3+CH3<=>OCH3A1CH3+CH4 1.80E+11 0.00E+00 7.70E+03
HOCH3A1CH3+A1-<=>OCH3A1CH3+A1 4.90E+12 0.00E+00 4.40E+03
HOCH3A1CH3+C5H5<=>OCH3A1CH3+C5H6 4.90E+11 0.00E+00 9.40E+03
HOCH3A1CH3+C3H5-A<=>OCH3A1CH3+C3H6 4.90E+11 0.00E+00 9.40E+03
HOCH3A1CH3+C4H5-I<=>OCH3A1CH3+C4H6 4.90E+11 0.00E+00 9.40E+03
HOCH3A1CH3+C4H5-N<=>OCH3A1CH3+C4H6 4.90E+11 0.00E+00 9.40E+03
HOCH3A1CH3+A1O<=>OCH3A1CH3+A1OH 4.90E+11 0.00E+00 9.40E+03
HOCH3A1CH3+P-C6H4CH3<=>OCH3A1CH3+A1CH3 7.90E+13 0.00E+00 1.20E+04
HOCH3A1CH3+O-C6H4CH3<=>OCH3A1CH3+A1CH3 7.90E+13 0.00E+00 1.20E+04

!***** DMCPD *****

!!CHAOS ET AL.
!!PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)
2007

DMCPDR+H(+M) = DMCPD(+M) 2.60E+14 0 0

LOW /4.400E+80 -18.28 12994/

TROE /0.0680 400.7 4135.8 5501.9/

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

!ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998

DMCPD+O2 = DMCPDR+HO2 4.00E+13 0 37150

!ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998

DMCPD+HO2 = DMCPDR+H2O 2.10E+04 2.6 12900

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPD+OH = DMCPDR+H2O 3.08E+06 2 0

 !
 !1992TSA3-8 (C3H6+H)
 DMCPD+H = DMCPDR+H2 3.40E+05 2.5 2484 !MM X2

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPD+H = C4H6-2+C3H5-A 3.87E+36 -6.18 32890 !! 7.74E+36
 -6.18 32890 RATE /2

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPD+O = DMCPDR+OH 4.80E+04 2.71 1100

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPD+C2H3 = DMCPDR+C2H4 0.12 4 0

 !EMDEE ET AL.
 !J. PHYS. CHEM. 1992, 96, 2151-2161
 DMCPD+A1O = DMCPDR+A1OH 3.16E+11 0 8000

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPD+CH3 = DMCPDR+CH4 0.18 4 0

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPD+A1- = DMCPDR+A1 0.1 4 0
 !
 !1997BUR/DVI505-514
 DMCPD+C3H5-A = DMCPDR+C3H6 5.50E+10 0 5505 !!/2

 !LIN J COMPUT CHEM 21 415-425 2000
 DMCPDR = C4H5-I+C3H4-P 1.98E+68 -15 124900

 !ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998
 DMCPDR+O = C3H5-S+C3H4-P+CO 3.20E+13 -0.17 440

 DMCPDR+OH = C3H6+C3H4-P+CO 4.00E+14 0 4500

 !
 !

DMCPDR+O2 = O+2C3H4-P+HCO 4.367E+03 2.399 50549.7
!WAGNON1@LLNL.GOV! FROM ROBINSON CNF 158 (2011) 666-686 12.00E+18 -2.48
10970 !!
!NOTE CH2CHCHCO IS VINYLKETENE.

!

!

!ZHONG & BOZZELI J PHYS CHEM A 102:00:00 3537 1998

DMCPDR+HO2 = 2C3H4-P+HCO+OH 6.86E+13 2.52E-01 5.09E+03 !!

!

DMCPDR=>A1CH3+H 3.000E+12 0.000 50400.0 !WAGNON1@LLNL.GOV! DUBNIKOVA
JPCA 106 (2002) 8173-8183

!

!

!!

!

!

!XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXX

!

!

!

!O-XYLENE

! ***** INITIATIONS

O-XYL (+M) <=> O-CH3A1CH2+H (+M) 5.56E+15 1.70E-01 9.12E+04
LOW/ 2.00E+98 -2.29E+01 9.99E+04 /
TROE/ 6.55E-02 1.51E+01 1.00E+10 7.60E+07 /

!

O-XYL (+M) <=> O-C6H4CH3+CH3 (+M) 3.90E+27 -3.16E+00 1.07E+05

LOW/ 1.00E+98 -2.30E+01 1.22E+05 /
TROE/ 7.05E-01 1.00E+10 4.60E+02 8.21E+09 /

!

CH3C6H3CH3+H (+M)=O-XYL (+M) 1.00E+14 0.00E+00 0.00E+00
LOW / 6.60E+75 -1.63E+01 7.00E+03 /
TROE / 1.00E+00 1.00E-01 5.85E+02 6.11E+03 /
H2/2.000/ H2O/6.000/ CH4/2.000/ CO/1.500/ CO2/2.000/ C2H6/3.000/

!!

! ***** SUBSTITUTIONS

O-XYL+H=A1CH3+CH3 1.90E+06 2 943 !
O-XYL+OH=O-HO A1CH3+CH3 1.57E+03 2.88E+00 3.22E+03

!ABSTRACTIONS

O-XYL+H<=>O-CH3A1CH2+H2 12.94 3.98E+00 3.38E+03 !!
O-XYL+O<=>O-CH3A1CH2+OH 15.08E+04 2.57 3.15E+03 !!A*2 FOR
DEGNERECY, LI ET AL., J. PHYS. CHEM. A 2016, 120, 3424 3432

!O-XYL+OH<=>O-CH3A1CH2+H2O 3.54E+05 2.39 -602 !COMMENT KUKKADAPU:
1.77E+05 2.39 -602 !!A/1.35 !!! !! A/1.35 !! !! 3540002.39E+00 -
6.02E+02

O-XYL+OH<=>O-CH3A1CH2+H2O 1.77E+05 2.39 -602 ! Nicolas Delort A/2
O-XYL+O2<=>O-CH3A1CH2+HO2 8.72E+7 2.50E+00 4.60E+04 !

O-XYL+HO2<=>O-CH3A1CH2+H2O2 4.201E+13 0 1.89E+04
O-XYL+CH3<=>O-CH3A1CH2+CH4 5.12E+00 3.80E+00 7.40E+03 !! LI ET AL., J. PHYS. CHEM. A 2016, 120, 3424 3432
O-XYL+CH3O2=O-CH3A1CH2+CH3O2H 0.146 4.12E+00 1.28E+04
O-XYL+HCO<=>O-CH3A1CH2+CH2O 7.54E+13 0.00E+00 2.38E+04
O-XYL+C2H3<=>O-CH3A1CH2+C2H48E+12 0.00E+00 8.00E+03
O-XYL+C3H5-A<=>O-CH3A1CH2+C3H6 7.94E+11 0.00E+00 2.05E+04
O-XYL+C3H3<=>O-CH3A1CH2+C3H4-P 7.94E+11 0.00E+00 2.05E+04
O-XYL+C4H5-I<=>O-CH3A1CH2+C4H6 7.94E+11 0.00E+00 2.05E+04
O-XYL+C4H5-N<=>O-CH3A1CH2+C4H6 7.94E+11 0.00E+00 2.05E+04
!O-XYL+C5H5<=>O-CH3A1CH2+C5H6 3.2E+12 0 11100
O-XYL+C5H5<=>O-CH3A1CH2+C5H61.086E+13 0.00E+00 2.09E+04
O-XYL+A1-<=>O-CH3A1CH2+A1 0.536 3.95 877.06
O-XYL+A1O<=>O-CH3A1CH2+A1OH 1.086E+13 0.00E+00 2.09E+04
O-XYL+O-C6H4CH3<=>O-CH3A1CH2+A1CH3 1.58E+14 0.00E+00 1.20E+04
O-XYL+P-C6H4CH3<=>O-CH3A1CH2+A1CH3 1.58E+14 0.00E+00 1.20E+04
O-XYL+A1OO=O-CH3A1CH2+A1OOH 20400 2.50E+00 1.23E+04

!Nicolas Delort removed!
!O-XYL+OA1CH3<=>O-CH3A1CH2+HOA1CH3 1.6E+11 0.00E+00 1.51E+04

O-XYL+A1CH2OO<=>O-CH3A1CH2+A1CH2OOH 8E+11 0.00E+00 1.40E+04
O-XYL+A1CH2O<=>O-CH3A1CH2+A1CH2OH 1.086E+13 0.00E+00 2.09E+04
O-XYL+O-HOA1CH2<=>O-CH3A1CH2+O-HOA1CH3 3.2E+11 0.00E+00 1.51E+04
O-XYL+P-HOA1CH2<=>O-CH3A1CH2+P-HOA1CH3 3.2E+11 0.00E+00 1.51E+04
!
O-XYL+H=CH3C6H3CH3+H2 1.60E+08 1.83E+00 1.44E+04! LI ET AL., J. PHYS. CHEM. A 2016, 120, 3424 3432!
O-XYL+O<=>CH3C6H3CH3+OH 2.02E+06 2.44E+00 9.14E+03!! LI ET AL., J. PHYS. CHEM. A 2016, 120, 3424 3432,A*4/5 FOR DEGENERACY

O-XYL+OH<=>CH3C6H3CH3+H2O 1.09E+04 2.69E+00 6.20E+02

O-XYL+HO2<=>CH3C6H3CH3+H2O2 2.20E+12 0.00E+00 28811.5
O-XYL+CH3<=>CH3C6H3CH3+CH4 1.75E-04 5.00E+00 1.23E+04
!
!
O-CH3A1CH2=O-XYLYLE+H 2.00E+14 0.00 6.74E+04 !! J. PHYS. CHEM. A, VOL. 113, NO. 38, 2009, LP RATE USED AS PLOG RATE NOT PROVIDED.
O-XYLYLE+O=O-CHOA1CH2+H 9.00E+008 1.450 -860.0 !!
O-XYLYLE=BZCYBUT 2.20E+12 0.00 2.93E+04
BZCYBUT=A1C2H3 1.24E+15 0.00 7.43E+04 !! .
!Nicolas Delort ! O-CH3A1CH2+C2H2=C5H5-C5H5+H 3.20E+12 0.00 1.38E+04 !!
SAME AS A1CH2+C2H2...GOK ADDITION,, NEED MORE INFO ABOUT THIS PATH..
!PLOG/3.947E-02 1.54E+31 -5.60 22640.0/
!PLOG/3.947E-02 1.40E+08 0.91 10080.0/ ! fit btw. 500 and 2500 K with MAE of 0.6%, 1.6%
!PLOG/1.000E+00 2.24E+36 -6.98 27250.0/
!PLOG/1.000E+00 1.08E+55 -11.29 72720.0/ ! fit btw. 500 and 2500 K with MAE of 1.0%, 3.7%
!PLOG/1.000E+01 6.32E+194 -47.77 254800.0/
!PLOG/1.000E+01 1.85E+42 -8.50 34890.0/ ! fit btw. 500 and 2500 K with MAE of 4.9%, 14.6%
!PLOG/1.000E+02 5.70E+44 -8.96 43510.0/
!PLOG/1.000E+02 7.19E+175 -52.00 76360.0/ ! fit btw. 500 and 2500 K with MAE of 5.6%, 15.5%
!
!

O-CH3A1CH2=C7H6+CH3 1.00E+15 0.00 7.55E+04 !! LP RATE USED AS PLOG
RATE NOT PROVIDED. J. PHYS. CHEM. A, VOL. 113, NO. 38, 2009

!!

!

!

!***** BENZYL+O

O-XYL+O<=>OCH3A1CH3+H 1.66E+07 1.8 3974

O-XYL+O=HOCH3A1CH3 3.86E+22 -2.56 14993

DUP

O-XYL+O=HOCH3A1CH3 8.00E+20 -2.6 6684

DUP

!

O-XYL+O=DMCPD+CO 4.82E+15 -4.90E-01 1.50E+04

O-CH3A1CH2+O<=>A1CH3+HCO 10.50E+12 0.329 686 !!A*1.5 DA

SILVA&BOZZELLI, PHYS. CHEM. CHEM. PHYS., 2012, 14, 16143 16154

O-CH3A1CH2+O<=>O-CH3A1CHO+H 4.25E+13 0.0723 732 !! DA SILVA&BOZZELLI,

PHYS. CHEM. CHEM. PHYS., 2012, 14, 16143 16154

!

O-XYL+OH<=>HOCH3A1CH3+H 2.51E+01 3.37E+00 4.72E+03

!

O-CH3A1CH2+O2=O-CH3A1CH2OO 3.16E+07 1.77E+00 2.52E+02

PLOG / 0.1 3.28E+46 -11.59 9.00E+03 /!! MURAKAMI_BENZYL

PLOG / 1 2.82E+45 -10.974 9.730E+03 /!!

MURAKAMI_BENZYL!!

PLOG / 10 9.56E+38 -8.765 8.43E+03 /!! MURAKAMI_BENZYL!

PLOG / 100 4.60E+31 -6.36 6.51E+03 /!! MURAKAMI_BENZYL

!! !

O-CH3A1CH2OO=O-CH3A1CHO+OH 1.00E+00 0.00E+00 0.00E+00

PLOG/ 0.1 1.54E+47 -13.01 4.12E+04/ !! REFIT BY GOUTHAM,

PLOG/ 1 6.65E+45 -11.77 4.36E+04/ !! REFIT BY GOUTHAM,

PLOG/ 10 7.17E+45 -11.03 4.77E+04/ !! REFIT BY GOUTHAM,

PLOG/ 100 5.46E+46 -10.43 5.35E+04/ !! REFIT BY GOUTHAM,

!

O-CH3A1CH2OO=O-OA1CH3+CH2O 1.00E+00 0.00E+00 0.00E+00

PLOG/ 0.1 3.59333E+47 -13.01 4.12E+04/ !! REFIT BY GOUTHAM,

PLOG/ 1 1.55167E+46 -11.77 4.36E+04/ !! REFIT BY GOUTHAM,

PLOG/ 10 1.673E+46 -11.03 4.77E+04/ !! REFIT BY GOUTHAM,

PLOG/ 100 1.274E+47 -10.43 5.35E+04/ !! REFIT BY GOUTHAM,

!

O-CH3A1CH2+O2=O-CH3A1CH2O+O 6.30E+12 0.00E+00 4.00E+04

O-CH3A1CH2OO+H=O-CH3A1CH2O+OH 3.80E+14 -0.19 1.89E+03

O-CH3A1CH2OO+H=O-CH3A1CH2OOH 4.35E+60 -15.92 1.14E+04

O-CH3A1CH2OO+H=O-CH3A1CH2+HO2 1.96E+04 2.47 1.43E+03

O-CH3A1CH2OO+O-CH3A1CH2OO=>2O-CH3A1CH2O+O2 6.30E+10 0.00E+00 -

7.25E+02

! ***** BENZYL+HO2

O-CH3A1CH2OOH<=>O-CH3A1CH2O+OH 1.00E+00 1.00E+00

1.00E+00

PLOG / 1.00E-03 9.39E+69 -1.77E+01 5.80E+04 /

PLOG / 1.00E-03 9.93E+35 -8.71E+00 5.69E+04 /

PLOG / 1.00E-02 3.42E+67 -1.66E+01 5.92E+04 /

PLOG / 1.00E-02 5.84E+40 -9.72E+00 6.07E+04 /

PLOG / 1.00E-01 9.00E+60 -1.43E+01 5.84E+04 /

PLOG /	1.00E-01	9.54E+41	-9.67E+00	6.35E+04	/
PLOG /	1.00E+00	1.48E+50	-1.08E+01	5.53E+04	/
PLOG /	1.00E+00	3.94E+36	-7.71E+00	6.33E+04	/
PLOG /	1.00E+01	1.20E+38	-6.99E+00	5.10E+04	/
PLOG /	1.00E+01	1.04E+26	-4.31E+00	6.01E+04	/
PLOG /	1.00E+02	1.88E+29	-4.28E+00	4.75E+04	/
PLOG /	1.00E+02	1.80E+16	-1.27E+00	5.66E+04	/
O-CH3A1CH2OOH<=>O-CH3A1CHO+H2O				1.00E+00	1.00E+00
	1.00E+00				
PLOG /	1.00E-03	5.23E+53	-1.36E+01	5.78E+04	/
PLOG /	1.00E-02	2.81E+52	-1.28E+01	5.95E+04	/
PLOG /	1.00E-01	7.04E+46	-1.08E+01	5.92E+04	/
PLOG /	1.00E+00	3.91E+36	-7.41E+00	5.64E+04	/
PLOG /	1.00E+01	3.68E+24	-3.64E+00	5.22E+04	/
PLOG /	1.00E+02	3.87E+15	-8.70E-01	4.87E+04	/
!!					
!! A1CH2+HO2<=>A1CH2O+OH	1.00E+97		-2.50E+01	4.40E+04	
!! DUP					
!! A1CH2+HO2<=>A1CH2O+OH	1.00E+35		-6.00E+00	2.00E+04	
!! DUP					
!					
O-CH3A1CH2+HO2<=>O-CH3A1CH2OOH	3.750E+30		-6.00	2.50E+03	!! MARCO FIT,
A					
!					
!!					
O-CH3A1CH2+HO2<=>O-CH3A1CH2O+OH	1.00E+97		-2.50E+01	4.40E+04	!!
DUP					
O-CH3A1CH2+HO2<=>O-CH3A1CH2O+OH	1.00E+35		-6.00E+00	2.00E+04	!! C
DUP					
!!!!					
!					
O-CH3A1CH2+HO2<=>O-CH3A1CHO+H2O				1.00E+00	1.00E+00
	1.00E+00				
PLOG /	1.00E-03	5.06E-03	3.88E+00	4.11E+02	/
PLOG /	1.00E-02	2.02E-01	3.43E+00	1.46E+03	/
PLOG /	1.00E-01	7.38E+03	2.13E+00	4.66E+03	/
PLOG /	1.00E+00	2.51E+09	6.10E-01	9.47E+03	/
PLOG /	1.00E+01	2.66E+09	7.30E-01	1.25E+04	/
PLOG /	1.00E+02	1.24E+02	2.93E+00	1.17E+04	/
O-CH3A1CH2OO+HO2<=>O-CH3A1CH2OOH+O2				2.00E+11	0.00E+00
	-1.30E+03				
O-CH3A1CH2OOH+H=>O-CH3A1CHO+H2+OH				6.47E+00	3.98E+00
	3.38E+03				
O-CH3A1CH2OOH+OH=>O-CH3A1CHO+H2O+OH				3.00E+05	2.39E+00
	-6.02E+02				
O-CH3A1CH2OOH+O2=>O-CH3A1CHO+HO2+OH				2.18E+07	2.50E+00
	4.60E+04				
O-CH3A1CH2OOH+HO2=>O-CH3A1CHO+H2O2+OH				2.45E-05	5.26E+00
	7.48E+03				
O-CH3A1CH2OOH+CH3=>O-CH3A1CHO+CH4+OH				2.94E+11	0.00E+00
	9.25E+03				
O-CH3A1CH2+CH3O2=O-CH3A1CH2O+CH3O				5.00E+12	0 0

O-CH3A1CH2+C2H5O2=O-CH3A1CH2O+C2H5O 5.00E+12 0.00E+00
0.00E+00

!

!

!!!!

O-CH3A1CH2+O-CH3A1CH2=O-XYLDIMER 1.55E+024 -3.784 2.03E+03 !! A*2,
XYLENE RATE_RATE FROM MATSUGI AND
MYOSHI_DOI:10.1016/J.CPLETT.2011.11.043!! !!

!

!

O-XYLDIMER+OH=O-XYLDIMERJ+H2O 39.0E+005 2.200 -
437.18

O-XYLDIMER+O2=O-XYLDIMERJ+HO2 2.80E+12 0.00 35000.0

O-XYLDIMERJ+HO2=O-CH3A1CH2+O-CH3A1CHO+OH 5.00E+12 0.00 0.000E+00

O-CH3A1CH2OO=O-XYLQOOH 10.01E+08 0.85 2.08E+04 !!A*1.5,CANNEAUX ET
AL., J. PHYS. CHEM. A, VOL. 113, NO. 12, 2009

!

!! ***** SEC O2 TO O-CH2TOLCH2OOH ADDED BY GOUTHAM

O-XYLQOOH+O2=>O-XYLSECO2 1.382E+41 -9.44 9020.0 !!

MURAKAMI_HP_LIMIT !!

PLOG / 0.1 3.28E+46 -11.59 9.00E+03 /!! MURAKAMI_BENZYL

PLOG / 1 2.82E+45 -10.974 9.730E+03 /!! MURAKAMI_BENZYL

PLOG / 10 9.56E+38 -8.765 8.43E+03 /!! MURAKAMI_BENZYL!

PLOG / 100 4.60E+31 -6.36 6.51E+03 /!! MURAKAMI_BENZYL

O-XYLSECO2=>O-XYLQOOH+O2 1.382E+41 -9.44 9020.0 !!

PLOG / 0.1 5.62E+46 -10.99 3.05E+04 /!! MURAKAMI_BENZYL!!

PLOG / 1 5.62E+46 -10.68 3.17E+04 /!! MURAKAMI_BENZYL!!

PLOG / 10 5.62E+46 -10.33 3.40E+04 /!! MURAKAMI_BENZYL!!

PLOG / 100 5.62E+46 -10.69 3.15E+04 /!! MURAKAMI_BENZYL!!

O-XYLSECO2=OH+O-XYLKET 10.50E+08 0.85 1.98E+04 !!CANNEAUX ET AL.,
J. PHYS. CHEM. A, VOL. 113, NO. 12, 2009

!!

O-XYLKET=>OH+CHOA1CH2OJ +1.0000000E+016 +0.0000000E+000 +4.2300000E+04

PLOG / +1.0000000E-003

+9.3900000E+069 -1.7680000E+001 +5.8006000E+004 /

PLOG / +1.0000000E-003

+9.9300000E+035 -8.7100000E+000 +5.6852000E+004 /

PLOG / +1.0000000E-002

+3.4200000E+067 -1.6560000E+001 +5.9187000E+004 /

PLOG / +1.0000000E-002

+5.8400000E+040 -9.7200000E+000 +6.0734000E+004 /

PLOG / +1.0000000E-001

+9.0000000E+060 -1.4260000E+001 +5.8390000E+004 /

PLOG / +1.0000000E-001

+9.5400000E+041 -9.6700000E+000 +6.3536000E+004 /

PLOG / +1.0000000E+000

+1.4800000E+050 -1.0770000E+001 +5.5271000E+004 /

PLOG / +1.0000000E+000

+3.9400000E+036 -7.7100000E+000 +6.3309000E+004 /

PLOG / +1.0000000E+001

+1.2000000E+038 -6.9900000E+000 +5.0953000E+004 /

```

PLOG / +1.0000000E+001
+1.0400000E+026 -4.3100000E+000 +6.0142000E+004 /
PLOG / +1.0000000E+002
+1.8800000E+029 -4.2800000E+000 +4.7518000E+004 /
PLOG / +1.0000000E+002
+1.8000000E+016 -1.2700000E+000 +5.6552000E+004 /
!
O-XYLQOOH=>O-XYLET+OH 2.28E+30 -5.40 2.98E+04 !! MURAKAMI RATE

!O-XYLET+OH=>CHOA1CH2+H2O 77.70E+005 2.200 -437.18
O-XYLET+OH=>O-CHOA1CH2+H2O 233.1E+005 2.200 -437.18 ! Nicolas
Delort A*3
O-XYLET+HO2=>O-CHOA1CH2+H2O2 2.353E-4 4.91966 3684.27444 !!
2.50E+12 0.00 0.00 !!
!
O-CHOA1CH2+HO2=>CHOA1CH2OJ+OH 1.00E+97 -2.50E+01 4.40E+04 !!
DUP !!
O-CHOA1CH2+HO2=>CHOA1CH2OJ+OH 1.00E+35 -6.00E+00 2.00E+04 !! C
DUP
!

O-CHOA1CH2=O-CH3A1CO 1.40E+00 3.20 1.6558E+04 !! A/5,3.09E+73 -
18.22 69670
P-CHOA1CH2=P-CH3A1CO 1.40E+00 3.20 1.6558E+04 !! A/5,3.09E+73 -
18.22 69670

!
! ***** A1CHO / A1CH2O *****
O-CHOA1CH2+O=A1CHO+HCO 10.50E+12 0.329 686 !! 1.5*DA SILVA&BOZZELLI,
PHYS. CHEM. CHEM. PHYS., 2012, 14, 16143 16154
O-CHOA1CH2+O=CHOA1CHO+H 4.25E+13 0.0723 732 !! 1.5*DA SILVA&BOZZELLI,
PHYS. CHEM. CHEM. PHYS., 2012, 14, 16143 16154
CHOA1CH2OJ=>CHOA1CHO+H +3.0400000E+032 -6.6650000E+000
+2.1880000E+004 !\AUTHOR: !\REF: !!
PLOG / +1.0000000E-002 +3.0400000E+032 -6.6650000E+000 +2.1880000E+004 /
PLOG / +1.0000000E-001 +6.1300000E+031 -6.2610000E+000 +2.2360000E+004 /
PLOG / +1.0000000E+000 +5.2600000E+028 -5.0810000E+000 +2.2250000E+004 /
PLOG / +1.0000000E+001 +1.6800000E+022 -2.9010000E+000 +2.0760000E+004 /
PLOG / +1.0000000E+002 +2.4400000E+017 -1.3070000E+000 +1.9540000E+004 /
!
!
!\AUTHOR: !\REF: !G. DA SILVA AND J W. BOZZELLI 2009 JPC 113
CHOA1CH2OJ => A1CO+CH2O
+4.5900000E+043 -9.5130000E+000 +3.9050000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+4.5900000E+043 -9.5130000E+000 +3.9050000E+004 /
PLOG / +1.0000000E-001
+2.8800000E+038 -7.7860000E+000 +3.7770000E+004 /
PLOG / +1.0000000E+000
+7.2100000E+033 -6.2100000E+000 +3.6850000E+004 /
PLOG / +1.0000000E+000
+7.2100000E+033 -6.2100000E+000 +3.6850000E+004 /
PLOG / +1.0000000E+001
+1.3200000E+027 -4.0090000E+000 +3.5070000E+004 /
PLOG / +1.0000000E+002
+1.0800000E+021 -2.0570000E+000 +3.3310000E+004 /
!YJ
!\AUTHOR: !\REF: !G. DA SILVA AND J W. BOZZELLI 2009 JPC 113

```

CHO1CH2OJ => A1CHO+HCO
 +2.5700000E+031 -6.2150000E+000 +2.5760000E+004 !\AUTHOR: !\REF:
 PLOG / +1.0000000E-002
 +2.5700000E+031 -6.2150000E+000 +2.5760000E+004 /
 PLOG / +1.0000000E-001
 +5.2700000E+031 -6.1530000E+000 +2.6880000E+004 /
 PLOG / +1.0000000E+000
 +2.3700000E+032 -6.0950000E+000 +2.8810000E+004 /
 PLOG / +1.0000000E+001
 +3.8200000E+031 -5.6630000E+000 +2.9840000E+004 /
 PLOG / +1.0000000E+002
 +2.0400000E+028 -4.5760000E+000 +2.9200000E+004 /
 !
 !
 !
 !
 CHO1CHO+OH=> CHO1CO+H2O 3.10E+13 0.00 2760 !! !! RATE FROM
 STANFORD, WANG ET AL., 36 (2017),151-160!!! KUKKADAPU1@LLNL.GOV!! !! GOK
 REFIT TO RATE
 CHO1CHO+HO2 =>CHO1CO+H2O2 1.1773E-4 4.91966 3684.27444 !\AUTHOR:
 !\REF:J. MENDES, C-W ZHOU, AND H. J. CURRAN. JPCA, 2014, 118, 12089-
 12104. !\COMMENT: !!3.01E+12 0 11920
 CHO1CHO+O2 =>CHO1CO+HO2 2.000E+013 0.000 40700.0
 !\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
 !\COMMENT:
 CHO1CO=>A1CO+CO 1.370E+21 -2.179 3.941E+04
 !
 ! ***** [__]A1C2H3 / [__]A1C2H5

 O-CH3A1CH2+CH3=>O-CH3A1C2H5 0.600E+013 +0.0000000E+000 +2.2100000E+002
 O-CH3A1C2H5+O2=O-CH3A1CHCH3+HO2 2.000E+013 0.000 37190.0 !! !!GOK
 CORRECTION, RATE FROM C4H8-1+O2_NO TUNING...
 O-CH3A1C2H5+O=O-CH3A1CHCH3+OH 3.9E+9 1.0 -1100.0
 O-CH3A1C2H5+H=O-CH3A1CHCH3+H2 +3.9700000E+002 +3.4400000E+000
 +3.1200000E+003 !\AUTHOR: !\REF
 O-CH3A1C2H5+HO2=O-CH3A1CHCH3+H2O2 2.7E+11 0.0 12000.0 !\AUTHOR: !\REF:
 !BOUNACEUR ET AL INT J CHEM KINET 37: 25-49, 2005
 O-CH3A1C2H5+CH3=O-CH3A1CHCH3+CH4 +3.6900000E+000 +3.3100000E+000
 +4.0020000E+003
 O-CH3A1CHCH3+O2=O-CH3A1CHOOCH3 2.69E+05 2.29 -1400 !ALTARAWNEH ET
 AL.,, PROC. COMBUST. INST 34 (2013) 315--323. !!
 O-CH3A1C2H5=O-CH3A1C2H3+H2 5.010E+12 0.00 63988.0 ! CLARK AND
 PRICE 1970 CAN. J. CHEM. VOL. 48
 O-CH3A1CHOOCH3=O-CH3A1C2H3+HO2 +7.0000000E+011 +0.0000000E+000
 +1.5000000E+004
 O-CH3A1C2H3+OH=O-CH2A1C2H3+H2O 1.77E+05 2.39 -602
 O-CH3A1C2H3+O2=O-CH2A1C2H3+HO2 21800000 2.50E+00 4.60E+04 !! P
 O-CH3A1C2H5+OH=O-CH3A1CHCH3+H2O 31.10E+005 2.200 -437.18 !!
 O-CH3A1C2H3+O=O-C6H4CH3+CH3CO +3.50E+013 +0.0000000E+000 +2.8320000E+003
 !! NIST WEBSITE RATE, KUKKADAPU1@LLNL.GOV

 P-CH3A1C2H5+O2=P-CH3A1CHCH3+HO2 2.000E+013 0.000 37190.0 !! !!GOK
 CORRECTION, RATE FROM C4H8-1+O2_NO TUNING...
 P-CH3A1C2H5+O=P-CH3A1CHCH3+OH 3.9E+9 1.0 -1100.0
 P-CH3A1C2H5+H=P-CH3A1CHCH3+H2 +3.9700000E+002 +3.4400000E+000
 +3.1200000E+003 !\AUTHOR: !\REF

P-CH3A1C2H5+HO2=P-CH3A1CHCH3+H2O2 2.7E+11 0.0 12000.0 !\AUTHOR: !\REF:
!BOUNACEUR ET AL INT J CHEM KINET 37: 25-49, 2005
P-CH3A1C2H5+CH3=P-CH3A1CHCH3+CH4 +3.6900000E+000 +3.3100000E+000
+4.0020000E+003
P-CH3A1CHCH3+O2=P-CH3A1CHOOCH3 2.69E+05 2.29 -1400 !ALTARAWNEH ET
AL.,, PROC. COMBUST. INST 34 (2013) 315--323. !!
P-CH3A1C2H5=P-CH3A1C2H3+H2 5.010E+12 0.00 63988.0 ! CLARK AND
PRICE 1970 CAN. J. CHEM. VOL. 48
P-CH3A1CHOOCH3=P-CH3A1C2H3+HO2 +7.0000000E+011 +0.0000000E+000
+1.5000000E+004
P-CH3A1C2H3+OH=P-CH2A1C2H3+H2O 1.77E+05 2.39 -602
P-CH3A1C2H3+O2=P-CH2A1C2H3+HO2 21800000 2.50E+00 4.60E+04 !! P
P-CH3A1C2H5+OH=P-CH3A1CHCH3+H2O 31.10E+005 2.200 -437.18 !!
P-CH3A1C2H3+O=P-C6H4CH3+CH3CO +3.50E+013 +0.0000000E+000 +2.8320000E+003
!! NIST WEBSITE RATE, KUKKADAPU1@LLNL.GOV
!!!!
O-CH2A1C2H3+HO2=OH+O-C2H3A1CH2O 1.00E+97 -2.50E+01 4.40E+04 !!
DUP !! !!
O-CH2A1C2H3+HO2=OH+O-C2H3A1CH2O 1.00E+35 -6.00E+00 2.00E+04 !!
DUP
P-CH2A1C2H3+HO2=OH+P-C2H3A1CH2O 1.00E+97 -2.50E+01 4.40E+04 !!
DUP !! !!
P-CH2A1C2H3+HO2=OH+P-C2H3A1CH2O 1.00E+35 -6.00E+00 2.00E+04 !!
DUP
!
!
!
O-C2H3A1CH2O=O-C2H3A1CHO+H
+3.0400000E+032 -6.6650000E+000 +2.1880000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+3.0400000E+032 -6.6650000E+000 +2.1880000E+004 /
PLOG / +1.0000000E-001
+6.1300000E+031 -6.2610000E+000 +2.2360000E+004 /
PLOG / +1.0000000E+000
+5.2600000E+028 -5.0810000E+000 +2.2250000E+004 /
PLOG / +1.0000000E+001
+1.6800000E+022 -2.9010000E+000 +2.0760000E+004 /
PLOG / +1.0000000E+002
+2.4400000E+017 -1.3070000E+000 +1.9540000E+004 /
!
O-C2H3A1CH2O=O-C6H4C2H3+CH2O +4.5900000E+043 -9.5130000E+000
+3.9050000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+4.5900000E+043 -9.5130000E+000 +3.9050000E+004 /
PLOG / +1.0000000E-001
+2.8800000E+038 -7.7860000E+000 +3.7770000E+004 /
PLOG / +1.0000000E+000
+7.2100000E+033 -6.2100000E+000 +3.6850000E+004 /
PLOG / +1.0000000E+001
+1.3200000E+027 -4.0090000E+000 +3.5070000E+004 /
PLOG / +1.0000000E+002
+1.0800000E+021 -2.0570000E+000 +3.3310000E+004 /
!
O-C2H3A1CH2O=A1C2H3+HCO
+2.5700000E+031 -6.2150000E+000 +2.5760000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+2.5700000E+031 -6.2150000E+000 +2.5760000E+004 /

PLOG / +1.0000000E-001
+5.2700000E+031 -6.1530000E+000 +2.6880000E+004 /
PLOG / +1.0000000E+000
+2.3700000E+032 -6.0950000E+000 +2.8810000E+004 /
PLOG / +1.0000000E+001
+3.8200000E+031 -5.6630000E+000 +2.9840000E+004 /
PLOG / +1.0000000E+002
+2.0400000E+028 -4.5760000E+000 +2.9200000E+004 /
!
O-C2H3A1CHO+H=O-C2H3A1CO+H2 1.3100000E+005 +2.5800000E+000
+1.2200000E+003 !\AUTHOR: !\REF:
O-C2H3A1CHO+OH=O-C2H3A1CO+H2O 61329.9 2.65 -4586.4
O-C2H3A1CHO+HO2=O-C2H3A1CO+H2O2 3.010E+012 0.000 11920.0
O-C2H3A1CHO+O2=O-C2H3A1CO+HO2 2.000E+013 0.000 40700.0
!\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
!\COMMENT:
O-C2H3A1CHO+O=O-C2H3A1CO+OH 5.9400000E+012 +0.0000000E+000
+1.8680000E+003
O-C2H3A1CO=>O-C6H4C2H3+CO 1.30E+21 -2.18E+00 3.94E+04!!

P-C2H3A1CH2O=P-C2H3A1CHO+H
+3.0400000E+032 -6.6650000E+000 +2.1880000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+3.0400000E+032 -6.6650000E+000 +2.1880000E+004 /
PLOG / +1.0000000E-001
+6.1300000E+031 -6.2610000E+000 +2.2360000E+004 /
PLOG / +1.0000000E+000
+5.2600000E+028 -5.0810000E+000 +2.2250000E+004 /
PLOG / +1.0000000E+001
+1.6800000E+022 -2.9010000E+000 +2.0760000E+004 /
PLOG / +1.0000000E+002
+2.4400000E+017 -1.3070000E+000 +1.9540000E+004 /
!
P-C2H3A1CH2O=P-C6H4C2H3+CH2O +4.5900000E+043 -9.5130000E+000
+3.9050000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+4.5900000E+043 -9.5130000E+000 +3.9050000E+004 /
PLOG / +1.0000000E-001
+2.8800000E+038 -7.7860000E+000 +3.7770000E+004 /
PLOG / +1.0000000E+000
+7.2100000E+033 -6.2100000E+000 +3.6850000E+004 /
PLOG / +1.0000000E+001
+1.3200000E+027 -4.0090000E+000 +3.5070000E+004 /
PLOG / +1.0000000E+002
+1.0800000E+021 -2.0570000E+000 +3.3310000E+004 /
!
P-C2H3A1CH2O=A1C2H3+HCO
+2.5700000E+031 -6.2150000E+000 +2.5760000E+004 !\AUTHOR: !\REF:
PLOG / +1.0000000E-002
+2.5700000E+031 -6.2150000E+000 +2.5760000E+004 /
PLOG / +1.0000000E-001
+5.2700000E+031 -6.1530000E+000 +2.6880000E+004 /
PLOG / +1.0000000E+000
+2.3700000E+032 -6.0950000E+000 +2.8810000E+004 /

PLOG / +1.0000000E+001
+3.8200000E+031 -5.6630000E+000 +2.9840000E+004 /
PLOG / +1.0000000E+002
+2.0400000E+028 -4.5760000E+000 +2.9200000E+004 /
!
P-C2H3A1CHO+H=P-C2H3A1CO+H2 1.3100000E+005 +2.5800000E+000
+1.2200000E+003 !\AUTHOR: !\REF:
P-C2H3A1CHO+OH=P-C2H3A1CO+H2O 61329.9 2.65 -4586.4
P-C2H3A1CHO+HO2=P-C2H3A1CO+H2O2 3.010E+012 0.000 11920.0
P-C2H3A1CHO+O2=P-C2H3A1CO+HO2 2.000E+013 0.000 40700.0
!\AUTHOR: !\REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)
!\COMMENT:
P-C2H3A1CHO+O=P-C2H3A1CO+OH 5.9400000E+012 +0.0000000E+000
+1.8680000E+003
P-C2H3A1CO=>P-C6H4C2H3+CO 1.30E+21 -2.18E+00 3.94E+04!!

!
!

!-----
!Autres réac d'autres blocs
OCH3A1CH3=>CO+DMCPDR 2.50E+14 0.00 5.48E+04 !! CARSTENSEN IJCK 44
(2012) 75-89
!deja presente delumpée !O-CH3A1C2H3+H=C9H8+H+H2 3.980E+02
3.44 3120.0 ! MARINOV 1996

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

!
!+++++
!
+ +
!
+ <=== Anisole
MECHANISM FROM BUTTGEN 2020 AND WAGNON 2018 ==> +
!
+ +
!
!+++++

!\SUBMECH: \A1OCH3 (ANISOLE) by Buttgen 2020

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

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

A1OCH3<=>A1O+CH3 +3.1700000E+015
+0.0000000E+000 +6.3208500E+004 !\AUTHOR: R.D.B. !\REF: I.W.C.E.
Arends, R. Louw, P. Mulder, Kinetic study of the thermolysis of anisole
in a hydrogen atmosphere, J. Phys. Chem. 97 (30) (1993) 7914-7925.
!\Comment: A * Upper limit uncertainty

A1OCH2+H<=>A1OCH3 +1.0000000E+014
+0.0000000E+000 +0.0000000E+000 !\AUTHOR: R.D.B. !\REF: Esstimation
!\COMMENT: Estimation for Radical Recombination

!

!\REACTIONCLASS: \IPSO-ADDITIO \A
\N \EA

!

!A1OCH3+H<=>A1+CH3O +2.2300000E+013
+0.0000000E+000 +7.9300000E+003 !\AUTHOR: R.D.B. !\REF: M. Nowakowska, O.
Herbinet, A. Dufour, P.-A. Glaude, Combust. Flame 161 (2014) 1474-1488.
!\COMMENT: Taken from Nowakowska et al. model, however, no clear
Reference in that mechanism given!

!A1OCH3+OH<=>A1OH+CH3O +7.8000000E+002
+2.8800000E+000 +3.2200000E+003 !\AUTHOR: R.D.B. !\REF: M. Nowakowska, O.
Herbinet, A. Dufour, P.-A. Glaude, Combust. Flame 161 (2014) 1474-1488.
!\COMMENT: Reference in Nowakowska et al. model: K1B SETA JPCA 110 (2006)
5081-5090

!A1OCH3+CH3<=>A1CH3+CH3O +9.6400000E+010
+0.0000000E+000 +8.0000000E+003 !\AUTHOR: R.D.B. !\REF: M. Nowakowska, O.
Herbinet, A. Dufour, P.-A. Glaude, Combust. Flame 161 (2014) 1474-1488.
!\COMMENT: Taken from Nowakowska et al. model, however, only "as
addition of CH3 on C=C PAG" as reference give

!A1OCH3+H=A1OH+CH3 3.49E+07
2.53E+00 4.77E+03!A*100 best value for pyro

!A1OCH3+H=A1OH+CH3 3.49E+06
2.53E+00 4.77E+03!A*10

!A1OCH3+H=A1OH+CH3 1.75E+06
2.53E+00 4.77E+03!A*5 Wagnon's parameters best value for oxi

!A1OCH3+H=A1OH+CH3 8.75E+05
2.53E+00 4.77E+03!A*2.5 Wagnon's parameters

!A1OCH3+CH3=A1OH+C2H5 +9.6400000E+010
+0.0000000E+000 +8.0000000E+003! As for A1OCH3+CH3<=>A1CH3+CH3O looks not
bad but not so usefull

!A1OCH3+CH3O=A1OH+C2H5O 1E13 0 0!

Absolutely inefficient. CH3O goes fast to formaldehyde.

!Original rate from Wagnon.However Ax5 good for speciation. But decreases
reactivity for IDT ST

A1OCH3+H=A1OH+CH3 3.49E+05

2.53E+00 4.77E+03 !\AUTHOR: R.D.B. !\REF: S.W. Wagnon, S. Thion,
E.J.K. Nilsson, M. Mehl, Z. Serinyel, K. Zhang, P. Dagaut, A.A. Konnov,
G. Dayma, W.J. Pitz, Combust. Flame 189 (2018) 325-336 !\COMMENT:Comment
in Wagnon et al. Model "E-3KCAL/MOL ESTIMATE AS REVRATE OF A1+OH=A1OH+H
K1B SETA JPCA 110 (2006) 5081-5090"

!

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

!ABSTRACTIONS CONSIDERED BY: OH;H;O;HO2;CH3;O2;!CH3O2;!CH3O;!O2CHO;!OCHO

!

A1OCH3+OH<=>A1OCH2+H2O +1.7916000E+002
+3.0607000E+000 -1.3637000E+003 !\AUTHOR:R.D.B. !\REF: Calculations of
this study at CBS-QB3 Level of Theory !

$\text{A1OCH3+H} \rightleftharpoons \text{A1OCH2+H2}$ +5.4874000E+006
+2.2086000E+000 +6.6105000E+003 !\AUTHOR:R.D.B. !\REF: Calculations of
this study at CBS-QB3 Level of Theory !
 $\text{A1OCH3+HO2} \rightleftharpoons \text{A1OCH2+H2O2}$ +8.6404500E-003
+4.2995000E+000 +1.1067000E+004 !\AUTHOR:R.D.B. !\REF: Calculations of
this study at CBS-QB3 Level of Theory ! A*1,5
 $\text{A1OCH3+CH3} \rightleftharpoons \text{A1OCH2+CH4}$ +1.0545700E-001
+3.9964000E+000 +8.7155000E+003 !\AUTHOR:R.D.B. !\REF: Calculations of
this study at CBS-QB3 Level of Theory !

$\text{A1OCH3+O} \rightleftharpoons \text{A1OCH2+OH}$ +1.1800000E+000
+4.0900000E+000 +2.5454100E+003 !\AUTHOR: R.D.B. !\REF:
YINGJIA_TEST_22/10/2015 !Narayanaswamy et al. Combustion and Flame 157
(2010) 1879-1898 !\COMMENT: In analogy to: $\text{A1CH3+O2} \rightleftharpoons \text{A1CH2+OH}$
! $\text{A1OCH3+O2} \rightleftharpoons \text{A1OCH2+HO2}$ +2.0500000E+013
+0.0000000E+000 +4.4910000E+004 !\AUTHOR: R.D.B. !\REF: U. Burke,
Combust. Flame 162 (2015) 315-330. !\Original_REF:S.L. FISCHER 32 (2000)
713-740. !\COMMENT: !\COMMENT_RENE: A/2 FROM DME TO ANISOLE
 $\text{A1OCH3+O2} \rightleftharpoons \text{A1OCH2+HO2}$ +2.1000000E+013
+0.0000000E+000 +4.7900000E+004 !\AUTHOR: R.D.B. !\REF: M. Nowakowska,
O. Herbinet, A. Dufour, P.-A. Glaude, Combust. Flame 161 (2014) 1474-
1488. !\COMMENT:
 $\text{A1OCH3+CH3O2} \rightleftharpoons \text{A1OCH2+CH3O2H}$ +1.9020000E-004
+4.6400000E+000 +1.0556000E+004 !\AUTHOR: R.D.B. !\REF: U. Burke,
Combust. Flame 162 (2015) 315-330. !\Original_REF:S.L. FISCHER 32 (2000)
713-740. !\COMMENT: A/3: FROM DME TO ANISOLE In Analogy to DME+HO2 :
3.17E-3 4.64 10556.025, A/2 for half the -CH3 Groups, and A/3 for HO2 to
CH3O2 (steric hinderence) and another A/5 because high impact ==> A/10
 $\text{A1OCH3+CH3O} \rightleftharpoons \text{A1OCH2+CH3OH}$ +3.0100000E+011
+0.0000000E+000 +4.0740000E+003 !\AUTHOR: R.D.B. !\REF: U. Burke,
Combust. Flame 162 (2015) 315-330. !\Original_REF:S.L. FISCHER 32 (2000)
713-740. !\COMMENT: A/2: FROM DME TO ANISOLE
! $\text{A1OCH3+O2CHO} \rightleftharpoons \text{A1OCH2+HO2CHO}$ +2.2125000E+004
+2.6000000E+000 +1.3910000E+004 !\AUTHOR: R.D.B. !\REF: U. Burke,
Combust. Flame 162 (2015) 315-330. !\Original_REF:S.L. FISCHER 32 (2000)
713-740. !\COMMENT: A/2: FROM DME TO ANISOLE
 $\text{A1OCH3+OCHO} \rightleftharpoons \text{A1OCH2+HOCHO}$ +5.0000000E+012
+0.0000000E+000 +1.7690000E+004 !\AUTHOR: R.D.B. !\REF: U. Burke,
Combust. Flame 162 (2015) 315-330. !\Original_REF:S.L. FISCHER 32 (2000)
713-740. !\COMMENT: A/2: FROM DME TO ANISOLE
 $\text{A1OCH3+C2H5} \rightleftharpoons \text{C2H6+A1OCH2}$ +3.0000000E+011
+0.0000000E+000 +9.2000000E+003 !\AUTHOR: R.D.B. !\REF: M. Nowakowska,
O. Herbinet, A. Dufour, P.-A. Glaude, Combust. Flame 161 (2014) 1474-
1488. !\COMMENT: Taken from Nowakowska et al. model, however, no clear
Reference in that mechanism given! "(AS 3 H TERTIAIRE EXGAS)"
 $\text{A1OCH3+A1CH2O} \rightleftharpoons \text{A1OCH2+A1CH2OH}$ +3.0100000E+011
+0.0000000E+000 +4.0740000E+003 !\AUTHOR: Y.F. !\REF: !\Comment: as
CH3O
 $\text{A1OH+A1OCH2} \rightleftharpoons \text{A1OCH3+A1O}$ +1.8000000E+011
+0.0000000E+000 +7.7000000E+003 !\AUTHOR: Y.F. !\REF: !\Comment: as
A1OH+CH3 Mulcahy65 NISTervoir
 $\text{A1OCH3+A1-} \rightleftharpoons \text{A1+A1OCH2}$ +3.0000000E+011
+0.0000000E+000 +3.8510000E+003 !\AUTHOR: Y.F. !\REF: !\Comment: !
as 3* H secondary in C3H8+phenyl Park2004 NIST

$\text{A1OCH3+H} \rightleftharpoons \text{C6H4OCH3+H2}$
+3.9100000E+008 +1.8000000E+000 +1.6352770E+004 !\AUTHOR: R.D.B. !\REF:

YINGJIA_TEST_22/10/2015 !Narayanaswamy et al. Combustion and Flame 157
(2010) 1879-1898 !\COMMENT: In analogy to: A1CH3+H=C6H4CH3+H2
A1OCH3+O<=>C6H4OCH3+OH
+2.6000000E+013 +0.0000000E+000 +1.4698850E+004 !\AUTHOR: R.D.B. !\REF:
YINGJIA_TEST_22/10/2015 !Narayanaswamy et al. Combustion and Flame 157
(2010) 1879-1898 !\COMMENT: In analogy to: A1CH3+O<=>C6H4CH3+OH
A1OCH3+OH<=>C6H4OCH3+H2O
+6.1290000E+003 +2.6910000E+000 +1.2400000E+003 !\AUTHOR: R.D.B. !\REF:
YINGJIA_TEST_22/10/2015 !NARAYANASWAMY ET AL. COMBUSTION AND FLAME 157
(2010) 1879-1898 !\COMMENT: In analogy to: A1CH3+OH<=>C6H4CH3+H2O
(!COMMENT: 0.5A 1.361E4 BY YINGJIA) !A*0.9 and Ea*2
A1OCH3+HO2<=>C6H4OCH3+H2O2
+3.6100000E+012 +0.0000000E+000 +3.0982000E+004 !\AUTHOR: R.D.B. !\REF:
YINGJIA_TEST_22/10/2015 =>!M. Altarawneh CNF 2010 A1+HO2 /4 !\COMMENT:
In analogy to: A1CH3+HO2<=>C6H4CH3+H2O2
A1OCH3+CH3<=>C6H4OCH3+CH4 +1.0925000E-
004 +5.0000000E+000 +1.2300000E+004 !\AUTHOR: R.D.B. !\REF:
YINGJIA_TEST_22/10/2015 !SAKAI ET AL. PCI 2009 32:411-418 ! !\COMMENT:
Comment by Yingjia: 0.5A_4.37E-4 In analogy to: A1CH3+CH3<=>C6H4CH3+CH4
!A/2
A1OH+C6H4OCH3<=>A1O+A1OCH3 +7.9000000E+013
+0.0000000E+000 +1.2000000E+004 !\AUTHOR: R.D.B. !\REF: !BOUNACEUR ET
AL INT J CHEM KINET 37: 25-49, 2005

A1OCH2+HO2<=>A1OCH2O+OH +5.8100000E+021
-2.5260000E+000 +1.1457500E+004 !\AUTHOR: Y.F !\REF: Thion butanone
addition on resonance stabilized radical and O-O split

!A1OCH2O<=>A1O+CH2O +8.6750000E+010
+6.1000000E-001 +1.0172000E+003 !\AUTHOR: Y.F !\REF: Thion beta-
scission of ketonoxyl radical
A1O+CH2O=>A1OCH2O 3.000E+011 0.000 7960.0! Nicolas
Delort A*3 on CH3O+CH2O<=>CH3OCH2O
!

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

A1CYCH2O<=>A1OCH2 +3.1600000E+012
+2.3300000E-001 +9.7100000E+003 !\AUTHOR: Y.F !\REF: Da Silva and
Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS8
REV /
+8.7800000E+010 +4.4200000E-001 +1.9030000E+004 / !\AUTHOR: Y.F !\REF:
!\Comment: Defined REV because of RMG approximate thermo for A1CYCH2O (1-
oxaspiro[2.5]octa-4,7-dien-5-yl)

A1CH2O<=>A1CYCH2O +1.1700000E+011
+3.9800000E-001 +1.1170000E+004 !\AUTHOR: Y.F !\REF: Da Silva and
Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS7
REV /
+1.2700000E+013 -3.1000000E-002 +1.6800000E+003 / !\AUTHOR: Y.F !\REF:
!\Comment: Defined REV because of RMG approximate thermo for A1CYCH2O (1-
oxaspiro[2.5]octa-4,7-dien-5-yl)

A1OCH2<=>A1-+CH2O +2.6100000E+014
+5.4000000E-002 +3.9280000E+004 !\AUTHOR: Y.F !\REF: Da Silva and
Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS9

A1CH2O<=>A1-+CH2O +1.0900000E+014
+1.5700000E-001 +3.1160000E+004 !\AUTHOR: Y.F !\REF: Da Silva and
Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS6
A1CH2O<=>A1CHO+H +5.0700000E+008
+1.5600000E+000 +1.6850000E+004 !\AUTHOR: Y.F !\REF: Da Silva and
Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS1

A1CH2O<=>PC6H4CHO
+1.6700000E+008 +1.4260000E+000 +1.9260000E+004 !\AUTHOR: Y.F !\REF:
Da Silva and Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS4
REV / +3.1600000E-
008 +1.1530000E+000 +2.4540000E+004 / !\AUTHOR: Y.F !\REF:
!\Comment: Defined REV because of RMG approximate thermo for PC6H4CHO
(2,5-cyclohexadien-4-formyl-1-yl)

PC6H4CHO<=>A1CHO+H
+2.6700000E+007 +1.6020000E+000 +2.3550000E+004 !\AUTHOR: Y.F !\REF:
Da Silva and Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment: TS5
REV / +9.1000000E-
018 +1.9840000E+000 +6.0700000E+003 / !\AUTHOR: Y.F !\REF:
!\Comment: Defined REV because of RMG approximate thermo for PC6H4CHO
(2,5-cyclohexadien-4-formyl-1-yl)

PC6H4CHO<=>A1+HCO
+6.7200000E+012 +2.2900000E-001 +1.7220000E+004 !\AUTHOR: Y.F !\REF:
Da Silva and Bozzelli, J Phys Chem A 2009;113(25):6979-86. !\Comment:
TS10
REV / +2.6500000E-
022 +2.7880000E+000 +1.1070000E+004 / !\AUTHOR: Y.F !\REF:
!\Comment: Defined REV because of RMG approximate thermo for PC6H4CHO
(2,5-cyclohexadien-4-formyl-1-yl)

A1O+CH3=C6H4OH+CH3 +1.2920000E-
031 +1.3200000E+001 +1.5580000E+004 !\AUTHOR: Y.F !\REF: S.W.
Wagon, S. Thion, E.J.K. Nilsson, M. Mehl, Z. Serinyel, K. Zhang, P.
Dagaut, A.A. Konnov, G. Dayma, W.J. Pitz, Combust. Flame 189 (2018) 325-
336 !\Comment: Comment in Wagon Model: "APPARENT RATE QRRK PECULLAN JPCA
101 (1997) 3305-3316"
!

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

A1OCH2+O2<=>A1OCH2OO +1.0000000E+000
+1.0000000E+000 +1.0000000E+000 !\AUTHOR:R.D.B !\Comment: Burke et al.
Combust. Flame 162 (2015) 315-330. !\REF: BURKE, CNF 2014 !\COMMENT: BASED
ON T. YAMADA, J.W. BOZZELLI, T.H. LAY, INTERNATIONAL JOURNAL OF CHEMICAL
KINETICS, 32 (2000) 435-452 AND S.L. FISCHER, F.L. DRYER, H.J. CURRAN,
INTERNATIONAL JOURNAL OF CHEMICAL KINETICS, 32 (2000) 713-740. A-FACTOR -
55%.
PLOG / +1.0000000E-003
+1.1200000E+018 -3.3700000E+000 -4.2940000E+003 /
PLOG / +1.0000000E-002
+1.3300000E+021 -3.9500000E+000 -2.6150000E+003 /
PLOG / +1.0000000E+000
+1.1300000E+028 -5.2400000E+000 +4.0880000E+003 /

PLOG / +2.0000000E+000
+3.9100000E+027 -5.0000000E+000 +4.5120000E+003 /
PLOG / +1.0000000E+001
+2.7500000E+024 -3.8700000E+000 +4.2900000E+003 /
PLOG / +2.0000000E+001
+2.9700000E+022 -3.2300000E+000 +3.7810000E+003 /
PLOG / +5.0000000E+001
+5.1900000E+019 -2.3500000E+000 +2.9080000E+003 /
PLOG / +1.0000000E+002
+5.4300000E+017 -1.7300000E+000 +2.2100000E+003 /

C6H4OCH3+O2=>OOA1OCH3

+3.2100000E+132 -3.8080000E+001 +3.3960000E+004 !\AUTHOR:R.D.B. !\REF:
da Silva et al. J. Phys. Chem. A 111 (2007) 8663-8676 !\Comment: In
analogy to: C6H4CH3+O2=>O-O2A1CH3

PLOG / +1.0000000E-002
+1.1300000E+090 -2.7980000E+001 -1.8900000E+003 /
PLOG / +1.0000000E-001
+6.5100000E+107 -3.2050000E+001 +1.2220000E+004 /
PLOG / +1.0000000E+000
+3.2100000E+132 -3.8080000E+001 +3.3960000E+004 /
PLOG / +1.0000000E+001
+6.5700000E+179 -4.9680000E+001 +8.1660000E+004 /
PLOG / +1.0000000E+002
+1.4700000E+184 -5.0240000E+001 +9.2040000E+004 /

OOA1OCH3=>C6H4OCH3+O2

+1.5200000E+034 -6.5600000E+000 +4.8790000E+004 !\AUTHOR:R.D.B. !\REF:
da Silva et al. J. Phys. Chem. A 111 (2007) 8663-8676 !\Comment: In
analogy to: O-O2A1CH3=>C6H4CH3+O2

PLOG / +1.0000000E-002
+4.6000000E+027 -5.3400000E+000 +4.4420000E+004 /
PLOG / +1.0000000E-001
+2.7800000E+029 -5.5500000E+000 +4.5160000E+004 /
PLOG / +1.0000000E+000
+1.5200000E+034 -6.5600000E+000 +4.8790000E+004 /
PLOG / +1.0000000E+001
+3.2700000E+041 -8.2500000E+000 +5.6050000E+004 /
PLOG / +1.0000000E+002
+9.4700000E+041 -8.0100000E+000 +5.9770000E+004 /

!

!\REACTIONCLASS: \RO and RO2_Classes \A
\N \EA
!

C6H4OCH3+O2=P-C6H4O2+CH3O

+3.1450000E+012 -1.8000000E-001 -1.2160000E+003 !\AUTHOR:R.D.B.
!\REF: da Silva et al. J. Phys. Chem. A 111 (2007) 8663-8676 !\Comment:
In analogy to: C6H4CH3+O2=OA1CH2+OH; Changed A*0.75 and Ea*1.5 to account
for: Steric repulsion of -OCH3 Group and stabilising effect of +M
Effect

PLOG / +1.0000000E-002
+2.9580000E+009 +6.5000000E-001 -3.3600000E+003 /
PLOG / +1.0000000E-001
+4.2330000E+009 +6.0000000E-001 -3.2480000E+003 /

PLOG / +1.0000000E+000
+3.1450000E+012 -1.8000000E-001 -1.2160000E+003 /
PLOG / +1.0000000E+001
+1.4790000E+024 -3.3600000E+000 +1.1225000E+004 /
PLOG / +1.0000000E+002
+3.1620000E+040 -7.7700000E+000 +3.1175000E+004 /

OOA1OCH3=P-C6H4O2+CH3O

+1.7255000E+045 -1.0170000E+001 +5.0275000E+004 !\AUTHOR:R.D.B.
!\REF: da Silva et al. J. Phys. Chem. A 111 (2007) 8663-8676 !\Comment:

In analogy to: O-O2A1CH3=OA1CH2+OH

PLOG / +1.0000000E-002
+4.7430000E+029 -6.6000000E+000 +2.9462500E+004 /
PLOG / +1.0000000E-001
+3.3235000E+038 -8.6900000E+000 +4.0175000E+004 /
PLOG / +1.0000000E+000
+1.7255000E+045 -1.0170000E+001 +5.0275000E+004 /
PLOG / +1.0000000E+001
+1.8190000E+044 -9.5000000E+000 +5.4300000E+004 /
PLOG / +1.0000000E+002
+5.1170000E+033 -6.2500000E+000 +4.9337500E+004 /

!C6H4OCH3+O2=OA1O+CH3O

+3.7000000E+012 -1.8000000E-001 -1.5200000E+003 !\AUTHOR:R.D.B. !\REF:
da Silva et al. J. Phys. Chem. A 111 (2007) 8663-8676 !\Comment: In

analogy to: C6H4CH3+O2=OA1CH2+OH;

!PLOG / +1.0000000E-002
+3.4800000E+009 +6.5000000E-001 -4.2000000E+003 /
!PLOG / +1.0000000E-001
+4.9800000E+009 +6.0000000E-001 -4.0600000E+003 /
!PLOG / +1.0000000E+000
+3.7000000E+012 -1.8000000E-001 -1.5200000E+003 /
!PLOG / +1.0000000E+001
+1.7400000E+024 -3.3600000E+000 +8.9800000E+003 /
!PLOG / +1.0000000E+002
+3.7200000E+040 -7.7700000E+000 +2.4940000E+004 /

!

!OOA1OCH3=OA1O+CH3O

+2.0300000E+045

-1.0170000E+001 +4.0220000E+004 !\AUTHOR:R.D.B. !\REF: da Silva et al.
J. Phys. Chem. A 111 (2007) 8663-8676 !\Comment: In analogy to: O-
O2A1CH3=OA1CH2+OH

!PLOG / +1.0000000E-002
+5.5800000E+029 -6.6000000E+000 +2.3570000E+004 /
!PLOG / +1.0000000E-001
+3.9100000E+038 -8.6900000E+000 +3.2140000E+004 /
!PLOG / +1.0000000E+000
+2.0300000E+045 -1.0170000E+001 +4.0220000E+004 /
!PLOG / +1.0000000E+001
+2.1400000E+044 -9.5000000E+000 +4.3440000E+004 /
!PLOG / +1.0000000E+002
+6.0200000E+033 -6.2500000E+000 +3.9470000E+004 /

!R+RO2<=>RO+RO

A1OCH2+A1OCH2OO<=>A1OCH2O+A1OCH2O +7.0000000E+012
+0.0000000E+000 -1.0000000E+003 !\AUTHOR: R.D.B. !\REF: ESTIMATE
!\COMMENT:

!RO2+HO2<=>ROOH+O2
A1OCH2OO+HO2=A1OCH2OOH+O2 +2.0000000E+011
+0.0000000E+000 -1.3000000E+003 !\AUTHOR: R.D.B. !\REF: Proc. Combust.
Inst. 34 (2013) 297-305! \COMMENT: In Analogy to A1CH2OO+HO2<=>BZCOOH+O2

!RO2+H2O2<=>RO2H+HO2
A1OCH2OO+H2O2<=>A1OCH2OOH+HO2 +2.4000000E+012
+0.0000000E+000 +1.0000000E+004 !\AUTHOR: R.D.B. !\REF: WARNING NO
REFERENCE !\COMMENT: In analogy to: AC5H11O2+H2O2<=>AC5H11O2H+HO2.
Problematic: No reference in analogy given

!RO2+Ch3O2<=>RO+CH3O+O2
A1OCH2OO+CH3O2<=>A1OCH2O+CH3O+O2 +1.4000000E+016
-1.6100000E+000 +1.8600000E+003 !\AUTHOR: R.D.B. !\REF: WARNING NO
REFERENCE !\COMMENT: In analogy to: AC5H11O2+CH3O2=>AC5H11O+CH3O+O2
Problematic: No reference in analogy given

!

!\REACTIONCLASS: \RO2_Decomposition \A
\N \EA
!

!IC_R: O2-Addition Products decomposition reactions. These reactions are taken from analogies by benzene.

!IC_R: It has a big influence on the IDT simulation results, if the reaction A1OCH2OO = leads either to A1O+HOCHO (slow) or A1OO+CH2O (very fast)

!IC_R: The reaction forming A1OO+CH2O leads to a slight S-Curveature in the simulation results

!IC_R: Especially of interests, for future low-temperature investigations; e.g. with DME.

A1OCH2OO=A1O+HOCHO +1.0000000E+000
+0.0000000E+000 +0.0000000E+000 !\AUTHOR: R.D.B. !\REF: MURAKAMI ET AL.
J. PHYS. CHEM. A 2007, 111, 13200-13208 CHANNEL D !\COMMENT: in analogy
to A1CH2OO=A1O+CH2O

PLOG / +1.0000000E-001

+9.8190000E+059 -1.6131000E+001 4.036918E+04 /!

PLOG / +1.0000000E+000

+2.8250000E+053 -1.3630000E+001 3.991664E+04 /!

PLOG / +1.0000000E+001

+1.4940000E+042 -9.7850000E+000 3.754594E+04 /!

PLOG / +1.0000000E+002

+3.5470000E+032 -6.5880000E+000 3.513952E+04 /!

A1OCH2OO=A1OO+CH2O +1.0000000E-001
+0.0000000E+000 +0.0000000E+000 !\AUTHOR: R.D.B. !\REF: MURAKAMI ET AL.
J. PHYS. CHEM. A 2007, 111, 13200-13208 CHANNEL D !\COMMENT: in analogy
to A1CH2OO=A1O+CH2O

PLOG / +1.0000000E-001

+9.8190000E+058 -1.6131000E+001 4.036918E+04 /!

PLOG / +1.0000000E+000
 +2.8250000E+051 -1.3630000E+001 3.991664E+04 /!
 PLOG / +1.0000000E+001
 +1.4940000E+041 -9.7850000E+000 3.754594E+04 /!
 PLOG / +1.0000000E+002
 +3.5470000E+031 -6.5880000E+000 3.513952E+04 /!

A1OCH2O=C5H5+CH2O+CO2 +7.5000000E-
 001 +0.0000000E+000 +0.0000000E+000 !\AUTHOR: R.D.B. !\REF: !MURAKAMI ET
 AL. J. PHYS. CHEM. A 2007, 111, 13200-13208 CHANNEL D !\COMMENT: NEW
 alternative decomposition route! Analogy might be questionable! A*0.75
 PLOG / +1.0000000E-001
 +7.3642500E+059 -1.6131000E+001 +4.2369180E+004 /
 PLOG / +1.0000000E+000
 +2.1187500E+053 -1.3630000E+001 +4.1916640E+004 /
 PLOG / +1.0000000E+001
 +1.1205000E+042 -9.7850000E+000 +3.9545940E+004 /
 PLOG / +1.0000000E+002
 +2.6602500E+032 -6.5880000E+000 +3.7139520E+004 /

!RO2+RO2<=>RO+RO+O2
 A1OCH2O+A1OCH2O=>O2+A1OCH2O+A1OCH2O +1.3070000E+014 -
 1.0670000E+000 -3.6630000E+002 !\AUTHOR: R.D.B. !\REF: U. Burke, K.P.
 Somers, P. O'Toole, C.M. Zinner, N. Marquet, G. Bourque, E.L. Petersen,
 W.K. Metcalfe, Z. Serinyel, H.J. Curran Combustion and Flame (2015)
 162(2) 315-330 !\COMMENT: In analogy to:
 CH3OCH2O2+CH3OCH2O2=>O2+CH3OCH2O+CH3OCH2O

A1OCH2+O2<=>A1OCHO+OH +0.5000000E+000
 +1.0000000E+000 +1.0000000E+000 !\AUTHOR:R.D.B !\REF: BURKE, CNF 2014
 !\COMMENT: BASED ON T. YAMADA, J.W. BOZZELLI, T.H. LAY, INTERNATIONAL
 JOURNAL OF CHEMICAL KINETICS, 32 (2000) 435-452 !\Comment: In Analogy to:
 CH2OCH2O2H+O2<=>HO2CH2OCHO+OH
 PLOG / +1.0000000E-003
 +5.9000000E+020 -2.8800000E+000 +3.2340000E+003 /
 PLOG / +1.0000000E-002
 +2.0600000E+023 -3.5900000E+000 +5.1160000E+003 /
 PLOG / +1.0000000E+000
 +4.4500000E+029 -5.2900000E+000 +1.2791000E+004 /
 PLOG / +2.0000000E+000
 +2.4400000E+028 -4.9200000E+000 +1.2891000E+004 /
 PLOG / +1.0000000E+001
 +9.4200000E+023 -3.6800000E+000 +1.2049000E+004 /
 PLOG / +2.0000000E+001
 +1.0400000E+022 -3.1600000E+000 +1.1505000E+004 /
 PLOG / +5.0000000E+001
 +6.9500000E+019 -2.6000000E+000 +1.0861000E+004 /
 PLOG / +1.0000000E+002
 +3.9600000E+018 -2.3100000E+000 +1.0500000E+004 /

!A1OCHO+H<=>A1OCH2O +4.6100000E+007
 +1.7100000E+000 +7.0900000E+003 !\AUTHOR:R.D.B !\REF: AramcoMech2.0
 !\REF: HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010 !\Comment: In
 analogy to: CH3CHO+H<=>C2H5O
 A1OCH2O<=>A1OCHO+H 3.300E+013 0.004 26136.3 !
 Nicolas Delort as CH3OCH2O<=>CH3OCHO+H
 A1OCH2O+O2<=>A1OCHO+HO2 +4.2800000E+010
 +0.0000000E+000 +1.0970000E+003 !\AUTHOR:R.D.B !\REF: AramcoMech2.0

!\REF: HARTMANN ET AL. 1990 !\Comment: In analogy
to:C2H5O+O2<=>CH3CHO+HO2

!IC_R: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN ANALOGY TO METHYLFORMATE

A1OCHO+C2H3=C2H4+A1OCO +2.0000000E+011
+0.0000000E+000 +1.6800000E+004 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+C2H5=C2H6+A1OCO +2.5000000E+010
+0.0000000E+000 +1.0400000E+004 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+CH3=CH4+A1OCO +1.3530000E+004
+2.2600000E+000 +7.2870000E+003 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+CH3O=CH3OH+A1OCO +5.4750000E+010
+0.0000000E+000 +5.0000000E+003 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+CH3O2=CH3O2H+A1OCO +2.8000000E+012
+0.0000000E+000 +1.7690000E+004 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+H=H2+A1OCO +6.5000000E+005
+2.4000000E+000 +4.4710000E+003 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+HO2=H2O2+A1OCO +2.8000000E+012
+0.0000000E+000 +1.7690000E+004 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF
OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-
1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN
ANALOGY TO METHYLFORMATE

A1OCHO+O=OH+A1OCO +2.3850000E+004
+2.7100000E+000 +2.1060000E+003 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM
METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K.
WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF

OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN ANALOGY TO METHYLFORMATE

A1OCHO+O2=HO2+A1OCO +1.0000000E+013
+0.0000000E+000 +5.1050000E+004 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K. WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN ANALOGY TO METHYLFORMATE

A1OCHO+OH=H2O+A1OCO +2.3400000E+007
+1.6100000E+000 -3.5000000E+001 !\AUTHOR: R.D.B. !\COMMENT: TAKEN FROM METHYLFORMATE!\REF:FISHER E. M., W. J. PITZ, H. J. CURRAN, AND C. K. WESTBROOK, "DETAILED CHEMICAL KINETIC MECHANISMS FOR COMBUSTION OF OXYGENATED FUELS," PROCEEDINGS OF THE COMBUSTION INSTITUTE 28, P. 1579-1586, 2000 !\COMMENT: H-ATOM ABSTRACTION BY RADICALS FROM THE FORMATE IN ANALOGY TO METHYLFORMATE

!CO2+A1-<=>A1OCO
+1.5000000E+011 +0.0000000E+000 +3.6730000E+004 ! In analogy:
!CO2+CH3=CH3OCO 1.500E+11 0.000 36730.0 !3 NDME (LLNL) ! !REF:
PRIVATE COMMUNICATION FROM S.J. KLIPPENSTEIN
!OR!

A1OCO<=>CO2+A1- +8.6910000E+017
-1.8100000E+000 1.3656700E+004 !\AUTHOR:R.D.B !\REF: AramcoMech2.0
!\REF: No Reference Given !\Comment: In analogy to: CH3OCO<=>CH3+CO2
PLOG/ 0.0500
+9.7200000E+012 -1.3100000E+000 9.4167000E+003/
PLOG/ 1.0000
+1.2500000E+016 -1.8300000E+000 1.1340800E+004/
PLOG/ 10.0000
+1.0400000E+018 -2.1000000E+000 1.2826900E+004/
PLOG/ 100.0000
+8.6900000E+017 -1.8100000E+000 1.3656700E+004/

A1OCO<=>A1O+CO +8.6910000E+017
-1.8100000E+000 +1.3656700E+004 !\AUTHOR:R.D.B !\REF: AramcoMech2.0
!\REF: No Reference Given !\Comment: In analogy to: CH3OCO<=>CH3O+CO
PLOG / +5.0000000E-002
+1.0300000E+003 +1.2900000E+000 +2.5401000E+004 /
PLOG / +1.0000000E+000
+4.0900000E+005 +8.1000000E-001 +2.1969100E+004 /
PLOG / +1.0000000E+001
+9.0200000E+014 -1.7200000E+000 +2.1767500E+004 /
PLOG / +1.0000000E+002
+2.8250000E+022 -3.4400000E+000 +2.3592400E+004 /

!OA1O<=>C2H2+C2H2+CO+CO
+6.3100000E+014 +0.0000000E+000 +6.7160000E+004 !\AUTHOR:R.D.B. !\REF:
YUAN ET AL. CNF 2015 3-21 !\REF: DORRESTIJN1997 !\Comment: In analogy to:
OA1CH2=A1+CO

C6H4OCH3<=>1-C6H4+CH3O
+6.1100000E+045 -8.8570000E+000 +9.4350600E+004 !1997 MADDEN ET AL.
RRKM A1-=O-C6H4+H !IC_R: In analogy to toluene
PLOG / +5.0000000E-001
+6.1100000E+045 -8.8570000E+000 +9.4350600E+004 /

PLOG / +1.0000000E+000
+8.0000000E+041 -7.7200000E+000 +9.2300300E+004 /
PLOG / +1.0000000E+001
+1.6600000E+030 -4.3180000E+000 +8.5756900E+004 /

!***** !Nicolas Delort formation of guaiacol from anisole!

A1OCH3+O=HOA1OCH3 2.961E+24 -2.820 21906.9
!WAGNON1@LLNL.GOV! A*5/6 AS 10ATM C6H6+O=C6H5OH K1B PATHWAY TAATJES JPCA
114 (2010) 3355-3370

!A1OCH3+HO2=>HOA1OCH3+OH 2.961E+24 -2.820 21906.9 ! Nicolas
Delort
!A1OCH3+HO2=>HOA1OCH3+OH 5.84E+35 -5.89 34534.1 ! Nicolas
Delort test as A1+O=A1OH 50 atm

A1OCH3+OH=>HOA1OCH3+H 0.65e13 0.0 10.6e3 !Nowakowska
2014 -estimated from C6H6#+R2OH with A/2!
!A1OCH3+OH=HOA1OCH3+H 1.104E+02 3.249 5590.0
!WAGNON1@LLNL.GOV! A*5/6 AS C6H6+OH=C6H5OH+H K1B SETA JPCA 110 (2006)
5081-5090
!H+HOA1OCH3=OH+A1OCH3 1.0000e+13
0.000 6500.00 ! Nicolas Delort from CRECK

C6H4OCH3+O2=OA1OCH3+O +9.1800000E+020 -2.3000000E+000 +7.3700000E+003
!!Nicolas Delort :analogy with C6H4CH3+O2=OA1CH3+O - AUTHORS: SILVA ET
AL. JPC, 2007, 111:8663-8676
PLOG / 1.00E-02 1.05E+18 -1.61E+00 5.06E+03 /
PLOG / 1.00E-01 2.00E+18 -1.68E+00 5.32E+03 /
PLOG / 1.00E+00 3.67E+20 -2.30E+00 7.37E+03 /
PLOG / 1.00E+01 2.91E+29 -4.72E+00 1.56E+04 /
PLOG / 1.00E+02 6.08E+42 -8.30E+00 2.91E+04 /

HOA1OCH3+A1OCH2=A1OCH3+OA1OCH3 +1.8000000E+011
+0.0000000E+000 +7.7000000E+003! Nicolas Delort as A1OH+A1OCH2=A1OCH3+A1O
C6H4OCH3+O=OA1OCH3 1.0E14 0.0 0.0 ! in
Wagnon and Nowakowska mech
C6H4OCH3+OH=HOA1OCH3 3.000E+13 0.000 0.0
!WAGNON1@LLNL.GOV! AS C6H4CH3+OH=HOC6H4CH3 ?ESTIMATE BY? SAKAI PROC
COMBUST INST 32 (2009) 411-418
!*****

!=====
=====
!\ENDSUBMECH: \A1OCH3
!=====

!*** ETHYLPHENOL TO BENZOFURAN REACTIONS (Wagnon)

P-HOA1CH2+CH3=P-HOA1C2H5 1.190E+12 0.000 221.0
!WAGNON1@LLNL.GOV! AS A1CH2+CH3=A1C2H5 ?YINGJIA ESTIMATE?
A1C2H5+O=P-HOA1C2H5 2.961E+24 -2.820 21906.9
!WAGNON1@LLNL.GOV! A*5/6 AS 10ATM A1+O=A1OH K1B PATHWAY TAATJES JPCA 114
(2010) 3355-3370

$\text{A1C2H5+OH=P-HOA1C2H5+H}$ 1.104E+02 3.249 5590.0
 !WAGNON1@LLNL.GOV! A*5/6 AS A1+OH=A1OH+H K1B SETA JPCA 110 (2006) 5081-5090

$\text{P-HOA1C2H5+O2=P-HOA1C2H4+HO2}$ 3.000E+13 0.000 52000.0
 !WAGNON1@LLNL.GOV! DH298K=52.0KCAL/MOL, A=DEG*1E13
 $\text{P-HOA1C2H5+O=P-HOA1C2H4+OH}$ 9.800E+05 2.430 4750.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+O=A1CH2CH2+OH}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+H=P-HOA1C2H4+H2}$ 6.650E+05 2.540 6756.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+H=A1CH2CH2+H2}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+OH=P-HOA1C2H4+H2O}$ 5.270E+09 0.970 1586.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+OH=A1CH2CH2+H2O}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+HO2=P-HOA1C2H4+H2O2}$ 2.380E+04 2.550 16490.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+HO2=A1CH2CH2+H2O2}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+CH3=P-HOA1C2H4+CH4}$ 4.520E-01 3.650 7154.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+CH3=A1CH2CH2+CH4}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+CH3O2=P-HOA1C2H4+CH3O2H}$ 1.190E+04 2.550 16490.0
 !WAGNON1@LLNL.GOV! A/2 AS $\text{HOA1C2H5+HO2=HOA1C2H4+H2O2}$

$\text{P-HOA1C2H5+O2=P-HOA1C2H4-S+HO2}$ 2.000E+13 0.000 37400.0
 !WAGNON1@LLNL.GOV! DH298K=37.4KCAL/MOL, A=DEG*1E13
 $\text{P-HOA1C2H5+O=P-HOA1C2H4-S+OH}$ 6.600E+05 2.430 1210.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+O=A1CHCH3+OH}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+H=P-HOA1C2H4-S+H2}$ 3.970E+02 3.440 3120.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+H=A1CHCH3+H2}$ ESTIMATE BY ERGUT COMBUST FLAME 144 (2006) 757-772
 $\text{P-HOA1C2H5+OH=P-HOA1C2H4-S+H2O}$ 5.170E+09 1.000 870.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+OH=A1CHCH3+H2O}$ ESTIMATE BY ERGUT COMBUST FLAME 144 (2006) 757-772
 $\text{P-HOA1C2H5+HO2=P-HOA1C2H4-S+H2O2}$ 6.800E+03 2.550 10114.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+HO2=A1CHCH3+H2O2}$?WALKER?
 $\text{P-HOA1C2H5+CH3=P-HOA1C2H4-S+CH4}$ 3.690E+00 3.310 4002.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+CH3=A1CHCH3+CH4}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{P-HOA1C2H5+CH3O2=P-HOA1C2H4-S+CH3O2H}$ 3.400E+03 2.550 10114.0
 !WAGNON1@LLNL.GOV! A/2 AS $\text{HOA1C2H5+HO2=HOA1C2H4-S+H2O2}$

$\text{P-HOA1C2H3+H=P-HOA1C2H4}$ 2.500E+11 0.500 2620.0
 !WAGNON1@LLNL.GOV! ANALOGY TO A1C2H3+H=A1CH2CH2 2.500E+11 0.500 2620.0 FROM LLNL MECHANISM RATE
 $\text{P-HOA1C2H4=C6H4OH+C2H4}$ 1.000E+15 0.000 36600.0
 !WAGNON1@LLNL.GOV! ESTIMATE
 $\text{P-HOA1C2H3+H=P-HOA1C2H4-S}$ 1.370E+26 -3.790 8012.0
 !WAGNON1@LLNL.GOV! AS 100ATM C4H8-1+H=SC4H9 ARAMCO2.0

$\text{O-HOA1CH2+CH3=O-HOA1C2H5}$ 1.190E+12 0.000 221.0
 !WAGNON1@LLNL.GOV! AS A1CH2+CH3=A1C2H5 ?YINGJIA ESTIMATE?
 $\text{A1C2H5+O=O-HOA1C2H5}$ 2.961E+24 -2.820 21906.9
 !WAGNON1@LLNL.GOV! A*5/6 AS 10ATM A1+O=A1OH K1B PATHWAY TAATJES JPCA 114 (2010) 3355-3370

$\text{A1C2H5+OH=O-HOA1C2H5+H}$ 1.104E+02 3.249 5590.0
 !WAGNON1@LLNL.GOV! A*5/6 AS A1+OH=A1OH+H K1B SETA JPCA 110 (2006) 5081-5090

$\text{O-HOA1C2H5+O2=O-HOA1C2H4+HO2}$ 3.000E+13 0.000 52000.0
 !WAGNON1@LLNL.GOV! DH298K=52.0KCAL/MOL, A=DEG*1E13
 $\text{O-HOA1C2H5+O=O-HOA1C2H4+OH}$ 9.800E+05 2.430 4750.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+O=A1CH2CH2+OH}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+H=O-HOA1C2H4+H2}$ 6.650E+05 2.540 6756.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+H=A1CH2CH2+H2}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+OH=O-HOA1C2H4+H2O}$ 5.270E+09 0.970 1586.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+OH=A1CH2CH2+H2O}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+HO2=O-HOA1C2H4+H2O2}$ 2.380E+04 2.550 16490.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+HO2=A1CH2CH2+H2O2}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+CH3=O-HOA1C2H4+CH4}$ 4.520E-01 3.650 7154.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+CH3=A1CH2CH2+CH4}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+CH3O2=O-HOA1C2H4+CH3O2H}$ 1.190E+04 2.550 16490.0
 !WAGNON1@LLNL.GOV! A/2 AS $\text{HOA1C2H5+HO2=HOA1C2H4+H2O2}$

$\text{O-HOA1C2H5+O2=O-HOA1C2H4-S+HO2}$ 2.000E+13 0.000 37400.0
 !WAGNON1@LLNL.GOV! DH298K=37.4KCAL/MOL, A=DEG*1E13
 $\text{O-HOA1C2H5+O=O-HOA1C2H4-S+OH}$ 6.600E+05 2.430 1210.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+O=A1CHCH3+OH}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+H=O-HOA1C2H4-S+H2}$ 3.970E+02 3.440 3120.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+H=A1CHCH3+H2}$ ESTIMATE BY ERGUT COMBUST FLAME 144 (2006) 757-772
 $\text{O-HOA1C2H5+OH=O-HOA1C2H4-S+H2O}$ 5.170E+09 1.000 870.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+OH=A1CHCH3+H2O}$ ESTIMATE BY ERGUT COMBUST FLAME 144 (2006) 757-772
 $\text{O-HOA1C2H5+HO2=O-HOA1C2H4-S+H2O2}$ 6.800E+03 2.550 10114.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+HO2=A1CHCH3+H2O2}$?WALKER?
 $\text{O-HOA1C2H5+CH3=O-HOA1C2H4-S+CH4}$ 3.690E+00 3.310 4002.0
 !WAGNON1@LLNL.GOV! AS $\text{A1C2H5+CH3=A1CHCH3+CH4}$?ESTIMATE BY? MEHL PROC COMB INST 33 (2011) 201-208
 $\text{O-HOA1C2H5+CH3O2=O-HOA1C2H4-S+CH3O2H}$ 3.400E+03 2.550 10114.0
 !WAGNON1@LLNL.GOV! A/2 AS $\text{HOA1C2H5+HO2=HOA1C2H4-S+H2O2}$

$\text{O-HOA1C2H3+H=O-HOA1C2H4}$ 2.500E+11 0.500 2620.0
 !WAGNON1@LLNL.GOV! ANALOGY TO A1C2H3+H=A1CH2CH2 2.500E+11 0.500 2620.0 FROM LLNL MECHANISM RATE
 $\text{O-HOA1C2H4=C6H4OH+C2H4}$ 1.000E+15 0.000 36600.0
 !WAGNON1@LLNL.GOV! ESTIMATE
 $\text{O-HOA1C2H3+H=O-HOA1C2H4-S}$ 1.370E+26 -3.790 8012.0
 !WAGNON1@LLNL.GOV! AS 100ATM C4H8-1+H=SC4H9 ARAMCO2.0

$\text{O-HOA1C2H5+O2=>C8H8O+HO2+H}$ 1.000E+13 0.000 38900.0
 !WAGNON1@LLNL.GOV! AS A1OH+O2=A1O+HO2
 $\text{O-HOA1C2H5+H=>C8H8O+H2+H}$ 1.150E+14 0.000 12400.0
 !WAGNON1@LLNL.GOV! AS A1OH+H=A1O+H2 HE JPC 92 (1988) 2196-2201
 $\text{O-HOA1C2H5+O=>C8H8O+OH+H}$ 1.300E+13 0.000 2900.0
 !WAGNON1@LLNL.GOV! AS A1OH+O=A1O+OH BAULCH COMBUST FLAME 98 (1994) 59-79

O-HOAlC2H5+OH=>C8H8O+H2O+H 0.695E+08 1.400 -960.0
!WAGNON1@LLNL.GOV! AS A1OH+OH=A1O+H2O SHANDROSS INT SYMP COMBUST 26
(1996) 711-719
O-HOAlC2H5+HO2=>C8H8O+H2O2+H 1.373E+00 3.798 10439.8
!WAGNON1@LLNL.GOV! AS A1OH+HO2=A1O+H2O2 ESTIMATE
O-HOAlC2H5+CH3=>C8H8O+CH4+H 8.732E-01 3.494 4392.4
!WAGNON1@LLNL.GOV! AS A1OH+CH3=A1O+CH4 ESTIMATE
O-HOAlC2H5+CH3O2=>C8H8O+CH3O2H+H 6.865E-01 3.798 10439.8
!WAGNON1@LLNL.GOV! A/2 AS HOAlC2H5+HO2=>C8H8O+H2O2+H

O-HOAlC2H3+O2=>C8H6O+HO2+H 1.000E+13 0.000 38900.0
!WAGNON1@LLNL.GOV! AS A1OH+O2=A1O+HO2
O-HOAlC2H3+H=>C8H6O+H2+H 1.150E+14 0.000 12400.0
!WAGNON1@LLNL.GOV! AS A1OH+H=A1O+H2 HE JPC 92 (1988) 2196-2201
O-HOAlC2H3+O=>C8H6O+OH+H 1.300E+13 0.000 2900.0
!WAGNON1@LLNL.GOV! AS A1OH+O=A1O+OH BAULCH COMBUST FLAME 98 (1994) 59-79
O-HOAlC2H3+OH=>C8H6O+H2O+H 0.695E+08 1.400 -960.0
!WAGNON1@LLNL.GOV! AS A1OH+OH=A1O+H2O SHANDROSS INT SYMP COMBUST 26
(1996) 711-719
O-HOAlC2H3+HO2=>C8H6O+H2O2+H 1.373E+00 3.798 10439.8
!WAGNON1@LLNL.GOV! AS A1OH+HO2=A1O+H2O2 ESTIMATE
O-HOAlC2H3+CH3=>C8H6O+CH4+H 8.732E-01 3.494 4392.4
!WAGNON1@LLNL.GOV! AS A1OH+CH3=A1O+CH4 ESTIMATE
O-HOAlC2H3+CH3O2=>C8H6O+CH3O2H+H 6.865E-01 3.798 10439.8
!WAGNON1@LLNL.GOV! A/2 AS HOAlC2H3+HO2=>C8H6O+H2O2+H

!HOAlC2H3 du bloc benzofuran de Wagnon
P-HOAlC2H3+H=A1C2H3+OH 6.977E+04 2.533 3954.2
!WAGNON1@LLNL.GOV! AS REVRATE OF A1+OH=A1OH+H K1B SETA JPCA 110 (2006)
5081-5090
P-HOAlC2H3=C6H4OH+C2H3 1.000E+15 0.000 116500.0
!WAGNON1@LLNL.GOV! ESTIMATE

O-HOAlC2H3+H=A1C2H3+OH 6.977E+04 2.533 3954.2
!WAGNON1@LLNL.GOV! AS REVRATE OF A1+OH=A1OH+H K1B SETA JPCA 110 (2006)
5081-5090
O-HOAlC2H3=C6H4OH+C2H3 1.000E+15 0.000 116500.0
!WAGNON1@LLNL.GOV! ESTIMATE
C8H8O=O-HOAlC2H3 4.540E+14 0.000 68300.0
!WAGNON1@LLNL.GOV! DUBNIKOVA JPCA 106 (2002) 9278-9283

!*** METHYL METHOXYBENZENE REACTIONS (Wagnon)
C6H4OCH3+CH3=P-CH3A1OCH3 2.000E+13 0.000 0.0
!WAGNON1@LLNL.GOV! AS C6H4CH3+CH3=O-XYL
!CH3A1OCH3=OA1CH3+CH3 1.240E+16 0.000 66270.0
!WAGNON1@LLNL.GOV! AS A1OCH3=A1O+CH3 PW
P-CH3A1OCH3=P-OA1CH3+CH3 1.240E+16 0.000 66270.0 !

P-CH3A1OCH3+O2=P-CH3A1OCH2+HO2 3.000E+13 0.000 50100.0
!WAGNON1@LLNL.GOV! DH298K=50.1KCAL/MOL, A=DEG*1E13
P-CH3A1OCH3+O=P-CH3A1OCH2+OH 3.875E+08 1.360 2250.0
!WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+O=CH3OCH2+OH ARAMCO2.0 [FITTED BY
CURRAN TO NIST DATA]

P-CH3A1OCH3+H=P-CH3A1OCH2+H2 3.862E+06 2.090 3384.0
 !WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+H=CH3OCH2+H2 ARAMCO2.0 [FITTED BY
 CURRAN TO NIST DATA]
 P-CH3A1OCH3+OH=P-CH3A1OCH2+H2O 4.676E+05 2.290 -780.7
 !WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+OH=CH3OCH2+H2O ARAMCO2.0 [FISCHER ET
 AL. INT. J. CHEM. KINET. 32 (2000) 713-740]
 P-CH3A1OCH3+HO2=P-CH3A1OCH2+H2O2 15.850E-04 4.640 11656.0
 !WAGNON1@LLNL.GOV! E+1.1KCAL/MOL AS A/2 OF CH3OCH3+HO2=CH3OCH2+H2O2
 ARAMCO2.0 [MENDES ET AL. J. PHYS. CHEM. A 118 (2014) 1300-1308]
 P-CH3A1OCH3+CH3=P-CH3A1OCH2+CH4 3.510E+00 3.780 9687.1
 !WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+CH3=CH3OCH2+CH4 ARAMCO2.0 [TRANTER
 ET AL. J. PHYS. CHEM. A 116 (2012) 7287-7292]
 P-CH3A1OCH3+CH3O2=P-CH3A1OCH2+CH3O2H 7.925E-04 4.640 11656.0
 !WAGNON1@LLNL.GOV! A/2 AS HOA1OCH3+HO2=HOA1OCH2+H2O2
 P-CH3A1OCH3+A1O=P-CH3A1OCH2+A1OH 4.169E+11 0.000 16060.0
 !WAGNON1@LLNL.GOV! AS A1OCH3+A1O=A1OCH2+A1OH ESTIMATE BY ARENDS JPC 97
 (1993) 7914-7925

P-CH3A1OCH3+O2=P-CH2A1OCH3+HO2 3.000E+13 0.000 39900.0
 !WAGNON1@LLNL.GOV! DH298K=39.9KCAL/MOL, A=DEG*1E13
 P-CH3A1OCH3+O=P-CH2A1OCH3+OH 1.180E+00 4.090 2545.4
 !WAGNON1@LLNL.GOV! AS A1CH3+O<=>A1CH2+OH NARAYANASWAMY COMBUST FLAME 157
 (2010) 1879-1898
 P-CH3A1OCH3+H=P-CH2A1OCH3+H2 6.470E+00 3.980 3384.0
 !WAGNON1@LLNL.GOV! AS A1CH3+H<=>A1CH2+H2 ?YINGJIA?
 P-CH3A1OCH3+OH=P-CH2A1OCH3+H2O 1.770E+05 2.390 -602.0
 !WAGNON1@LLNL.GOV! AS A1CH3+OH<=>A1CH2+H2O SETA JPCA 110 (2006) 5081-5090
 P-CH3A1OCH3+HO2=P-CH2A1OCH3+H2O2 2.100E+13 0.000 18900.0
 !WAGNON1@LLNL.GOV! AS A1CH3+HO2<=>A1CH2+H2O2 ALTARAWNEH J COMP CHEM 32
 (2011) 1725-1733
 P-CH3A1OCH3+CH3=P-CH2A1OCH3+CH4 4.220E+14 0.000 22256.2
 !WAGNON1@LLNL.GOV! AS A1CH3+CH3<=>A1CH2+CH4 ?YINGJIA?
 P-CH3A1OCH3+CH3O2=P-CH2A1OCH3+CH3O2H 1.050E+13 0.000 18900.0
 !WAGNON1@LLNL.GOV! A/2 AS CH3A1OCH3+HO2=CH2A1OCH3+H2O2
 P-CH3A1OCH3+A1O=P-CH2A1OCH3+A1OH 5.430E+12 0.000 20923.0
 !WAGNON1@LLNL.GOV! AS A1CH3+A1O=A1CH2+A1OH SAKAI PROC COMBUST INST 32
 (2009) 411-418

P-CH2A1OCH3=P-CH3A1OCH2 2.700E+12 0.000 30100.0
 !WAGNON1@LLNL.GOV! AS O-OA1OCH3 H-TRANSFER PATHWAY ROBICHAUD J CHEM PHYS
 140 (2014) 234302

P-CH3A1OCH2=P-C6H4CH3+CH2O 2.610E+14 0.054 39280.0
 !WAGNON1@LLNL.GOV! AS A1OCH2=A1-+CH2O HPL DA SILVA JPCA 113 (2009) 6979-
 6986
 P-CH3A1OCH2=P-CH3A1CYCH2O 4.390E+10 0.442 19030.0
 !WAGNON1@LLNL.GOV! A/2 AS A1OCH2=A1CYCH2O HPL DA SILVA JPCA 113 (2009)
 6979-6986
 P-CH3A1CYCH2O=P-CH3A1CH2O 1.270E+13 -0.031 1680.0
 !WAGNON1@LLNL.GOV! AS A1CYCH2O=A1CH2O HPL DA SILVA JPCA 113 (2009) 6979-
 6986

P-CH3A1OCH3+H=P-HOA1CH3+CH3 6.977E+04 2.533 954.2
 !WAGNON1@LLNL.GOV! E-3KCAL/MOL ESTIMATE AS REVRATE OF A1+OH=A1OH+H K1B
 SETA JPCA 110 (2006) 5081-5090
 P-CH3A1OCH3+H=A1CH3+CH3O 6.977E+04 2.533 3954.2
 !WAGNON1@LLNL.GOV! AS REVRATE OF A1+OH=A1OH+H K1B SETA JPCA 110 (2006)
 5081-5090

P-CH3A1OCH3+OH=P-HOA1CH3+CH3O 0.783E+03 2.884 3221.3
 !WAGNON1@LLNL.GOV! AS A1CH3+OH<=>A1OH+CH3 K2C SETA JPCA 110 (2006) 5081-5090
 P-CH3A1OCH3+CH3=P-XYL+CH3O 0.888E+00 3.455 9797.6
 !WAGNON1@LLNL.GOV! A/2 AS REVRATE OF A1CH3+OH<=>A1OH+CH3 K2C SETA JPCA 110 (2006) 5081-5090

 P-CH3A1OCH3+H=A1OCH3+CH3 9.490E+05 2.000 944.0
 !WAGNON1@LLNL.GOV! AS A1CH3+H<=>A1+CH3 ELLIS COMBUST FLAME 132 (2003) 291-304
 P-CH3A1OCH3+OH=HOA1OCH3+CH3 0.783E+03 2.884 3221.3
 !WAGNON1@LLNL.GOV! AS A1CH3+OH<=>A1OH+CH3 K2C SETA JPCA 110 (2006) 5081-5090

 P-CH3A1OCH2+O2=P-CH3A1OCH2OO 1.130E+28 -5.240 4088.0
 !WAGNON1@LLNL.GOV! AS CH3OCH2+O2=CH3OCH2OO ARAMCO2.0
 !CH3A1OCH2+O2=CH3A1OCH2OO 4.520E+12 0.000 0.0
 !WAGNON1@LLNL.GOV! AS A1CH2CH2+O2=A1CH2CH2OO ?ESTIMATE BY? MEHL PROC COMBUT INST 33 (2011) 201-208
 P-CH3A1OCH2OO=>P-OA1CH3+HCO+OH 7.674E+36 -7.577 47350.2
 !WAGNON1@LLNL.GOV! AS A1CH2OO=>A1CHO+OH CHANNEL B 1ATM MURAKAMI JPCA 111 (2007) 13200-13208
 !CH3A1OCH2OO=>O-O2A1CH3+CH2O 2.009E+08 1.100 30100.0
 !WAGNON1@LLNL.GOV! AS 5MEMBERED RING RO2=QOOH, C6H13O2-1<=>C6H12OOH1-2
 !Nicolas Delort!CH3A1OCH2OO=>O-O2A1CH3+CH2O 1.774E+32 -6.588
 21390.0 !WAGNON1@LLNL.GOV! A/2, -15.75KCAL SINCE 5M VS 4M-RING MATHEU IJCK 35 (2003) SUP MAT, AS A1CH2OO=>A1O+CH2O CHANNEL D 1ATM MURAKAMI JPCA 111 (2007) 13200-13208
 P-CH3A1OCH2+HO2=P-CH3A1OCH2OOH 5.000E+12 0.000 0.0
 !WAGNON1@LLNL.GOV! AS A1CH2CH2+HO2=>A1CH2+CH2O+OH ?BOUNACEUR IJCK 37 (2005) 25-49?
 P-CH3A1OCH2OOH=>P-OA1CH3+CH2O+OH 7.810E+22 -3.500 23156.0
 !WAGNON1@LLNL.GOV! AS CH2OCH2O2H=>CH2O+CH2O+OH ARAMCO2.0
 P-CH3A1OCH2OO+HO2=P-CH3A1OCH2OOH+O2 2.000E+11 0.000 -1300.0
 !WAGNON1@LLNL.GOV! AS A1CH2OO+HO2=BZCOOH+O2 HERBINET PROC COMBUST INST 34 (2013) 297-305

!ortho-----

C6H4OCH3+CH3=O-CH3A1OCH3 2.000E+13 0.000 0.0
 !WAGNON1@LLNL.GOV! AS C6H4CH3+CH3=O-XYL
 !CH3A1OCH3=OA1CH3+CH3 1.240E+16 0.000 66270.0
 !WAGNON1@LLNL.GOV! AS A1OCH3=A1O+CH3 PW
 O-CH3A1OCH3=O-OA1CH3+CH3 1.240E+16 0.000 66270.0 !

 O-CH3A1OCH3+O2=O-CH3A1OCH2+HO2 3.000E+13 0.000 50100.0
 !WAGNON1@LLNL.GOV! DH298K=50.1KCAL/MOL, A=DEG*1E13
 O-CH3A1OCH3+O=O-CH3A1OCH2+OH 3.875E+08 1.360 2250.0
 !WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+O=CH3OCH2+OH ARAMCO2.0 [FITTED BY CURRAN TO NIST DATA]
 O-CH3A1OCH3+H=O-CH3A1OCH2+H2 3.862E+06 2.090 3384.0
 !WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+H=CH3OCH2+H2 ARAMCO2.0 [FITTED BY CURRAN TO NIST DATA]
 O-CH3A1OCH3+OH=O-CH3A1OCH2+H2O 4.676E+05 2.290 -780.7
 !WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+OH=CH3OCH2+H2O ARAMCO2.0 [FISCHER ET AL. INT. J. CHEM. KINET. 32 (2000) 713-740]

O-CH3A1OCH3+HO2=O-CH3A1OCH2+H2O2 15.850E-04 4.640 11656.0
!WAGNON1@LLNL.GOV! E+1.1KCAL/MOL AS A/2 OF CH3OCH3+HO2=CH3OCH2+H2O2
ARAMCO2.0 [MENDES ET AL. J. PHYS. CHEM. A 118 (2014) 1300-1308]
O-CH3A1OCH3+CH3=O-CH3A1OCH2+CH4 3.510E+00 3.780 9687.1
!WAGNON1@LLNL.GOV! AS A/2 OF CH3OCH3+CH3=CH3OCH2+CH4 ARAMCO2.0 [TRANTER
ET AL. J. PHYS. CHEM. A 116 (2012) 7287-7292]
O-CH3A1OCH3+CH3O2=O-CH3A1OCH2+CH3O2H 7.925E-04 4.640 11656.0
!WAGNON1@LLNL.GOV! A/2 AS HOA1OCH3+HO2=HOA1OCH2+H2O2
O-CH3A1OCH3+A1O=O-CH3A1OCH2+A1OH 4.169E+11 0.000 16060.0
!WAGNON1@LLNL.GOV! AS A1OCH3+A1O=A1OCH2+A1OH ESTIMATE BY ARENDS JPC 97
(1993) 7914-7925

O-CH3A1OCH3+O2=O-CH2A1OCH3+HO2 3.000E+13 0.000 39900.0
!WAGNON1@LLNL.GOV! DH298K=39.9KCAL/MOL, A=DEG*1E13
O-CH3A1OCH3+O=O-CH2A1OCH3+OH 1.180E+00 4.090 2545.4
!WAGNON1@LLNL.GOV! AS A1CH3+O<=>A1CH2+OH NARAYANASWAMY COMBUST FLAME 157
(2010) 1879-1898
O-CH3A1OCH3+H=O-CH2A1OCH3+H2 6.470E+00 3.980 3384.0
!WAGNON1@LLNL.GOV! AS A1CH3+H<=>A1CH2+H2 ?YINGJIA?
O-CH3A1OCH3+OH=O-CH2A1OCH3+H2O 1.770E+05 2.390 -602.0
!WAGNON1@LLNL.GOV! AS A1CH3+OH<=>A1CH2+H2O SETA JPCA 110 (2006) 5081-5090
O-CH3A1OCH3+HO2=O-CH2A1OCH3+H2O2 2.100E+13 0.000 18900.0
!WAGNON1@LLNL.GOV! AS A1CH3+HO2<=>A1CH2+H2O2 ALTARAWNEH J COMP CHEM 32
(2011) 1725-1733
O-CH3A1OCH3+CH3=O-CH2A1OCH3+CH4 4.220E+14 0.000 22256.2
!WAGNON1@LLNL.GOV! AS A1CH3+CH3<=>A1CH2+CH4 ?YINGJIA?
O-CH3A1OCH3+CH3O2=O-CH2A1OCH3+CH3O2H 1.050E+13 0.000 18900.0
!WAGNON1@LLNL.GOV! A/2 AS CH3A1OCH3+HO2=CH2A1OCH3+H2O2
O-CH3A1OCH3+A1O=O-CH2A1OCH3+A1OH 5.430E+12 0.000 20923.0
!WAGNON1@LLNL.GOV! AS A1CH3+A1O=A1CH2+A1OH SAKAI PROC COMBUST INST 32
(2009) 411-418

C8H8O+H=O-CH3A1OCH2 3.270E+25 -3.510 8145.0
!WAGNON1@LLNL.GOV! AS 100ATM C4H8-2+H=SC4H9 ARAMCO2.0
C8H8O+H=O-CH2A1OCH3 3.270E+25 -3.510 8145.0
!WAGNON1@LLNL.GOV! AS 100ATM C4H8-2+H=SC4H9 ARAMCO2.0

O-CH2A1OCH3=O-CH3A1OCH2 2.700E+12 0.000 30100.0
!WAGNON1@LLNL.GOV! AS O-OA1OCH3 H-TRANSFER PATHWAY ROBICHAUD J CHEM PHYS
140 (2014) 234302

O-CH3A1OCH2=O-C6H4CH3+CH2O 2.610E+14 0.054 39280.0
!WAGNON1@LLNL.GOV! AS A1OCH2=A1-+CH2O HPL DA SILVA JPCA 113 (2009) 6979-
6986
O-CH3A1OCH2=O-CH3A1CYCH2O 4.390E+10 0.442 19030.0
!WAGNON1@LLNL.GOV! A/2 AS A1OCH2=A1CYCH2O HPL DA SILVA JPCA 113 (2009)
6979-6986
O-CH3A1CYCH2O=O-CH3A1CH2O 1.270E+13 -0.031 1680.0
!WAGNON1@LLNL.GOV! AS A1CYCH2O=A1CH2O HPL DA SILVA JPCA 113 (2009) 6979-
6986

O-CH3A1OCH3+H=O-HOA1CH3+CH3 6.977E+04 2.533 954.2
!WAGNON1@LLNL.GOV! E-3KCAL/MOL ESTIMATE AS REVRATE OF A1+OH=A1OH+H K1B
SETA JPCA 110 (2006) 5081-5090
O-CH3A1OCH3+H=A1CH3+CH3O 6.977E+04 2.533 3954.2
!WAGNON1@LLNL.GOV! AS REVRATE OF A1+OH=A1OH+H K1B SETA JPCA 110 (2006)
5081-5090

O-CH3A1OCH3+OH=O-HOA1CH3+CH3O 0.783E+03 2.884 3221.3
!WAGNON1@LLNL.GOV! AS A1CH3+OH<=>A1OH+CH3 K2C SETA JPCA 110 (2006) 5081-5090

O-CH3A1OCH3+CH3=O-XYL+CH3O 0.888E+00 3.455 9797.6
!WAGNON1@LLNL.GOV! A/2 AS REVRATE OF A1CH3+OH<=>A1OH+CH3 K2C SETA JPCA 110 (2006) 5081-5090

O-CH3A1OCH3+H=A1OCH3+CH3 9.490E+05 2.000 944.0
!WAGNON1@LLNL.GOV! AS A1CH3+H<=>A1+CH3 ELLIS COMBUST FLAME 132 (2003) 291-304

O-CH3A1OCH3+OH=HOA1OCH3+CH3 0.783E+03 2.884 3221.3
!WAGNON1@LLNL.GOV! AS A1CH3+OH<=>A1OH+CH3 K2C SETA JPCA 110 (2006) 5081-5090

O-CH3A1OCH2+O2=O-CH3A1OCH2OO 1.130E+28 -5.240 4088.0
!WAGNON1@LLNL.GOV! AS CH3OCH2+O2=CH3OCH2OO ARAMCO2.0
!CH3A1OCH2+O2=CH3A1OCH2OO 4.520E+12 0.000 0.0
!WAGNON1@LLNL.GOV! AS A1CH2CH2+O2=A1CH2CH2OO ?ESTIMATE BY? MEHL PROC COMBUT INST 33 (2011) 201-208

O-CH3A1OCH2OO=>O-OA1CH3+HCO+OH 7.674E+36 -7.577 47350.2
!WAGNON1@LLNL.GOV! AS A1CH2OO=>A1CHO+OH CHANNEL B 1ATM MURAKAMI JPCA 111 (2007) 13200-13208

!CH3A1OCH2OO=>O-O2A1CH3+CH2O 2.009E+08 1.100 30100.0
!WAGNON1@LLNL.GOV! AS 5MEMBERED RING RO2=QOOH, C6H13O2-1<=>C6H12OOH1-2
!Nicolas Delort!CH3A1OCH2OO=>O-O2A1CH3+CH2O 1.774E+32 -6.588
21390.0 !WAGNON1@LLNL.GOV! A/2, -15.75KCAL SINCE 5M VS 4M-RING MATHEU IJCK 35 (2003) SUP MAT, AS A1CH2OO=>A1O+CH2O CHANNEL D 1ATM MURAKAMI JPCA 111 (2007) 13200-13208

O-CH3A1OCH2+HO2=O-CH3A1OCH2OOH 5.000E+12 0.000 0.0
!WAGNON1@LLNL.GOV! AS A1CH2CH2+HO2=>A1CH2+CH2O+OH ?BOUNACEUR IJCK 37 (2005) 25-49?

O-CH3A1OCH2OOH=>O-OA1CH3+CH2O+OH 7.810E+22 -3.500 23156.0
!WAGNON1@LLNL.GOV! AS CH2OCH2O2H=>CH2O+CH2O+OH ARAMCO2.0

O-CH3A1OCH2OO+HO2=O-CH3A1OCH2OOH+O2 2.000E+11 0.000 -1300.0
!WAGNON1@LLNL.GOV! AS A1CH2OO+HO2=BZCOOH+O2 HERBINET PROC COMBUST INST 34 (2013) 297-305

!from xylene mech of Wagnon (NOT IN KUKKADAPU MODEL)

O-CH3A1CH2+O=O-CH3A1CH2O 2.28E+14 0.00E+00 0.00E+00
P-CH3A1CH2+O=P-CH3A1CH2O 2.28E+14 0.00E+00 0.00E+00

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<=== GUAIACOL

MECHANISM FROM NOWAKOWSKA 2018 ==> +

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OA1OH+CH3=HOA1OCH3 5.e12 0.0 0.0
!anisole<=CH3+C6H5O

HOA1OCH2+H=HOA1OCH3 1.0E14 0.0 0.0 !estimated R+H
Allara1980!

OA1OCH3+H=HOA1OCH3 !estimated!	1e14	0.0	0.0	
OA1OH+H=HOA1OH	1e14	0.0	0.0 !	
OA1OCH3=>CO+CH3+C5H4O 2011 DUPLICATE	3.3e14	0.0	58000	!Carstensen
OA1OCH3=>CO+CH3+C5H4O DUPLICATE	2.1e14	0.0	59600	!Carstensen 2011
!Bimolecular initiation!				
HOA1OCH3+O2=HOA1OCH2+HO2 !estimated as Delta H reaction at 800K!	2.1E13	0.0	50169	
HOA1OCH3+O2=OA1OCH3+HO2 !estimated as Delta H reaction at 800K!	7.0e12	0.0	38410	
!Decomposition HOA1OH				
HOA1OH=>H2O+CO+C2H2+C3H2 Altarawneh et al. JPCA2010	7.43E12	0.91	78900.0	!
HOA1OH=>CO+C5H5OH Altarawneh et al. JPCA2010	1.91E11	0.61	67560.0	!
HOA1OH+H=A1OH+OH Nicolas Delort from CRECK 2019	2.0000e+13	0.000	5100.00	!
H+CATECHOL=OH+C6H5OH CH3+HOA1OH=OH+O-HOA1CH3 Nicolas Delort CRECK	1.8000e+12	0.000	15000.00	!
! H-abstr on pyrocatechol of Nowakowska 2018 are replaced by CRECK rate constants				
! H-abst pyrochatecol Nowakowska 2018				
!HOA1OH+H=OA1OH+H2 !<ALZUETA00>!A*2	2.4E14	0.0	12.4E3	
!HOA1OH+O=OA1OH+OH !<ALZUETA00>!A*2	2.6E13	0.0	2.9E3	
!HOA1OH+OH=OA1OH+H2O !<SHANDROSS96>!A*2	2.8E8	1.4	-0.96E3	
!HOA1OH+HO2=OA1OH+H2O2 !<ALZUETA00>!A*2	2.0E12	0.0	10.0E3	
!HOA1OH+CH3=OA1OH+CH4 !<MULCAHY65>!A*2	3.6E11	0.0	7.7E3	
!HOA1OH+A1=OA1OH+A1 !<ALZUETA00>!A*2	9.8E12	0.0	4.4E3	
!HOA1OH+C5H5=OA1OH+C5H6 !mf <Lovell(1989)>A*2	5.34e14	0.0	25.238e3	
!HOA1OH+C3H5-A=OA1OH+C3H6 !mf <Lovell(1989)>A*2	5.34e14	0.0	25.238e3	
!HOA1OH+C4H5-I=OA1OH+C4H6 !mf <Lovell(1989)>A*2	5.34e14	0.0	25.238e3	
!HOA1OH+CH3O2=OA1OH+CH3O2H CH3O2+H2O2=CH3O2H+HO2 with A*2	4.8E12	0.0	9.9E3	!as
!HOA1OH+CH3O=OA1OH+CH3OH	2E12	0.0	0.0	! est.
!HOA1OH+A1O=OA1OH+A1OH	4E12	0.0	0.0	! 4.17 as
HOA1OH+CH3O=OA1OH+CH3OH				
!from CRECK				
HOA1OH+H=OA1OH+H2	2.4000e+07	2.000	2719.45	
HOA1OH+O=OA1OH+OH	1.8800e+07	2.000	1169.32	

HOA1OH+OH=OA1OH+H2O	1.2000e+10	1.000	-412.31	
HOA1OH+HO2=OA1OH+H2O2	6.4000e+06	2.000	13892.46	
HOA1OH+CH3=OA1OH+CH4	2.4000e+05	2.000	3755.29	
HOA1OH+A1=OA1OH+A1	2.9600e+08	1.000	1117.36	
HOA1OH+C5H5=OA1OH+C5H6	2.7200e+05	2.000	12129.83	
HOA1OH+C3H5-A=OA1OH+C3H6	4.3120e+05	2.000	10972.41	
HOA1OH+C4H5-I=OA1OH+C4H6	2.1600e+05	2.000	3293.91	
HOA1OH+CH3O2=OA1OH+CH3O2H	6.0800e+05	2.000	10779.70	
HOA1OH+CH3O=OA1OH+CH3OH	6.0800e+05	2.000	10779.70	
A1O+HOA1OH=A1OH+OA1OH	4.3200e+05	2.000	10623.62	
HOA1OH+O2=OA1OH+HO2	7e11	0.0	30441	!estimated as Delta
H reaction at 298K!				
OA1OH=CO+C5H4OH	6.17E+78	-18.794	90504.0	!as
A1O=bicycle				
OA1OH=H+O-C6H4O2	7.63E+14	0.0	71930.0	!Altarawneh
et al. JPCA2010				
!already in colibri!C5H4O+H=C5H4OH			1.74E06	2.2
7512.0	!as H+CH3CHO	Sivaramakrishnan	JPCA2010	
!formation of methylcatechols (like cresols)!				
!OA1OH+CH3=HOA1OHCH3-4	2.31e72	-17.37	38.78e3	
!Pecullan_1997! +0kcal A/10				
!OA1OH+CH3=HOA1OHCH3-4	4.62e73	-17.37	38.78e3	
!Nicolas Delort A*2 with A1O+CH3=cresol				
OA1OH+CH3=HOA1OHCH3-4	6.9e72	-17.37	38.78e3	!
Nicolas Delort A*3				
OA1OH+CH3=OA1OHCH3-1+H	3.33e39	-7.78	31.67e3	!as
A1O+CH3=OC6H4CH3+H				
OA1OH+CH3=OA1OHCH3-2+H	3.33e39	-7.78	31.67e3	!as
A1O+CH3=OC6H4CH3+H !				
!methatheses as HOC6H4CH3+R!				
HOA1OHCH3-4+H=OA1OHCH3-1+H2	2.4E14	0.0	9.4E3	
!<estimated(s)>!A*2 -3kcal				
HOA1OHCH3-4+O=OA1OHCH3-1+OH	2.6E13	0.0	2.9E3	
!<estimated(s)>!A*2				
HOA1OHCH3-4+OH=OA1OHCH3-1+H2O	2.8E8	1.4	-0.96E3	
!<estimated(s)>!A*2				
HOA1OHCH3-4+HO2=OA1OHCH3-1+H2O2	2.0E12	0.0	10.0E3	
!<estimated(s)>!A*2				
HOA1OHCH3-4+CH3=OA1OHCH3-1+CH4	3.6E11	0.0	4.7E3	
!<estimated(s)>! A*2 -3kcal				
HOA1OHCH3-4+A1=OA1OHCH3-1+A1	9.8E12	0.0	4.4E3	
!<estimated(s)>!A*2				
HOA1OHCH3-4+C5H5=OA1OHCH3-1+C5H6	9.8E11	0.0	9.4E3	
!<estimated(s)>!A*2				
HOA1OHCH3-4+C3H5-A=OA1OHCH3-1+C3H6	9.8E11	0.0	9.4E3	
!<estimated(s)>!A*2				
HOA1OHCH3-4+C4H5-I=OA1OHCH3-1+C4H6	9.8E11	0.0	9.4E3	
!<estimated(s)>!A*2				
!HOA1OHCH3-4+A1O=OA1OHCH3-1+A1OH	9.8E11	0.0	9.4E3	
!<estimated(s)>!A*2				

HOA1OHCH3-4+A1O=OA1OHCH3-1+A1OH Delort A*3	29.4E11	0.0	9.4E3	! Nicolas
HOA1OHCH3-4+OA1OH=OA1OHCH3-1+HOA1OH !<estimated(s)>! A*2	9.8E11	0.0	9.4E3	
HOA1OHCH3-4+CH3O2=OA1OHCH3-1+CH3O2H CH3O2+H2O2=CH3O2H+HO2 with A*2	4.8E12	0.0	9.9E3	!as
HOA1OHCH3-4+CH3O=OA1OHCH3-1+CH3OH	1E12	0.0	0.0	! est.
HOA1OHCH3-4+O2=OA1OHCH3-1+HO2 reaction a 298K a/10 A/2	3.5e11	0.0	29281	!as drH
HOA1OHCH3-4+C6H4OH=OA1OHCH3-1+A1OH HOA1OHCH3-4+A1-=OA1OHCH3-1+A1	9.8E12	0.0	4.4E3	! 4.17 as
OA1OHCH3-1+H=HOA1OHCH3-4	1e14	0.0	0.0	!as cresols
HOA1OHCH3-4+H=OA1OHCH3-2+H2 !<estimated(s)>!A*2	2.4E14	0.0	9.4E3	
HOA1OHCH3-4+O=OA1OHCH3-2+OH !<estimated(s)>!A*2	2.6E13	0.0	2.9E3	
HOA1OHCH3-4+OH=OA1OHCH3-2+H2O !<estimated(s)>!A*2	2.8E8	1.4	-0.96E3	
HOA1OHCH3-4+HO2=OA1OHCH3-2+H2O2 !<estimated(s)>!A*2	2.0E12	0.0	10.0E3	
HOA1OHCH3-4+CH3=OA1OHCH3-2+CH4 !<estimated(s)>! A*2 -3kcal	3.6E11	0.0	4.7E3	
HOA1OHCH3-4+A1-=OA1OHCH3-2+A1 !<estimated(s)>!A*2	9.8E12	0.0	4.4E3	
HOA1OHCH3-4+C5H5=OA1OHCH3-2+C5H6 !<estimated(s)>!A*2	9.8E11	0.0	9.4E3	
HOA1OHCH3-4+C3H5-A=OA1OHCH3-2+C3H6 !<estimated(s)>!A*2	9.8E11	0.0	9.4E3	
HOA1OHCH3-4+C4H5-I=OA1OHCH3-2+C4H6 !<estimated(s)>!A*2	9.8E11	0.0	9.4E3	
!HOA1OHCH3-4+A1O=OA1OHCH3-2+A1OH !<estimated(s)>!A*2	9.8E11	0.0	9.4E3	
HOA1OHCH3-4+A1O=OA1OHCH3-2+A1OH Delort A*3	29.4E11	0.0	9.4E3	! Nicolas
HOA1OHCH3-4+OA1OH=OA1OHCH3-2+HOA1OH !<estimated(s)>! A*2	9.8E11	0.0	9.4E3	
HOA1OHCH3-4+CH3O2=OA1OHCH3-2+CH3O2H !as CH3O2+H2O2=CH3O2H+HO2 with A*2	4.8E12	0.	9.9E3	
HOA1OHCH3-4+CH3O=OA1OHCH3-2+CH3OH HOA1OH	1E12	0.0	0.0	! as
HOA1OHCH3-4+O2=OA1OHCH3-2+HO2 reaction a 298K a/10 A/2	3.5e11	0.0	28561	!as drH
HOA1OHCH3-4+C6H4OH=OA1OHCH3-2+A1OH HOA1OHCH3-4+A1-=OA1OHCH3-2+A1	9.8E12	0.0	4.4E3	! 4.17 as
OA1OHCH3-2+H=HOA1OHCH3-4	1e14	0.0	0.0	!as cresols
!ipso addition sur HOA1OHCH3-4! HOA1OHCH3-4+H=HOA1OH+CH3 HOC6H4CH3+H=A1OH+CH3!	5.8E13	0.0	8.1E3	!as

!methatheses sur OCH3 du HOA1OCH3!

HOA1OCH3+H=HOA1OCH2+H2	3.6e08	1.5	6905	! EV
HOA1OCH3+CH3=HOA1OCH2+CH4	5.01e11	0	1.05e4	!Mulcahy
HOA1OCH3+OH=HOA1OCH2+H2O	3.6e+06	2.0	-855	! Evans
Polanyi				
HOA1OCH3+HO2=HOA1OCH2+H2O2	4.2e3	2.69	16592.2	! Evans
Polanyi				
HOA1OCH3+C2H5=HOA1OCH2+C2H6	3.0E+11	0.0	9.2E3	! as 3 H
tertiaire Exgas				
HOA1OCH3+C5H5=HOA1OCH2+C5H6	5.4E+00	3.3	17.2E3	! as 3 H
tertiaire par Y. Exgas				
HOA1OCH3+A1-=HOA1OCH2+A1	3E+11	0.0	3851	! as 3*
H secondary in C3H8+phenyl				Park2004 NIST
HOA1OCH2+HOA1OH=HOA1OCH3+OA1OH	1.8E+11	0.0	7.7E3	! as
C6H5OH+CH3				Mulcahy65 NIST
HOA1OCH3+O=HOA1OCH2+OH	3.0E+13	0.0	3.28E3	! as 3
H tertiaire Exgas				
HOA1OCH3+CH3O=CH3OH+HOA1OCH2	2.16e11	0	4500	!estimation as
secondary H!				
HOA1OCH3+CH3O2=HOA1OCH2+CH3O2H	4.5e12	0	17500	!comme
une methatheses du H secondaire sur				
HOA1OCH3+C4H5-N=HOA1OCH2+C4H6	5e11	0	7600	!as
methathese sur H allkyliques par V				
!methatheses sur OH du HOA1OCH3 (constantes from phenol) !				
HOA1OCH3+H=OA1OCH3+H2	1.2E14	0.0	12.4E3	
!<ALZUETA00>!				
HOA1OCH3+CH3=OA1OCH3+CH4	1.8E11	0.0	7.7E3	
!<MULCAHY65>!				
HOA1OCH3+OH=OA1OCH3+H2O	1.4E8	1.4	-0.96E3	
!<SHANDROSS96>!				
HOA1OCH3+HO2=OA1OCH3+H2O2	1.0E12	0.0	10.0E3	
!<ALZUETA00>!				
HOA1OCH3+C5H5=OA1OCH3+C5H6	2.67e14	0.0	25.238e3	!mf
<Lovell Int. J. Chem. Kinet.21(1989)547>				
HOA1OCH3+A1-=OA1OCH3+A1	4.9E12	0.0	4.4E3	
!<ALZUETA00>!				
HOA1OCH3+O=OA1OCH3+OH	1.3E13	0.0	2.9E3	
!<ALZUETA00>!				
HOA1OCH3+C3H5-A=OA1OCH3+C3H6	2.67e14	0.0	25.238e3	
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>				
HOA1OCH3+C4H5-I=OA1OCH3+C4H6	2.67e14	0.0	25.238e3	
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>				
HOA1OCH3+OA1OH=OA1OCH3+HOA1OH	1.05e11	0.0	11500	! as
HOC6H4CH3+A1O=OC6H4CH3+A1OH from Pecullan +2kcal				
!HOA1OCH3+OA1OH=OA1OCH3+HOA1OH	0.5e11	0.0	11500	! 4.16 A/2
HOA1OCH3+CH3O=CH3OH+OA1OCH3	1E12	0.0	1240.0	
! est lower				
HOA1OCH3+CH3O2=OA1OCH3+CH3O2H	1.0E12	0.0	10.0E3	
!as HO2				
HOA1OCH3+C4H5-N=OA1OCH3+C4H6	5e11	0	5300	
!as methathese sur H allyliques par V				
!Nicolas Delort from Wagnon A1OCH3+A1O				
HOA1OCH3+A1O=HOA1OCH2+A1OH	4.169E+11	0.000	16060.0	
HOA1OCH3+A1O=OA1OCH3+A1OH	4.900E+11	0.000	9400.0	

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!isomerisation!
OA1OCH3=HOA1OCH2          5.02e9    1.0      25e3    !estimation
correlation Benson!

!formation of benzaldehyde 2 hydroxy !
HOA1OCH2=CH2O+C6H4OH      2.61e14    0.054    39.28e3
!Silva et Bozzelli 2009

!Nicolas Delort - delumping!
!HOA1OCH2=HOA1CH2O          8.78e10    0.442    21.03e3  !Silva
et Bozzelli 2009 +2 H-bond in reactant
HOA1OCH2=HOA1CYCH2O      4.390E+10    0.442    19030.0
!WAGNON1@LLNL.GOV! A/2 AS C6H5OCH2=C6H5CYCH2O HPL DA SILVA JPCA 113
(2009) 6979-6986
HOA1CYCH2O=HOA1CH2O      1.270E+13   -0.031    1680.0
!WAGNON1@LLNL.GOV! AS C6H5CYCH2O=C6H5CH2O HPL DA SILVA JPCA 113 (2009)
6979-6986

HOA1CH2O=HOA1CHO+H        5.26e28    -5.081    22.25e3  !Silva et
Bozzelli 2009
HOA1CH2O=A1OH+HCO         2.37e32    -6.095    28.81e3  !Silva
et Bozzelli 2009
HOA1CH2O=CH2O+C6H4OH      7.21e33    -6.21     36.85e3
!Silva et Bozzelli 2009

HOA1CH2O+H=HOA1CHO+H2     1e13        0.0       0.0      !estimated
HOA1CH2O+CH3=HOA1CHO+CH4  1e12        0.0       0.0      !estimated
HOA1CH2O+A1-=HOA1CHO+A1  1e12        0.0       0.0      !estimated

C6H4OH+HOA1OCH3=A1OH+HOA1OCH2  3E+11    0.0       3851    !as
anisole+A1-=A1+A1-OCH2
C6H4OH+HOA1OCH3=A1OH+OA1OCH3  4.9E12    0.0       4.4E3    !as A1OH+A1-
=A1O+A1 !<ALZUETA00>!

!H-abstraction on OH from hydroxybenzalehyde
HOA1CHO+H=OA1CHO+H2       1.2E14     0.0       12.4E3   !as phenol
HOA1CHO+CH3=OA1CHO+CH4    1.8E11     0.0       7.7E3    !
HOA1CHO+O=OA1CHO+OH       1.3E13     0.0       2.9E3    !
HOA1CHO+OH=OA1CHO+H2O     1.4E8      1.4       -0.96E3  !
HOA1CHO+HO2=OA1CHO+H2O2   1.0E12     0.0       10.0E3   !

OA1CHO=HOA1CO              5.02e9     1.0       25e3     ! as OA1OCH3=HOA1OCH2

OA1CHO=C5H4CHO+CO          6.17E+78   -18.794    90504.0  !as
A1O=bicycle
C5H4CHO=C5H5CO             2e13       0          40e3
!estimated PAG
C5H5CO=C5H5+CO             5.27E14    0.0       29.01e3  ! as
C6H5CO=A1-+CO

!Ips0 additions!
HOA1OCH3+H=A1OH+CH3O      2.23e13    0.0       10930
!as phenol +3kcal
HOA1OCH3+CH3=O-HOA1CH3+CH3O  9.64e10    0.0       8e03
!as addition of CH3 on C=C PAG

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HOA1OCH3+OH=HOA1OH+CH3O 7.8E02 2.88 3.22E3 !as
toluene +OH=phenol+ch3 Seta2006 NIST

!!Decomposition of OA1OH via formation of orthoquinone!!!
!OA1OH+O2=O-C6H4O2+HO2 1.0E13 0.0 19051 !
estimation as DrH thermo MIT
OA1OH+O2=O-C6H4O2+HO2 0.5E+13 0.0 38800.0 !
Nicolas Delort as A1OH+O2=A1O+HO2

OA1OH+O=C5H4OH+CO2 1e13 0 0 !as
A1O+O=C5H5+CO2
OA1OHCH3-2+O=HOC5H3CH3+CO2 1e13 0 0 !as
A1O+O=C5H5+CO2
OA1OHCH3-1+O=HOC5H3CH3+CO2 1e13 0 0 !as
A1O+O=C5H5+CO2

OA1OH+HO2=O-C6H4O2+H2O2 3e11 0 0 !estimated
as C2H5 + HO2 = C2H4 + H2O2 (nist)

OA1OHCH3-2+O2=OC6H3 (O) CH3+HO2 1.0E13 0.0 21872 !as
DRH
OA1OHCH3-1+O2=OC6H3 (O) CH3+HO2 1.0E13 0.0 21152 !as
DRH

OC6H3 (O) CH3+H=>C2H3+C3H4-P+2CO 5.2E13 0.0 3.2E3 !O-
C6H4O2+H=>2CO+C2H2+C2H3
OC6H3 (O) CH3+H=>CH3+C4H4+2CO 5.2E13 0.0 3.2E3 !O-
C6H4O2+H=>2CO+C2H2+C2H3
OC6H3 (O) CH3+OH=>2CO+CH3+C4H2+H2O 4.4E6 2.0 1.4E3 !O-
C6H4O2+OH=>H2O+2CO+C2H2+R9C2H
OC6H3 (O) CH3+OH=>C3H4-P+CO+HCO+CH2CO 5.48e12 0 -1040! as
d'addition des radicaux sur la double liaison exgas

OC6H3 (O) CH3=OC5H3CH3+CO 1.0E12 0.0 40.0E3 !as
O-C6H4O2=>C5H4O+CO !<ALZUETA00>!
OC5H3CH3=>C2H2+CO+C3H4-P 5.7E32 -6.76 68.5E3 !as
C5H4O=>2C2H2+CO

OA1OHCH3-2=HOC5H3CH3+CO 6.17E+78 -18.794 90504.0 !as
A1O=bicycle
OA1OHCH3-1=HOC5H3CH3+CO 6.17E+78 -18.794 90504.0 !as
A1O=bicycle

OC5H3CH3+H=HOC5H3CH3 1.74E06 2.2 7512.0 !as
H+CH3CHO Sivaramakrishnan JPCA2010

OC5H3CH3+H=>CH3+C4H4+CO 2.6E13 0.0 3.2E3!as
C5H4O+H=CO+C4H5-N
OC5H3CH3+H=>C2H3+C3H4-P+CO 2.6E13 0.0 3.2E3!as
C5H4O+H=CO+C4H5-N
OC5H3CH3+O=>C2H2+C3H4-P+CO2 1.0E13 0.0 2.0E3 ! as
C5H4O+O=C4H4+CO2

OC5H3CH3+H=>A1O+H2 1.74E05 2.5 2510.0 ! H-abst
3HpY Exgas

!OC5H3CH3+OH=>A1O+H2O 3.0E06 2.0 -298.0 ! H-abst
 3HpY Exgas
 OC5H3CH3+OH=>A1O+H2O 6.0E06 2.0 -298.0 ! Nicolas
 Delort A*2

OC5H3CH3+CH3=>A1O+CH4 2.22E00 3.5 5670.0 ! H-abst
 3HpY Exgas

!++++
 +++++
 +
 !
 +++++
 ! +
 +
 ! + <=== 1.3-BENZODIOXOLE / BENZODIOXOLE-
 2-ONE MECHANISM ==> +
 ! +
 +
 !
 +++++

A1OCH2O+H=A1CYOCH2O1-2+H2 1.7E+14 0.0 16000.0 ! as
 A1OH+H=C6H4OH+H2
 A1OCH2O+O=A1CYOCH2O1-2+OH 2.0e+13 0.0 14700.0 ! as
 A1OH+O=C6H4OH+OH
 A1OCH2O+OH=A1CYOCH2O1-2+H2O 1.4e+13 0.0 4600.0 ! as
 A1OH+OH=C6H4OH+H2O
 A1OCH2O+CH3=A1CYOCH2O1-2+CH4 2.0e+12 0.0 15000.0 ! as
 A1OH+CH3=C6H4OH+CH4
 A1OCH2O+HO2=A1CYOCH2O1-2+H2O2 4.0e+11 0.0 28900.0 ! as
 A1OH+HO2=C6H4OH+H2O2

!A1CYOCH2O1-2+H=HOA1OCH2 3.270E+25 -3.510 8145.0 ! as
 C8H8O+H=O-CH3A1OCH2
 !A1CYOCH2O1-2+H=OA1OCH3 3.270E+25 -3.510 8145.0 ! as
 C8H8O+H=O-CH2A1OCH3
 A1CYOCH2O1-2+H=HOA1OCH2 0.8E+25 -3.510 8145.0 ! A/4
 A1CYOCH2O1-2+H=OA1OCH3 0.8E+25 -3.510 8145.0 ! A/4

A1OCH2O=A1CYOCH2O1-2+H 4.99E+08 1.31 6543.0 !
 A1+OH=A1OH+H
 A1CYOCHO1-2+H=A1OCHO +2.2300000E+013 +0.0000000E+000
 +7.9300000E+003 ! ipso addition of H on OCH like A1OCH3+H<=>A1+CH3O from
 Nowakowska 2014
 A1CYOCHO1-2+H=A1CYOCH2O1-2 1E13 0.0 0.0 ! terminaison

!H-abstr on -OCH2O-
 A1CYOCH2O1-2+OH=>A1CYOCHO1-2+H2O +1.7916000E+002
 +3.0607000E+000 -1.3637000E+003 ! A1OCH3+OH<=>A1OCH2+H2O
 A1CYOCH2O1-2+H=>A1CYOCHO1-2+H2 +5.4874000E+006
 +2.2086000E+000 +6.6105000E+003 ! as A1OCH3+H<=>A1OCH2+H2
 A1CYOCH2O1-2+HO2=>A1CYOCHO1-2+H2O2 +8.6404500E-003
 +4.2995000E+000 +1.1067000E+004 ! as A1OCH3+HO2<=>A1OCH2+H2O2
 A1CYOCH2O1-2+CH3=>A1CYOCHO1-2+CH4 +1.0545700E-001
 +3.9964000E+000 +8.7155000E+003 ! as A1OCH3+CH3<=>A1OCH2+CH4

$A1CYOCH2O1-2+O=>A1CYOCHO1-2+OH$ +1.1800000E+000
+4.0900000E+000 +2.5454100E+003 ! as $A1OCH3+O<=>A1OCH2+OH$
 $A1CYOCH2O1-2+O2=>A1CYOCHO1-2+HO2$ +2.1000000E+013
+0.0000000E+000 +4.7900000E+004 ! as $A1OCH3+O2<=>A1OCH2+HO2$
 $A1CYOCH2O1-2+CH3O2=>A1CYOCHO1-2+CH3O2H$ +1.9020000E-004
+4.6400000E+000 +1.0556000E+004 ! as $A1OCH3+CH3O2<=>A1OCH2+CH3O2H$
 $A1CYOCH2O1-2+CH3O=>A1CYOCHO1-2+CH3OH$ +3.0100000E+011
+0.0000000E+000 +4.0740000E+003 ! as $A1OCH3+CH3O<=>A1OCH2+CH3OH$
 $A1CYOCH2O1-2+OCHO=>A1CYOCHO1-2+HOCHO$ +5.0000000E+012
+0.0000000E+000 +1.7690000E+004 ! as $A1OCH3+OCHO<=>A1OCH2+HOCHO$
 $A1CYOCH2O1-2+C2H5=>C2H6+A1CYOCHO1-2$ +3.0000000E+011
+0.0000000E+000 +9.2000000E+003 ! as $A1OCH3+C2H5<=>C2H6+A1OCH2$
 $A1CYOCH2O1-2+A1CH2O=>A1CYOCHO1-2+A1CH2OH$ +3.0100000E+011
+0.0000000E+000 +4.0740000E+003 ! as $A1OCH3+A1CH2O<=>A1OCH2+A1CH2OH$
 $A1OH+A1CYOCHO1-2=A1CYOCH2O1-2+A1O$ +1.8000000E+011
+0.0000000E+000 +7.7000000E+003 ! as $A1OH+A1OCH2=A1OCH3+A1O$
 $A1CYOCH2O1-2+A1=>A1+A1CYOCHO1-2$ +3.0000000E+011
+0.0000000E+000 +3.8510000E+003 ! as $A1OCH3+A1-=A1+A1OCH2$

!benzodioxole to benzodioxole-2-one

$A1CYOCHO1-2+HO2=A1CYOCHOO1-2+OH$ 1.000E+013 0.000 0.0
! as $CH2OH+HO2<=>HOCH2O+OH$
 $A1CYOCHO1-2+O2=A1CYOCHOO1-2+O$ 7.546E+012 0.000 28320.0
! as $CH3+O2<=>CH3O+O$
 $A1CYOCHOO1-2=A1CYOCO01-2+H$ +5.0700000E+008 +1.5600000E+000
+1.6850000E+004 ! as $A1CH2O<=>A1CHO+H$

!HOA1OCH2 -> HOA1OCHO -> benzodioxole-2-one

$HOA1OCH2+HO2=HOA1OCH2O+OH$ +5.8100000E+021 -2.5260000E+000
+1.1457500E+004 ! as $A1OCH2+HO2<=>A1OCH2O+OH$
 $HOA1OCH2+O2=HOA1OCH2OO$ +1.0000000E+000 +1.0000000E+000
+1.0000000E+000 ! as $A1OCH2+O2<=>A1OCH2OO$
PLOG / +1.0000000E-003
+1.1200000E+018 -3.3700000E+000 -4.2940000E+003 /
PLOG / +1.0000000E-002
+1.3300000E+021 -3.9500000E+000 -2.6150000E+003 /
PLOG / +1.0000000E+000
+1.1300000E+028 -5.2400000E+000 +4.0880000E+003 /
PLOG / +2.0000000E+000
+3.9100000E+027 -5.0000000E+000 +4.5120000E+003 /
PLOG / +1.0000000E+001
+2.7500000E+024 -3.8700000E+000 +4.2900000E+003 /
PLOG / +2.0000000E+001
+2.9700000E+022 -3.2300000E+000 +3.7810000E+003 /
PLOG / +5.0000000E+001
+5.1900000E+019 -2.3500000E+000 +2.9080000E+003 /
PLOG / +1.0000000E+002
+5.4300000E+017 -1.7300000E+000 +2.2100000E+003 /

!HOA1OCH2OO=HOA1OCHO+OH 1.4E+10 1.0 37.5E3 ! as
 $A1CH2OO=A1CHO+OH$
! Plog/1.0 1.4E+09 1.0 37.5E3/ !
! Plog/10.0 1.6E+10 1.0 37.5E3/ !
! Plog/50.0 3.2E+10 1.0 37.5E3/ !
 $HOA1OCH2OO=HOA1OCHO+OH$ 1.6E+10 1.0 37.5E3 ! 10 atm
 $HOA1OCH2OO+H=HOA1OCH2O+OH$ 3.80E14 -0.19 1.89E3 ! as
 $A1CH2OO+H=A1CH2O+OH$

HOA1OCH2O=HOA1OCHO+H 3.300E+013 0.004 26136.3 ! as
A1OCH2O<=>A1OCHO+H

!H-abstr HOA1OCHO+ R = HOA1OCO+ RH

HOA1OCHO+C2H3=C2H4+HOA1OCO +2.0000000E+011 +0.0000000E+000
+1.6800000E+004 ! as A1OCHO+C2H3=C2H4+A1OCO
HOA1OCHO+C2H5=C2H6+HOA1OCO +2.5000000E+010 +0.0000000E+000
+1.0400000E+004 ! as A1OCHO+C2H5=C2H6+A1OCO
HOA1OCHO+CH3=CH4+HOA1OCO +1.3530000E+004 +2.2600000E+000
+7.2870000E+003 ! as A1OCHO+CH3=CH4+A1OCO
HOA1OCHO+CH3O=CH3OH+HOA1OCO +5.4750000E+010 +0.0000000E+000
+5.0000000E+003 ! as A1OCHO+CH3O=CH3OH+A1OCO
HOA1OCHO+CH3O2=CH3O2H+HOA1OCO +2.8000000E+012 +0.0000000E+000
+1.7690000E+004 ! as A1OCHO+CH3O2=CH3O2H+A1OCO
HOA1OCHO+H=H2+HOA1OCO +6.5000000E+005 +2.4000000E+000
+4.4710000E+003 ! as A1OCHO+H=H2+A1OCO
HOA1OCHO+HO2=H2O2+HOA1OCO +2.8000000E+012 +0.0000000E+000
+1.7690000E+004 ! as A1OCHO+HO2=H2O2+A1OCO
HOA1OCHO+O=OH+HOA1OCO +2.3850000E+004 +2.7100000E+000
+2.1060000E+003 ! as A1OCHO+O=OH+A1OCO
HOA1OCHO+O2=HO2+HOA1OCO +1.0000000E+013 +0.0000000E+000
+5.1050000E+004 ! as A1OCHO+O2=HO2+A1OCO
HOA1OCHO+OH=H2O+HOA1OCO +2.3400000E+007 +1.6100000E+000
-3.5000000E+001 ! as A1OCHO+OH=H2O+A1OCO

!H-abstr HOA1OCHO+ R = OA1OCHO+ RH

HOA1OCHO+H=OA1OCHO+H2 1.2E14 0.0 12.4E3 !
as HOA1OCH3+H=OA1OCH3+H2
HOA1OCHO+CH3=OA1OCHO+CH4 1.8E11 0.0 7.7E3 !
as HOA1OCH3+CH3=OA1OCH3+CH4
HOA1OCHO+OH=OA1OCHO+H2O 1.4E8 1.4 -0.96E3
! as HOA1OCH3+OH=OA1OCH3+H2O
HOA1OCHO+HO2=OA1OCHO+H2O2 1.0E12 0.0 10.0E3 ! as
HOA1OCH3+HO2=OA1OCH3+H2O2
HOA1OCHO+C5H5=OA1OCHO+C5H6 2.67e14 0.0 25.238e3 ! as
HOA1OCH3+C5H5=OA1OCH3+C5H6
HOA1OCHO+A1-=OA1OCHO+A1 4.9E12 0.0 4.4E3
! as HOA1OCH3+A1-=OA1OCH3+A1
HOA1OCHO+O=OA1OCHO+OH 1.3E13 0.0 2.9E3
! as HOA1OCH3+O=OA1OCH3+OH
HOA1OCHO+C3H5-A=OA1OCHO+C3H6 2.67e14 0.0 25.238e3
! as HOA1OCH3+C3H5-A=OA1OCH3+C3H6
HOA1OCHO+C4H5-I=OA1OCHO+C4H6 2.67e14 0.0 25.238e3
! as HOA1OCH3+C4H5-I=OA1OCH3+C4H6
HOA1OCHO+OA1OH=OA1OCHO+HOA1OH 1.05e11 0.0 11500
! as HOA1OCH3+OA1OH=OA1OCH3+HOA1OH
HOA1OCHO+CH3O=CH3OH+OA1OCHO 1E12 0.0 1240.0 ! as
HOA1OCH3+CH3O=CH3OH+OA1OCHO
HOA1OCHO+CH3O2=OA1OCHO+CH3O2H 1.0E12 0.0 10.0E3 !
as HOA1OCH3+CH3O2=OA1OCH3+CH3O2H
HOA1OCHO+C4H5-N=OA1OCHO+C4H6 5e11 0 5300
! as HOA1OCH3+C4H5-N=OA1OCH3+C4H6
HOA1OCHO+O2=OA1OCHO+HO2 7.0e12 0.0 38410
! as HOA1OCH3+O2=OA1OCH3+HO2

A1CYOCOO1-2+H=HOA1OCO 3.270E+25 -3.510 8145.0 ! as C8H8O+H=O-
CH3A1OCH2

A1CYOCOO1-2+H=OA1OCHO 3.270E+25 -3.510 8145.0 ! as C8H8O+H=O-CH2A1OCH3

OA1OCHO=HOA1OCO 5.02e9 1.0 25e3 ! as OA1OCH3=HOA1OCH2

A1CYOCOO1-2+H=A1OCO2 +2.2300000E+013 +0.0000000E+000
+7.9300000E+003! as A1OCH3+H<=>A1+CH3O in Nowakowska 2014

A1OCO2<=>A1O+CO2 +8.6910000E+017 -1.8100000E+000
+1.3656700E+004 ! AS A1OCO<=>A1O+CO
PLOG / +5.0000000E-002
+1.0300000E+003 +1.2900000E+000 +2.5401000E+004 /
PLOG / +1.0000000E+000
+4.0900000E+005 +8.1000000E-001 +2.1969100E+004 /
PLOG / +1.0000000E+001
+9.0200000E+014 -1.7200000E+000 +2.1767500E+004 /
PLOG / +1.0000000E+002
+2.8250000E+022 -3.4400000E+000 +2.3592400E+004 /

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!A1OCH2CHCH2+H=A1OCH2+C2H4 1.000E+000 1.000 1.0 ! as
C3H6+H<=>C2H4+CH3
!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
!A1OCH2CHCH2+H=A1OCH2+C2H4 1.000E+000 1.000 1.0 ! as
C3H6+H<=>C2H4+CH3
!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

!A1OCH2+C2H2=>A1OCH2CHCH 1.780E+042 -10.400 13647.0 ! as
CH3+C2H2<=>C3H5-S
!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/

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!DUP
!A1OCH2+C2H2=>A1OCH2CHCH          1.780E+042   -10.400   13647.0 ! as
CH3+C2H2<=>C3H5-S
!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

!A1OCHCHCH2=A1OCH2CHCH          1.300E+055   -14.530   73800.0 ! as C3H5-
A<=>C3H5-S
!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/

!A1O+C3H4-P=>A1OCHCCH3          0.4E+10          0.0        460 ! as
A1O+C2H2=>C8H6O+H ~ A1O+C#C-R
!!A1O+C3H4-P=>A1OCHCCH3          4E+10          0.0        460 ! A*10
!A1OCHCHCH2=A1OCHCCH3          3.900E+059   -15.420   75400.0 ! as C3H5-
A<=>C3H5-T
!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/
!A1OCHCCH3+H=A1OCHCHCH2+H      2.11E+17          -1.08E+00   1.29E+03
! as C3H5-T+H<=>C3H5-A+H
!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
!A1OCHCCH3+H=A1OCHCHCH2+H      6.41E+03          2.61E+00   -3778.4
! as C3H5-T+H<=>C3H5-A+H
!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

!!A1OCH2CHCH2+H=A1O+C3H6
!A1OCH2CHCH2=A1O+C3H5-A          +3.1700000E+015 +0.0000000E+000
+6.3208500E+004 ! as A1OCH3<=>A1O+CH3
!!A1O+C3H5-A=>A1OCH2CHCH2      1e13  0.0  0.0

!!H abstraction A1OCH2CHCH2+R=A1OCHCHCH2+RH
!A1OCH2CHCH2+O2=A1OCHCHCH2+HO2          1.500E+013      0.000
50150.0 ! AS C2H5OH+O2<=>SC2H4OH+HO2
!A1OCH2CHCH2+O=A1OCHCHCH2+OH          1.450E+005      2.470
876.0 ! AS C2H5OH+O<=>SC2H4OH+OH

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!A1OCH2CHCH2+H=A1OCHCHCH2+H2	8.790E+004	2.680
2910.0 ! AS C2H5OH+H<=>SC2H4OH+H2		
!A1OCH2CHCH2+OH=A1OCHCHCH2+H2O	7.520E+004	2.490
-1474.1 ! AS C2H5OH+OH<=>SC2H4OH+H2O		
!A1OCH2CHCH2+HO2=A1OCHCHCH2+H2O2	2.450E-005	5.260
7475.1 ! AS C2H5OH+HO2<=>SC2H4OH+H2O2		
!A1OCH2CHCH2+CH3=A1OCHCHCH2+CH4	1.993E+001	3.370
7634.0 ! AS C2H5OH+CH3<=>SC2H4OH+CH4		
!A1OCH2CHCH2+CH3O2=A1OCHCHCH2+CH3O2H	1.225E-005	
5.260 7475.1 ! AS C2H5OH+CH3O2<=>SC2H4OH+CH3O2H		
!A1OCH2CHCH2+C2H5=A1OCHCHCH2+C2H6	5.000E+010	
0.000 10400.0 ! AS C2H5OH+C2H5<=>SC2H4OH+C2H6		

!A1CYOCHCHCH2=A1OCHCHCH2	+3.1600000E+012	+2.3300000E-001
+9.7100000E+003 ! AS A1CYCH2O<=>A1OCH2		
! REV /		+8.7800000E+010
+4.4200000E-001 +1.9030000E+004 /		

!A1CH2CHCHO=A1CYOCHCHCH2	+1.1700000E+011	+3.9800000E-001
+1.1170000E+004 ! AS A1CH2O<=>A1CYCH2O		
! REV /		+1.2700000E+013 -
3.1000000E-002 +1.6800000E+003 /		

!! H abstraction A1CH2CHCHO+R=A1CHCHCHO+RH

!A1CH2CHCHO+H=A1CHCHCHO+H2	3.31E+07	2.0	5345.3
! AS A1C2H5+H=A1CHCH3+H2			
!A1CH2CHCHO+CH3=A1CHCHCHO+CH4	1.1E+12	0.0	9100.0
! AS A1C2H5+CH3=A1CHCH3+CH4			
!A1CH2CHCHO+OH=A1CHCHCHO+H2O	3.5E9	1.0	-1.13E3 ! AS
A1C2H5+OH=A1CHCH3+H2O			
!A1CH2CHCHO+O=A1CHCHCHO+OH	3.9E+9	1.0	-1100.0
! AS A1C2H5+O=A1CHCH3+OH			
!A1CH2CHCHO+HO2=A1CHCHCHO+H2O2	6.80E+03	2.50	10114.0
! AS A1C2H5+HO2=A1CHCH3+H2O2			
!A1CH2CHCHO+O2=A1CHCHCHO+HO2	1.81E+12	0.0	39740.0
! AS A1C2H5+O2=A1CHCH3+HO2			