



JOOcy(CCOCC) != o(#1)/ch2/ch(/o/o.)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 HOOcy(COCCJ) != o(#1)/ch(/o/o/h)/ch./ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 HOOcy(COCCJC) != o(#1)/ch(/o/o/h)/ch2/ch./ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 HOOcy(COCJCC) != o(#1)/ch(/o/o/h)/ch2/ch2/ch./1 thermo  
 Hans-Heinrich Carstensen (this work)  
 HOOcy(CCJOCC) != o(#1)/ch./ch(/o/o/h)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 HOOcy(CCOCCJ) != o(#1)/ch2/ch(/o/o/h)/ch./ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 HOOcy(CCOCJC) != o(#1)/ch2/ch(/o/o/h)/ch2/ch./1 thermo  
 Hans-Heinrich Carstensen (this work)  
 O\*cy(COCCC) != o(#1)/c(/o)/ch2/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 O\*cy(CCOCC) != o(#1)/ch2/c(/o)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 CYCOJCCCO != o(#1)/ch(/o.)/ch./ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 CYCCOJCCO != o(#1)/ch./ch(/o.)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 CYCO2HCCCO != o(#1)/ch(/o/o/h)/ch2/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 CYCCO2HCCO != o(#1)/ch2/ch(/o/o/h)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 bicy(O)(CCCOC) != o(#1)/ch(#2)/ch(/o/2)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 bicy(O)(CCOCC) != o(#1)/ch(#2)/ch2/ch(/o/2)/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 Qcy(COC(OOJ)CC) != o(#1)/ch(/o/o/h)/ch2/ch2/ch(o/o.)/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 Qcy(COCC(OOJ)C) != o(#1)/ch(/o/o/h)/ch2/ch(o/o.)/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 Qcy(COCCC(OOJ)) != o(#1)/ch(/o/o/h)/ch(o/o.)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 JOOcy(CCOCC(Q)) != o(#1)/ch2/ch(/o/o/h)/ch(o/o.)/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 JOOcy(COCC(Q)C) != o(#1)/ch(o/o.)/ch(/o/o/h)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 JOOcy(COCCC(Q)) != o(#1)/ch2/ch(/o/o/h)/ch2/ch(o/o.)/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 OHCCCCHO != o//ch/ch2/ch2/ch//o thermo  
 Hans-Heinrich Carstensen (this work)  
 CJC(OOH)CCHO != .ch2/ch(/o/o/h)ch2/ch//o thermo  
 Hans-Heinrich Carstensen (this work)  
 OHCCcy(COC) != ch(/o)/ch2/ch(#1)/o/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 CYC\*OCO2HCCO != o(#1)/ch(/o)/ch(o/o/h)/ch2/ch2/1 thermo  
 THERM (updated 2016)  
 CYC\*OCCO2HCO != o(#1)/ch(/o)/ch2/ch(o/o/h)/ch2/1 thermo  
 THERM (updated 2016)  
 CYC\*OCCCO2HO != o(#1)/ch(/o)/ch2/ch2/ch(o/o/h)/1 thermo  
 THERM (updated 2016)  
 CYCO2HC\*OCCO != o(#1)/ch(o/o/h)/ch(/o)/ch2/ch2/1 thermo  
 THERM (updated 2016)  
 CYCC\*OCO2HCO != o(#1)/ch2/ch(/o)/ch(o/o/h)/ch2/1 thermo  
 THERM (updated 2016)

CYCC\*OCCO2HO != o(#1)/ch2/ch(/o)/ch2/ch(o/o/h)/1 thermo  
 THERM (updated 2016)  
 THFOOH14J2 != o(#1)/ch(/o/o/h)/ch./ch2/ch(/o/o/h)/1 thermo  
 THERM (updated 2016)  
 THFOOH13J2 != o(#1)/ch(/o/o/h)/ch./ch(/o/o/h)/ch2/1 thermo  
 THERM (updated 2016)  
 THFOOH13J4 != o(#1)/ch(/o/o/h)/ch2/ch(/o/o/h)/ch./1 thermo  
 THERM (updated 2016)  
 THFOOH12J3 != o(#1)/ch(/o/o/h)/ch(/o/o/h)/ch./ch2/1 thermo  
 THERM (updated 2016)  
 THFOOH23J1 != o(#1)/ch./ch(/o/o/h)/ch(/o/o/h)/ch2/1 thermo  
 THERM (updated 2016)  
 THFOOH1X3 != o(#1)/ch(/o/o/h)/ch2/ch//ch/1 thermo  
 THERM (updated 2016)  
 THFOOH1X2 != o(#1)/ch(/o/o/h)/ch//ch/ch2/1 thermo  
 THERM (updated 2016)  
 THFOOH2X3 != o(#1)/ch2/ch(/o/o/h)/ch//ch/1 thermo  
 THERM (updated 2016)  
 C3H6CHO1O2 != o//ch/ch2/ch2/ch2/o/o. thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1Q4J != o//c./ch2/ch2/ch2/o/o/h thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1Q3J != o//ch/ch./ch2/ch2/o/o/h thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1Q2J != o//ch/ch2/ch./ch2/o/o/h thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1Q4O2 != o//c(/o/o.)/ch2/ch2/ch2/o/o/h thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1Q3O2 != o//ch/ch(/o/o.)/ch2/ch2/o/o/h thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1Q2O2 != o//ch/ch2/ch(/o/o.)/ch2/o/o/h thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1\*O4Q != o//c(/o/o/h)/ch2/ch2/ch2//o thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1\*O3Q != o//ch/ch(/o/o/h)/ch2/ch2//o thermo  
 Veloo et al. C&F 2013  
 C3H6CHO1\*O2Q != o//ch/ch2/ch(/o/o/h)/ch2//o thermo  
 Veloo et al. C&F 2013  
 NC3H7CO3 != ch3/ch2/ch2/c(/o)/o/o. thermo  
 Veloo et al. C&F 2013  
 !  
 !THF high temperature (this work)  
 !  
 cy(OCCCC) != o(#1)/ch2/ch2/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 cy(OCJCCC) != o(#1)/ch(/o/o/h)/ch2/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 cy(OCCJCC) != o(#1)/ch2/ch(/o/o/h)/ch2/ch2/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 cy(OC\*CCC) != o(#1)/ch2/ch2/ch//ch/1 thermo  
 Hans-Heinrich Carstensen (this work)  
 cy(OCC\*CC) != c(#1)(/h)/ch2/o/ch2/ch//1 thermo  
 Hans-Heinrich Carstensen (this work)  
 C\*COCCHO != ch2//ch/o/ch2/ch//o thermo  
 Hans-Heinrich Carstensen (this work)  
 C\*CCCOH != ch2//ch/ch2/ch2/o/h thermo  
 Hans-Heinrich Carstensen (this work)

CY(OCOCC*C)	!= o(#1)/ch//ch/ch2/o/ch2/1	thermo
THERM (updated 2016)		
CY(OCJOCC*C)	!= o(#1)/ch//ch/ch2/o/ch./1	thermo
THERM (updated 2016)		
!		
!THF high temperature - Tran et al. 2015		
C3H6CHO-1	!= .ch2/ch2/ch2/ch//o	thermo Tran
et al C&F 2015		
C2H3OC2H4	!= .ch2/ch2/o/ch//ch2	thermo Tran
et al C&F 2015		
AC3H5OCH2	!= .ch2/o/ch2/ch//ch2	thermo Tran
et al C&F 2015		
CH2CHCH2CH2O	!= .o/ch2/ch2/ch//ch2	thermo Tran
et al C&F 2015		
C4H5O-2	!= o(#1)/ch//ch/ch2/ch(./)1	thermo Tran
et al C&F 2015		
C4H5O-3	!= o(#1)/ch//ch/ch(./)ch2/1	thermo Tran
et al C&F 2015		
FURAN	!= o(#1)/ch//ch/ch//ch/1	thermo Tran
et al C&F 2015		
CYC3H5(CHO)	!= ch(//o)/ch(#1)/ch2/ch2/1	thermo Tran
et al C&F 2015		
SC3H5CHO	!= ch3/ch//ch/ch//o	thermo Tran
et al C&F 2015		
CHCHCH2CHO	!= o//ch/ch2/ch//ch(./)	thermo Tran
et al C&F 2015		
CH2CHCHCHO	!= ch2//ch/ch//ch/o(./)	thermo Tran
et al C&F 2015		
CHCHCHCHOH	!= ch(./)//ch/ch//ch/oh	thermo Tran
et al C&F 2015		
CH3CHCHCO	!= ch3/ch//ch/c(./)//o	thermo Tran
et al C&F 2015		
CH3CH2CHCHO	!= .ch(/ch//o)/ch2/ch3	thermo Tran
et al C&F 2015		
CH3CH2CH2CO	!= .c(//o)/ch2/ch2/ch3	thermo Tran
et al C&F 2015		
CH3CH2OCCH2	!= .c(//ch2)/o/ch2/ch3	thermo Tran
et al C&F 2015		
CH3CH2OCHCH	!= .ch//ch/o/ch2/ch3	thermo Tran
et al C&F 2015		
CH3OCHCHCH2	!= .ch(/ch//ch2)/o/ch3	thermo Tran
et al C&F 2015		
CH3OCH2CCH2	!= .c(//ch2)/ch2/o/ch3	thermo Tran
et al C&F 2015		
CH3OCH2CHCH	!= .ch//ch/ch2/o/ch3	thermo Tran
et al C&F 2015		
CH2CHOCHCH3	!= .ch(/ch3)/o/ch//ch2	thermo Tran
et al C&F 2015		
CH3CHCOCH3	!= .c(/o/ch3)//ch/ch3	thermo Tran
et al C&F 2015		
CH3CHCHOCH2	!= .ch2/o/ch//ch/ch3	thermo Tran
et al C&F 2015		
CH3OCHCCH3	!= .c(/ch3)//ch/o/ch3	thermo Tran
et al C&F 2015		
CH3OCHCCH2	!= ch3/o/ch//c//ch2	thermo Tran
et al C&F 2015		
CH2CCHCHO	!= ch2//c//ch/ch//o	thermo Tran
et al C&F 2015		

FURYL-2	!= o(#1)/c(.)//ch/ch//ch/1	thermo Tran
et al C&F 2015		
FURYL-3	!= o(#1)/ch//c(.)//ch//ch/1	thermo Tran
et al C&F 2015		
CHCHCHO	!= ch(.)//ch/ch//o	thermo Tran
et al C&F 2015		
CHCHCHCO	!= ch(.)//ch/ch//c//o	thermo Tran
et al C&F 2015		
CHCCHCHO	!= ch///c/ch//ch/o(.)	thermo Tran
et al C&F 2015		
CHCCHCO	!= ch///c/ch//c//o	thermo Tran
et al C&F 2015		

!

!Other high temperature species (YF 2017)

O*cy(COCCC)	C*CCC(*O)OH	O*CYCCJCCO	O*CYCCCCJCO
O*CYCCCCJO	C*CC(*O)OCJ	C*CCOCJ(*O)	C(*O)CCCJ(*O)
C*COCC(*O)CJ	O*CYCC*CCO	O*CYCCC*CO	O*CCC*C*O
O*CC*CC*O	O*CYCCJCOHCO	O*CYCCCCOHCJO	O*CYCC*CCJO
O*CYCCJC*CO	O*CJC*CC*O	CHCHCHO	O*C*CC*COJ
O*cy(CCOCC)	O*CYCCJCOC	O*CYCCCJOC	O*CYCCCCOCJ
O*CYCC*COCC	O*CYCC*COCCJ	O*CYCCOHCJOC	CHOCHO
O*CC(*O)C*CJ	CHOCO	O*CYCC*COCC	C*CCOCHO
C*CCJOC*O	AC3H5CHO	AC3H5CO	C*COCCJCHO
C*COCCJO	CHOCH2CHO	CHOCH2CO	

!

!Base C0-C4 Metcalfe et al. Int. J. Chem. Kinet. 2013

H	H2	O	O2
OH	OH*	H2O	N2
HO2	H2O2	AR	CO
CO2	CH2O	HCO	HO2CHO
HCOH	O2CHO	HOCHO	OCHO
HOCH2O2H	HOCH2O2	OCH2O2H	HOCH2O
CH3OH	CH2OH	CH3O	CH3O2H
CH3O2	CH4	CH3	CH2
CH2(S)	C	CH	CH*
C2H6	C2H5	C2H4	C2H3
C2H2	C2H	CH3CHO	C2H3OH
C2H2OH	CH3CO	CH2CHO	O2CH2CHO
HO2CH2CO	CH2CO	HCCO	HCCOH
CH3CO3H	CH3CO3	CH3CO2	C2H5OH
C2H5O	PC2H4OH	SC2H4OH	O2C2H4OH
C2H5O2H	C2H5O2	C2H4O2H	C2H4O1-2
C2H3O1-2	CH3COCH3	CH3COCH2	CH3COCH2O2
C3KET21	C*CCHO	C2H3CO	C2H5CHO
C2H5CO	CH3OCH3	CH3OCH2	CH3OCH2O2
CH2OCH2O2H	CH3OCH2O2H	CH3OCH2O	O2CH2OCH2O2H
HO2CH2OCHO	OCH2OCHO	HOCH2OCO	CH3OCHO
CH3OCO	CH2OCHO	HE	C3H8
IC3H7	NC3H7	C3H6	C3H5-A
C3H5-S	C3H5-T	C3H4-P	C3H4-A
C3H3	C3H5O	C3H6OOH1-2	C3H6OOH1-3
C3H6OOH2-1	C3H6OOH1-2O2	C3H6OOH1-3O2	C3H6OOH2-1O2
C3H6OOH2-2	NC3H7O2H	IC3H7O2H	NC3H7O2
IC3H7O2	NC3H7O	IC3H7O	C3H6O1-2
C3H6O1-3	C3KET12	C3KET13	C3H51-2-3OOH
C3H52-1-3OOH	C3H6OH1-2	HOC3H6O2	CH3CHCO
AC3H5OOH	C2H3OOH	CC3H4	H2CC
C4H10	C4H8-1	C4H8-2	PC4H9

SC4H9	C4H71-1	C4H71-2	C4H71-3
C4H71-4	C4H72-2	C4H6	PC4H9O2H
SC4H9O2H	PC4H9O2	SC4H9O2	PC4H9O
SC4H9O	C4H7O	C4H8O1-2	C4H8O1-3
C4H8O1-4	C4H8O2-3	PC4H8OH	SC4H8OH
C4H8OH-1O2	C4H8OH-2O2	C4H8OOH1-1	C4H8OOH1-2
C4H8OOH1-3	C4H8OOH1-4	C4H8OOH2-1	C4H8OOH2-2
C4H8OOH2-3	C4H8OOH2-4	C4H8OOH1-2O2	C4H8OOH1-3O2
C4H8OOH1-4O2	C4H8OOH2-1O2	C4H8OOH2-3O2	C4H8OOH2-4O2
NC4KET12	NC4KET13	NC4KET14	NC4KET21
NC4KET23	NC4KET24	C2H5COCH3	C2H5COCH2
CH2CH2COCH3	CH3CHCOCH3	C2H3COCH3	CH3CHOOCOCH3
CH2CHOOHCOCH3	NC3H7CHO	NC3H7CO	C3H6CHO-1
C3H6CHO-2	C3H6CHO-3	C2H5CHCO	SC3H5CHO
SC3H5CO	CH2CH2CHO	IC4H10	IC4H9
TC4H9	IC4H8	IC4H7	TC4H9O2
IC4H9O2	TC4H8O2H-I	IC4H8O2H-I	IC4H8O2H-T
IC4H8O	CC4H8O	IC4H9O	TC4H9O
IC4H9O2H	TC4H9O2H	IC4H7O	IC4H8OH
IO2C4H8OH	IC3H7CHO	TC3H6CHO	IC3H7CO
IC3H6CHO	TC4H8OOH-IO2	IC4H8OOH-IO2	IC4H8OOH-TO2
IC4KETII	IC4KETIT	IC4H7OH	IC4H6OH
IC3H5CHO	IC3H5CO	TC3H6OCHO	IC3H6CO
IC4H7OOH	TC3H6OHCHO	C3H6OH2-1	IC3H5OH
TC3H6O2CHO	TC3H6O2HCO	IC3H5O2HCHO	CH2CCH2OH
TC4H8CHO	O2C4H8CHO	O2HC4H8CO	C3H5OH
TIC4H7Q2-I	IIC4H7Q2-T	IIC4H7Q2-I	CH2O2H
C4H4	C4H3-I	C4H3-N	C4H612
C4H2	C4H5-I	C4H5-N	CH3CHCHCO
CH2CHCHCHO	C4H6O25	C2H3CHOCH2	C4H5-2
C4H6-2	C4H6O23	CH3CHCHCHO	C4H4O
H2C4O	C2H3OCH2	H2C4O	C6H6
C*CCJC*C	C5H6	C6H5	C6H2
C6H3	L-C6H4	C-C6H4	C6H5O
C6H5OH	P-C6H4O2	O-C6H4O2	P-C6H3O2
C5H6	C5H5	C5H4O	C5H5O
C5H5OH	C5H4OH	C5H3O	C6H5OO
C6H5OOH	OC6H4OH	C6H4OH	O-OC6H5OJ
P-OC6H5OJ	CTCC*CCJ	C5H6-L	CJ*CC*CC*O
C*CC*CCJ*O	CJ*CC*O	C5H7	OC5H7O
C*CCJC*COH	C*CC*CCJ	C*CC*CC	C*CC*CCOH
C*CCJC*O	OC4H6O	OC4H5O	HOCO
HOC*CC*O	HOC*CCJ*O	O2CCHOOJ	C2H3OCH2
C6H10	C6H9-A	C3H2	C3H2 (S)
C3H2C	H2CCC (S)	C3H3O	C3H3O2H
C2HCHO	CH3COCH2O	C6H5CH3	C6H5CH2
PC3H4OH-2	SC3H4OH	SC3H5OH	CH3CHCHO
SC3H4OH	C6H11	AC4H7OOH	HOC4H6

!
   
CYC\*CCOHC O HC (\*O)OOH cy(O)13cy(CCCOC) C\*CCC(OJ)OOH
   
!

END

REACTIONS

!\*\*\*\*\*!

!\*\*\* Sub-mechanism THF \*\*\*!

!\*\*\*\*\*!

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!*** Low temperature ***!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!*** Addition of o2 to alkylradical R+O2=RO2 ***!
!
cy(OCJCCC)+O2=JOOcy(COCCC)          0.346E+15 -0.92 -
130!Cai opt /3 o in alpha position
cy(OCCJCC)+O2=JOOcy(CCOCC)         1.039E+15 -0.92 -
130!Cai opt
!
!*** H-atom shift from alpha position ROO=ketone+OH ***!
!
JOOcy(COCCC)=O*cy(COCCC)+OH         7.4E+06  1.79
37000!Carstensen calculations
REV/ 9.4E-01 3.36 76100/
JOOcy(CCOCC)=O*cy(CCOCC)+OH        1.9E+06  1.99
38200!Carstensen calculations
REV/ 6.8E-01 3.45 64700/
!
!*** H-atom shift from beta position ROO=QOOH ***!
!
JOOcy(COCCC)=HOOcy(COCCCJ)         1.1E+07  1.57
28400!Carstensen calculations
REV/ 8.0E+10 0.18 17900/
JOOcy(CCOCC)=HOOcy(CCJOCC)         1.8E+07  1.39
22900!Carstensen calculations
REV/ 6.4E+08 0.72 16900/
JOOcy(CCOCC)=HOOcy(CCOCCJ)         1.5E+07  1.57
31300!Carstensen calculations
REV/ 1.8E+08 0.98 17600/
!
!*** H-atom shift from gamma position ROO=QOOH ***!
!
JOOcy(COCCC)=HOOcy(COCCJC)         6.6E+06  1.51
24700!Carstensen calculations
REV/ 6.0E+10 -0.02 14900/
!JOOcy(COCCC)=HOOcy(COCJCC)         3.7E+07  1.26
18300!Carstensen calculations
!REV/ 6.4E+11 -0.21 11800/
JOOcy(COCCC)=HOOcy(COCJCC)         7.2E+07  1.26
18300!Carstensen calculations*2
REV/ 12.8E+11 -0.21 11800/
JOOcy(CCOCC)=HOOcy(CCOCJC)         1.6E+07  1.28
20200!Carstensen calculations
REV/ 1.5E+08 0.78 11300/
!
!*** cyclic ether formation ***!
!
HOOcy(COCCCJ)=bicy(O)(CCCOC)+OH    2.0E+15  -0.57
13300!Carstensen calculations
REV/ 1.4E+05 2.28 25500/
HOOcy(CCJOCC)=bicy(O)(CCCOC)+OH    1.8E+12   0.21
7700!Carstensen calculations
REV/ 4.3E+04 2.37 22200/
HOOcy(CCOCCJ)=bicy(O)(CCOCC)+OH    2.2E+11   0.46
11200!Carstensen calculations
REV/ 2.6E+04 2.54 27200/

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HOOcy(COCCJC)=cy(O)13cy(CCCOC)+OH 9.1E+13 -0.47 27500!Carstensen
calculations! nov 2017
REV/1.6E+04 2.51 28800/
!
!*** beta-scission (radical in gamma position from -COOH)***!
!
HOOcy(COCJCC)=OHCCCCHO+OH 2.3E+14 -0.23
20100!Carstensen calculations! Updated by HHC/1.5
REV/ 2.2E+01 2.43 45700/
HOOcy(CCOCCJC)=C*COCCCHO+OH 3.5E+11 0.06
33300!Carstensen calculations
REV/ 1.5E-01 3.47 59900/
HOOcy(COCCJC)=C*CCOCHO+OH 1.3E+11 0.64
21800!Carstensen calculations
REV/ 2.6E+02 2.12 36500/
!HOOcy(CCOCCJC)=CJC(OOH)CCHO 9.5E+11 0.49
21700!Carstensen calculations
!REV/ 1.8E+11 -0.19 17200/
HOOcy(COCCJC)=C*CCOCHO+OH 3.5E+13 0.06 33300!Carstensen calculations!
Updated by HHC, nov2017
REV/ 1.5E-01 3.47 59900/
HOOcy(COCCJC)=C*CCC(OJ)OOH 9.1E+13 -0.47 27500!Carstensen calculations!
Updated by HHC, nov2017
REV/ 1.6E+04 2.51 28800/
!
!*** QOOH=Alkene+HO2 HO2 loss ***!
!
HOOcy(COCCCJ)=cy(OC*CCC)+HO2 1.6E+13 0.12
18800!Carstensen calculations
REV/ 2.2E-01 3.63 3600/
HOOcy(CCOCCJ)=cy(OCC*CC)+HO2 1.0E+13 0.16 16100!
Carstensen calculations
REV/ 3.5E+02 2.89 8100/
HOOcy(CCJOCC)=cy(OC*CCC)+HO2 5.6E+13 -0.02
17400!Carstensen calculations
REV/ 2.8E+02 2.80 4400/
!
!*** ROO=Alkene+HO2 concerted elimination ***!
!
JOOcy(COCCC)=cy(OC*CCC)+HO2 3.3E+09 1.15
28300!Carstensen calculations
REV/ 3.5E-01 3.27 2630/
JOOcy(CCOCC)=cy(OC*CCC)+HO2 2.1E+08 1.35
30400!Carstensen calculations
REV/ 3.7E-02 3.5 11500/
JOOcy(CCOCC)=cy(OCC*CC)+HO2 4.4E+08 1.24
28500!Carstensen calculations
REV/ 1.9E-01 3.38 6700/
!
!*** QOOH addition to O2 ***!
!
HOOcy(COCCCJ)+O2=Qcy(COCCC(OOJ)) 4.449E+14 -0.92 -
130!Cai opt
HOOcy(COCCJC)+O2=Qcy(COCC(OOJ)C) 4.449E+14 -0.92 -130
HOOcy(COCJCC)+O2=Qcy(COC(OOJ)CC) 1.483E+14 -0.92 -
130!/3 O in alpha
HOOcy(CCJOCC)+O2=JOOcy(COCCC(Q)) 1.483E+14 -0.92 -
130!/3 O in alpha

```



HOOcy(CCOCCJ)+O2=JOOcy(CCOCC(Q))	4.449E+14	-0.92	-130
HOOcy(CCOCJC)+O2=JOOcy(COCC(Q)C)	1.483E+14	-0.92	-
130!/3 O in alpha			
!			
!*** Isomerization of OOQOOH and formation of carbonyloxydroperoxide and OH ***!			
!			
Qcy(COCCC(OOJ))=CYC*OCO2HCCO+OH	1.8E+07	1.39	
22900!Carstensen calculations			
REV/ 6.4E+08 0.72 16900/			
Qcy(COCC(OOJ)C)=CYC*OCCO2HCO+OH	1.6E+07	1.28	
20200!Carstensen calculations			
REV/ 1.5E+08 0.78 11300/			
Qcy(COC(OOJ)CC)=CYC*OCCCO2HO+OH	3.7E+07	1.26	
18300!Carstensen calculations			
REV/ 6.4E+11 -0.21 11800/			
JOOcy(COCCC(Q))=CYCO2HC*OCCO+OH	1.1E+07	1.57	
28400!Carstensen calculations			
REV/ 8.0E+10 0.18 17900/			
JOOcy(CCOCC(Q))=CYCC*OCO2HCO+OH	1.5E+07	1.57	
31300!Carstensen calculations			
REV/ 1.8E+08 0.98 17600/			
JOOcy(COCC(Q)C)=CYCC*OCCO2HO+OH	6.6E+06	1.51	
24700!Carstensen calculations			
REV/ 6.0E+10 -0.02 14900/			
!			
!*** Isomerization of OOQOOH forming HOOPOOH radical ***			
!			
Qcy(COC(OOJ)CC)=THFOOH14J2	6.6E+06	1.51	
24700!Carstensen calculations			
REV/ 6.0E+10 -0.02 14900/			
DUP			
Qcy(COC(OOJ)CC)=THFOOH14J2	1.1E+07	1.57	
28400!Carstensen calculations			
REV/ 8.0E+10 0.18 17900/			
DUP			
Qcy(COCC(OOJ)C)=THFOOH13J2	1.5E+07	1.57	
31300!Carstensen calculations			
REV/ 1.8E+08 0.98 17600/			
Qcy(COCC(OOJ)C)=THFOOH13J4	1.8E+07	1.39	
22900!Carstensen calculations			
REV/ 6.4E+08 0.72 16900/			
Qcy(COCCC(OOJ))=THFOOH12J3	1.5E+07	1.57	
31300!Carstensen calculations			
REV/ 1.8E+08 0.98 17600/			
JOOcy(COCCC(Q))=THFOOH12J3	6.6E+06	1.51	
24700!Carstensen calculations			
REV/ 6.0E+10 -0.02 14900/			
JOOcy(CCOCC(Q))=THFOOH23J1	3.7E+07	1.26	
18300!Carstensen calculations			
REV/ 6.4E+11 -0.21 11800/			
DUP			
JOOcy(CCOCC(Q))=THFOOH23J1	1.8E+07	1.39	
22900!Carstensen calculations			
REV/ 6.4E+08 0.72 16900/			
DUP			
JOOcy(COCC(Q)C)=THFOOH13J4	3.7E+07	1.26	
18300!Carstensen calculations			

```

REV/ 6.4E+11 -0.21 11800/
JOOcy(COCC(Q)C)=THFOOH13J2          1.5E+07      1.57
31300!Carstensen calculations
REV/ 1.8E+08 0.98 17600/
!
!*** HOOPOOH=Alkene+HO2 HO2 loss ***!
!
THFOOH14J2=THFOOH1X3+HO2          1.6E+13      0.12
18800!Carstensen calculations
REV/ 2.2E-01 3.63 3600/
THFOOH13J2=THFOOH1X2+HO2          1.0E+13      0.16
16100! Carstensen calculations
REV/ 3.5E+02 2.89 8100/
THFOOH13J4=THFOOH1X3+HO2          5.6E+13     -0.02
17400!Carstensen calculations
REV/ 2.8E+02 2.80 4400/
THFOOH12J3=THFOOH1X2+HO2          1.0E+13      0.16
16100! Carstensen calculations
REV/ 3.5E+02 2.89 8100/
THFOOH23J1=THFOOH2X3+HO2          5.6E+13     -0.02
17400!Carstensen calculations
REV/ 2.8E+02 2.80 4400/
!
!*** OOQOOH=Alkene+HO2 concerted elimination ***!
!
Qcy(COC(OOJ)CC)=THFOOH1X3+HO2      3.3E+09      1.15
28300!Carstensen calculations
REV/ 3.5E-01 3.27 2630/
Qcy(COCC(OOJ)C)=THFOOH1X3+HO2      2.1E+08      1.35
30400!Carstensen calculations
REV/ 3.7E-02 3.5 11500/
Qcy(COCC(OOJ)C)=THFOOH1X2+HO2      4.4E+08      1.24
28500!Carstensen calculations
REV/ 1.9E-01 3.38 6700/
Qcy(COCCC(OOJ))=THFOOH1X2+HO2      4.4E+08      1.24
28500!Carstensen calculations
REV/ 1.9E-01 3.38 6700/
JOOcy(CCOCC(Q))=THFOOH2X3+HO2      2.1E+08      1.35
30400!Carstensen calculations
REV/ 3.7E-02 3.5 11500/
JOOcy(COCC(Q)C)=THFOOH2X3+HO2      3.3E+09      1.15
28300!Carstensen calculations
REV/ 3.5E-01 3.27 2630/
!
!*** Decompostion of hydroperoxide dihydrofurans
!
THFOOH1X3=HCO+C*CCHO+OH            3.87e+021   -1.82
44588.5
THFOOH1X2=HCO+C*CCHO+OH            3.87e+021   -1.82
44588.5
THFOOH2X3=HCO+C*CCHO+OH            3.87e+021   -1.82
44588.5
!
!*** Decomposition of carbonyl hydroperoxide ***!
!
CYC*OCO2HCCO=CH2O+CH2CO+HCO+OH     3.87e+021   -1.82
44588.5

```

CYC*OCCO2HCO=CH2O+CH2CO+HCO+OH 44588.5	3.87e+021	-1.82		
CYC*OCCCO2HO=CH2O+CH2CO+HCO+OH 44588.5	3.87e+021	-1.82		
CYCO2HC*OCCO=CH2O+CH2CO+HCO+OH 44588.5	3.87e+021	-1.82		
CYCC*OCO2HCO=CH2O+CH2CO+HCO+OH 44588.5	3.87e+021	-1.82		
CYCC*OCCO2HO=CH2O+CH2CO+HCO+OH 44588.5	3.87e+021	-1.82		
!				
CYC*OCO2HCCO=CH3CHO+CHOCO+OH 44588.5	3.87e+021	-1.82		
CYC*OCCO2HCO=CH3CHO+CHOCO+OH 44588.5	3.87e+021	-1.82		
CYC*OCCCO2HO=CH3CHO+CHOCO+OH 44588.5	3.87e+021	-1.82		
CYCO2HC*OCCO=CH3CHO+CHOCO+OH 44588.5	3.87e+021	-1.82		
CYCC*OCO2HCO=CH3CHO+CHOCO+OH 44588.5	3.87e+021	-1.82		
CYCC*OCCO2HO=CH3CHO+CHOCO+OH 44588.5	3.87e+021	-1.82		
!				
!*** Cyclic ether reactions with OH and HO2 ***!				
!				
bicy(O) (CCCOC)+OH=>H2O+C2H4O1-2+HCCO 0.0 !TRI2016 CLASS29 CYCLIC ETHER REACTIONS WITH OH AND HO2	6.064E+12	0.0		
bicy(O) (CCCOC)+OH=>H2O+C*CCHO+HCO 0.0 !TRI2016 CLASS29 CYCLIC ETHER REACTIONS WITH OH AND HO2	6.064E+12	0.0		
!				
bicy(O) (CCCOC)+H=>H2+C2H4O1-2+HCCO !HHC Calculations	7.0E+06	2.24	4500	
bicy(O) (CCCOC)+H=>H2+C*CCHO+HCO !HHC Calculations	5.2E+07	1.96	11400	
!				
bicy(O) (CCCOC)+CH3=>CH4+C2H4O1-2+HCCO !HHC Calculations	8.7E+02	3.08	7300	
bicy(O) (CCCOC)+CH3=>CH4+C*CCHO+HCO !HHC Calculations	1.5E+03	2.94	11700	
!				
bicy(O) (CCCOC)+HO2=>H2O2+C2H4O1-2+HCCO !HHC Calculations	6.7E+00	3.67	9200	
bicy(O) (CCCOC)+HO2=>H2O2+C*CCHO+HCO !HHC Calculations	1.2E+03	3.12	18400	
!				
bicy(O) (CCOCC)+OH=>H2O+C*CCHO+HCO 0.0 !TRI2016 CLASS29 CYCLIC ETHER REACTIONS WITH OH AND HO2 DUP	6.064E+12	0.0		
bicy(O) (CCOCC)+OH=>H2O+C*CCHO+HCO 0.0 !TRI2016 CLASS29 CYCLIC ETHER REACTIONS WITH OH AND HO2 DUP	6.064E+12	0.0		
bicy(O) (CCOCC)+OH=>H2O+C2H4O1-2+HCCO 0.0 !TRI2016 CLASS29 CYCLIC ETHER REACTIONS WITH OH AND HO2 DUP	6.064E+12	0.0		
bicy(O) (CCOCC)+OH=>H2O+C2H4O1-2+HCCO 0.0 !TRI2016 CLASS29 CYCLIC ETHER REACTIONS WITH OH AND HO2 DUP	6.064E+12	0.0		

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!
bicy(O) (CCOCC)+H=>H2+C*CCHO+HCO          2.9E+07  1.97  13500
!HHC Calculations
DUP
bicy(O) (CCOCC)+H=>H2+C*CCHO+HCO          2.4E+07  1.98  10900
!HHC Calculations
DUP
bicy(O) (CCOCC)+H=>H2+C2H4O1-2+HCCO        9.8E+06  2.12   7200
!HHC Calculations
DUP
bicy(O) (CCOCC)+H=>H2+C2H4O1-2+HCCO        9.5E+06  2.15   5900
!HHC Calculations
DUP
!
bicy(O) (CCOCC)+CH3=>CH4+C*CCHO+HCO        8.1E+02  2.94  13000
!HHC Calculations
DUP
bicy(O) (CCOCC)+CH3=>CH4+C*CCHO+HCO        6.6E+02  2.96  11400
!HHC Calculations
DUP
bicy(O) (CCOCC)+CH3=>CH4+C2H4O1-2+HCCO      5.2E+02  3.03   8900
!HHC Calculations
DUP
bicy(O) (CCOCC)+CH3=>CH4+C2H4O1-2+HCCO      1.4E+02  3.22   7900
!HHC Calculations
DUP
!
bicy(O) (CCOCC)+HO2=>H2O2+C*CCHO+HCO       2.8E+02  3.25  21400
!HHC Calculations
DUP
bicy(O) (CCOCC)+HO2=>H2O2+C*CCHO+HCO       5.7E+02  3.17  17700
!HHC Calculations
DUP
bicy(O) (CCOCC)+HO2=>H2O2+C2H4O1-2+HCCO    1.0E+01  3.31  13900
!HHC Calculations
DUP
bicy(O) (CCOCC)+HO2=>H2O2+C2H4O1-2+HCCO     4.8E-02  4.24   9900
!HHC Calculations
DUP
!
cy(O)13cy(CCCOC)=C*CCOCHO                   1.5E+11  1.01  49200
!HHC Calculations
REV/ 3.7E+06 1.43 74500/
!
!Low temperature reaction class
!*** R+HO2<=>RO+OH ***!
cy(OCJCCC)+HO2=CYCOJCCCO+OH                 4.892E+12  0.00 -
1000.0 !TRI2016 CLASS 13 R+HO2<=>RO+OH REACTIONS
cy(OCCJCC)+HO2=CYCCOJCCO+OH                 4.892E+12  0.00 -
1000.0 !TRI2016 CLASS 13 R+HO2<=>RO+OH REACTIONS
!
!*** R+CH3O2<=>RO+CH3O ***!
cy(OCJCCC)+CH3O2=CYCOJCCCO+CH3O             7.000E+12  0.00 -
1000.0 !TRI2016 CLASS 14 R+CH3O2<=>RO+CH3O REACTIONS
cy(OCCJCC)+CH3O2=CYCCOJCCO+CH3O             7.000E+12  0.00 -
1000.0 !TRI2016 CLASS 14 R+CH3O2<=>RO+CH3O REACTIONS
!
!*** addition of alkyl radical to alkyl peroxy radical ***!

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JOOcy(COCCC)+cy(OCJCCC)=CYCOJCCCO+CYCOJCCCO      7.000E+12    0.00  -
1000.0 !TRI2016 CLASS 12 ADDITION OF ALKYL RADICAL TO ALKYL PEROXY
RADICAL (ROO) TO FORM TWO RO RADICALS
JOOcy(COCCC)+cy(OCCJCC)=CYCOJCCCO+CYCCOJCCO      7.000E+12    0.00  -
1000.0 !TRI2016 CLASS 12 ADDITION OF ALKYL RADICAL TO ALKYL PEROXY
RADICAL (ROO) TO FORM TWO RO RADICALS
JOOcy(CCOCC)+cy(OCJCCC)=CYCOJCCCO+CYCCOJCCO      7.000E+12    0.00  -
1000.0 !TRI2016 CLASS 12 ADDITION OF ALKYL RADICAL TO ALKYL PEROXY
RADICAL (ROO) TO FORM TWO RO RADICALS
JOOcy(CCOCC)+cy(OCCJCC)=CYCCOJCCO+CYCCOJCCO      7.000E+12    0.00  -
1000.0 !TRI2016 CLASS 12 ADDITION OF ALKYL RADICAL TO ALKYL PEROXY
RADICAL (ROO) TO FORM TWO RO RADICALS
!
!*** Bimolecular reactions between alkylperoxy radical and ho2
ROO+HO2=ROOH+O2 ***!
JOOcy(COCCC)+HO2=CYCO2HCCCO+O2                    1.75E+10    0.0   -3275
!TRI2016 CLASS 17 BIMOLECULAR REACTIONS BETWEEN ALKYLPEROXY RADICAL AND
HO2 ROO+HO2<=>ROOH+O2
JOOcy(CCOCC)+HO2=CYCCO2HCCO+O2                    1.75E+10    0.0   -3275
!TRI2016 CLASS 17 BIMOLECULAR REACTIONS BETWEEN ALKYLPEROXY RADICAL AND
HO2 ROO+HO2<=>ROOH+O2
!
!*** Bimolecular reactions between alkylperoxy radicals and h2o2
ROO+H2O2<=>ROOH+HO2 ***!
JOOcy(COCCC)+H2O2=CYCO2HCCCO+HO2                  2.40E+12    0.0  1.0E+04
!TRI2016 CLASS 18 BIMOLECULAR REACTIONS BETWEEN ALKYLPEROXY RADICALS AND
H2O2 ROO+H2O2<=>ROOH+HO2
JOOcy(CCOCC)+H2O2=CYCCO2HCCO+HO2                  2.40E+12    0.0  1.0E+04
!TRI2016 CLASS 18 BIMOLECULAR REACTIONS BETWEEN ALKYLPEROXY RADICALS AND
H2O2 ROO+H2O2<=>ROOH+HO2
!
!*** RO2+CH3O2=>RO+CH3O+O2 ***!
JOOcy(COCCC)+CH3O2=>CYCOJCCCO+CH3O+O2             1.40E+16    -1.61  1860
!TRI2016 CLASS19 RO2+CH3O2<=>RO+CH3O+O2
JOOcy(CCOCC)+CH3O2=>CYCCOJCCO+CH3O+O2             1.40E+16    -1.61  1860
!TRI2016 CLASS19 RO2+CH3O2<=>RO+CH3O+O2
!
!*** ROO+ROO<=>RO+RO+O2 ***!
JOOcy(COCCC)+JOOcy(COCCC)=CYCOJCCCO+CYCOJCCCO+O2 1.400E+16    -1.61  1860
!TRI2016 CLASS20 ROO+ROO<=>RO+RO+O2
JOOcy(COCCC)+JOOcy(CCOCC)=CYCOJCCCO+CYCCOJCCO+O2 1.400E+16    -1.61  1860
!TRI2016 CLASS20 ROO+ROO<=>RO+RO+O2
JOOcy(CCOCC)+JOOcy(CCOCC)=CYCCOJCCO+CYCCOJCCO+O2 1.400E+16    -1.61  1860
!TRI2016 CLASS20 ROO+ROO<=>RO+RO+O2
!
!*** ROOH<=>RO+OH ***!
CYCO2HCCCO=CYCOJCCCO+OH                            1.000E+16    0.00  39000
!TRI2016 CLASS21 ROOH<=>RO+OH
CYCCO2HCCO=CYCCOJCCO+OH                            1.000E+16    0.00  39000
!TRI2016 CLASS21 ROOH<=>RO+OH
!
!*** Alkyloxy radical decomposition ***!
!
CYCOJCCCO=C2H4+CH2O+HCO                             4.4E+12     0.38   9400
!HHC calculations O*cy(COC(OJ)CC) => HC(*O)OC(*O)CCJ
CYCCOJCCO=C2H4+CH2O+HCO                             1.4E+12     0.45  20000
!HHC calculations O*cy(COC(OJ)CC) => OHCCCC(*O)OJ
!

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!H abstraction 2-mthf aachen
cy(OCCJCC)+H=cy(OCC*CC)+H2          5.00E+13    0.00
0.0
cy(OCCJCC)+OH=cy(OCC*CC)+H2O        1.00E+13    0.00
0.0
cy(OCCJCC)+O=cy(OCC*CC)+OH          3.00E+13    0.00
0.0
cy(OCCJCC)+CH3=cy(OCC*CC)+CH4       2.00E+12    0.00
0.0
cy(OCCJCC)+CH3O=cy(OCC*CC)+CH3OH    8.00E+12    0.00
0.0
cy(OCCJCC)+H=cy(OC*CCC)+H2          5.00E+13    0.00
0.0
cy(OCCJCC)+OH=cy(OC*CCC)+H2O        1.00E+13    0.00
0.0
cy(OCCJCC)+O=cy(OC*CCC)+OH          3.00E+13    0.00
0.0
cy(OCCJCC)+CH3=cy(OC*CCC)+CH4       2.00E+12    0.00
0.0
cy(OCCJCC)+CH3O=cy(OC*CCC)+CH3OH    8.00E+12    0.00
0.0
cy(OCJCCC)+H=cy(OC*CCC)+H2          5.00E+13    0.00
0.0
cy(OCJCCC)+OH=cy(OC*CCC)+H2O        1.00E+13    0.00
0.0
cy(OCJCCC)+O=cy(OC*CCC)+OH          3.00E+13    0.00
0.0
cy(OCJCCC)+CH3=cy(OC*CCC)+CH4       2.00E+12    0.00
0.0
cy(OCJCCC)+CH3O=cy(OC*CCC)+CH3OH    8.00E+12    0.00
0.0
!
cy(OCJCCC)+O2=cy(OC*CCC)+HO2        2.00E+24    -3.9
7099.9!Cai et al. C&F 2017
cy(OCCJCC)+O2=cy(OC*CCC)+HO2        2.00E+24    -3.9
7099.9!Cai et al. C&F 2017
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!*** Haute température ***!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!
!*****
!***THF oxidation***
!*****
!
!***Thermal decomposition***
!
!---UPDATES HHC!---!
!
cy(OCCCC)=C*CCCOH                    1.3E+05 2.57 75900 !
HHC Calculations
REV/ 7.9E+03 2.02 66600/
C*CCCOH=C3H6+CH2O                    2.2E+08 0.93 37900 !
HHC Calculations
REV/ 8.2E-04 3.90 22600/
cy(OCCCC)=C2H4+CH3CHO                 1.1E+10 1.57 85300 !
HHC Calculations
REV/ 2.2E-03 4.06 66400/

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cy(OCCCC)=C3H6+CH2O          6.3E+10 1.51 91800 !
HHC Calculations
REV/ 3.0E-03 4.13 67000/
cy(OCCCC)=C*CCOC            1.7E+05 2.61 85900 !
HHC Calculations
REV/ 8.9E+00 3.07 66300/
!
!---END UPDATES---!
!
!***Unimolecular initiation***
!
H+cy(OCJCCC)=cy(OCCCC)      1.00E+14 0.00 0.0
!TRA2015
H+cy(OCCJCC)=cy(OCCCC)     1.00E+14 0.00 0.0
!TRA2015
!
!***Amorçage bimoléculaire***
!
cy(OCCCC)+O2=cy(OCJCCC)+HO2 1.338E+13 0.00
45640.0 !cai opt
cy(OCCCC)+O2=cy(OCCJCC)+HO2 1.338E+13 0.00
49640.0 !cai opt
!
!***H-abstraction (metathesis)***
!
cy(OCCCC)+C3H6CHO-1=cy(OCJCCC)+NC3H7CHO 3.2E+00 3.71 6200 !
HHC Calculations
cy(OCCCC)+C3H6CHO-1=cy(OCCJCC)+NC3H7CHO 8.3E-02 3.89 7700 !
HHC Calculations
!
cy(OCCCC)+CH2CH2CHO=cy(OCJCCC)+C2H5CHO 4.9E-02 3.99 4600 !
HHC Calculations
cy(OCCCC)+CH2CH2CHO=cy(OCCJCC)+C2H5CHO 1.4E+00 3.54 8200 !
HHC Calculations
!
cy(OCCCC)+OH=cy(OCJCCC)+H2O 6.93E+11 0.41 213.6
!GIR2016
cy(OCCCC)+OH=cy(OCCJCC)+H2O 4.12E+03 3.02 -913.8
!GIR2016
!
cy(OCCCC)+H=cy(OCJCCC)+H2 1.16E+07 2.0154
3203.8013 ! MARCO abinitio T
cy(OCCCC)+H=cy(OCCJCC)+H2 1.27E+04 2.8453
4185.0571 ! MARCO abinitio TS
!
cy(OCCCC)+O=cy(OCJCCC)+OH 6.80E+08 1.5
385.0 !VER2015
cy(OCCCC)+O=cy(OCCJCC)+OH 6.80E+08 1.5
3677.5 !VER2015
!
cy(OCCCC)+CH3=cy(OCJCCC)+CH4 8.37E-04 4.60
4113.80 ! MARCO abinitio TS_
cy(OCCCC)+CH3=cy(OCCJCC)+CH4 4.27E-06 5.26
4378.68 ! MARCO abinitio T
!
cy(OCCCC)+HO2=cy(OCJCCC)+H2O2 7.79E+00 3.53 7890
! CHA 2MTHF TST with Exact Solution for Torsional Motions

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cy(OCCCC)+HO2=>cy(OCCJCC)+H2O2          7.21E-02      4.13 11460
! CHA 2MTHF TST with Exact Solution for Torsional Motions
!
cy(OCCCC)+HCO=>cy(OCJCCC)+CH2O          2.2E+0007    1.900
17000.0 ! ME 52 CN
cy(OCCCC)+HCO=>cy(OCCJCC)+CH2O          2.2E+0007    1.900
17000.0 ! ME 53 CN
!
cy(OCCCC)+CH2OH=>cy(OCJCCC)+CH3OH        1.2E+0002    2.950
12000.0 ! ME 54 CN
cy(OCCCC)+CH2OH=>cy(OCCJCC)+CH3OH        1.2E+0002    2.950
12000.0 ! ME 55 CN
!
cy(OCCCC)+CH3O=>cy(OCJCCC)+CH3OH        2.9E+0011    0.000 4500.0
! ME 56 CN
cy(OCCCC)+CH3O=>cy(OCCJCC)+CH3OH        2.9E+0011    0.000 4500.0
! ME 57 CN
!
cy(OCCCC)+CH3O2=>cy(OCJCCC)+CH3O2H      6.0E+0012    0.000
17500.0 ! ME 58 CN
cy(OCCCC)+CH3O2=>cy(OCCJCC)+CH3O2H      6.0E+0012    0.000
17500.0 ! ME 59 CN
!
cy(OCCCC)+C2H5=>cy(OCJCCC)+C2H6          4.0E+0011    0.000
11000.0 ! ME 60 CN
cy(OCCCC)+C2H5=>cy(OCCJCC)+C2H6          4.0E+0011    0.000
11000.0 ! ME 61 CN
!
!*****
!***tetrahydrofuanyl radicals***
!*****
!***isomerization***!
!
cy(OCJCCC)=cy(OCCJCC)                    2.2E+081.56  43800 !
HHC Calculations: Independent pathways (1)
REV/ 3.1E+08 1.42 39400/
DUP
cy(OCJCCC)=cy(OCCJCC)                    1.3E+071.72  46500 !
HHC Calculations: Independent pathways (2)
REV/ 1.9E+07 1.58 42100/
DUP
!
!***Beta-scission (ring opening)***
!
cy(OCJCCC)=C3H6CHO-1                      4.5E+11 0.56 22200 !
HHC Calculations
REV/ 6.0E+06 1.03 18100/
C3H6CHO-1=CH2CHO+C2H4                    2.4E+10 0.94 21200 !
HHC Calculations *2
REV/14.4E+03 2.56 5400/
C3H6CHO-1=CH3CH2CHCHO                    1.30E+01 3.08 25615.2
!VER2015-MARCO abinitio TS17a new
C3H6CHO-1=CH3CH2CH2CO                    2.8E+05 1.73 14100 ! HHC
Calculations
REV/1.3E+05 1.96 26400/
C3H6CHO-1+HO2=NC3H7CHO+O2                6.1E+00 3.24 -6200 ! HHC
Calculations
REV/3.5E+02 3.34 46800/

```



```

!
!C3H6CHO-1 by VELOO (butanal mech)
!
C3H6CHO-1+O2=C3H6CHO1O2          9.000e+18  -2.50  0.000e+00 ! Buda
et al., Combust Flame, 142 (2005) 170-186 (ks)
C3H6CHO1O2=C3H6CHO1Q4J          8.480e+06   1.00  1.650e+04 !#1
Buda et al., Combust Flame, 142 (2005) 170-186 (cyc sat à 7 + 1HalD)
C3H6CHO1Q4J=CO+C2H4+CH2O+OH      3.65E+12   0.6   15122.9
!VER2015-MARCO ABINITIO TS18A DE 40
C3H6CHO1O2=C3H6CHO1Q3J          9.872e+07   1.00  2.500e+04 !#2
Buda et al., Combust Flame, 142 (2005) 170-186 (cyc sat à 6 + 2Hs)
C3H6CHO1Q3J=C*CCHO+CH2O+OH      6.635E+013  -0.160  29900.0!REF:GREEN
2003 = C4H8OOH1-3=>OH+CH2O+C3H6
C3H6CHO1O2=C3H6CHO1Q2J          5.746e+08   1.00  3.250e+04 !#3
Buda et al., Combust Flame, 142 (2005) 170-186 (cyc sat à 5 + 2Hs)
AC3H5CHO+HO2=C3H6CHO1Q2J        1.000E+011   0.000
11000.0!Metcalf = C4H8-1+HO2<=>C4H8OOH1-2
C3H6CHO1Q4J+O2=C3H6CHO1Q4O2      9.000e+18  -2.50   0.0 !
#1
C3H6CHO1Q3J+O2=C3H6CHO1Q3O2      1.050e+19  -2.50  0.000e+00 !Buda
et al., Combust Flame, 142 (2005) 170-186 (ks+kt)
C3H6CHO1Q2J+O2=C3H6CHO1Q2O2      1.800e+19  -2.50  0.000e+00 !Buda
et al., Combust Flame, 142 (2005) 170-186 (2ks)
C3H6CHO1Q4O2=>C3H6CHO1*O4Q+OH     1.772e+07   1.00  20000.0 ! 2s,7
#1
C3H6CHO1Q3O2=>C3H6CHO1*O3Q+OH     9.872e+07   1.00  2.300e+04 !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat à 6 + 2Hs)-2kcal
C3H6CHO1Q2O2=>C3H6CHO1*O2Q+OH     5.746e+08   1.00  3.050e+04 !Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat à 5 + 2Hs)-2kcal
C3H6CHO1*O4Q=>OH+CO2+C2H4+HCO     1.000e+16   0.0   43000.0 ! #1
C3H6CHO1*O3Q=>CHOCHO+CH2CHO+OH    1.000e+16   0.00  4.300e+04 !#2
C3H6CHO1*O2Q=>CHOCH2CHO+HCO+OH    5.000e+15   0.00  4.300e+04 !#3
C3H6CHO1*O2Q=>CHOCHO+CH2CHO+OH    5.000e+15   0.00  4.300e+04 !#3
!
CH3CH2CHCHO=>CH3+C*CCHO          2.0E+0013  0.00  31000.0
!VER2015-DE 26 CN
!CH3CH2CH2CO=>NC3H7+CO           3.65E+12   0.6   15122.9
!VER2015-MARCO ABINITIO TS18A DE 40
CH3CH2CH2CO=NC3H7+CO             1.3E+13    0.35  15300 ! HHC
Calculations
REV/5.2E+05 2.02 4400/
!
!VELOO (butanal mech)
CH3CH2CH2CO+O2=NC3H7CO3          1.750E+10   0.00  -3275.0
!29/06
NC3H7CO3=>C3H6+CO2+OH             5.746E+08   1.00  25000.0
!BUDA ET AL., COMBUST.FLAME, 142 (2005) 170-186 (CYC SAT À 6 + 2HS)
NC3H7CO3=>C3H6+CO+HO2             5.746E+08   1.00  25000.0
!BUDA ET AL., COMBUST.FLAME, 142 (2005) 170-186 (CYC SAT À 6 + 2HS)
NC3H7CO3=>C2H4+CH2CO+HO2          1.481E+08   1.00  25000.0
!BUDA ET AL., COMBUST.FLAME, 142 (2005) 170-186 (CYC SAT À 7 + 3HP)
!
CHOCH2CHO+OH=CHOCH2CO+H2O        4.600E+10   0.73  -1100.0 ! IDEM
CH3HCO+OH *2
CHOCH2CHO+H=CHOCH2CO+H2          8.200E+09   1.16  2405.0 ! IDEM
CH3HCO+H *2
CHOCH2CHO+HO2=CHOCH2CO+H2O2      6.000E+12   0.0   12000.0 ! IDEM
CH3HCO+HO2 *2

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CHOCH2CHO+CH3=CHOCH2CO+CH4 CH3HCO+CH3 *2	1.520E+01	3.4	3740.0	! IDEM
CHOCH2CHO+O2=CHOCH2CO+HO2 CH3HCO+O2 *2	6.000E+13	0.0	39200.0	! IDEM
CHOCH2CO=CH2CHO+CO C2H5CO= CURRAN	1.834E+15	-0.73	12910.0	! IDEM
!				
cy(OCJCCC)=C2H3OC2H4		6.8E+11	0.66	33000 !
HHC Calculations				
REV/ 3.5E+09 0.43 12100/				
!C2H3OC2H4=CH3CH2OCCH2		2.90E+08	1.00	16940.0
!VER2015-IS 8 KB MARCO this corresp				
C2H3OC2H4=CH3CH2OCCH2		1.45E+08	1.00	16940.0
!VER2015-IS 8 KB MARCO this corresp/2				
CH3CH2OCCH2=CH2CHOCHCH3		3.30E+09	1.00	42640.0
!VER2015-IS 13 KB				
CH2CHOCHCH3=>C2H3+CH3CHO		2.00E+13	0.00	24000.0
!VER2015-DE 31 MARCO N				
CH3CH2OCCH2=>C2H5+CH2CO		8.50E+12	0.00	28000.0
!VER2015-DE 27 CN				
C2H3OC2H4=CH3CH2OCHCH		5.70E+08	1.00	14040.0
!VER2015-IS 9 KB MARCO this corresp				
CH3CH2OCHCH=CH2CHOCHCH3		3.30E+09	1.00	16540.0
!VER2015-IS 14 KB ! Attention				
CH3CH2OCHCH=>C2H5O+C2H2		8.50E+12	0.00	28000.0
!VER2015-DE 28 CN				
C2H3OC2H4=>CH2CHO+C2H4		9.82E+09	0.93	17132.7
!VER2015-MARCO abinitio TS				
!				
cy(OCCJCC)=>AC3H5OCH2		4.5E+10	0.71	32365.5
!VER2015-(MARCO TS6a DE 45) /2				
AC3H5OCH2=CH3OCHCHCH2		1.09E-32	12.4	8730.0
!VER2015-MARCO Abinitio				
CH3OCHCHCH2=CH3CHCHOCH2		6.18E-09	5.79	19600.0
!VER2015-MARCO ABINI				
CH3CHCHOCH2=CH3OCHCCH3		1.70E+09	1.00	24540.0
!VER2015-IS 18 KB ! Attention				
CH3OCHCCH3=>CH3O+C3H4-P		8.50E+12	0.00	28000.0
!VER2015-DE 35 CN				
CH3CHCHOCH2=>C3H5-S+CH2O		2.00E+13	0.00	24000.0
!VER2015-DE 34 MARCO N				
CH3OCHCHCH2=CH3OCH2CHCH		1.9E+10	1.00	52300.0
!VER2015-IS 15 KB ! Attention				
CH3OCH2CHCH=>C2H2+CH3+CH2O		2.0E+13	0.00	33000.0
!VER2015-As R27C5H9V=>R19C3H7+C2H2T EXGAS				
CH3OCHCHCH2=CH3CHCOCH3		9.7E+09	1.00	44300.0
!VER2015-IS 16 KB ! Attention				
CH3CHCOCH3=CH3CHCHOCH2		5.0E+09	1.00	42640.0
!VER2015-IS 17 KB				
CH3CHCOCH3=>CH3+CH3CHCO		8.5E+12	0.00	28000.0
!VER2015-DE 33 CN				
CH3OCHCHCH2=>CH3+C*CCHO		4.3E+12	0.00	33200.0
!VER2015-DE 29 CN				
CH3OCHCHCH2+O2=>CH3OCHCCH2+HO2		1.0E+12	0.00	22730.0
!VER2015-OX 41 CN				
AC3H5OCH2=CH3OCH2CCH2		2.9E+08	1.00	24940.0
!VER2015-IS 11 KB				

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CH3OCH2CCH2=>CH3O+C3H4-A                8.5E+12    0.00  28000.0
!VER2015-DE 30 CN
AC3H5OCH2=CH3OCH2CHCH                    5.7E+08    1.00  20040.0
!VER2015-IS 12 KB ! Attention
AC3H5OCH2=>C3H5-A+CH2O                    9.78E+07   1.50  15114.7
!VER2015-MARCO abinitio TS8a
!
cy(OCCJCC)=CH2CHCH2CH2O                    2.0E+12  0.27  31100  !
HHC Calculations /2
REV/ 3.5E+09 0.44 14200/
CH2CHCH2CH2O=C3H5-A+CH2O                  2.4E+11  0.58   6700  !
HHC Calculations
REV/ 1.3E+03 2.59 10700/
!
!***Second H-abstr -> DHF***
!
!Rien de satisfaisant chez FEN2016 et VER2015, car parallele avec
nc3h7... trouver une autre comparaison avec un ether!
!
!***Radical H loss -> DHF***
!
cy(OCJCCC)=cy(OC*CCC)+H                    2.80E+04   2.70  45675.2
!VER2015 (TS15a Marco abiniti) close to SIM2012 (see WUR2014?)
cy(OCCJCC)=cy(OC*CCC)+H                    9.18E+09   1.14  32896.9
!VER2015 (TS13a Marco abiniti) close to SIM2012 (see WUR2014?)
cy(OCCJCC)=cy(OCC*CC)+H                    1.65E+10   1.10  35716.8
!VER2015 (TS14a abinitio Marc) close to SIM2012 (see WUR2014?)
!
!*****
!***DHF dihydrofurans***
!*****
!
!*** (2,3)-dihydrofuran***
!
cy(OC*CCC)+O2=C4H5O-2+HO2                  1.40E+13   0.00  47600.0
!VER2015-INGHAM 94!C5H8#+O2
cy(OC*CCC)+O2=C4H5O-3+HO2                  1.40E+12   0.00  35600.0
!VER2015-INGHAM 94!A/2 C5H
cy(OC*CCC)+H=C4H5O-2+H2                    9.00E+06   2.00   5000.0
!VER2015-BUDA05 C5H8#+R1H=C
cy(OC*CCC)+H=C4H5O-3+H2                    5.40E+04   2.50  -1900.0
!VER2015-HEYBERGER02 A/2 C5
cy(OC*CCC)+O=C4H5O-2+OH                    2.60E+13   0.00   5200.0
!VER2015-BUDA05 C5H8#+B1O=C
cy(OC*CCC)+O=C4H5O-3+OH                    8.80E+10   0.70   3250.0
!VER2015-HEYBERGER02 A/2 C
cy(OC*CCC)+OH=C4H5O-2+H2O                  2.60E+06   2.00   -770.0
!VER2015-BUDA05 C5H8#+R2OH=
cy(OC*CCC)+OH=C4H5O-3+H2O                  3.00E+06   2.00  -1520.0
!VER2015-HEYBERGER02 A/2 C5
cy(OC*CCC)+HO2=C4H5O-2+H2O2                4.00E+11   0.00  15500.0
!VER2015-A-I-19 ALKYLIC
cy(OC*CCC)+HO2=C4H5O-3+H2O2                6.40E+03   2.60  12400.0
!VER2015-A-I-19 ALKYLIC
cy(OC*CCC)+CH3=C4H5O-2+CH4                 2.00E+11   0.00   9600.0
!VER2015-BUDA05 C5H8#+R4CH3
cy(OC*CCC)+CH3=C4H5O-3+CH4                 1.00E+11   0.00   7300.0
!VER2015-HEYBERGER02 A/2

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cy(OC*CCC)=FURAN+H2                5.80E+13    0.00    82600.0
!VER2015-NIST LIFSHITZ
cy(OC*CCC)+OH=>CH2O+C2H4+HCO        2.70E+12    0.00   -1100.0
!VER2015-HEYBERGER02 R2OH+C
!cy(OC*CCC)+OH=>CH2O+C2H4+HCO        2.2E+13    0.0    -
970.0!Atkinson, Alvarez-Idaboy et al. J. Am. Chem. Soc., Vol. 122, No.
15, 2000 !*2
!
!*** (2,5)-dihydrofuran***
!
cy(OCC*CC)=FURAN+H2                1.00E+13    0.00   49530.0
!VER2015-NIST LIFSHITZ
cy(OCC*CC)+O2=C4H5O-3+HO2          2.80E+12    0.00   35600.0
!VER2015-INGHAM 94! C5H8#
cy(OCC*CC)+H=C4H5O-3+H2            1.08E+05    2.50  -1900.0
!VER2015-HEYBERGER02 C5H8#+
cy(OCC*CC)+O=C4H5O-3+OH            1.76E+11    0.70   3250.0
!VER2015-HEYBERGER02 C5H8#+
cy(OCC*CC)+OH=C4H5O-3+H2O          6.00E+06    2.00  -1520.0
!VER2015-HEYBERGER02 C5H8#
cy(OCC*CC)+HO2=C4H5O-3+H2O2        1.28E+04    2.60  12400.0
!VER2015-A-I-19 ALKYLIC
cy(OCC*CC)+CH3=C4H5O-3+CH4         2.00E+11    0.00   7300.0
!VER2015-HEYBERGER02 C5H8#
cy(OCC*CC)+OH=>CH2O+C2H4+HCO        2.70E+12    0.00  -1100.0
!VER2015-HEYBERGER02 R2OH+C
!cy(OCC*CC)+OH=>CH2O+C2H4+HCO        2.2E+13    0.0    -
970.0!Atkinson, Alvarez-Idaboy et al. J. Am. Chem. Soc., Vol. 122, No.
15, 2000 !*2
!
!***Addition on double bond***
cy(OC*CCC)+O<=>CHOCHO+C2H4          3.000e+12    0.000
0.00!Cai et al. C&F 2017
cy(OC*CCC)+O<=>C*CCHO+CH2O          3.000e+12    0.000    0.00
cy(OCC*CC)+O<=>C*CCHO+CH2O          6.000e+12    0.000    0.00
!
!!*** Cyclic ether formation via cyclization of diradical QOOH<=>CYCLIC
ETHER + OH ***!
cy(OC*CCC)+HO2<=>bicy(O) (CCOC)+OH          1.130E+019
-1.680 23587.0!Propene Burke 2014
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/
cy(OCC*CC)+HO2<=>bicy(O) (CCOCC)+OH          1.130E+019
-1.680 23587.0
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/
!
!*****!
!* Reactions of C4H5O and derived radicals *!
!*****!
!
!***isomerization***
C4H5O-2=C4H5O-3                3.34E+09    1.00   39100.0
!VER2015-as C4H7-1=C4H7Y!

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!
!***ring opening***
!
C4H5O-2=CHCHCH2CHO          4.44E+12    0.32    34745.0
!VER2015-Pr. Fournet
C4H5O-3=CH2CHCHCHO          1.05E+13    0.085   22555.0
!VER2015-CBSQ-B3 high pressu
!
!***H abstraction and O addition+ring opening***
!
C4H5O-2+O2=HO2+FURAN        2.60E+11    0.00    2500.0
!VER2015-similar to C5H7#+O2
C4H5O-3+O2=HO2+FURAN        1.58E+12    0.00    15200.0
!VER2015-similar to C5H7#Y+O
C4H5O-2+O=C*CCHO+HCO        5.50E+13    0.00     0.0
!VER2015-B10+R11C2H5=CH3CHO+
C4H5O-3+O=C2H2+CH2O+HCO     5.50E+13    0.00     0.0
!VER2015-B10+R11C2H5=CH3CHO+
C4H5O-2+H=cy(OC*CCC)        1.00E+14    0.00     0.0
!VER2015-Est.
C4H5O-3+H=cy(OC*CCC)        1.00E+14    0.00     0.0
!VER2015-Est.
C4H5O-3+H=cy(OCC*CC)        1.00E+14    0.00     0.0
!VER2015-Est.
C4H5O-2+HO2=H2O2+FURAN      5.50E+13    0.00
0.0!TSANG
C4H5O-3+HO2=H2O2+FURAN      5.5E+13    0.00
0.0!TSANG*2
!
!***derived radical of C4H5O***
!
CHCHCH2CHO=C2H2+CH2CHO       3.70E10     0.957   23912.0
!VER2015-Pr. Fournet
CHCHCH2CHO=CO+C3H5-A         1.40E06     1.326   6190.0
!VER2015-Pr. Fournet
!
CH2CHCHCHO=CHCHCHCHOH        2.20E11     0.435   35127.0
!VER2015-CBSQ-B3 high pressu
CH2CHCHCHO=CO+C3H5-A         4.85E12     0.261   47443.0
!VER2015-CBSQ-B3 high pres
CH2CHCHCHO=SC3H5CO           1.81E09     0.985   28846.0
!VER2015-Pr. Fournet
CHCHCHCHOH=C2H2+CH2CHO       1.20E15     0.102   48750.0
!VER2015-CBSQ-B3 high pressu
!CH2CHCHCHO+H=C3H6CHO-1      1.00E14     0.000   0.0
!VER2015-est.
!CH2CHCHCHO+CH3=C5H8O        1.50E13     0.000   0.0
!VER2015-est. YF:C5H8O not included in the study (ch2//ch/ch(/ch3)/cho)
!
!*****
!*****!
!* System (2,3)-dihydrofuran cy(OC*CCC), Cyclopropancarboxaldehyde
CYC3H5(CHO) and 2-butenal SC3H5CHO      *!
!*****
!*****!
!
!Isomerisation: SC3H5CHO (2-Butenal); cy(OC*CCC) (2,3 dihydrofuran);
CYC3H5(CHO) (Cyclopropancarboxaldehyde)

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cy(OC*CCC)=>SC3H5CHO          4.57E+14   0.00   63570.0
!VER2015-DUBNIKOVA AND LIFSHITZ 2002 JPCA 106
cy(OC*CCC)=CYC3H5(CHO)        12.62E+14  0.00   56300.0
!VER2015-DUBNIKOVA AND LIFSHITZ 2002 JPCA 106 *2
CYC3H5(CHO)=>SC3H5CHO          4.07E+14   0.00   58880.0
!VER2015-DUBNIKOVA AND LIFSHITZ 2002 JPCA 106
!
!Consumption of SC3H5CHO (2-Butenal)
!
!Unimolecular decomposition
HCO+C3H5-S=>SC3H5CHO          1.80E+13   0.0    0.0
!VER2015-as acrolein
SC3H5CHO=>CH3+C2H2+HCO        1.58E+17   0.0    99400.0
!VER2015-1985DEA4600-4608!as C4H8-2/2
SC3H5CHO=>C3H6+CO              1.51E+13   0.0
50700.0 !VER2015-2007CHA/DOM307-312!in C0-C4 base
!SC3H5CHO=>C3H6+CO              3.16E+13   0.0
59600.0 !VER2015-1986GRE/COL434
!metathesis
SC3H5CHO+OH=>CH3CHCHCO+H2O     1.00E+13   0.0    0.0
!VER2015-<MARINOV>! as acrolein
SC3H5CHO+O=>CH3CHCHCO+OH       7.20E+12   0.0    2000.0
!VER2015-<MARINOV>! as acrolein
SC3H5CHO+H=>CH3CHCHCO+H2       4.00E+13   0.0    4200.0
!VER2015-<MARINOV>! as acrolein
SC3H5CHO+CH3=>CH3CHCHCO+CH4    2.608e+6   1.78    5911.0
!VER2015-Curran! as acrolein
SC3H5CHO+HO2=>CH3CHCHCO+H2O2   1.00E+12   0.0    10000.0
!VER2015-Exgas rule
SC3H5CHO+O2=>CH3CHCHCO+HO2     3.00E+13   0.0    36000.0
!VER2015-<MARINOV>! as acrolein
!
SC3H5CHO+H=>CH2CHCHCHO+H2       1.70E+05   2.5     2.5E3
!VER2015-<TSAnG91>! as C3H6Y
SC3H5CHO+CH3=>CH2CHCHCHO+CH4    2.20E+00   3.5     5.7E3
!VER2015-<TSAnG91>! as C3H6Y
SC3H5CHO+C2H5=>CH2CHCHCHO+C2H6  2.20E+00   3.5     6.6E3
!VER2015-<TSAnG91>! as C3H6Y
SC3H5CHO+O=>CH2CHCHCHO+OH       1.70E+11   0.7     5.9E3
!VER2015-<TSAnG91>! as C3H6Y
SC3H5CHO+OH=>CH2CHCHCHO+H2O     3.10E+06   2.0    -0.3E3
!VER2015-<TSAnG91>! as C3H6Y
SC3H5CHO+O2=>CH2CHCHCHO+HO2     1.90E+12   0.0    39.0E3
!VER2015-<WALKER93>! as C3H6Y
SC3H5CHO+HO2=>CH2CHCHCHO+H2O2   9.60E+03   2.6    13.9E3
!VER2015-<TSAnG91>! as C3H6Y
!H additions:
SC3H5CHO+H=>C3H6+HCO            2.00E+13   0.0    3.50E3
!VER2015-<MARINOV>! as acrolein
SC3H5CHO+H=>C*CCHO+CH3          1.32E+13   0.0    3.26E3
!VER2015-Exgas
!O additions:
SC3H5CHO+O=>CH3CHCO+HCO+H       5.00E+07   1.76    0.08E3
!VER2015-<MARINOV>!as acrolein
!OH additions:
SC3H5CHO+OH=>C2H5CHO+HCO        1.37E+12   0.00   -1040.0
!VER2015-Exgas rule! to check products
!

```

!Consumption of CYC3H5(CHO) (CYCLOPROPANECARBOXALDEHYDE)

!				
CYC3H5(CHO)=HCO+C3H5-A		7.00E+15	0.0	8.17E4
!VER2015-1992BAU/COB411-429	!as CH3CHO			
CYC3H5(CHO)+H=>CO+C3H5-A+H2		1.31E+05	2.58	1220.0
!VER2015-Klippenstein et al.2010	!as CH3CHO			
CYC3H5(CHO)+OH=>CO+C3H5-A+H2O		2.30E+10	0.73	-1100.0
!VER2015-Konnov 2005!	!as CH3CHO			
CYC3H5(CHO)+O=>CO+C3H5-A+OH		1.40E+13	0.0	2.3E3
!VER2015-(219,-219)<CAVANAGH9	!as CH3CHO			
CYC3H5(CHO)+CH3=>CO+C3H5-A+CH4		2.00E-06	5.6	2.5E3
!VER2015-(216,-216)<BAULCH94>	!as CH3CHO			
CYC3H5(CHO)+C2H3=>CO+C3H5-A+C2H4		8.10E+10	0.0	3.7E3
!VER2015-(217,-217)<SCHERZER8	!as CH3CHO			
CYC3H5(CHO)+C2H5=>CO+C3H5-A+C2H6		1.30E+12	0.0	8.5E3
!VER2015-(218,-218)<HOHLEIN70	!as CH3CHO			
!				
CYC3H5(CHO)+H=>CH2CHCHCHO+H2		9.0E+06	2.00	5000.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+H=>CH2CHCHCHO+H2		9.0E+06	2.00	5000.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+OH=>CH2CHCHCHO+H2O		2.6E+06	2.00	-770.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+OH=>CH2CHCHCHO+H2O		2.6E+06	2.00	-770.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+CH3=>CH2CHCHCHO+CH4		2.0E+11	0.00	9600.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+CH3=>CH2CHCHCHO+CH4		2.0E+11	0.00	9600.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+O=>CH2CHCHCHO+OH		2.6E+13	0.00	5200.0
!VER2015-Exgas rule				
Duplicate				
CYC3H5(CHO)+O=>CH2CHCHCHO+OH		2.6E+13	0.00	5200.0
!VER2015-Exgas rule				
Duplicate				
!				
CYC3H5(CHO)+H=>H2+C3H4-A+HCO		2.5E4	2.50	-2790.0
!VER2015-Exgas rule				
CYC3H5(CHO)+OH=>H2O+C3H4-A+HCO		1.3E6	2.00	-2620.0
!VER2015-Exgas rule				
CYC3H5(CHO)+O=>OH+C3H4-A+HCO		3.4E10	0.70	1330.0
!VER2015-Exgas rule				
CYC3H5(CHO)+CH3=>CH4+C3H4-A+HCO		5.0E10	0.70	5600.0
!VER2015-Exgas rule				
!				
!				
!				
!*****!				
!*** AC3H5CHO REACTIONS ***!	AramcoMech_1.3			
!*****!				
AC3H5CHO=C3H5-A+HCO		1.813E+19	-1.08	6.848E+04
REV /		1.000E+13	0.00	0.000E+00 /

```

AC3H5CHO+OH=AC3H5CO+H2O 3.370E+12 0.00 6.160E+02
    REV / 2.181E+12 0.00 3.215E+04 /
AC3H5CHO+OH=CH2CHCHCHO+H2O 3.120E+06 2.00 -2.980E+02
    REV / 1.246E+08 1.79 3.493E+04 /
AC3H5CHO+HO2=AC3H5CO+H2O2 3.000E+12 0.00 1.192E+04
    REV / 1.152E+13 -0.33 1.199E+04 /
AC3H5CHO+HO2=CH2CHCHCHO+H2O2 9.630E+03 2.60 1.391E+04
    REV / 2.283E+06 2.06 1.767E+04 /
AC3H5CHO+CH3O2=AC3H5CO+CH3O2H 1.000E+12 0.00 1.192E+04
    REV / 1.579E+13 -0.51 1.127E+04 /
AC3H5CHO+CH3O2=CH2CHCHCHO+CH3O2H 1.990E+12 0.00 1.705E+04
    REV / 1.939E+15 -0.72 2.009E+04 /
AC3H5CO=C3H5-A+CO 6.199E+15 -1.09 -3.300E+02
    REV / 1.500E+11 0.00 4.810E+03 /
!*****!
!*** CH2CHCHCHO REACTIONS ***! AramcoMech_1.3
!*****!
CH2CHCHCHO+HO2=C*CCHO+HCO+OH 8.910E+12 0.00 0.000E+00
    REV / 0.000E+00 0.00 0.000E+00 /
CH2CHCHCHO+H=AC3H5CHO 1.00E+14 0.0 00.
!ESTIMATED
!
!*****!
!* Reactions of FURAN *!
!*****!
!Réaction FURAN+HO2?
!
!**unimolecular initiation
!*rupture of C-C and C-H
FURAN=CH2CCHCHO 6.04E+58 -13.4 94049.0
!VER2015-Prof.Fournet low
CH2CCHCHO=HCO+C3H3 3.59E+14 0.0 69880.0
!VER2015-Sendt2000 A/2.2
CH2CCHCHO=CO+C3H4-P 7.96E+62 -15.35 64415.0
!VER2015-Prof.Fournet 0.047b
FURAN=C2H2+CH2CO 7.5E+73 -17.4 113325.0
!VER2015-Prof.Fournet low *2
!
H+FURYL-2=FURAN 1.00E+14 0.00 0.0
!VER2015-Est. by analogy with
H+FURYL-3=FURAN 1.00E+14 0.00 0.0
!VER2015-Est. by analogy with
!
!**bimolecular initiation
FURAN+O2=FURYL-2+HO2 2.00E+13 0.00 70680.0
!VER2015-A-I-3 secondary A*2
FURAN+O2=FURYL-3+HO2 2.00E+13 0.00 70880.0
!VER2015-A-I-3 secondary A*2
!
!**reaction with H atoms
FURAN+H=C4H5O-2 2.60E+13 0.00 3200.0
!VER2015-as C4H6Z2+R1H=C4H7-
FURAN+H=C4H5O-3 2.60E+13 0.00 1560.0
!VER2015-as C4H6Z2+R1H=C4H7Y
!
!**reaction with OH atoms
FURAN+OH=C*CCHO+HCO 8.22E+12 0.00 -1040.0
!VER2015-Table A-I-5 *3

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FURAN+OH=CHCHCHO+CH2O          5.48E+12   0.00   -1040.0
!VER2015-Table A-I-5 *2
!
FURAN+HO2<=>FURYL-2+H2O2  1.83E+12  0.00E+00  2.89E+04
FURAN+HO2<=>FURYL-3+H2O2  1.83E+12  0.00E+00  2.89E+04
!
!**H-abstraction
FURAN+H=FURYL-2+H2          8.20E+05   2.50   12280.0
!VER2015-A-I-20 secondary A*
FURAN+H=FURYL-3+H2          8.20E+05   2.50   12280.0
!VER2015-A-I-20 secondary A*
FURAN+O=FURYL-2+OH          2.40E+11   0.70    8960.0
!VER2015-A-I-20 secondary A*2
FURAN+O=FURYL-3+OH          2.40E+11   0.70    8960.0
!VER2015-A-I-20 secondary A*2
FURAN+OH=FURYL-2+H2O        4.40E+06   2.00    2780.0
!VER2015-A-I-20 secondary A*2
FURAN+OH=FURYL-3+H2O        4.40E+06   2.00    2780.0
!VER2015-A-I-20 secondary A*2
FURAN+CH3=FURYL-2+CH4       1.36E+00   3.50   12900.0
!VER2015-A-I-20 secondary A*
FURAN+CH3=FURYL-3+CH4       1.36E+00   3.50   12900.0
!VER2015-A-I-20 secondary A*
!
!*****!
!* Reactions of furyl radicals *!
!*****!
!
!isomerization
FURYL-3=FURYL-2             1.50E+13   0.00   67800.0
!as  iC4H5=nC4H5 <LE
!
!reaction with O2
FURYL-2+O2=CO+C2H3+CO2      4.50E+16  -1.39   1000.0
!O2+R10C2H3V=H
FURYL-2+O2=>CHCHCHO+CO+O     3.30E+11  -0.29  10000.0
!O2+R10C2H3V=B10+R13
FURYL-3+O2=CO+C2H3+CO2      4.50E+16  -1.39   1000.0
!O2+R10C2H3V=H
FURYL-3+O2=>C2H2+HCO+CO+O    3.30E+11  -0.29  10000.0
!O2+R10C2H3V=B10+R13
!
!reaction with O
FURYL-2+O=CHCHCHO+CO         3.00E+13   0.00    0.0
!B10+R10C2H3V=CH2COZ
FURYL-3+O=C2H2+HCO+CO        3.00E+13   0.00    0.0
!B10+R10C2H3V=CH2COZ
!
!**beta-scission decomposition
FURYL-2=CHCHCHCO            1.81E+13   0.34   34511.0
!CBSQ-B3 high pressu
FURYL-3=CHCCHCHO            1.05E+13   0.31   31215.0
!CBSQ-B3 high pressu
!
CHCHCHO+H=C*CCHO             1.00E+14   0.00    0.0
!est.!
!

```

CHCHCHCO=C2H2+HCCO	5.30E+15	-0.23	34234.0
!CBSQ-B3 high pressu			
CHCHCHCO=CHCCHCO+H	8.72E+11	0.71	38680.0
!CBSQ-B3 high pressu			
!			
CHCCHCHO=CO+C3H3	1.46E+12	0.34	48401.0
!CBSQ-B3 high pr			
CHCCHCHO=CHCCHCO+H	1.03E+12	0.72	51949.0
!CBSQ-B3 high pressu			
CHCCHCO+H=C3H3+CO	1.32E+13	0.00	3260.0
!Exgas!			
!			
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
! Decomposition of species yielded by THF Oxidation !			
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!			
!			
!*****!			
!*** CJC (OOH) CCHO ***!			
!*****!			
!			
CJC (OOH) CCHO=OHCCcy (COC)+OH	3.980E+012	0.000	17000.0!Approx. C4H8OOH2-
1<=>C4H8O1-2+OH			
CJC (OOH) CCHO=AC3H5CHO+HO2	1.000E+011	0.000	11750.0! Approx. C4H8-
1+HO2<=>C4H8OOH2-1			
!			
!*****!			
!*** OHCCcy (COC) ***!			
!*****!			
!			
OHCCcy (COC)=HCO+C3H5O	7.00E+15	0.0	
8.17E4 !Approx. CY (C3H5) CHO VER2015-1992BAU/COB411-429 !as CH3CHO			
OHCCcy (COC)+OH=>CH2O+C3H3O+H2O	5.000E+012	0.000	
0.0!Approx. C4H8O1-2			
OHCCcy (COC)+H=>CH2O+C3H3O+H2	5.000E+012	0.000	
0.0!Approx. C4H8O1-2			
OHCCcy (COC)+O=>CH2O+C3H3O+OH	5.000E+012	0.000	
0.0!Approx. C4H8O1-2			
OHCCcy (COC)+HO2=>CH2O+C3H3O+H2O2	1.000E+013	0.000	
15000.0!Approx. C4H8O1-2			
OHCCcy (COC)+CH3O2=>CH2O+C3H3O+CH3O2H	1.000E+013	0.000	
19000.0!Approx. C4H8O1-2			
OHCCcy (COC)+CH3=>CH2O+C3H3O+CH4	2.000E+011	0.000	
10000.0!Approx. C4H8O1-2			
!			
!*** OHCCCCHO ***! SEE CURRAN			
!REF:ANALOGY WITH ACETALDEHYDE			
OHCCCCHO+O2<=>C (*O) CCCJ (*O) +HO2	1.200E+005	2.500	37560.0
!CURRAN			
OHCCCCHO+OH<=>C (*O) CCCJ (*O) +H2O	2.000E+006	1.800	-1300.0
!CURRAN			
!			
OHCCCCHO+H<=>C (*O) CCCJ (*O) +H2	4.140E+009	1.120	2320.0
!CURRAN			
OHCCCCHO+O<=>C (*O) CCCJ (*O) +OH	5.940E+012	0.000	1868.0
!CURRAN			
!REF:HALF OF CH2O+HO2			
OHCCCCHO+HO2<=>C (*O) CCCJ (*O) +H2O2	4.090E+004	2.500	10200.0
!CURRAN			

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!REF:ANALOGY WITH ACETALDEHYDE
OHCCCCHO+CH3<=>C (*O) CCCJ (*O) +CH4      2.890E-003  4.620   3210.0
!CURRAN
OHCCCCHO+CH3O<=>C (*O) CCCJ (*O) +CH3OH     1.000E+012  0.000   3300.0
!CURRAN
!REF:PITZ ESTIMATE
OHCCCCHO+CH3O2<=>C (*O) CCCJ (*O) +CH3O2H   4.090E+004  2.500  10200.0
!CURRAN
C (*O) CCCJ (*O) <=>CH2CH2CHO+CO           1.000E+011  0.000   9600.0
!CURRAN
!
!*** C*CCOCHO ***!
!
C*CCOCHO+O2=C*CCJOC*O+HO2                 2.80E+12    0.00   35600.0
!=25DHF
C*CCOCHO+H=C*CCJOC*O+H2                   1.08E+05    2.50   -1900.0
!=25DHF
C*CCOCHO+O=C*CCJOC*O+OH                   1.76E+11    0.70    3250.0
!=25DHF
C*CCOCHO+OH=C*CCJOC*O+H2O                 6.00E+06    2.00   -1520.0
!=25DHF
C*CCOCHO+HO2=C*CCJOC*O+H2O2               1.28E+04    2.60   12400.0
!=25DHF
C*CCOCHO+CH3=C*CCJOC*O+CH4                2.00E+11    0.00    7300.0
!=25DHF
C*CCJOC*O=C*CCHO+HCO                       2.537E+19  -1.79  1.826E+04
!NUIG DEE =C2H5OC2H4S
!
!*** C*COCCHO ***!
!
!
C*COCCHO+H=C*COCJCHO+H2  1.148e+06  2.49  2.330e+03!CURRAN, diethylether
C*COCCHO+O2=C*COCJCHO+HO2  5.200e+13  0.00  4.680e+04!CURRAN, diethylether
C*COCCHO+HO2=C*COCJCHO+H2O2  2.948e+04  2.60  1.391e+04!CURRAN, diethylether
C*COCCHO+OH=C*COCJCHO+H2O  2.260e+03  2.93  4.040e+03!CURRAN, diethylether
C*COCCHO+O=C*COCJCHO+OH  5.620e+13  0.00  5.200e+03!CURRAN, diethylether
C*COCCHO+CH3=C*COCJCHO+CH4  3.012e+00  3.46  5.480e+03!CURRAN, diethylether
C*COCJCHO=CHOCHO+C2H3  6.818e+16  -1.34  2.693e+04!CURRAN, diethylether
!
C*COCCHO+H=C*COCCJO+H2  4.000E+013    0.000    4200.0
C*COCCHO+O2=C*COCCJO+HO2  1.005E+013    0.000   40700.0
C*COCCHO+HO2=C*COCCJO+H2O2  2.800E+012    0.000   13600.0
C*COCCHO+OH=C*COCCJO+H2O  2.690E+010    0.760    -340.0
C*COCCHO+O=C*COCCJO+OH  5.000E+012    0.000   1790.0
C*COCCHO+CH3=C*COCCJO+CH4  2.608E+006    1.780    5911.0
C*COCCJO=CH2CHO+CH2CO  2.537e+19  -1.79  1.826e+04
!
HOOCy (CCJOCC) =CY (OCOCC*C) +OH  0.9E+12  0.21  7700!Carstensen calculations /2
HOOCy (COCCJ) =CY (OCOCC*C) +OH  1.1E+11  0.46  11200!Carstensen calculations
/2
!
CY (OCOCC*C) +OH=CY (OCJOCC*C) +H2O      6.93E+11    0.41
213.6 !GIR2016
CY (OCOCC*C) +H=CY (OCJOCC*C) +H2      1.16E+07    2.0154    3203.8013    !
MARCO abinitio T
CY (OCOCC*C) +O=CY (OCJOCC*C) +OH      6.80E+08  1.5
385.0 !VER2015

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CY (OCOCC*C)+CH3=CY (OCJOCC*C)+CH4      8.37E-04      4.60  4113.80  ! MARCO
abinitio TS_
CY (OCOCC*C)+HO2=CY (OCJOCC*C)+H2O2      1.264E+02      3.37  11720      !
Alkane (C4H10) -2kcal/mol
!
CY (OCJOCC*C)=CH2CO+CH2CHO  1.05E+13    0.085  22555.0 !VER2015-CBSQ-B3
high pressure = C4H5O-3=CH2CHCHCHO
!
!***C*CCC (OJ) OOH***
!
C*CCC (OJ) OOH=C3H5-A+HC (*O) OOH  7.7E+10  0.58  1100!Carstensen calculations
nov 2017
REV/1.9E+01  3.12  18100/
C*CCOCHO=CO2+C3H6  4.0E+07    1.40    48300!!Carstensen calculations nov
2017
REV/ 7.3E-01  3.33  69500/
!
!
!*** O*cy (COCCC) ***!
!
!!!!!!!!!!!!!!!!!!!!CLASS 1 UNIMOLECULAR DECOMPOSITION
REACTIONS!!!!!!!!!!!!!!!!!!!!
O*cy (COCCC)=C*CCC (*O) OH      1.1E+07      1.97    61100.
!SUD2016=GVL TSTDG HHC DEC 2014
O*CYCCJCCO+H=O*cy (COCCC)      1.0E+14      0.00    0.000
!SUD2016=GVL ESTIM. 2013
O*CYCCCJCO+H=O*cy (COCCC)      1.0E+14      0.00    0.000
!SUD2016=GVL ESTIM. 2013
O*CYCCCCJO+H=O*cy (COCCC)      1.0E+14      0.00    0.000
!SUD2016=GVL ESTIM. 2013
!
!!!!!!!!!!!!!!!!!!!!CLASS 2 ABSTRACTION REACTIONS!!!!!!!!!!!!!!!!!!!!
H+O*cy (COCCC)=H2+O*CYCCCCJO    5.80E+05    2.49    2330.00
!FEN2016=2MTHF
H+O*cy (COCCC)=H2+O*CYCCCJCO    1.5E+07      2.07    7400.
!SUD2016=GVL TSTDG HHC 2014; COMBINED ATS+STS
H+O*cy (COCCC)=H2+O*CYCCJCCO    1.1E+07      2.07    6100.
!SUD2016=GVL TSTDG HHC 2014; COMBINED ATS+STS
CH3+O*cy (COCCC)=CH4+O*CYCCCCJO  1.22e+3    2.818  8721
!FEN2016=2MTHF
CH3+O*cy (COCCC)=CH4+O*CYCCCJCO  4.1E+02      3.04    9000.
!SUD2016=GVL TSTDG HHC 2014; COMBINED ATS+STS
CH3+O*cy (COCCC)=CH4+O*CYCCJCCO  4.6E+02      3.01    7100.
!SUD2016=GVL TSTDG HHC 2014; COMBINED ATS+STS
O*cy (COCCC)+OH<=>O*CYCCJCCO+H2O  9.3E+03      1.03    2.602E+03
!SUD2016=GVL!!Rates FROM De BRUYCKER ET AL.
O*cy (COCCC)+OH<=>O*CYCCCJCO+H2O  17.22E+05    0.40    5.358E+03
!SUD2016=GVL
O*cy (COCCC)+OH<=>O*CYCCCCJO+H2O  4.670E+07      1.61    -
380.0!FEN2016=2MTHF
O*cy (COCCC)+HO2<=>O*CYCCJCCO+H2O2  2.516E+02    3.37    11720.00
!SUD2016=GVL!!!ALL FROM OPT CAI -2KCAL
O*cy (COCCC)+HO2<=>O*CYCCCJCO+H2O2  2.516E+02    3.37    13720.00
!SUD2016=GVL
O*cy (COCCC)+HO2<=>O*CYCCCCJO+H2O2  2.10E+10    0.53    9790
!FEN2016=2MTHF
O*cy (COCCC)+O<=>O*CYCCJCCO+OH      5.520E+05    2.450    2.830E+03
!SUD2016=GVL ALPHA FROM N-BUTANOL

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O*cy(COCCC)+O<=>O*CYCCCJCO+OH	5.520E+05	2.450	2.830E+03	
!SUD2016=GVLSEC 2MH				
O*cy(COCCC)+O<=>O*CYCCCCJO+OH	5.620e+13	0.00	5.200e+03	
!FEN2016=2MTHF				
O*cy(COCCC)+O2<=>O*CYCCJCCO+HO2	2.000E+13	0.000	4.980E+04	
!SUD2016=GVLSEC 2MH				
O*cy(COCCC)+O2<=>O*CYCCCJCO+HO2	2.000E+13	0.000	4.980E+04	
!SUD2016=GVLSEC 2MH				
O*cy(COCCC)+O2<=>O*CYCCCCJO+HO2	2.0E13	0.0	45640	
!FEN2016=2MTHF				
!				
!!!!!!!!!!!!!!!!!!!!CLASS 3 ALKYL RADICAL DECOMPOSITION!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
O*CYCCCCJO=C(*O)CCCJ(*O)	3.3E+12	0.37	29400.	
!SUD2016=GVL TSTDG HHC JAN 2015				
C(*O)CCCJ(*O)=CH2CHO+CH2CO	4.1E+10	0.78	32100.	
!SUD2016=GVL TSTDG HHC DEC 2014				
O*CYCCCCJO=C*COC(*O)CJ	5.5E+11	0.67	34500.	
!SUD2016=GVL TSTDG HHC JAN 2015				
C*COC(*O)CJ=CH2CHO+CH2CO	3.1E+10	0.81	27500.	
!SUD2016=GVL TSTDG HHC JAN 2015				
O*CYCCCJCO=C*CCOCJ(*O)	4.7E+12	0.27	33800.	
!SUD2016=GVL TSTDG HHC JAN 2015 (EQ PLUS AX)				
C*CCOCJ(*O)=C3H5-A+CO2	2.2E+12	0.18	7300.	
!SUD2016=GVL TSTDG HHC JAN 2015				
DUPLICATE				
C*CCOCJ(*O)=C3H5-A+CO2	2.2E+12	0.18	7300.	
!SUD2016=GVL TSTDG HHC JAN 2015				
DUPLICATE				
O*CYCCCJCO=C3H5-A+CO2	3.6E+12	0.11	28500.	
!SUD2016=GVL TSTDG HHC JAN 2015; VIA C-CC=CCC(=O)OJ				
DUPLICATE				
O*CYCCCJCO=C3H5-A+CO2	1.8E+13	-0.06	25800.	
!SUD2016=GVL TSTDG HHC JAN 2015; VIA T-CC=CCC(=O)OJ				
DUPLICATE				
O*CYCCJCCO=C*CC(*O)OCJ	2.4E+12	0.42	38800.	
!SUD2016=GVL TSTDG HHC JAN 2015				
C*CC(*O)OCJ=C2H3CO+CH2O	3.5E+10	0.69	21400.	
!SUD2016=GVL TSTDG HHC JAN 2015				
!				
!!!!!!!!!!!!!!!!!!!!CLASS 4 FUEL RADICAL ISOMERIZATION!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
O*CYCCJCCO=O*CYCCCJCO	1.1E+09	1.28	38200.	
!SUD2016=GVL TSTDG HHC JAN 2015				
O*CYCCCJCO=O*CYCCCCJO	4.8E+08	1.25	38300.	
!SUD2016=GVL TSTDG HHC JAN 2015				
!				
!!!!!!!!!!!!!!!!!!!!H ELIMINATION REACTIONS C-H BETA				
SCISSION!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!				
H+O*CYCC*CCO=O*CYCCCJCO	2.66E+08	1.584	3499.0	!
WUR2014 H adds on site C3				
H+O*CYCC*CCO=O*CYCCJCCO	2.29E+08	1.613	3664.0	!
WUR2014 H adds on site C4				
H+O*CYCC*CO=O*CYCCCCJO	4.01E+08	1.528	2719.9	!
WUR2014 H adds on site C4				
H+O*CYCC*CO=O*CYCCCJCO	2.08E+08	1.620	3805.0	!
WUR2014 H adds on site C5				
!				
O*CYCCJCCO+H=O*CYCC*CCO+H2	5.00E+13	0.00	0.00	!SUD2016=GVL
O*CYCCJCCO+OH=O*CYCC*CCO+H2O	1.00E+13	0.00	0.00	!SUD2016=GVL

O\*CYCCJCCO+O=O\*CYCC\*CCO+OH 3.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCJCCO+CH3=O\*CYCC\*CCO+CH4 2.00E+12 0.00 0.00!SUD2016=GVL  
O\*CYCCJCCO+O2=O\*CYCC\*CCO+HO2 4.00E+24 -3.90 7100.00!SUD2016=GVL  
O\*CYCCCJCO+H=O\*CYCC\*CCO+H2 5.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+OH=O\*CYCC\*CCO+H2O 1.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+O=O\*CYCC\*CCO+OH 3.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+CH3=O\*CYCC\*CCO+CH4 2.00E+12 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+O2=O\*CYCC\*CCO+HO2 4.00E+24 -3.90 7100.00!SUD2016=GVL  
O\*CYCCCJCO+H=O\*CYCCC\*CO+H2 5.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+OH=O\*CYCCC\*CO+H2O 1.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+O=O\*CYCCC\*CO+OH 3.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+CH3=O\*CYCCC\*CO+CH4 2.00E+12 0.00 0.00!SUD2016=GVL  
O\*CYCCCJCO+O2=O\*CYCCC\*CO+HO2 4.00E+24 -3.90 7100.00!SUD2016=GVL  
O\*CYCCCCJO+H=O\*CYCCC\*CO+H2 5.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCCJO+OH=O\*CYCCC\*CO+H2O 1.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCCJO+O=O\*CYCCC\*CO+OH 3.00E+13 0.00 0.00!SUD2016=GVL  
O\*CYCCCCJO+CH3=O\*CYCCC\*CO+CH4 2.00E+12 0.00 0.00!SUD2016=GVL  
O\*CYCCCCJO+O2=O\*CYCCC\*CO+HO2 4.00E+24 -3.90 7100.00!SUD2016=GVL

!  
!!!!!!!!!!!!!!!!!!!!!!!!WURMEL AND SIMMIE DIHYDROFURANONES!!!!!!!!!!!!!!!!!!!!!!!!!!!!

O\*CYCCC\*CO=C\*CCHO+CO 4.15E+13 0.360 53202.7 !WUR2015  
O\*CYCCC\*CO=O\*CCC\*C\*O 7.27E+10 0.879 56381.4 !WUR2015  
O\*CCC\*C\*O=C\*CCHO+CO 1.55E+11 0.739 47179.7 !WUR2015  
DUP  
O\*CCC\*C\*O=C\*CCHO+CO 1.38E+11 0.856 68116.6 !WUR2015  
DUP  
O\*CCC\*C\*O=CH3CHCO+CO 6.81E+10 1.156 77437.9 !WUR2015  
O\*CYCCC\*CO=O\*CC\*CC\*O 1.44E+11 0.742 57911.1 !WUR2015  
O\*CC\*CC\*O=C\*CCHO+CO 9.73E+09 1.456 81118.5 !WUR2015  
!O\*CYCCC\*CO=CYCOH\*CC\*CO 9.38E+02 3.043 65870.0 !WUR2015 CYCOH\*CC\*CO  
consumption?  
O\*CYCC\*CCO=O\*CCC\*C\*O 2.58E+10 0.992 51481.8 !WUR2015

!  
!!!!!!!!!!!!!!!!!!!!!!!!CLASS 5 H ABSTRACTION FROM ALKENE!!!!!!!!!!!!!!!!!!!!!!!!!!!!

O\*CYCC\*CCO+H=O\*CYCC\*CCJO+H2 3.38E+05 2.36 207.00!SUD2016=GVL  
O\*CYCC\*CCO+OH=O\*CYCC\*CCJO+H2O 2.76E+04 2.64 -1920.00!SUD2016=GVL  
O\*CYCC\*CCO+HO2=O\*CYCC\*CCJO+H2O2 4.82E+03 2.55 10500.00!SUD2016=GVL  
O\*CYCC\*CCO+O=O\*CYCC\*CCJO+OH 9.59E+12 0.00 1970.00!SUD2016=GVL  
O\*CYCC\*CCO+CH3=O\*CYCC\*CCJO+CH4 3.69E+00 3.31 4000.00!SUD2016=GVL  
!  
O\*CYCCC\*CO+H=O\*CYCCJC\*CO+H2 3.38E+05 2.36 207.00!SUD2016=GVL  
O\*CYCCC\*CO+OH=O\*CYCCJC\*CO+H2O 2.76E+04 2.64 -1920.00!SUD2016=GVL  
O\*CYCCC\*CO+HO2=O\*CYCCJC\*CO+H2O2 4.82E+03 2.55 10500.00!SUD2016=GVL  
O\*CYCCC\*CO+O=O\*CYCCJC\*CO+OH 9.59E+12 0.00 1970.00!SUD2016=GVL  
O\*CYCCC\*CO+CH3=O\*CYCCJC\*CO+CH4 3.69E+00 3.31 4000.00!SUD2016=GVL

!  
O\*CYCCC\*CO+H=>CO+C2H2+HCO+H2 2.67E+05 2.519 3513 ! WUR2014  
O\*CYCCC\*CO+H=>CO2+C3H3+H2 5.65E+07 1.97 19579 !  
WUR2014  
O\*CYCCC\*CO+H=>CO+CO+C2H3+H2 9.31E+06 2.137 18568 ! WUR2014  
O\*CYCCC\*CO+CH3=>CO+C2H2+HCO+CH4 3.25E+00 3.731 3380 !  
WUR2014  
O\*CYCCC\*CO+CH3=>CO2+C3H3+CH4 1.32E+01 3.671 16353 ! WUR2014  
O\*CYCCC\*CO+CH3=>CO+CO+C2H3+CH4 7.13E+01 3.678 15805 !  
WUR2014

!  
!!!!!!!!!!!!!!!!!!!!!!!!CLASS 6 ADDITION OF RADICAL SPECIES O AND OH TO  
ALKENE!!!!!!!!!!!!!!!!!!!!!!!!!!!!

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O*CYCC*CCO+OH=O*CYCCJCOHCO      2.30E+12   0.00  -1110.00 ! SUD2016
O*CYCCC*CO+OH=O*CYCCCOHCJO      2.30E+12   0.00  -1110.00 ! SUD2016
O*CYCCJCOHCO=CH2O+CO+CH2CHO      1.25E+10  0.79  26300.00 ! SUD2016
O*CYCCCOHCJO=CO+CH3CHO+HCO       1.25E+10  0.79  26300.00 ! SUD2016
O*CYCC*CCO+O=CH2O+HCO+HCCO       6.00E+12   0.00   0.00 ! SUD2016
O*CYCC*CCO+O=CO2+HCO+C2H3        6.00E+12   0.00   0.00 ! SUD2016
O*CYCCC*CO+O=CO+CH2CHO+HCO       3.00E+12   0.00   0.00 ! SUD2016
O*CYCCC*CO+O=CH2CO+CHOCHO        3.00E+12   0.00   0.00 !
SUD2016
O*CYCCC*CO+O=CO2+C*CCHO          3.00E+12   0.00   0.00 !
SUD2016
!
!!!!!!!!!!!!!!!!!!!!CLASS 8 ALKYL RADICAL DECOMPOSITIONS!!!!!!!!!!!!!!!!!!!!
O*CJC*CC*O<=>O*CYCC*CCJO  1.62E+12   0.00  18300.00! SUD2016
O*CJC*CC*O<=>CO+CHCHCHO   2.640E+15  -1.839  8489.00 ! SUD2016
O*CYCCJJC*CO<=>O*C*CC*COJ  5.0E+13   0.0  30951   ! SUD2016
O*C*CC*COJ<=>CO+CHCHCHO   2.640E+15  -1.839  8489.00! SUD2016
!
!*** O*cy(CCOCC) ***!
!
!***Bond scission of fuel***
!
!***H-abstraction from fuel *** 2-furanone considered as cyclopentanone
to give a try
!Bimolecular initiation
O*cy(CCOCC)+O2=O*CYCCJCOC+HO2  2.000E+13  0.000  4.980E+04
!SUD2016=GVLSEC 2MH
O*cy(CCOCC)+O2=O*CYCCCJOC+HO2  2.0E13   0.0   45640   !FEN2016=2MTHF
O*cy(CCOCC)+O2=O*CYCCCOCJ+HO2  2.0E13   0.0   45640   !FEN2016=2MTHF
!
!H abstr by OH, HO2, O, H and CH3 radicals (cf Zhou 2016)***
O*cy(CCOCC)+OH=O*CYCCJCOC+H2O  2.34E+03  3.04  -817 ! ZHO2016 radical in
alpha position from carbonyl
O*cy(CCOCC)+OH=O*CYCCCJOC+H2O  1.13E+05  2.58  -626 ! ZHO2016 radical in
beta position from carbonyl
O*cy(CCOCC)+OH=O*CYCCCOCJ+H2O  2.34E+03  3.04  -817 ! ZHO2016 radical in
alpha position from carbonyl
!
O*cy(CCOCC)+HO2=O*CYCCJCOC+H2O2  9.91E-04  4.27  5040 ! ZHO2016 radical in
alpha position from carbonyl
O*cy(CCOCC)+HO2=O*CYCCCJOC+H2O2  5.45E-02  4.27  5957 ! ZHO2016 radical in
beta position from carbonyl
O*cy(CCOCC)+HO2=O*CYCCCOCJ+H2O2  9.91E-04  4.27  5040 ! ZHO2016 radical in
alpha position from carbonyl
!
O*cy(CCOCC)+O=O*CYCCJCOC+OH  2.09E+05  2.501  3776.3 ! ZHO2016 radical in
alpha equatorial position from carbonyl
DUP
O*cy(CCOCC)+O=O*CYCCJCOC+OH  1.33E+05  2.389  2055.4 ! ZHO2016 radical in
alpha axial position from carbonyl
DUP
O*cy(CCOCC)+O=O*CYCCCJOC+OH  5.14E+04  2.629  2605.2 ! ZHO2016 radical in
beta equatorial position from carbonyl
DUP
O*cy(CCOCC)+O=O*CYCCCJOC+OH  7.03E+04  2.522  1577.4 ! ZHO2016 radical in
beta axial position from carbonyl
DUP

```

O\*cy(CCOCC)+O=O\*CYCCOCJ+OH 2.09E+05 2.501 3776.3 ! ZHO2016 radical in  
alpha equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+O=O\*CYCCOCJ+OH 1.33E+05 2.389 2055.4 ! ZHO2016 radical in  
alpha axial position from carbonyl  
DUP  
!  
O\*cy(CCOCC)+H=O\*CYCCJOC+H2 2.64E+06 2.185 4326.0 ! ZHO2016 radical in  
alpha equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+H=O\*CYCCJOC+H2 3.39E+06 2.121 2581.3 ! ZHO2016 radical in  
alpha axial position from carbonyl  
DUP  
O\*cy(CCOCC)+H=O\*CYCCCJOC+H2 2.05E+06 2.259 5879.5 ! ZHO2016 radical in  
beta equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+H=O\*CYCCCJOC+H2 1.71E+06 2.263 4421.6 ! ZHO2016 radical in  
beta axial position from carbonyl  
DUP  
O\*cy(CCOCC)+H=O\*CYCCOCJ+H2 2.64E+06 2.185 4326.0 ! ZHO2016 radical in  
alpha equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+H=O\*CYCCOCJ+H2 3.39E+06 2.121 2581.3 ! ZHO2016 radical in  
alpha axial position from carbonyl  
DUP  
!  
O\*cy(CCOCC)+CH3=O\*CYCCJOC+CH4 5.49E+01 3.270 6022.9 ! ZHO2016 radical in  
alpha equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+CH3=O\*CYCCJOC+CH4 3.38E+01 3.232 4469.4 ! ZHO2016 radical in  
alpha axial position from carbonyl  
DUP  
O\*cy(CCOCC)+CH3=O\*CYCCCJOC+CH4 8.48E+00 3.483 7935.0 ! ZHO2016 radical in  
beta equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+CH3=O\*CYCCCJOC+CH4 9.69E+00 3.468 6859.5 ! ZHO2016 radical in  
beta axial position from carbonyl  
DUP  
O\*cy(CCOCC)+CH3=O\*CYCCOCJ+CH4 5.49E+01 3.270 6022.9 ! ZHO2016 radical in  
alpha equatorial position from carbonyl  
DUP  
O\*cy(CCOCC)+CH3=O\*CYCCOCJ+CH4 3.38E+01 3.232 4469.4 ! ZHO2016 radical in  
alpha axial position from carbonyl  
DUP  
!  
!\*\*\*Isomerization of radicals\*\*\*  
!  
O\*CYCCJOC=O\*CYCCCJOC 2.66E+13 0.0 20393 ! ZHO2016  
!  
!\*\*\*ring opening of alkyl radical\*\*\* seule l'étape cinétiquement  
limitante est conservée donc globalisation  
!  
O\*CYCCJOC=CH2O+C2H3CO 1.32E+14 0.0 40511.5 ! ZHO2016  
!O\*CYCCJOC=CH2CHCO+CH2O 9.50E+13 0.0 36687.4 ! ZHO2016  
!  
O\*CYCCOCJ=CHOCO+C2H4 2.64E+14 0.0 40511.5 ! ZHO2016 \*2 2.64E+14 0.0  
40511.5  
!



```

O*CYCCCJOC=CH2CHO+CH2CO 2.78E+13 0.0 33006.7 ! ZHO2016 *2
!
!***H loss from alkyl radical to form alkene***
!
O*CYCCJOC+H=O*CYCC*COCH2 5.00E+13 0.00 0.00!SUD2016=GVL
O*CYCCJOC+OH=O*CYCC*COCH2O 1.00E+13 0.00 0.00!SUD2016=GVL
O*CYCCJOC+O=O*CYCC*COCH2OH 3.00E+13 0.00 0.00!SUD2016=GVL
O*CYCCJOC+CH3=O*CYCC*COCH2CH4 2.00E+12 0.00 0.00!SUD2016=GVL
O*CYCCJOC+O2=O*CYCC*COCH2HO2 4.00E+24 -3.90 7100.00!SUD2016=GVL
!
O*CYCCCJOC+H=O*CYCC*COCH2 5.00E+13 0.00 0.00!SUD2016=GVL
O*CYCCCJOC+OH=O*CYCC*COCH2O 1.00E+13 0.00 0.00!SUD2016=GVL
O*CYCCCJOC+O=O*CYCC*COCH2OH 3.00E+13 0.00 0.00!SUD2016=GVL
O*CYCCCJOC+CH3=O*CYCC*COCH2CH4 2.00E+12 0.00 0.00!SUD2016=GVL
O*CYCCCJOC+O2=O*CYCC*COCH2HO2 4.00E+24 -3.90 7100.00!SUD2016=GVL
!
!***alkene reactions***
!
O*CYCC*COCH2+H=O*CYCC*COCH2J+H2 3.38E+05 2.36 207.00!SUD2016=GVL
O*CYCC*COCH2+OH=O*CYCC*COCH2J+H2O 2.76E+04 2.64 -1920.00!SUD2016=GVL
O*CYCC*COCH2+HO2=O*CYCC*COCH2J+H2O2 4.82E+03 2.55 10500.00!SUD2016=GVL
O*CYCC*COCH2+O=O*CYCC*COCH2J+OH 9.59E+12 0.00 1970.00!SUD2016=GVL
O*CYCC*COCH2+CH3=O*CYCC*COCH2J+CH4 3.69E+00 3.31 4000.00!SUD2016=GVL
!
O*CYCC*COCH2+OH=O*CYCCOHCJOC 2.30E+12 0.00 -1110.00 ! SUD2016
O*CYCCOHCJOC=HCO+CH2O+CH2CO 1.25E+10 0.79 26300.00 ! SUD2016
!
O*CYCC*COCH2+O=HCO+HCO+CH2CO 6.00E+12 0.00 0.00 ! SUD2016
O*CYCC*COCH2+O=CHOCHO+CH2CO 6.00E+12 0.00 0.00 ! SUD2016
!
!***6-beta-scission of alkenyl radical***
!
O*CYCC*COCH2=O*CC(*O)C*CH 1.62E+12 0.00 18300.00! SUD2016
O*CC(*O)C*CH=C2H2+CHOCO 2.640E+15 -1.839 8489.00 ! SUD2016
!
CHOCHO (+M)=CH2O+CO (+M) 4.270E+12 0.00 50600.0 !
MARINOV 1995
LOW / 8.91E+16 0.00 49200.0 / !
MARINOV 1995
CHOCHO (+M)=CO+CO+H2 (+M) 1.072E+14 0.00 55100.0
!(MARINOV94, SAITO:JPC 88, 1182 (1984)
LOW / 2.57E+16 0.00 38400.0 /
CHOCHO+OH=CHOCO+H2O 1.000E+13 0.00 0.0
!(MARINOV94)
CHOCHO+O=CHOCO+OH 7.240E+12 0.00 1970.0
!(MARINOV94)
CHOCHO+H=CH2O+HCO 1.000E+12 0.00 0.0
!(MARINOV94)
CHOCHO+HO2=CHOCO+H2O2 1.700E+12 0.00 10700.0
!(MARINOV94)
CHOCHO+CH3=CHOCO+CH4 1.740E+12 0.00 8440.0
!(MARINOV94)
CHOCHO+O2=HCO+CO+HO2 6.300E+13 0.00 30000.0
!(MARINOV94)
CHOCO=HCO+CO 2.000E+07 0.00 0.0
!(MARINOV94)
CHOCO+O2=CO+CO+HO2 6.300E+13 0.00 30000.0 !

```



TROE/ 7.000E-001 1.000E-030 1.000E+030 1.000E+030/

!REF:LPL \* 1.5 AK  
H+O2 (+HE) <=>HO2 (+HE) 4.650E+012 0.440  
0.0  
LOW/ 9.192E+018 -1.200  
0.0/

TROE/ 5.900E-001 1.000E-030 1.000E+030 1.000E+030/  
HO2+H<=>OH+OH 7.079E+013 0.000  
295.0

!REF:MICHAEL SUTHERLAND 2000  
H2+O2<=>H+HO2 5.176E+005 2.433  
53502.0

!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)  
HO2+O<=>OH+O2 3.250E+013 0.000  
0.0

!REF:KEYSER, J. PHYS. CHEM. 92:1193 (1988) REDUCED BY 15%  
HO2+OH<=>H2O+O2 2.456E+013 0.000  
-497.0

!REF:HIPPLER ET AL. J.CHEM.PHYS 93 1755-1760 (1990)  
HO2+HO2<=>H2O2+O2 1.300E+011 0.000  
-1630.0  
DUP

!REF:REDUCED BY 13%  
HO2+HO2<=>H2O2+O2 3.658E+014 0.000  
12000.0  
DUP

!REF:TROE, COMBUST. FLAME, 158:594-601 (2011)

!REF:RATE CONSTANT IS FOR N2  
H2O2 (+H2O) <=>OH+OH (+H2O) 2.000E+012 0.900  
48749.0  
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  
LOW/ 2.490E+024 -2.300  
48749.0/

TROE/ 4.300E-001 1.000E-030 1.000E+030/  
H2O/ 0.00/ CO2/ 1.60/ N2/ 1.50/ O2/ 1.20/ HE/ 0.65/ H2O2/ 7.70/

!REF:EFFICIENCIES FOR H2 AND CO TAKEN FROM LI ET AL., INT. J. CHEM.  
KINET. 36:566-575 (2004)  
H2/ 3.70/ CO/ 2.80/

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
H2O2+H<=>H2O+OH 2.410E+013 0.000  
3970.0

!REF: ELLINGSON J. PHYS. CHEM. (2007) 111, (51), 13554-13566

H2O2+H<=>H2+HO2 6000.0	2.150E+010	1.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
H2O2+O<=>OH+HO2 3970.0	9.550E+006	2.000
!REF: HONG ET AL. J. PHYS. CHEM. A 114 (2010) 5718-5727		
H2O2+OH<=>H2O+HO2 318.0	1.740E+012	0.000
DUP		
H2O2+OH<=>H2O+HO2 7269.0	7.590E+013	0.000
DUP		
!REF:MEULLER 99 * 0.76		
CO+O(+M)<=>CO2(+M) 2384.0	1.362E+010	0.000
LOW/ 4191.0/	1.173E+024	-2.790
H2/ 2.00/ H2O/ 12.00/ CO/ 1.75/ CO2/ 3.60/ AR/ 0.70/ HE/ 0.70/		
!REF:86TSA/ HAM * 0.44		
CO+O2<=>CO2+O 47700.0	1.119E+012	0.000
!REF: JOSHI AND WANG IJCK (2006), 38, (1), 57-73.		
CO+OH<=>CO2+H -355.7	7.015E+004	2.053
DUP		
CO+OH<=>CO2+H 331.8	5.757E+012	-0.664
DUP		
!REF:YOU ET AL. J. PHYS. CHEM. A 2007, 111, 4031-4042		
CO+HO2<=>CO2+OH 17940.0	1.570E+005	2.180
!REF:LI ET AL. IJCK 2007 *1.2		
HCO+M<=>H+CO+M 14870.0	5.700E+011	0.660
H2/ 2.00/ H2O/ 6.00/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/ 3.00/		
!REF:TIMONEN ET AL., JPC, 92:651 (1988)		
HCO+O2<=>CO+HO2 410.0	7.580E+012	0.000
HCO+H<=>CO+H2 0.0	7.340E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
HCO+O<=>CO+OH 0.0	3.020E+013	0.000
HCO+O<=>CO2+H 0.0	3.000E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
HCO+OH<=>CO+H2O 0.0	3.011E+013	0.000

!REF:TIMONEN ET AL., JPC, 92:651 (1988)

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
HCO+HO2=>CO2+H+OH 3.000E+013 0.000  
0.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
HCO+HCO=>H2+CO+CO 3.000E+012 0.000  
0.0

!REF:MULENKO, S.A. REV. ROUM. PHYS. 32, 173 (1987)  
HCO+CH3<=>CH4+CO 2.650E+013 0.000  
0.0

!REF:N. K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109, 7902-7914 (2005)  
CH2O+O2<=>HCO+HO2 8.070E+015 0.000  
53420.0

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

!REF:ANALOGY WITH CH3O2+CH2O TSANG/ HAMPSON 1986  
CH2O+O2CHO<=>HCO+HO2CHO 1.990E+012 0.000  
11660.0

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

!REF:  
H+CO2<=>OCHO 7.500E+013 0.000  
29000.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
HCO+HCO<=>CH2O+CO 1.800E+013 0.000  
0.0

!REF:OH\* KATHROTIA ET AL. COMB & FLAME 2010  
H+O+M<=>M+OH\* 1.500E+013 0.000  
5975.0  
H2/ 1.00/ H2O/ 6.50/ O2/ 0.40/ N2/ 0.40/ AR/ 0.35/  
OH\*+H2O<=>OH+H2O 5.930E+012 0.500  
-860.0  
OH\*+H2<=>OH+H2 2.950E+012 0.500  
-444.0  
OH\*+N2<=>OH+N2 1.080E+011 0.500  
-1242.0  
OH\*+OH<=>OH+OH 6.010E+012 0.500  
-764.0  
OH\*+H<=>OH+H 1.310E+012 0.500  
-167.0  
OH\*+AR<=>OH+AR 1.690E+012 0.000  
4135.0  
OH\*<=>OH 1.450E+006 0.000  
0.0

OH*+O2<=>OH+O2 -478.0	2.100E+012	0.500
OH*+CO2<=>OH+CO2 -968.0	2.750E+012	0.500
OH*+CO<=>OH+CO -787.0	3.230E+012	0.500
OH*+CH4<=>OH+CH4 -635.0	3.360E+012	0.500
CH+O2<=>CO+OH* 0.0	4.040E+013	0.000
C2H+O<=>CO+CH* 0.0	6.200E+012	0.000
C+H+M<=>CH*+M 6940.0	6.000E+014	0.000

!REF:DEVRIENDT, VAN LOOK, CEURSTERS, AND PEETERS, CHEM PHYS LETT. 261 (1996) 450, C2H+O2

C2H+O2<=>CO2+CH* 0.0	2.170E+010	0.000
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!REF:HWANG, GARDINER, FRENKLACH, HIDAKA, COMB. FL. 67, 65-75 (1987)

CH*+M<=>CH+M		
CH*+AR<=>CH+AR 0.0	4.000E+011	0.500
CH*+H2O<=>CH+H2O 0.0	5.300E+013	0.000
CH*+CO<=>CH+CO 0.0	2.440E+012	0.500
CH*+CO2<=>CH+CO2 -1694.0	2.410E-001	4.300
CH*+O2<=>CH+O2 -1720.0	2.480E+006	2.140
CH*+H2<=>CH+H2 1361.0	1.470E+014	0.000
CH*+CH4<=>CH+CH4 167.0	1.730E+013	0.000
CH*<=>CH 0.0	1.860E+006	0.000
CH*+N2<=>CH+N2 -381.0	3.030E+002	3.400

!REF:LASKIN ET AL. IJCK 32 589-614 2000

HCO+H (+M) <=> CH2O (+M) -260.0	1.090E+012	0.480
LOW/ 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) 79600.0	1.350E+024	-2.570
LOW/ 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/	4.300E+007	1.500
	5.070E+027	-3.420

!REF:V. VASUDEVAN ET AL. IJCK. 37: 98--109 (2005).

CH2O+OH<=>HCO+H2O -1055.0	7.820E+007	1.630
!REF:IRDAM ET AL., IJCK 1993, 25, 285		
CH2O+H<=>HCO+H2 2740.0	5.740E+007	1.900
!REF:CURRAN FIT TO NIST DATABASE		
CH2O+O<=>HCO+OH 2260.0	6.260E+009	1.150
!REF:BAULCH ET AL.		
!REF:JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA:		
!REF:34, 3, 757-1397 2005		
CH2O+CH3<=>HCO+CH4 4312.0	3.830E+001	3.360
!REF:J. PHYS. CHEM. A 109, 12027-12035, 2005		
CH2O+HO2<=>HCO+H2O2 11520.0	1.880E+004	2.700
!REF:PHIL TAYLOR CH3CHO+OH X 1.5		
!REF:26TH INTL. COMBUSTION SYMP. P 497--504.		
CH2O+OH<=>HOCH2O 0.0	4.500E+015	-1.100
!REF:CURRAN ESTIMATE		
HOCH2O<=>HOCHO+H 14900.0	1.000E+014	0.000
!REF:BLAKE ET AL. J. CHEM. SOC. B: 10, 1923 (1971)		
HOCHO<=>CO+H2O 60470.0	2.450E+012	0.000
HOCHO<=>CO2+H2 48520.0	2.950E+009	0.000
!REF:CURRAN ESTIMATE		
OCHO+HO2<=>HOCHO+O2 -3275.0	3.500E+010	0.000
!REF:MARINOV ESTIMATE		
HOCHO+OH=>H2O+CO2+H 916.0	2.620E+006	2.060
HOCHO+OH=>H2O+CO+OH -962.0	1.850E+007	1.510
HOCHO+H=>H2+CO2+H 4868.0	4.240E+006	2.100
!REF:MARINOV ESTIMATE		
HOCHO+H=>H2+CO+OH 2988.0	6.030E+013	-0.350
HOCHO+CH3=>CH4+CO+OH 2200.0	3.900E-007	5.800
!REF: CURRAN ESTIMATE		

OCHO+H2O2<=>HOCHO+HO2 10000.0	2.400E+012	0.000
!REF:MARINOV ESTIMATE		
HOCHO+HO2=>H2O2+CO+OH 11920.0	1.000E+012	0.000
!REF:MARINOV ESTIMATE		
HOCHO+O=>CO+OH+OH 2975.0	1.770E+018	-1.900
!REF:CURRAN ESTIMATE		
CH2O+OCHO<=>HOCHO+HCO 13600.0	5.600E+012	0.000
!REF:HIPPLER ET AL. PCCP. 3: 3450--2458 (2001).		
CH3O(+M)<=>CH2O+H(+M) 26170.0	6.800E+013	0.000
LOW/ 24307.0/	1.867E+025	-3.000
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/		
!REF:WANTUCK, P.J. E AL. J. PHYS. CHEM. 91, 4653 (1987)		
CH3O+O2<=>CH2O+HO2 -5501.0	4.380E-019	9.500
!REF:FITTSCHEN, C., J. CHIM. PHYS. 95: 2129 (1998).		
CH2O+CH3O<=>CH3OH+HCO 2294.0	6.620E+011	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
CH3+CH3OH<=>CH4+CH3O 6935.0	1.440E+001	3.100
!REF:		
CH3O+CH3<=>CH2O+CH4 0.0	1.200E+013	0.000
!REF:HOYERMANN ET AL., 18TH SYMPOSIUM		
CH3O+H<=>CH2O+H2 0.0	2.000E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
CH3O+HO2<=>CH2O+H2O2 0.0	3.010E+011	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
CH2O+H(+M)<=>CH2OH(+M) 3600.0	5.400E+011	0.454
LOW/ 6530.0/	1.270E+032	-4.820
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/		
!REF:GROTHER, H. H. ET AL., J. PHYS. CHEM. 92: 4028 (1988).		
CH2OH+O2<=>CH2O+HO2 0.0	1.510E+015	-1.000



DUP		
CH2OH+O2<=>CH2O+HO2	2.410E+014	0.000
5017.0		
DUP		
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH2OH+H<=>CH2O+H2	6.000E+012	0.000
0.0		
!REF:NORTON, T.S ET AL., IJCK. (1991).		
CH2OH+HO2<=>CH2O+H2O2	1.200E+013	0.000
0.0		
!REF:T. J. HELD ET AL. IJCK. 30: 805--830 (1998)		
CH2OH+HCO<=>CH2O+CH2O	1.800E+014	0.000
0.0		
!REF:NORTON, T.S ET AL., IJCK. (1991).		
CH2OH+CH3O<=>CH2O+CH3OH	2.400E+013	0.000
0.0		
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+HCO<=>CH2OH+CH2O	9.630E+003	2.900
13110.0		
OH+CH2OH<=>H2O+CH2O	2.400E+013	0.000
0.0		
O+CH2OH<=>OH+CH2O	4.200E+013	0.000
0.0		
CH2OH+CH2OH<=>CH2O+CH3OH	3.000E+012	0.000
0.0		
!REF:CURRAN ESTIMATE		
CH2OH+HO2<=>HOCH2O+OH	1.000E+013	0.000
0.0		
CH2O+HO2<=>OCH2O2H	1.500E+011	0.000
11900.0		
OCH2O2H<=>HOCH2O2	3.000E+011	0.000
8600.0		
HOCH2O2+HO2<=>HOCH2O2H+O2	3.500E+010	0.000
-3275.0		
HOCH2O+OH<=>HOCH2O2H	1.000E+013	0.000
0.0		
!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950		
!REF:NEGLECTING HCOH CHANNELS AS THEY ARE NOT IMPORTANT		
CH3OH (+M) <=> CH3+OH (+M)	2.084E+018	-0.615
92540.6		
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		
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		

LOW/ 105230.3/ TROE/ -7.391E+001 3.705E+004 4.150E+004 5.220E+003/	3.390E+042	-7.244
!REF:J. CHEM. PHYS. 134, 094302 (2011)		
CH3OH+H<=>CH2OH+H2 5440.0	3.070E+005	2.550
CH3OH+H<=>CH3O+H2 10300.0	1.990E+005	2.560
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+O<=>CH2OH+OH 3080.0	3.880E+005	2.500
!REF:XU ET AL. PROC 31 2007 159-166		
CH3OH+OH<=>CH2OH+H2O -806.7	3.080E+004	2.650
CH3OH+OH<=>CH3O+H2O -763.0	1.500E+002	3.030
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
CH3OH+O2<=>CH2OH+HO2 44900.0	2.050E+013	0.000
!REF:CURRAN ESTIMATE		
CH3OH+HO2<=>CH2OH+H2O2 10530.0	1.080E+004	2.550
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
CH3OH+CH3<=>CH2OH+CH4 7172.0	3.190E+001	3.170
CH3O+CH3OH<=>CH2OH+CH3OH 4074.0	3.000E+011	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
CH3O+CH3O<=>CH3OH+CH2O 0.0	6.030E+013	0.000
!REF:GRI		
CH3+H(+M)<=>CH4(+M) 383.0	1.270E+016	-0.630
LOW/ 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/	2.477E+033	-4.760
!REF:BAULCH, D.L.; ET AL., J. PHYS. CHEM. REF. DATA (2005)		
CH4+H<=>CH3+H2 9587.0	6.140E+005	2.500
!REF:CURRAN, FIT TO NIST DATABASE		
CH4+OH<=>CH3+H2O 2190.0	5.830E+004	2.600
!REF:GRI 3.0		

CH4+O<=>CH3+OH 1.020E+009 1.500  
8600.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.

!REF:X1.5  
CH4+HO2<=>CH3+H2O2 1.695E+001 3.740  
21010.0

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

!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950

!REF:ONLY INCLUDING TRANS HCOH FOR SIMPLICITY, DO NOT HAVE TO COMBINE THE K'S.

!REF:IT'S NOT REALLY SIGNIFICANT ANYWAY

CH3+OH<=>CH2(S)+H2O 4.936E+014 -0.669  
-445.8  
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/

!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950

CH3+OH<=>CH2O+H2 3.502E+005 1.441  
-3244.0  
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/

!REF:INCREASED BY FACTOR OF 2 TO IMPROVE AGREEMENT WITH CH4 FLAMESPEED

CH3+OH<=>CH2OH+H 1.621E+010 0.965  
3210.0  
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/

!REF:FROM JASPER/ KLIPP, J. PHYS. CHEM A 111, 19, 3932-3950

CH3+OH<=>H+CH3O 1.186E+009 1.016  
11940.0  
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  
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					
!REF:MARINOV 1996					
HCOH+OH<=>HCO+H2O				2.000E+013	0.000
0.0					
HCOH+H<=>CH2O+H				2.000E+014	0.000
0.0					
HCOH+O=>CO2+H+H				5.000E+013	0.000
0.0					
HCOH+O=>CO+OH+H				3.000E+013	0.000
0.0					
HCOH+O2=>CO2+H+OH				5.000E+012	0.000
0.0					
HCOH+O2<=>CO2+H2O				3.000E+013	0.000
0.0					
!REF: JASPER/ KLIPPENSTEIN PROC COMBUST INST 32 (2009) 279-286					
CH3+HO2<=>CH3O+OH				1.000E+012	0.269
-687.5					
CH3+HO2<=>CH4+O2				1.160E+005	2.230
-3022.0					
!REF:HARDING AND KLIPPENSTEIN 2B04, 30TH SYMP 2004.					
CH3+O<=>CH2O+H				5.540E+013	0.050
-136.0					
!REF:N. K. SRINIVASAN ET AL., J. PHYS. CHEM. A 109, 7902-7914 (2005)					
CH3+O2<=>CH3O+O				7.546E+012	0.000
28320.0					
!REF: PERSONAL COMMUNICATION, STEVE KLIPPENSTEIN					
CH3+O2<=>CH2O+OH				2.641E+000	3.283
8105.0					
!REF:R.X. FERNANDES ET AL., J PHYS. CHEM. A, (2006) 110:4442-4449.					
CH3+O2 (+M) <=> CH3O2 (+M)				7.812E+009	0.900
0.0					
LOW/				6.850E+024	-3.000
0.0/					
TROE/	6.000E-001	1.000E+003	7.000E+001	1.700E+003/	
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)					
CH3O2+CH2O<=>CH3O2H+HCO				1.990E+012	0.000
11660.0					
!REF:NEW FIT FROM HJC					
!REF:X1.5					
CH4+CH3O2<=>CH3+CH3O2H				9.600E-001	3.770
17810.0					
!REF:TSANG, JPC REF. DATA, 16:471 (1987)					
CH3OH+CH3O2<=>CH2OH+CH3O2H				1.810E+012	0.000
13710.0					

!REF:KEIFFER, M. ET AL., J. CHEM. SOC. FARADAY TRANS. 2: 84, 505 (1988)  
CH3O2+CH3<=>CH3O+CH3O 5.080E+012 0.000  
-1411.0

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

!REF:LIGHTFOOT ET AL. J. CHEM. SOC. FARA TRANS. 1991, 87(19), 3213--3220.  
CH3O2+CH3O2=>CH2O+CH3OH+O2 3.110E+014 -1.610  
-1051.0  
CH3O2+CH3O2=>O2+CH3O+CH3O 1.400E+016 -1.610  
1860.0  
CH3O2+H<=>CH3O+OH 9.600E+013 0.000  
0.0  
CH3O2+O<=>CH3O+O2 3.600E+013 0.000  
0.0  
CH3O2+OH<=>CH3OH+O2 6.000E+013 0.000  
0.0  
CH3O2H<=>CH3O+OH 6.310E+014 0.000  
42300.0

!REF:GRI  
CH2 (S) +N2<=>CH2+N2 1.500E+013 0.000  
600.0  
CH2 (S) +AR<=>CH2+AR 9.000E+012 0.000  
600.0  
CH2 (S) +H<=>CH+H2 3.000E+013 0.000  
0.0  
CH2 (S) +O<=>CO+H2 1.500E+013 0.000  
0.0  
CH2 (S) +O<=>HCO+H 1.500E+013 0.000  
0.0  
CH2 (S) +OH<=>CH2O+H 3.000E+013 0.000  
0.0  
CH2 (S) +H2<=>CH3+H 7.000E+013 0.000  
0.0  
CH2 (S) +O2=>H+OH+CO 2.800E+013 0.000  
0.0  
CH2 (S) +O2<=>CO+H2O 1.200E+013 0.000  
0.0  
CH2 (S) +H2O<=>CH2+H2O 3.000E+013 0.000  
0.0  
CH2 (S) +CO<=>CH2+CO 9.000E+012 0.000  
0.0  
CH2 (S) +CO2<=>CH2+CO2 7.000E+012 0.000  
0.0  
CH2 (S) +CO2<=>CH2O+CO 1.400E+013 0.000  
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000  
CH2+H (+M) <=>CH3 (+M) 2.500E+016 -0.800  
0.0  
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/

!REF:GRI 3.0

CH2+O2<=>HCO+OH	1.060E+013	0.000
1500.0		
CH2+O2=>CO2+H+H	2.640E+012	0.000
1500.0		
CH2+O=>CO+H+H	5.000E+013	0.000
0.0		
CH2+OH<=>CH+H2O	1.130E+007	2.000
3000.0		
CH+O2<=>HCO+O	3.300E+013	0.000
0.0		

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

C+OH<=>CO+H	5.000E+013	0.000
0.0		
C+O2<=>CO+O	5.000E+013	0.000
0.0		

!REF: GRI

CH+H<=>C+H2	1.100E+014	0.000
0.0		

!REF:MESSING ET AL., J. CHEM. PHYS. 74, 3874 (1981)

CH+O<=>CO+H	5.700E+013	0.000
0.0		

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

CH+OH<=>HCO+H	3.000E+013	0.000
0.0		
CH2+H<=>CH+H2	3.000E+013	0.000
0.0		

!REF:MAYER, S. W. ET AL., ELEVENTH INTERNATIONAL SYMPOSIUM ON COMBUSTION

!REF:BERGEAT ET AL., CHEM. PHYS. LETT. 480, 21 (2009)

CH+H2O<=>H+CH2O	1.774E+016	-1.220
23.8		

!REF:SMITH ET AL., GRI MECH VERSION 2.11

!REF:1/ 2 OF BERMAN, FLEMING, HARVEY AND LIN, 19TH SYMP. COMB. P. 73,  
1982

CH+CO2<=>HCO+CO	1.700E+012	0.000
685.0		

!REF:WANG ET AL., JPC A 107:11414 (2003)

CH3+CH3(+M)<=>C2H6(+M)	2.277E+015	-0.690
174.9		
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/		

!REF:GRI 3.0  
 C2H5+H(+M) $\rightleftharpoons$ C2H6(+M) 5.210E+017 -0.990  
 1580.0  
 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/  
 C2H6+H $\rightleftharpoons$ C2H5+H2 1.150E+008 1.900  
 7530.0

!REF: \*MIYOSHI, A. ET AL., CHEM. PHYS. LETT. 204, 241-247 (1993)  
 C2H6+O $\rightleftharpoons$ C2H5+OH 3.550E+006 2.400  
 5830.0

!REF:CURRAN, FIT TO NIST DATABASE  
 C2H6+OH $\rightleftharpoons$ C2H5+H2O 1.480E+007 1.900  
 950.0

!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)  
 C2H6+O2 $\rightleftharpoons$ C2H5+HO2 6.030E+013 0.000  
 51870.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
 C2H6+CH3 $\rightleftharpoons$ C2H5+CH4 5.550E-004 4.720  
 3231.0

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-  
 7054.  
 C2H6+HO2 $\rightleftharpoons$ C2H5+H2O2 3.460E+001 3.610  
 16920.0

!REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003  
 C2H6+CH3O2 $\rightleftharpoons$ C2H5+CH3O2H 1.940E+001 3.640  
 17100.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
 C2H6+CH3O $\rightleftharpoons$ C2H5+CH3OH 2.410E+011 0.000  
 7090.0  
 C2H6+CH $\rightleftharpoons$ C2H5+CH2 1.100E+014 0.000  
 -260.0

!REF:MILLER, J.A. AND BOWMAN, C.T.,

!REF:MECHANISM AND MODELING OF NITROGEN CHEMISTRY IN COMBUSTION, WSS/ CI,  
 AUTUMN 1988  
 CH2(S)+C2H6 $\rightleftharpoons$ CH3+C2H5 1.200E+014 0.000  
 0.0

!REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202

!REF:HP AND LP LIMIT\*0.7  
 C2H4+H(+M) $\rightleftharpoons$ C2H5(+M) 9.569E+008 1.463  
 1355.0  
 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/

!REF:

H2+CH3O2<=>H+CH3O2H 1.500E+014 0.000  
26030.0

H2+C2H5O2<=>H+C2H5O2H 1.500E+014 0.000  
26030.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
C2H4+C2H4<=>C2H5+C2H3 4.820E+014 0.000  
71530.0

!REF:ZHU, R.S. ET AL., J. CHEM. PHYS. 120:6566:6573 (2004)  
CH3+C2H5<=>CH4+C2H4 1.180E+004 2.450  
-2921.0

!REF:STEWART ET AL C&F 1989  
CH3+CH3<=>H+C2H5 4.740E+012 0.105  
10664.3

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/

!REF:CURRAN: FIT TO PRATT/ WOOD 84 AND PRATT/ VELDMAN 76  
C2H5+H<=>C2H4+H2 2.000E+012 0.000  
0.0

!REF:GRI 3.0  
C2H5+O<=>CH3CHO+H 1.100E+014 0.000  
0.0

!REF:CURRAN. BASED ON CH3+HO2<=>PRODUCTS  
C2H5+HO2<=>C2H5O+OH 1.100E+013 0.000  
0.0

!REF:CURRAN. BASED ON CH3+HO2<=>PRODUCTS  
CH3O2+C2H5<=>CH3O+C2H5O 8.000E+012 0.000  
-1000.0

!REF: HARTMANN ET AL. 1990  
C2H5O+O2<=>CH3CHO+HO2 4.280E+010 0.000  
1097.0

!REF: CURRAN ESTIMATE  
CH3+CH2O<=>C2H5O 3.000E+011 0.000  
6336.0

!REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010  
CH3CHO+H<=>C2H5O 4.610E+007 1.710  
7090.0

!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)  
C2H5O2+CH2O<=>C2H5O2H+HCO 1.990E+012 0.000  
11660.0



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!REF:BASED ON CH4+CH3O2
CH4+C2H5O2<=>CH3+C2H5O2H          1.810E+011      0.000
18480.0

!REF:TSANG, JPC REF. DATA, 16:471 (1987)
CH3OH+C2H5O2<=>CH2OH+C2H5O2H      1.810E+012      0.000
13710.0
C2H5O2+HO2<=>C2H5O2H+O2           1.750E+010      0.000
-3275.0

!REF:CARSTENSEN AND DEAN PROC COMBUST INST 30 (2005) 995-1003
C2H6+C2H5O2<=>C2H5+C2H5O2H        8.600E+000      3.760
17200.0
C2H5O2H<=>C2H5O+OH                 6.310E+014      0.000
42300.0
C2H5+O2<=>C2H5O2                   3.398E+053     -13.900
9279.0
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
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
DUP
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
DUP
C2H5+O2<=>C2H4O1-2+OH              1.303E+003      1.930
-502.7
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
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
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
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
PLOG/      0.0400      1.782E+032     -7.100     32840.0/
PLOG/      1.0000      2.701E+037     -8.470     35840.0/

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PLOG/	10.0000	1.980E+038	-8.460	37900.0/	
C2H5O2<=>C2H4O1-2+OH				5.778E+045	-11.900
4112.0					
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					
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					
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					
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/	
!REF:LIFSHITZ ET AL. 1983					
C2H4O1-2<=>CH3+HCO				3.630E+013	0.000
57200.0					
!REF:CURRAN, FIT TO NIST DATABASE					
C2H4O1-2<=>CH3CHO				7.407E+012	0.000
53800.0					
!REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984)					
C2H4O1-2+OH<=>C2H3O1-2+H2O				1.780E+013	0.000
3610.0					
C2H4O1-2+H<=>C2H3O1-2+H2				8.000E+013	0.000
9680.0					
!REF:ANALOGY WITH ETHENE					
C2H4O1-2+HO2<=>C2H3O1-2+H2O2				1.130E+013	0.000
30430.0					
C2H4O1-2+CH3O2<=>C2H3O1-2+CH3O2H				1.130E+013	0.000
30430.0					
C2H4O1-2+C2H5O2<=>C2H3O1-2+C2H5O2H				1.130E+013	0.000
30430.0					
!REF:BALDWIN ET AL., J. CHEM. SOC. FARADAY TRANS. 1, 80, 435 (1984)					
C2H4O1-2+CH3<=>C2H3O1-2+CH4				1.070E+012	0.000
11830.0					
C2H4O1-2+CH3O<=>C2H3O1-2+CH3OH				1.200E+011	0.000
6750.0					
C2H3O1-2<=>CH3CO				8.500E+014	0.000
14000.0					
C2H3O1-2<=>CH2CHO				1.000E+014	0.000
14000.0					
!REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL 114, NO. 2, 2010					
CH3CHO (+M) <=>CH3+HCO (+M)				2.450E+022	-1.740
86355.0					

LOW/ 95912.5/ TROE/ 2.490E-003 7.181E+002 6.089E+000 3.780E+003/ CH3CHO (+M) <=> CH4+CO (+M) 86355.0	1.030E+059	-11.300
LOW/ 95912.5/ TROE/ 2.490E-003 7.181E+002 6.089E+000 3.780E+003/	1.144E+058	-11.300
!REF:HARDING J. PHYS. CHEM., VOL. 114, NO. 2, 2010		
CH3CHO+H<=>CH3CO+H2 1220.0	1.310E+005	2.580
CH3CHO+H<=>CH2CHO+H2 5210.0	2.720E+003	3.100
!REF:CURRAN, FIT TO NIST DATABASE		
CH3CHO+O<=>CH3CO+OH 1868.0	5.940E+012	0.000
!REF:JUAN LI'S PHD THESIS		
CH3CHO+OH<=>CH3CO+H2O -619.0	3.370E+012	0.000
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3CHO+O2<=>CH3CO+HO2 39150.0	3.010E+013	0.000
!REF: GUPTA ET AL., PROC COMBUST INST 31 (2007) 167-174		
CH3CHO+CH3<=>CH3CO+CH4 1966.0	7.080E-004	4.580
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3CHO+HO2<=>CH3CO+H2O2 11920.0	3.010E+012	0.000
!REF:BAULCH ET AL., J. PHYS. CHEM. REF DATA, 21:411 (1992)		
CH3O2+CH3CHO<=>CH3O2H+CH3CO 11920.0	3.010E+012	0.000
CH3CHO+CH3CO3<=>CH3CO+CH3CO3H 11920.0	3.010E+012	0.000
!REF:TAYLOR ET AL. 1996		
CH3CHO+OH<=>CH3+HOCHO 0.0	3.000E+015	-1.076
CH3CHO+OH<=>CH2CHO+H2O 815.0	1.720E+005	2.400
!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781		
CH3CO (+M) <=> CH3+CO (+M) 16900.0	1.070E+012	0.630
LOW/ 14600.0/ TROE/ 6.290E-001 8.730E+009 5.520E+000 7.600E+007/	5.650E+018	-0.970
!REF:		
CH3CO+H<=>CH2CO+H2 0.0	2.000E+013	0.000

CH3CO+O<=>CH2CO+OH	2.000E+013	0.000
0.0		
CH3CO+CH3<=>CH2CO+CH4	5.000E+013	0.000
0.0		

!REF:

CH3CO+O2<=>CH3CO3	1.200E+011	0.000
-1100.0		
CH3CO3+HO2<=>CH3CO3H+O2	1.750E+010	0.000
-3275.0		
H2O2+CH3CO3<=>HO2+CH3CO3H	2.410E+012	0.000
9936.0		
CH4+CH3CO3<=>CH3+CH3CO3H	1.810E+011	0.000
18480.0		

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

!REF:ANALOGY TO CH3O2+CH2O

CH2O+CH3CO3<=>HCO+CH3CO3H	1.990E+012	0.000
11660.0		

!REF: ANALOGY TO C2H6+HO2

C2H6+CH3CO3<=>C2H5+CH3CO3H	1.700E+013	0.000
20460.0		

!REF:SAHETCHIAN ET AL. 1992

CH3CO3H<=>CH3CO2+OH	5.010E+014	0.000
40150.0		

!REF:ANALOGY TO CH3CO<=>CH3+CO

CH3CO2+M<=>CH3+CO2+M	4.400E+015	0.000
10500.0		

!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781

CH2CHO (+M) <=> CH2CO+H (+M)	1.430E+015	-0.150
45600.0		

!REF:LPL TIMES 2

LOW/	6.000E+029	-3.800
43423.9/		
TROE/ 9.850E-001 3.930E+002 9.800E+009 5.000E+009/		

!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781

CH2CHO (+M) <=> CH3+CO (+M)	2.930E+012	0.290
40300.0		
LOW/	9.520E+033	-5.070
41300.0/		
TROE/ 7.130E-017 1.150E+003 4.990E+009 1.790E+009/		

!REF:J. LEE, AND J.W. BOZZELLI. J. PHYS. CHEM. A, 2003, 107 (19), 3778-3791

CH2CHO+O2<=>O2CH2CHO	1.580E+077	-21.900
19350.0		
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					
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					
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					
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					
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					
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					
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					
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/	

!REF:LASKIN ET AL. IJCK 32 589-614 2000

CH2+CO (+M) <=> CH2CO (+M)				8.100E+011	0.000
0.0					
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/	

!REF:J. PHYS. CHEM. A 2006, 110, 5772-5781

!REF:DEFINED IN THE REVERSE FROM SJK, P DEPENDENCE FROM CHEMDIS

!REF:IMPORTANT FOR ACETONE FLAME SPEEDS

CH3CO (+M) <=>CH2CO+H (+M)	9.413E+007	1.917
44987.2		
LOW/	1.516E+051	-10.270
55390.0/		
TROE/ 6.009E-001 8.103E+009 6.677E+002 5.000E+009/		
!REF:WKM (SEE COMMENTS AT BEGINNING OF FILE 15/ 09/ 2011		
CH2CO+H<=>HCCO+H2	1.401E+015	-0.171
8783.2		
CH2CO+H<=>CH3+CO	7.704E+013	-0.171
4183.2		
!REF:CURRAN ESTIMATE		
CH2CO+O<=>CH2+CO2	1.750E+012	0.000
1350.0		
!REF:		
CH2CO+O<=>HCCO+OH	1.000E+013	0.000
8000.0		
CH2CO+OH<=>HCCO+H2O	1.000E+013	0.000
2000.0		
!REF:BROWN ET AL. CHEM. PHYS. LETT. 1989, 161, 491.		
CH2CO+OH<=>CH2OH+CO	2.000E+012	0.000
-1010.0		
!REF:WKM CALCULATION, CHEMICALLY ACTIVATED, APPEARS PRESSURE INDEPENDANT		
CH2CO+CH3<=>C2H5+CO	4.769E+004	2.312
9468.0		
CH2 (S) +CH2CO<=>C2H4+CO	1.600E+014	0.000
0.0		
HCCO+OH=>H2+CO+CO	1.000E+014	0.000
0.0		
HCCO+O=>H+CO+CO	8.000E+013	0.000
0.0		
!REF:GRI		
HCCO+H<=>CH2 (S) +CO	1.000E+014	0.000
0.0		
!REF:KLIPPENSTEIN 2002		
HCCO+O2=>OH+CO+CO	1.910E+011	-0.020
1020.0		
HCCO+O2=>CO2+CO+H	4.780E+012	-0.142
1150.0		
!REF:FULLE, D.; HIPPLER, H.; STRIEBEL, F.		
!REF:J. CHEM. PHYS. 108: 6709-6716 1998		
CH+CO+M<=>HCCO+M	7.570E+022	-1.900
0.0		
!REF:REG 2.11		
CH+CH2O<=>H+CH2CO	9.460E+013	0.000
-515.0		
CH+HCCO<=>CO+C2H2	5.000E+013	0.000
0.0		

!REF:GRI 3.0  
 C2H3+H (+M) <=> C2H4 (+M) 6.080E+012 0.270  
 280.0  
 LOW/ 1.400E+030 -3.860  
 3320.0/  
 TROE/ 7.820E-001 2.075E+002 2.663E+003 6.095E+003/  
 H2/ 2.00/ H2O/ 6.00/ AR/ 0.70/ CO/ 1.50/ CO2/ 2.00/ CH4/ 2.00/ C2H6/  
 3.00/ HE/ 0.70/

!REF:GRI  
 C2H4 (+M) <=> H2+H2CC (+M) 8.000E+012 0.440  
 88770.0  
 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/

!REF:KNYAZEV,V.D. ET AL.,J. PHYS. CHEM. 100, 11346-1135 (1996)  
 C2H4+H<=>C2H3+H2 5.070E+007 1.930  
 12950.0

!REF:BAULCH ET AL.

!REF:JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA:

!REF:34, 3, 757-1397 2005

!REF:MAKING BRANCHING RATIO 55:45  
 C2H4+O<=>CH3+HCO 7.453E+006 1.880  
 183.0  
 C2H4+O<=>CH2CHO+H 6.098E+006 1.880  
 183.0

!REF:J. PHYS. CHEM 109 2005 7489-7499 (PEETERS)

!REF: FROM STANFORD  
 C2H4+OH<=>C2H3+H2O 2.230E+004 2.745  
 2215.5

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

!REF:ETHENOL CHEMISTRY FROM CURRAN/ YASUNAGA

C2H3OH+O2<=>CH2CHO+HO2				5.310E+011	0.210
39830.0					
C2H3OH+O<=>CH2CHO+OH				1.875E+006	1.900
-860.0					
C2H3OH+OH<=>CH2CHO+H2O				3.330E+009	1.100
540.5					
C2H3OH+CH3<=>CH2CHO+CH4				2.030E-008	5.900
1052.0					
C2H3OH+CH3O2<=>CH2CHO+CH3O2H				3.400E+003	2.500
8922.0					

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

!REF:EXCEPT FOR SC2H4OH CHANNEL KEPT WKM CALCULATION

C2H3OH+H<=>CH2CHO+H2				1.480E+003	3.077
7220.0					
C2H3OH+H<=>C2H2OH+H2				2.470E+007	2.030
15200.0					
C2H3OH+H<=>PC2H4OH				3.010E+008	1.577
3670.0					

!REF:DA SILVA BOZZELLI CHEMICAL PHYSICS LETTERS 483 (2009) 25-29

C2H3OH+HO2<=>CH3CHO+HO2				1.490E+005	1.670
6810.0					

!REF:JU-XIANG SHAO THEOR CHEM ACC (2011) 128:341-348

!REF:CHANGED PRODUCTS FROM CH3+HCO

C2H3OH<=>CH3CHO				7.420E+046	-10.560
67420.0					
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/	

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

!REF:WKM 19/ 04/ 2010

!REF:TAKEN FROM SAN DIEGO MECH



!REF: MARINOV, 1995

!REF:CHECK EFFECT!!!!

C2H4+O2<=>C2H3+HO2 4.220E+013 0.000  
57623.1

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

C2H4+CH3O<=>C2H3+CH3OH 1.200E+011 0.000  
6750.0

!REF:WKM 22/ 04/ 2010

!REF:FROM BILL PITZ'S SUGGESTION

C2H4+CH3O2<=>C2H3+CH3O2H 8.590E+000 3.754  
27132.0

!REF:WKM 22/ 04/ 2010

!REF:FROM BILL PITZ'S SUGGESTION

C2H4+C2H5O2<=>C2H3+C2H5O2H 8.590E+000 3.754  
27132.0

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

C2H4+CH3CO3<=>C2H3+CH3CO3H 1.130E+013 0.000  
30430.0

!REF:PITZ ESTIMATE

C2H4+CH3O2<=>C2H4O1-2+CH3O 2.820E+012 0.000  
17110.0

C2H4+C2H5O2<=>C2H4O1-2+C2H5O 2.820E+012 0.000  
17110.0

!REF:BAULCH AND COBOS REDUCED BY A FACTOR OF 4

C2H4+HO2<=>C2H4O1-2+OH 5.575E+011 0.000  
17190.0

!REF:BUTLER, FLEMING, GOSS, LIN, ACS SYMP. SER. 134 (1980).

CH+CH4<=>C2H4+H 6.000E+013 0.000  
0.0

!REF:MARINOV ESTIMATE.

CH2(S)+CH3<=>C2H4+H 2.000E+013 0.000  
0.0

!REF:MILLER KLIPPENSTEIN PCCP 2004, 6, 1192-1202

C2H2+H(+M)<=>C2H3(+M) 1.710E+010 1.266  
2709.0

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/

!REF:N.M MARINOV ET AL., COMBUST. FLAME 114 (1998) 192-213

!REF:ADOPTING KLIPPENSTEIN'S PRODUCTS FOR ONE OF THE CHANNELS,

!REF:TO COMBAT OVER-PRODUCTION OF C2H2 IN ETHYLENE JSR

C2H3+O2<=>CH2O+HCO 4912.3	2.380E+027	-4.859
C2H3+O2<=>CH2CHO+O 3322.7	5.340E+012	-0.013
C2H3+O2=>H+CO+CH2O 2176.7	3.380E+014	-0.885
!REF:		
CH3+C2H3<=>CH4+C2H2 0.0	3.920E+011	0.000
!REF:86TSA/ HAM		
C2H3+H<=>C2H2+H2 0.0	9.000E+013	0.000
!REF:USC ESTIMATE		
C2H3+H<=>H2CC+H2 0.0	6.000E+013	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
C2H3+OH<=>C2H2+H2O 0.0	3.011E+013	0.000
C2H3+C2H3<=>C2H2+C2H4 0.0	9.600E+011	0.000
!REF: GRI 3.0		
C2H+H (+M) <=>C2H2 (+M) 0.0	1.000E+017	0.000
LOW/ 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/	3.750E+033	-4.800
!REF:GRI		
C2H+O<=>CH+CO 0.0	5.000E+013	0.000
C2H+OH<=>H+HCCO 0.0	2.000E+013	0.000
C2H+O2<=>HCO+CO 1500.0	5.000E+013	0.000
C2H+H2<=>H+C2H2 560.0	4.900E+005	2.500
!REF:99 LAS/ WAN		
C2H2 (+M) <=>H2CC (+M) 50750.0	8.000E+014	-0.520
LOW/ 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/	2.450E+015	-0.640
!REF:NGUYEN ET AL. J.PHYS.CHEM A 2006, 110, 6696-6706		
C2H2+O<=>CH2+CO 2472.0	7.395E+008	1.280
C2H2+O<=>HCCO+H 2472.0	2.958E+009	1.280

C2H2+HO2<=>CH2CO+OH 6.030E+009 0.000  
7949.0

!REF:SJK J. PHYS. CHEM A 2005, 109, 6045-6055

C2H2+OH<=>C2H+H2O 2.632E+006 2.140  
17060.0

C2H2+OH<=>HCCOH+H 2.800E+005 2.280  
12420.0

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

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

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

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/

!REF:GRI 3.0 AND USC II

C2H2+HCO<=>C2H3+CO 1.000E+007 2.000  
6000.0

C2H2+CH2<=>C3H3+H 1.200E+013 0.000  
6620.0

C2H2+CH2(S)<=>C3H3+H 2.000E+013 0.000  
0.0

C2H2+HCCO<=>C3H3+CO 1.000E+011 0.000  
3000.0

H2CC+H<=>C2H2+H 1.000E+014 0.000  
0.0

H2CC+OH<=>CH2CO+H 2.000E+013 0.000  
0.0

H2CC+O2<=>HCO+HCO 1.000E+013 0.000  
0.0

!REF:GRI 2.11

H+HCCOH<=>H+CH2CO 1.000E+013 0.000  
0.0

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

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

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

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/

C2H5OH+O2<=>PC2H4OH+HO2 2.000E+013 0.000  
52800.0

C2H5OH+O2<=>SC2H4OH+HO2 1.500E+013 0.000  
50150.0

!REF:SIVARAMAKRISHNAN J. PHYS. CHEM. A, VOL. 114, NO. 35, 2010  
C2H5OH+H<=>SC2H4OH+H2 8.790E+004 2.680  
2910.0

C2H5OH+H<=>PC2H4OH+H2 5.310E+004 2.810  
7490.0

C2H5OH+H<=>C2H5O+H2 9.450E+002 3.140  
8701.1

!REF: SMB 04/ 09/ 2013

!REF: Branching ratio changed for the underprediciotn of c2h4 in the JSR  
and flow reactor

C2H5OH+OH<=>SC2H4OH+H2O 7.520E+004 2.490  
-1474.1

C2H5OH+OH<=>PC2H4OH+H2O 3.760E+003 2.780  
-1810.2

C2H5OH+OH<=>C2H5O+H2O 5.810E-003 4.280  
-3560.0

!REF:ESTIMATED FROM CW ZHOU BUTANOL+OH

!REF: Mittal 2013 ( increased by 1.75 Zhou )

C2H5OH+HO2<=>SC2H4OH+H2O2 2.450E-005 5.260  
7475.1

C2H5OH+HO2<=>PC2H4OH+H2O2 3.986E-002 4.300  
15333.0

C2H5OH+HO2<=>C2H5O+H2O2 10533.1		6.470E-007	5.300	
!REF:ANAOLGY WITH C2H5OH+HO2				
C2H5OH+CH3O2<=>SC2H4OH+CH3O2H 7475.1		1.225E-005	5.260	
C2H5OH+CH3O2<=>PC2H4OH+CH3O2H 15333.0		1.995E-002	4.300	
C2H5OH+CH3O2<=>C2H5O+CH3O2H 10533.1		3.236E-007	5.300	
!REF:WU ET AL., J. PHYS. CHEM. A 2007, 111, 6693-6703				
C2H5OH+O<=>PC2H4OH+OH 4658.0		9.690E+002	3.230	
C2H5OH+O<=>SC2H4OH+OH 876.0		1.450E+005	2.470	
C2H5OH+O<=>C2H5O+OH 1727.0		1.460E-003	4.730	
!REF:XU, Z.F. ET AL., J. CHEM. PHYS. 120,6593-6599, 2004				
C2H5OH+CH3<=>PC2H4OH+CH4 12290.0		3.300E+002	3.300	
C2H5OH+CH3<=>SC2H4OH+CH4 7634.0		1.993E+001	3.370	
C2H5OH+CH3<=>C2H5O+CH4 7721.0		2.035E+000	3.570	
!REF:1/ 2 OF C4H10+C2H5				
C2H5OH+C2H5<=>PC2H4OH+C2H6 13400.0		5.000E+010	0.000	
!REF:ESTIMATE				
C2H5OH+C2H5<=>SC2H4OH+C2H6 10400.0		5.000E+010	0.000	
!REF:CURRAN, FIT TO NIST DATABASE				
!REF:WKM CALCULATION.				
SC2H4OH<=>CH3CHO+H 45049.0		5.690E+052	-13.380	
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 44323.0		5.400E+046	-11.630	
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					
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					
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/	
!REF:BASED ON C3H6OH+O2 REACTION					
O2C2H4OH<=>PC2H4OH+O2				3.900E+016	-1.000
30000.0					
!REF:					
O2C2H4OH=>OH+CH2O+CH2O				3.125E+009	0.000
18900.0					
!REF:DA SILVA J. PHYS. CHEM. A 2009, 113, 8923-8933					
SC2H4OH+O2<=>CH3CHO+HO2				5.260E+017	-1.638
869.0					
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					
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/	
!REF: SAXENA ET AL. PROCEEDINGS. 32 123-130 (2009)					
CH3COCH3<=>CH3CO+CH3				2.050E+058	-12.796
100030.1					
PLOG/	0.0100	2.050E+058	-12.796	100030.1/	
PLOG/	0.1000	3.300E+051	-10.574	98221.2/	
PLOG/	1.0000	1.310E+042	-7.657	94660.6/	
PLOG/	10.0000	2.160E+033	-4.989	90916.5/	
PLOG/	100.0000	9.400E+028	-3.669	89022.8/	
!REF:ESTIMATE					
CH3COCH3+OH<=>CH3COCH2+H2O				1.250E+005	2.483
445.0					

!REF:CURRAN ESTIMATE		
CH3COCH3+H<=>CH3COCH2+H2 5160.0	9.800E+005	2.430
!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98		
CH3COCH3+O<=>CH3COCH2+OH 4890.0	5.130E+011	0.211
!REF:		
CH3COCH3+CH3<=>CH3COCH2+CH4 9784.0	3.960E+011	0.000
!REF:ESTIMATE		
CH3COCH3+CH3O<=>CH3COCH2+CH3OH 6460.0	4.340E+011	0.000
!REF:A-FACTOR BY ANALOGY WITH C2H6+O2 AND EA FROM DHRXN		
CH3COCH3+O2<=>CH3COCH2+HO2 48500.0	6.030E+013	0.000
!REF:ANALOGY TO ETHANE		
CH3COCH3+HO2<=>CH3COCH2+H2O2 20460.0	1.700E+013	0.000
CH3COCH3+CH3O2<=>CH3COCH2+CH3O2H 20460.0	1.700E+013	0.000
!REF:WJP: BASED ON CH3+C2H4 ADDITION, CURRAN IJCK 2006		
CH2CO+CH3<=>CH3COCH2 6130.0	1.760E+004	2.480
CH3COCH2+HO2<=>CH3COCH2O+OH 0.0	2.410E+013	0.000
CH3COCH2+CH3O2<=>CH3COCH2O+CH3O 0.0	1.205E+013	0.000
CH3COCH2+H<=>CH3COCH3 0.0	1.000E+013	0.000
CH3COCH2O<=>CH3CO+CH2O 5108.0	5.000E+010	0.000
!REF:		
CH3COCH2+O2<=>CH3COCH2O2 -1100.0	1.200E+011	0.000
!REF:WESTBROOK ESTIMATE		
CH3COCH3+CH3COCH2O2<=>CH3COCH2+C3KET21 5000.0	1.000E+011	0.000
CH2O+CH3COCH2O2<=>HCO+C3KET21 9000.0	1.288E+011	0.000
HO2+CH3COCH2O2<=>C3KET21+O2 0.0	1.000E+012	0.000
!REF:ESTIMATE		
C2H3+HCO<=>C*CCHO 0.0	1.810E+013	0.000
!REF:BASED ON CH3CHO+H		
C*CCHO+H<=>C2H3CO+H2 3300.0	1.340E+013	0.000

C*CCHO+O<=>C2H3CO+OH 1868.0	5.940E+012	0.000
!REF:TAYLOR ET AL. 1996		
C*CCHO+OH<=>C2H3CO+H2O -962.0	9.240E+006	1.500
C*CCHO+O2<=>C2H3CO+HO2 40700.0	1.005E+013	0.000
!REF:BASED ON CH3CHO+HO2		
C*CCHO+HO2<=>C2H3CO+H2O2 11920.0	3.010E+012	0.000
C*CCHO+CH3<=>C2H3CO+CH4 5911.0	2.608E+006	1.780
!REF:ANALOGY WITH ACETALDEHYDE.		
C*CCHO+C2H3<=>C2H3CO+C2H4 8440.0	1.740E+012	0.000
!REF:ANALOGY WITH CH3CHO+CH3O		
C*CCHO+CH3O<=>C2H3CO+CH3OH 3300.0	1.000E+012	0.000
!REF:BASED ON CH3CHO+HO2		
C*CCHO+CH3O2<=>C2H3CO+CH3O2H 11920.0	3.010E+012	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
C2H3+CO<=>C2H3CO 4810.0	1.510E+011	0.000
!REF:		
C2H5+HCO<=>C2H5CHO 0.0	1.810E+013	0.000
!REF:ANALOGY WITH CH3CHO+H		
C2H5CHO+H<=>C2H5CO+H2 4200.0	4.000E+013	0.000
!REF:ANALOGY WITH CH3CHO+O		
C2H5CHO+O<=>C2H5CO+OH 1790.0	5.000E+012	0.000
!REF:ESTIMATE		
C2H5CHO+OH<=>C2H5CO+H2O -340.0	2.690E+010	0.760
!REF:FIT TO DATA ON NIST STANDARD REFERENCE DATABASE 17 -2Q98		
C2H5CHO+CH3<=>C2H5CO+CH4 5911.0	2.608E+006	1.780
!REF:ANALOGY WITH CH3CHO+HO2		
C2H5CHO+HO2<=>C2H5CO+H2O2 13600.0	2.800E+012	0.000
!REF:ANALOGY WITH CH3CHO+CH3O		
C2H5CHO+CH3O<=>C2H5CO+CH3OH 3300.0	1.000E+012	0.000



!REF:ANALOGY WITH CH3CHO+HO2 C2H5CHO+CH3O2<=>C2H5CO+CH3O2H 11920.0	3.010E+012	0.000
!REF:ACETALDEHYDE ANALOG C2H5CHO+C2H5<=>C2H5CO+C2H6 8000.0	1.000E+012	0.000
C2H5CHO+C2H5O<=>C2H5CO+C2H5OH 3300.0	6.026E+011	0.000
!REF:BASED ON CH3CHO+HO2 C2H5CHO+C2H5O2<=>C2H5CO+C2H5O2H 11920.0	3.010E+012	0.000
!REF:ESTIMATE C2H5CHO+O2<=>C2H5CO+HO2 40700.0	1.005E+013	0.000
!REF:BASED ON CH3CHO+HO2 C2H5CHO+CH3CO3<=>C2H5CO+CH3CO3H 11920.0	3.010E+012	0.000
!REF:!ANALOGY WITH ACETALDEHYDE C2H5CHO+C2H3<=>C2H5CO+C2H4 8440.0	1.700E+012	0.000
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986) C2H5+CO<=>C2H5CO 4810.0	1.510E+011	0.000
!REF:COOK ET AL. J. PHYS. CHEM A 2009, 113, 9974-9980 CH3OCH3 (+M) <=> CH3+CH3O (+M) 83890.0	4.380E+021	-1.570
LOW/ 42790.0/ TROE/ 4.540E-001 1.000E-030 2.510E+003/	7.520E+015	0.000
!REF:ARIF M, ET AL., J. PHYS. CHEM. A, 101, 13, 2436-2441 (1997). CH3OCH3+OH<=>CH3OCH2+H2O -651.7	6.324E+006	2.000
!REF:CURRAN, FIT TO NIST DATABASE CH3OCH3+H<=>CH3OCH2+H2 3384.0	7.721E+006	2.090
!REF:CURRAN 08 NIST FIT CH3OCH3+O<=>CH3OCH2+OH 2250.0	7.750E+008	1.360
!REF:BASED ON J. AGUILERA-IPARRAGUIRRE ET AL  !REF:J PHYS CHEM A (2008) 112(30): 7047-7054.  !REF:THE A-FACTOR FOR ABSTRACTION BY HO2 AND CH3O2 WAS MULTIPLIED BY 0.5 CH3OCH3+HO2<=>CH3OCH2+H2O2 12090.0	8.670E+002	3.010

CH3OCH3+CH3O2<=>CH3OCH2+CH3O2H 13190.0	3.120E+002	3.120
!REF:		
CH3OCH3+CH3<=>CH3OCH2+CH4 5700.0	1.445E-006	5.730
CH3OCH3+O2<=>CH3OCH2+HO2 44910.0	4.100E+013	0.000
!REF:ESTIMATE		
CH3OCH3+CH3O<=>CH3OCH2+CH3OH 4074.0	6.020E+011	0.000
!REF:		
CH3OCH3+CH3OCH2O2<=>CH3OCH2+CH3OCH2O2H 17690.0	5.000E+012	0.000
CH3OCH3+O2CHO<=>CH3OCH2+HO2CHO 13910.0	4.425E+004	2.600
CH3OCH3+OCHO<=>CH3OCH2+HOCHO 17690.0	1.000E+013	0.000
CH3OCH2<=>CH2O+CH3 25500.0	1.600E+013	0.000
!REF:ESTIMATE		
CH3OCH2+CH3O<=>CH3OCH3+CH2O 0.0	2.410E+013	0.000
CH3OCH2+CH2O<=>CH3OCH3+HCO 5862.0	5.490E+003	2.800
CH3OCH2+CH3CHO<=>CH3OCH3+CH3CO 8499.0	1.260E+012	0.000
CH3OCH2+O2<=>CH3OCH2O2 0.0	2.000E+012	0.000
!REF:!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
!REF:!1/ 2 CH3O2+CH2O<=>CH3O2H+HCO		
CH3OCH2O2+CH2O<=>CH3OCH2O2H+HCO 11660.0	1.000E+012	0.000
!REF:ESTIMATE		
CH3OCH2O2+CH3CHO<=>CH3OCH2O2H+CH3CO 13600.0	2.800E+012	0.000
CH3OCH2O2+CH3OCH2O2=>O2+CH3OCH2O+CH3OCH2O 0.0	1.547E+023	-4.500
CH3OCH2O+OH<=>CH3OCH2O2H 0.0	2.000E+013	0.000
CH3O+CH2O<=>CH3OCH2O 7960.0	1.000E+011	0.000
CH3OCH2O+O2<=>CH3OCHO+HO2 500.0	5.000E+010	0.000
!REF:		
CH3OCHO+H<=>CH3OCH2O 7838.0	1.000E+013	0.000
!REF:ESTIMATE EA EQUALS DELTAH+RS+EABS		
CH3OCH2O2<=>CH2OCH2O2H 21580.0	6.000E+010	0.000

!REF: ESTIMATE EA<=>DELTAU+EADDN.  
CH2OCH2O2H=>OH+CH2O+CH2O 1.500E+013 0.000  
20760.0

!REF:ESTIMATE  
CH2OCH2O2H+O2<=>O2CH2OCH2O2H 7.000E+011 0.000  
0.0  
O2CH2OCH2O2H<=>HO2CH2OCHO+OH 4.000E+010 0.000  
18580.0  
HO2CH2OCHO<=>OCH2OCHO+OH 2.000E+016 0.000  
40500.0

!REF:WKM RECOMMENDATION 8/ 9/ 2010

!REF:ESTIMATE  
CH2O+OCHO<=>OCH2OCHO 1.250E+011 0.000  
11900.0  
OCH2OCHO<=>HOCH2OCO 1.000E+011 0.000  
14000.0  
HOCH2O+CO<=>HOCH2OCO 1.500E+011 0.000  
4800.0  
CH2OH+CO2<=>HOCH2OCO 1.500E+011 0.000  
35720.0

!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.  
CH2OCHO+H<=>CH3OCHO 1.000E+014 0.000  
0.0  
CH3OCO+H<=>CH3OCHO 1.000E+014 0.000  
0.0

!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.  
CH3O+HCO<=>CH3OCHO 3.000E+013 0.000  
0.0

!REF:ESTIMATE  
CH3+OCHO<=>CH3OCHO 1.000E+013 0.000  
0.0  
CH3OCHO+O2<=>CH3OCO+HO2 1.000E+013 0.000  
49700.0  
CH3OCHO+O2<=>CH2OCHO+HO2 2.050E+013 0.000  
52000.0

!REF:ANOLOGY TO PROPANE  
CH3OCHO+OH<=>CH3OCO+H2O 1.580E+007 1.800  
934.0  
CH3OCHO+OH<=>CH2OCHO+H2O 5.270E+009 0.970  
1586.0

!REF:CURRAN ESTIMATE TSANG '88 PRIMARY H  
CH3OCHO+HO2<=>CH3OCO+H2O2 4.820E+003 2.600  
13910.0

!REF:CURRAN ESTIMATE TSANG '88 SECONDARY H  
CH3OCHO+HO2<=>CH2OCHO+H2O2 2.380E+004 2.550  
16490.0

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

CH3OCHO+O<=>CH3OCO+OH 2830.0	2.755E+005	2.450		
!REF: FIT TO COHEN/ WESTBERG '86				
CH3OCHO+O<=>CH2OCHO+OH 4750.0	9.800E+005	2.430		
!REF:1/ 2 TSANG'S C3H8+H				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+H<=>CH3OCO+H2 4471.0	6.500E+005	2.400		
CH3OCHO+H<=>CH2OCHO+H2 6756.0	6.650E+005	2.540		
!REF:C3H8+CH3<=>IC3H7+CH4				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+CH3<=>CH3OCO+CH4 5481.0	7.550E-001	3.460		
!REF:C3H8+CH3<=>NC3H7+CH4				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+CH3<=>CH2OCHO+CH4 7154.0	4.520E-001	3.650		
!REF:ESTIMATE				
CH3OCHO+CH3O<=>CH3OCO+CH3OH 5000.0	5.480E+011	0.000		
CH3OCHO+CH3O<=>CH2OCHO+CH3OH 6458.0	2.170E+011	0.000		
!REF:ANOLOGY WITH HO2				
CH3OCHO+CH3O2<=>CH3OCO+CH3O2H 13910.0	4.820E+003	2.600		
CH3OCHO+CH3O2<=>CH2OCHO+CH3O2H 16490.0	2.380E+004	2.550		
!REF:C3H8+HCO				
!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)				
CH3OCHO+HCO<=>CH3OCO+CH2O 17010.0	5.400E+006	1.900		
CH3OCHO+HCO<=>CH2OCHO+CH2O 18430.0	1.025E+005	2.500		
!REF:FISHER, E.M. ET AL., PROC. COMB. INST., VOL. 28, 2000.				
CH3OCO<=>CH2OCHO 40670.0	1.629E+012	-0.180		
!REF: PRIVATE COMMUNICATION FROM S.J. KLIPPENSTEIN				
CH3OCO<=>CH3+CO2 13656.7	8.691E+017	-1.810		
PLOG/	0.0500	9.720E+012	-1.310	9416.7/
PLOG/	1.0000	1.250E+016	-1.830	11340.8/
PLOG/	10.0000	1.040E+018	-2.100	12826.9/
PLOG/	100.0000	8.690E+017	-1.810	13656.7/

CH3OCO<=>CH3O+CO				8.691E+017	-1.810
13656.7					
PLOG/	0.0500	1.030E+003	1.290	25401.0/	
PLOG/	1.0000	4.090E+005	0.810	21969.1/	
PLOG/	10.0000	9.020E+014	-1.720	21767.5/	
PLOG/	100.0000	2.825E+022	-3.440	23592.4/	

!REF:PIERRE GLAUDE'S RATES

!REF: CURRAN ESTIMATE

CH2O+HCO<=>CH2OCHO				1.500E+011	0.000
11900.0					

!REF:OEHSCHLAEGER ET AL., PROC COMB INST 30 (2005) 1119-1127

C3H8(+M)<=>CH3+C2H5(+M)				1.290E+037	-5.840
97380.0					

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/	

!REF:ESTIMATE

NC3H7+H<=>C3H8				1.000E+014	0.000
0.0					

!REF:ESTIMATE

IC3H7+H<=>C3H8				1.000E+014	0.000
0.0					

!REF:

C3H8+O2<=>IC3H7+HO2				2.000E+013	0.000
49640.0					

C3H8+O2<=>NC3H7+HO2				6.000E+013	0.000
52290.0					

H+C3H8<=>H2+IC3H7				1.300E+006	2.400
4471.0					

H+C3H8<=>H2+NC3H7				3.490E+005	2.690
6450.0					

C3H8+O<=>IC3H7+OH				5.490E+005	2.500
3140.0					

C3H8+O<=>NC3H7+OH				3.710E+006	2.400
5505.0					

C3H8+OH<=>NC3H7+H2O				1.054E+010	0.970
1586.0					

C3H8+OH<=>IC3H7+H2O				4.670E+007	1.610
-35.0					

!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.

C3H8+HO2<=>IC3H7+H2O2				6.320E+001	3.370
13720.0					

C3H8+HO2<=>NC3H7+H2O2				4.080E+001	3.590
17160.0					

!REF:FIT TO NIST DATABASE

CH3+C3H8<=>CH4+IC3H7				6.400E+004	2.170
7520.0					

!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
CH3+C3H8<=>CH4+NC3H7	9.040E-001	3.650
7154.0		
!REF:FROM HAUTMAN, D. J., SANTORO, R. J., DRYER, F. L.,		
!REF:AND GLASSMAN, I., TO BE PUBLISHED.		
IC3H7+C3H8<=>NC3H7+C3H8	3.000E+010	0.000
12900.0		
C2H3+C3H8<=>C2H4+IC3H7	1.000E+011	0.000
10400.0		
C2H3+C3H8<=>C2H4+NC3H7	1.000E+011	0.000
10400.0		
C2H5+C3H8<=>C2H6+IC3H7	1.000E+011	0.000
10400.0		
C2H5+C3H8<=>C2H6+NC3H7	1.000E+011	0.000
10400.0		
!REF:DAGAUT ET AL., CST 71, 111(1990)		
C3H8+C3H5-A<=>NC3H7+C3H6	7.940E+011	0.000
20500.0		
C3H8+C3H5-A<=>IC3H7+C3H6	7.940E+011	0.000
16200.0		
!REF:DRYER ESTIMATE		
C3H8+CH3O<=>NC3H7+CH3OH	3.000E+011	0.000
7000.0		
C3H8+CH3O<=>IC3H7+CH3OH	3.000E+011	0.000
7000.0		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
!REF:SCALED AS PER CARSTENSEN ET AL		
CH3O2+C3H8<=>CH3O2H+NC3H7	1.386E+000	3.970
18280.0		
CH3O2+C3H8<=>CH3O2H+IC3H7	1.019E+001	3.580
14810.0		
C2H5O2+C3H8<=>C2H5O2H+NC3H7	1.386E+000	3.970
18280.0		
C2H5O2+C3H8<=>C2H5O2H+IC3H7	1.019E+001	3.580
14810.0		
!REF:ANALOGY TO C2H6+HO2		
NC3H7O2+C3H8<=>NC3H7O2H+NC3H7	1.700E+013	0.000
20460.0		
!REF:WALKER, R. W., REACTION KINETICS,		
!REF:VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975		
NC3H7O2+C3H8<=>NC3H7O2H+IC3H7	2.000E+012	0.000
17000.0		
!REF:ANALOGY TO C2H6+HO2		
IC3H7O2+C3H8<=>IC3H7O2H+NC3H7	1.700E+013	0.000
20460.0		

!REF:WALKER, R. W., REACTION KINETICS,

!REF:VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975

IC3H7O2+C3H8<=>IC3H7O2H+IC3H7 17000.0	2.000E+012	0.000
C3H8+CH3CO3<=>IC3H7+CH3CO3H 17000.0	2.000E+012	0.000

!REF:ANALOGY TO C2H6+HO2

C3H8+CH3CO3<=>NC3H7+CH3CO3H 20460.0	1.700E+013	0.000
C3H8+O2CHO<=>NC3H7+HO2CHO 16480.0	5.520E+004	2.550
C3H8+O2CHO<=>IC3H7+HO2CHO 13910.0	1.475E+004	2.600

!REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006

!REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST

IC3H7+H<=>C2H5+CH3 0.0	2.000E+013	0.000
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!REF:TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)

IC3H7+OH<=>C3H6+H2O 0.0	2.410E+013	0.000
IC3H7+O<=>CH3COCH3+H 0.0	4.818E+013	0.000
IC3H7+O<=>CH3CHO+CH3 0.0	4.818E+013	0.000

!REF:REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006

NC3H7+O2<=>C3H6+HO2 3000.0	3.000E-019	0.000
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!REF:ANALOGY WITH ACETALDEHYDE

C2H5CHO+NC3H7<=>C2H5CO+C3H8 8440.0	1.700E+012	0.000
C2H5CHO+IC3H7<=>C2H5CO+C3H8 8440.0	1.700E+012	0.000
C2H5CHO+C3H5-A<=>C2H5CO+C3H6 8440.0	1.700E+012	0.000

!REF:LASKIN ET AL. IJCK 32 589-614 2000

C2H3+CH3 (+M) <=> C3H6 (+M) 0.0	2.500E+013	0.000
LOW/ 9769.8/	4.270E+058	-11.940
TROE/ 1.750E-001 1.341E+003 6.000E+004 1.014E+004/ C3H5-A+H (+M) <=> C3H6 (+M) 0.0	1.000E+014	0.000
LOW/ 5967.8/	6.650E+059	-12.000
TROE/ 2.000E-002 1.097E+003 1.097E+003 6.860E+003/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/ C3H6 <=> C3H5-S+H 140000.0	7.710E+069	-16.090

C3H6<=>C3H5-T+H 5.620E+071 -16.580  
139300.0

!REF: ANALOGY WITH C2H4

C3H6+O<=>C2H5+HCO 7.450E+006 1.880  
183.0  
C3H6+O=>CH2CO+CH3+H 3.050E+006 1.880  
183.0  
C3H6+O=>CH3CHCO+H+H 3.050E+006 1.880  
183.0  
C3H6+O<=>C3H5-A+OH 5.240E+011 0.700  
5884.0  
C3H6+O<=>C3H5-S+OH 1.200E+011 0.700  
8959.1  
C3H6+O<=>C3H5-T+OH 6.030E+010 0.700  
7632.0

!REF: TOTAL RATE ZADOR (PHYS. CHEM. CHEM. PHYS., 2009, 11,  
11040-11053)/VASU(J. PHYS. CHEM. A 2010, 114, 11529-11537) ALTERED  
BRANCHING RATIO

C3H6+OH<=>C3H5-A+H2O 4.460E+006 2.072  
1050.8  
C3H6+OH<=>C3H5-S+H2O 1.860E+005 2.369  
2502.0  
C3H6+OH<=>C3H5-T+H2O 1.800E+006 1.979  
2235.2

!REF:Bill

!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+CH3O<=>C3H5-A+CH3OH 8.400E+010 0.000  
2600.0

!REF: C3 NUIG CALCULATION J.M

C3H6+HO2<=>C3H5-S+H2O2 9.570E+002 3.059  
20798.6  
C3H6+HO2<=>C3H5-T+H2O2 1.560E+004 2.820  
24427.9  
C3H6+HO2<=>IC3H7O2 1.050E-025 3.520  
5109.0  
PLOG/ 0.0130 8.280E+054 -14.710 21141.0/  
PLOG/ 0.9869 1.170E+042 -10.250 18891.0/  
PLOG/ 9.8700 1.170E+038 -8.770 18811.0/  
PLOG/ 98.6900 5.570E+022 -3.910 13896.0/  
C3H6+HO2<=>C3H6OOH2-1 4.850E-021 2.650  
11201.0  
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  
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				
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				
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/	
C3H6+HO2<=>C3H5-A+H2O2				3.070E-002	4.403
	13547.2				

!REF:LASKIN ET AL IJCK 32 589-614 2000

!REF: CURRAN EST

C3H6+H<=>NC3H7				1.000E+000	1.000
	0.0				
PLOG/	0.0013	7.990E+081	-23.161	22239.0/	
PLOG/	0.0400	4.240E+068	-18.427	19665.0/	
PLOG/	1.0000	1.040E+049	-11.500	15359.0/	
PLOG/	10.0000	6.200E+041	-8.892	14637.0/	
PLOG/	100.0000	-6.450E+031	-5.851	8177.8/	
DUP					
C3H6+H<=>NC3H7				1.000E+000	1.000
	0.0				
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	7.240E+026	-4.210	6825.0/	
DUP					
C3H6+H<=>C2H4+CH3				1.000E+000	1.000
	1.0				
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				
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				
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				

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						
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						
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						
C3H6+H<=>C3H5-A+H2				3.644E+005		2.455
4361.2						
C3H6+H<=>C3H5-T+H2				1.498E+002		3.381
8909.5						
C3H6+H<=>C3H5-S+H2				5.101E+002		3.234
12357.0						
DUP						
C3H6+H<=>C3H5-S+H2				3.969E+002		3.252
12007.0						
DUP						
C2H4+CH3<=>C2H3+CH4				9.760E+002		2.947
15148.0						
DUP						
C2H4+CH3<=>C2H3+CH4				8.130E-005		4.417
8835.8						
DUP						
!REF:LASKIN ET AL IJCK 32 589-614 2000						
!REF:ORIGINAL:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.						
!REF: KINETICS FROM FRANKLIN C GOLDSMITH J. PHYS. CHEM. A, 2012, 116						
(13), PP 3325-3346						
C3H5-A+HO2<=>C3H5O+OH				1.000E+011		0.000
0.0						
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						
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<=>C*CCHO+H2O				1.000E+011	0.000
0.0					
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<=>C*CCHO+H2O				1.000E+011	0.000
0.0					
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					
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					
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<=>C2H3OCH2				1.000E+011	0.000
0.0					
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					
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<=>C*CCHO+H				1.000E+011	0.000
0.0					
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						
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/		
C2H3OCH2<=>C2H3+CH2O					1.000E+011	0.000
0.0						
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/		
C2H3OCH2<=>CH2CH2CHO					1.000E+011	0.000
0.0						
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/		
C2H3OCH2<=>C*CCHO+H					1.000E+011	0.000
0.0						
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/		
C2H3OCH2<=>C2H4+HCO					1.000E+011	0.000
0.0						
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						
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<=>C*CCHO+H					1.000E+011	0.000
0.0						
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					
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<=>C*CCHO+H				1.000E+011	0.000
0.0					
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					
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/	

!REF: ESTIMATE C3 NUIG S. M. BURKE

C3H6+O2<=>C3H5-A+HO2				5.960E+019	-1.670
46192.1					
C3H6+O2<=>C3H5-S+HO2				2.000E+013	0.000
62270.0					
C3H6+O2<=>C3H5-T+HO2				1.000E+013	0.000
58770.0					

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

C3H6+CH3<=>C3H5-A+CH4				2.210E+000	3.500
5675.0					
C3H6+CH3<=>C3H5-S+CH4				1.348E+000	3.500
12850.0					
C3H6+CH3<=>C3H5-T+CH4				8.400E-001	3.500
11660.0					

!REF:!ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)

C3H6+C2H5<=>C3H5-A+C2H6				1.000E+011	0.000
9800.0					

!REF:ANALOGY TO C3H6+HO2

C3H6+CH3O2<=>C3H5-A+CH3O2H				7.680E-002	4.403
13547.2					
C3H6+CH3CO3<=>C3H5-A+CH3CO3H				7.680E-002	4.403
13547.2					

!REF:

!REF:ANALOGY TO C3H6+HO2

C3H6+C2H5O2<=>C3H5-A+C2H5O2H	7.680E-002	4.403
13547.2		
C3H6+NC3H7O2<=>C3H5-A+NC3H7O2H	7.680E-002	4.403
13547.2		
C3H6+IC3H7O2<=>C3H5-A+IC3H7O2H	7.680E-002	4.403
13547.2		

!REF: ZADOR PHYS. CHEM. CHEM. PHYS., 2009, 11, 11040-11053

C3H6+OH<=>C3H5OH+H	2.290E+013	0.070		
10580.0				
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				
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				
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				
PLOG/	0.0013	3.47E+06	1.53	4288/
PLOG/	0.0100	1.08E+07	1.34	4576/
PLOG/	0.0130	9.76E+06	1.33	4589/
PLOG/	0.0250	5.14E+06	1.36	4594/
PLOG/	0.1000	3.13E+05	1.69	4603/
PLOG/	0.1315	1.39E+05	1.80	4603/
PLOG/	1.0000	1.03E+02	2.83	4530/
PLOG/	10.0000	3.40E-02	3.89	4390/
PLOG/	100.0000	4.46E-06	5.03	4132/
!C3H6+OH<=>CH3CHO+CH3	6.930E+005	1.490		
-536.0				

!PLOG/	0.0013	6.930E+005	1.490	-536.0/
!PLOG/	0.0100	5.940E+003	2.010	-560.0/
!PLOG/	0.0130	1.100E+003	2.220	-680.0/
!PLOG/	0.0250	1.070E+002	2.500	-759.0/
!PLOG/	0.1000	7.830E-001	3.100	-919.0/
!PLOG/	0.1315	3.070E-001	3.220	-946.0/
!PLOG/	1.0000	3.160E-004	4.050	-1144.0/
!PLOG/	10.0000	7.590E-006	4.490	-680.0/
!PLOG/	100.0000	5.450E-005	4.220	1141.0/
C3H6+OH<=>CH3CHO+CH3	1.370e+12	0.00	-1.040e+03	!Heyberger et al., combust Flame, 126 (2001) 1780-1802
C3H6+OH<=>C2H5+CH2O	1.370e+12	0.00	-1.040e+03	!Heyberger et al., combust Flame, 126 (2001) 1780-1802
C3H6+OH<=>C3H6OH1-2			5.100E+054	-20.700
32402.0				
PLOG/	0.0013	2.300E+078	-20.700	32402.0/
PLOG/	0.0100	2.740E+077	-20.000	33874.0/
PLOG/	0.0130	1.070E+076	-19.580	32874.0/
PLOG/	0.0250	3.680E+073	-18.790	31361.0/
PLOG/	0.1000	1.040E+068	-17.010	27909.0/
PLOG/	0.1315	7.230E+066	-16.640	27162.0/
PLOG/	1.0000	1.950E+059	-14.170	23079.0/
PLOG/	10.0000	7.580E+053	-12.230	22976.0/
PLOG/	100.0000	1.430E+048	-10.230	23772.0/
DUP				
C3H6+OH<=>C3H6OH1-2			1.420E+036	-15.840
11594.0				
PLOG/	0.0013	6.410E+059	-15.840	11594.0/
PLOG/	0.0100	7.280E+059	-15.510	12898.0/
PLOG/	0.0130	2.790E+059	-15.340	12913.0/
PLOG/	0.0250	2.650E+058	-14.930	12936.0/
PLOG/	0.1000	1.350E+056	-14.040	12945.0/
PLOG/	0.1315	3.980E+055	-13.850	12887.0/
PLOG/	1.0000	1.550E+050	-12.040	11493.0/
PLOG/	10.0000	6.410E+041	-9.350	8921.0/
PLOG/	100.0000	2.300E+032	-6.310	6088.0/
DUP				
C3H6+OH<=>C3H6OH2-1			5.100E+054	-20.700
32402.0				
PLOG/	0.0013	2.140E+059	-15.840	11594.0/
PLOG/	0.0100	2.430E+059	-15.510	12898.0/
PLOG/	0.0130	9.300E+058	-15.340	12913.0/
PLOG/	0.0250	8.830E+057	-14.930	12936.0/
PLOG/	0.1000	4.500E+055	-14.040	12945.0/
PLOG/	0.1315	1.330E+055	-13.850	12887.0/
PLOG/	1.0000	5.180E+049	-12.040	11493.0/
PLOG/	10.0000	2.140E+041	-9.350	8921.0/
PLOG/	100.0000	7.650E+031	-6.310	6088.0/
DUP				
C3H6+OH<=>C3H6OH2-1			1.420E+036	-15.840
11594.0				
PLOG/	0.0013	7.680E+077	-20.700	32402.0/
PLOG/	0.0100	9.130E+076	-20.000	33874.0/
PLOG/	0.0130	3.550E+075	-19.580	32874.0/
PLOG/	0.0250	1.230E+073	-18.790	31361.0/
PLOG/	0.1000	3.450E+067	-17.010	27909.0/
PLOG/	0.1315	2.410E+066	-16.640	27162.0/
PLOG/	1.0000	6.500E+058	-14.170	23079.0/

PLOG/ 10.0000 2.530E+053 -12.230 22976.0/  
PLOG/ 100.0000 4.780E+047 -10.230 23772.0/  
DUP

!REF:Bill Sept 2013

!REF:For sc3h5oh, assume that the allyl hydrogen is abstracted and then C\*CCHO+h are formed.

!REF: Use rate primary allylic

!REF: Used rate of c3h6+r<=>c2h5-a+rh.

!REF: SAUDI ARAMCO MECH 1.3 (NO REFERENCE)

SC3H5OH+O2=>C\*CCHO+H+HO2 3.000E+013 0.000  
39100.0

!REF: TSANG 1991

SC3H5OH+OH=>C\*CCHO+H+H2O 3.100E+006 2.000  
-298.0

SC3H5OH+H=>C\*CCHO+H+H2 1.730E+005 2.500  
2492.0

SC3H5OH+O=>C\*CCHO+H+OH 1.750E+012 0.700  
5884.0

SC3H5OH+HO2=>C\*CCHO+H+H2O2 9.600E+003 2.600  
13900.0

SC3H5OH+CH3=>C\*CCHO+H+CH4 2.210E+000 3.500  
5675.0

!REF: USE HO2 ABSTRACTION RATE CONSTANT

SC3H5OH+CH3O2=>C\*CCHO+H+CH3O2H 9.600E+003 2.600  
13900.0

!REF: USED SECONDARY ALKYL H RATE FOR N-ALKANE+CH3O,

!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

!REF: 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+CH3O=>C\*CCHO+H+CH3OH 8.300E+010 0.000  
2600.0

!REF: FROM PROPANOL, MAN ET AL. CNF2013:

!REF: !DASILVA, BOZZELLI, CHEM. PHYS. LETT. 483 (2009) 25-29.  
SC3H5OH+HO2<=>C2H5CHO+HO2 1.490E+005 1.670  
6810.0

!REF: !DASILVA, ANGEW. CHEM. 122 (2010) 7685-7687

SC3H5OH+HOCHO<=>C2H5CHO+HOCHO 2.810E-002 3.286  
-4509.0

!REF: Sarathy et al. CnF2012

SC3H5OH<=>C2H5CHO 8.590E+011 0.318  
55900.0

!REF: WILK, CERNANSKY, PITZ, AND WESTBROOK, C&F 1988.

!C3H6OH1-2+O2<=>HOC3H6O2 1.200E+011 0.000  
-1100.0

!REF:

!HOC3H6O2=>CH3CHO+CH2O+OH 1.250E+010 0.000  
18900.0



!Dagaut isobutene 98

C3H6OH1-2+O2<=>HOC3H6O2 3.25E+26 -4.686 4294 !Dag98

PLOG/1.0000 3.25E+26 -4.686 4294/

PLOG/10.000 1.14E+22 -3.0 4343/

HOC3H6O2=>CH3CHO+CH2O+OH 1.00E+16 0.0 25000.0!Dag98

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589

C2H2+CH3<=>C3H5-A 8.200E+053 -13.320  
33200.0

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/

!REF: ANOLOGY WITH C3H5-A+HO2

C3H5-A+CH3O2<=>C3H5O+CH3O 1.000E+011 0.000  
0.0

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

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

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/

!REF:KLIPPENSTEIN & HARDING 2007

C3H5-A+H<=>C3H4-A+H2 1.232E+003 3.035  
2582.0

!REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.

C3H5-A+O<=>C\*CCHO+H 6.000E+013 0.000  
0.0

!REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.

C3H5-A+OH=>C\*CCHO+H+H 5.300E+037 -6.710  
29306.0

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/

!REF:TSANG, W. J.PHYS.CHEM.REF.DATA 1991, 20, 221.

C3H5-A+OH<=>C3H4-A+H2O 6.000E+012 0.000  
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000  
C3H5-A+CH3<=>C3H4-A+CH4 3.000E+012 -0.320  
-131.0

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).  
C3H5-A+C2H5<=>C2H6+C3H4-A 4.000E+011 0.000  
0.0  
C3H5-A+C2H5<=>C2H4+C3H6 4.000E+011 0.000  
0.0  
C3H5-A+C2H3<=>C2H4+C3H4-A 1.000E+012 0.000  
0.0

!REF:!WANG, J. PHYS. CHEM. REF. DATA 20, 221-273, (1991)

!REF:LASKIN ET AL. IJCK 32 589-614 2000  
C3H5-A+O2<=>C3H4-A+HO2 4.990E+015 -1.400  
22428.0  
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  
PLOG/ 1.0000 1.190E+015 -1.010 20128.0/  
PLOG/ 10.0000 7.140E+015 -1.210 21046.0/  
C3H5-A+O2<=>C\*CCHO+OH 1.820E+013 -0.410  
22859.0  
PLOG/ 1.0000 1.820E+013 -0.410 22859.0/  
PLOG/ 10.0000 2.470E+013 -0.450 23017.0/

!REF:LASKIN ET AL. IJCK 32 589-614 2000  
C3H5-A+HCO<=>C3H6+CO 6.000E+013 0.000  
0.0  
C2H3+CH3<=>C3H5-A+H 1.500E+024 -2.830  
18618.0

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589  
C3H5-A<=>C3H5-T 3.900E+059 -15.420  
75400.0  
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/

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589  
C3H5-A<=>C3H5-S 1.300E+055 -14.530  
73800.0  
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/

!REF: Analogy C2H3+O2 Klippenstein

C3H5-S+O2<=>CH3CHO+HCO 5748.4	3.100E+031	-5.944
C3H5-S+O2<=>CH3CHCHO+O 5142.9	5.380E+018	-2.140
C3H5-S+O2<=>C*CCHO+OH 5142.9	2.700E+019	-2.140

!REF:DAGAUT, P. ET AL., CST 71, 111(1990).

C3H5-S+H<=>C3H4-A+H2 0.0	3.333E+012	0.000
C3H5-S+CH3<=>C3H4-A+CH4 0.0	1.000E+011	0.000

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589

C2H2+CH3<=>C3H5-T 18000.0	6.800E+020	-4.160	18000.0/
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/

!REF:LASKIN ET AL. IJCK 32 589-614 2000

C3H5-S+H<=>C3H4-P+H2 0.0	3.340E+012	0.000
C3H5-S+O<=>C2H4+HCO 0.0	6.000E+013	0.000
C3H5-S+OH=>C2H4+HCO+H 0.0	5.000E+012	0.000
C3H5-S+HO2=>C2H4+HCO+OH 0.0	2.000E+013	0.000
C3H5-S+HCO<=>C3H6+CO 0.0	9.000E+013	0.000
C3H5-S+CH3<=>C3H4-P+CH4 0.0	1.000E+011	0.000

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589

C3H5-T<=>C3H5-S 52200.0	1.600E+044	-12.160	52200.0/
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/

!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589

C3H4-A+H<=>C3H5-S 15200.0	1.100E+030	-6.520	15200.0/
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/

!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)

C3H4-A+C3H4-A<=>C3H5-A+C3H3 64746.7	5.000E+014	0.000
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!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H5-T+O2<=>CH3COCH2+O		9.860E+025	-3.751	
11255.4				
C3H5-T+O2<=>CH3CO+CH2O		2.550E+020	-2.608	
1565.7				
C3H5-T+O2<=>C3H4-A+HO2		3.590E+010	-0.270	
-413.6				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H5-T+H<=>C3H4-P+H2		3.340E+012	0.000	
0.0				
C3H5-T+CH3<=>C3H4-P+CH4		1.000E+011	0.000	
0.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H5-T+O<=>CH3+CH2CO		6.000E+013	0.000	
0.0				
C3H5-T+OH=>CH3+CH2CO+H		5.000E+012	0.000	
0.0				
C3H5-T+HO2=>CH3+CH2CO+OH		2.000E+013	0.000	
0.0				
C3H5-T+HCO<=>C3H6+CO		9.000E+013	0.000	
0.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).				
C3H4-A+HO2=>CH2CO+CH2+OH		4.000E+012	0.000	
19000.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H4-A+O<=>C2H4+CO		2.000E+007	1.800	
1000.0				
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).				
C3H4-A+O<=>C2H2+CH2O		3.000E-003	4.610	
-4243.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H4-A+CH3<=>C3H3+CH4		1.300E+012	0.000	
7700.0				
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).				
C3H4-A+C3H5-A<=>C3H3+C3H6		2.000E+011	0.000	
7700.0				
!REF:LASKIN ET AL. IJCK 32 589-614 2000				
C3H4-A+C2H<=>C2H2+C3H3		1.000E+013	0.000	
0.0				
!REF:DAVIS AND LAW J. PHYS. CHEM. A 1999, 103, 5889-589				
C3H4-P+H<=>C3H5-A		1.100E+060	-14.560	
28100.0				
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/		
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
C3H4-P+C3H3<=>C3H4-A+C3H3				6.140E+006	1.740	
10450.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
C3H4-P+O<=>HCCO+CH3				7.300E+012	0.000	
2250.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
C3H4-P+O<=>C2H4+CO				1.000E+013	0.000	
2250.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
C3H4-P+C2H<=>C2H2+C3H3				1.000E+013	0.000	
0.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
C3H4-P+CH3<=>C3H3+CH4				1.800E+012	0.000	
7700.0						
!REF:PITZ ESTIMATE						
C2H+CH3<=>C3H4-P				8.000E+013	0.000	
0.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).						
C3H4-P+HO2=>C2H4+CO+OH				3.000E+012	0.000	
19000.0						
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).						
C3H4-P+O<=>C2H3+HCO				3.200E+012	0.000	
2010.0						
!REF:GLAUDE, P.A. ET AL, PROC. COMBUST. INST						
C3H4-P+O<=>C3H3+OH				7.650E+008	1.500	
8600.0						
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).						
C3H4-P+C2H3<=>C3H3+C2H4				1.000E+012	0.000	
7700.0						
C3H4-P+C3H5-A<=>C3H3+C3H6				3.000E+012	0.000	
7700.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
C3H3+O<=>CH2O+C2H				2.000E+013	0.000	
0.0						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						
!REF:LASKIN ET AL. IJCK 32 589-614 2000						

C3H3+HO2=>OH+CO+C2H3 0.0	8.000E+011	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H3+HCO<=>C3H4-A+CO 0.0	2.500E+013	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H3+HCO<=>C3H4-P+CO 0.0	2.500E+013	0.000
!REF:		
C2H5+C2H<=>C3H3+CH3 0.0	1.810E+013	0.000
!REF:DAGAUT, P. ET AL., CST 71, 111(1990).		
C3H4-A+HO2=>C2H4+CO+OH 14000.0	1.000E+011	0.000
C3H4-A+HO2<=>C3H3+H2O2 9632.8	3.580E-002	4.170
C3H4-A+CH3O2<=>C3H3+CH3O2H 9632.8	7.161E-002	4.170
C3H4-P+HO2<=>C3H3+H2O2 9632.8	9.550E-002	4.170
C3H4-P+CH3O2<=>C3H3+CH3O2H 9632.8	9.550E-002	4.170
!REF: ESTIMATE ATkinson 1984 C3 NUIG S.M.B		
C3H4-A+OH<=>CH2CCH2OH -304.0	1.110E+012	0.000
C3H4-A+OH<=>SC3H4OH -304.0	2.220E+012	0.000
!REF: ANALOGY with Curran 2006 alkyl decomp		
CH2CCH2OH<=>CH2O+C2H3 30460.0	9.240E+010	0.870
CH2CCH2OH<=>C*CCHO+H 36770.0	1.110E+011	0.480
CH2CCH2OH<=>HCO+C2H4 30460.0	9.240E+010	0.870
SC3H4OH<=>CH2CO+CH3 30460.0	9.240E+010	0.870
C3H4-A+H<=>C3H3+H2 5522.0	6.625E+003	3.095
!REF: analogies with c3h6 a and s		
C3H4-P+OH<=>C3H3+H2O 1059.6	4.940E+006	2.027
C3H4-A+OH<=>C3H3+H2O 1807.2	1.482E+005	2.492
C3H4-P+H<=>C3H3+H2 4821.0	3.572E+004	2.825
!REF: ESTIMATES C3 NUIG S.M.B from Atkinson 1982 and 1984		
C3H4-P+OH<=>PC3H4OH-2 0.0	3.930E+011	0.000
C3H4-P+OH<=>SC3H4OH 0.0	2.360E+012	0.000

!REF: Matheu et al. IJCK, 2003, 35, 95--119

PC3H4OH-2<=>CH3CHCHO 3.560E+010 0.880  
23238.0

!REF: Pelucchi ECM 2013

CH3CHCHO<=>C\*CCHO+H 4.164E+012 -0.020  
32410.0

CH3CHCHO<=>CH3CHCO+H 8.328E+012 -0.020  
32410.0

C3H3+H<=>C3H2+H2 2.140E+005 2.520  
7453.0

C3H3+H<=>C3H2(S)+H2 3.311E+013 0.195  
17579.0

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

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

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/

C3H4-A<=>C3H4-P 4.786E+048 -10.000  
88685.0

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

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

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

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

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

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/

C3H2(S)+M<=>C3H2+M 1.000E+013 0.000  
0.0

H2CCC(S)+O2<=>CO2+C2H2 1.000E+013 0.000  
0.0

C3H2 (S) +H<=>H2CCC (S) +H				1.000E+013	0.000
0.0					
C3H2C+O2<=>C2H2+CO2				1.000E+013	0.000
0.0					
!REF: MILLER ET AL. J. PHYS. CHEM. A 2008, 112, 9429-9438					
C3H4-A+H<=>C3H5-A				2.210E+061	-15.250
20076.0					
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					
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<=>C3H4-P+H				2.440E+010	1.040
2159.0					
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					
PLOG/	10.0000	1.790E+007	1.980	4521.0/	
PLOG/	100.0000	4.630E+004	2.620	4466.0/	
DUP					
C3H4-A+H<=>CH3+C2H2				3.740E+001	3.350
57.8					
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					
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-A+H<=>C3H5-T				6.440E+102	-27.510
51768.0					
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					
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-P+H<=>C3H5-T				8.850E+051	-13.040
12325.0					
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					
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					
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					
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					
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/	
CH3+C2H2<=>C3H5-S				1.780E+042	-10.400
13647.0					
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					
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					
C3H4-A+O2<=>C3H3+HO2				4.000E+013	0.000
41320.0					
C3H4-P+O2<=>C3H3+HO2				3.000E+013	0.000
42630.0					
C3H3+C3H3<=>C6H5+H				2.020E+033	-6.050
15940.0					
C3H3+C3H3<=>C6H6				1.640E+066	-15.902
27529.0					
DUP					
C3H3+C3H3<=>C6H6				1.200E+035	-7.435
5058.0					
DUP					
C3H3+OH<=>C3H2+H2O				2.000E+013	0.000
8000.0					
C3H3+OH<=>CH2O+C2H2				2.000E+012	0.000
0.0					
C3H3+OH<=>C2H3+HCO				1.000E+013	0.000
0.0					
C3H3+OH<=>C2H4+CO				1.000E+013	0.000
0.0					
C3H3+OH<=>C3H2(S)+H2O				1.000E+012	0.000
0.0					
C3H3+OH<=>H2CCC(S)+H2O				1.000E+012	0.000
0.0					
C3H3+O2<=>CH2CO+HCO				1.700E+005	1.700
1500.0					

!REF: ANALOGY WITH C3H5-A+HO2 !KINETICS FROM FRANKLIN C GOLDSMITH !J.  
 PHYS. CHEM. A, 2012, 116 (13), PP 3325-3346

C3H3+HO2<=>C3H3O+OH				1.000E+011	0.000
0.0					
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					
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					
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					
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<=>C2H2+CO				2.510E+014	0.000
68000.0					
C2H+HCO<=>C2HCHO				1.000E+013	0.000
0.0					
!REF:ESTIMATE					
CH3CHCO+OH<=>C2H5+CO2				1.730E+012	0.000
-1010.0					
CH3CHCO+OH<=>SC2H4OH+CO				2.000E+012	0.000
-1010.0					
CH3CHCO+H<=>C2H5+CO				4.400E+012	0.000
1459.0					
CH3CHCO+O<=>CH3CHO+CO				3.200E+012	0.000
-437.0					
!REF:					
NC3H7+HO2<=>NC3H7O+OH				7.000E+012	0.000
-1000.0					
IC3H7+HO2<=>IC3H7O+OH				7.000E+012	0.000
-1000.0					
CH3O2+NC3H7<=>CH3O+NC3H7O				7.000E+012	0.000
-1000.0					
CH3O2+IC3H7<=>CH3O+IC3H7O				7.000E+012	0.000
-1000.0					
!REF:					
NC3H7+O2<=>NC3H7O2				4.520E+012	0.000
0.0					
IC3H7+O2<=>IC3H7O2				7.540E+012	0.000
0.0					
!REF:ANALOGY TO CH2O+HO2					
NC3H7O2+CH2O<=>NC3H7O2H+HCO				5.600E+012	0.000
13600.0					
!REF:HALF OF CH2O+HO2					
NC3H7O2+CH3CHO<=>NC3H7O2H+CH3CO				2.800E+012	0.000
13600.0					
!REF:ANALOGY TO CH2O+HO2					
IC3H7O2+CH2O<=>IC3H7O2H+HCO				5.600E+012	0.000
13600.0					
!REF:HALF OF CH2O+HO2					
IC3H7O2+CH3CHO<=>IC3H7O2H+CH3CO				2.800E+012	0.000
13600.0					
!REF:					

NC3H7O2+HO2<=>NC3H7O2H+O2 -3275.0	1.750E+010	0.000
IC3H7O2+HO2<=>IC3H7O2H+O2 -3275.0	1.750E+010	0.000
!REF:ANALOGY TO C2H4+HO2		
C2H4+NC3H7O2<=>C2H3+NC3H7O2H 30430.0	1.130E+013	0.000
C2H4+IC3H7O2<=>C2H3+IC3H7O2H 30430.0	1.130E+013	0.000
!REF:ANALOGY TO CH3OH+HO2		
CH3OH+NC3H7O2<=>CH2OH+NC3H7O2H 19360.0	6.300E+012	0.000
CH3OH+IC3H7O2<=>CH2OH+IC3H7O2H 19360.0	6.300E+012	0.000
!REF:HALF OF CH2O+HO2		
C*CCHO+NC3H7O2<=>C2H3CO+NC3H7O2H 13600.0	2.800E+012	0.000
C*CCHO+IC3H7O2<=>C2H3CO+IC3H7O2H 13600.0	2.800E+012	0.000
!REF:ANALOGY TO CH4+HO2		
CH4+NC3H7O2<=>CH3+NC3H7O2H 24640.0	1.120E+013	0.000
CH4+IC3H7O2<=>CH3+IC3H7O2H 24640.0	1.120E+013	0.000
!REF:		
NC3H7O2+CH3O2=>NC3H7O+CH3O+O2 1860.0	1.400E+016	-1.610
IC3H7O2+CH3O2=>IC3H7O+CH3O+O2 1860.0	1.400E+016	-1.610
!REF:TSANG AND HAMPSON, J. PHYS. CHEM. REF. DATA, 15:1087 (1986)		
H2+NC3H7O2<=>H+NC3H7O2H 26030.0	3.010E+013	0.000
H2+IC3H7O2<=>H+IC3H7O2H 26030.0	3.010E+013	0.000
!REF:WESTBROOK ESTIMATE		
IC3H7O2+C2H6<=>IC3H7O2H+C2H5 20460.0	1.700E+013	0.000
NC3H7O2+C2H6<=>NC3H7O2H+C2H5 20460.0	1.700E+013	0.000
IC3H7O2+C2H5CHO<=>IC3H7O2H+C2H5CO 9500.0	2.000E+011	0.000
NC3H7O2+C2H5CHO<=>NC3H7O2H+C2H5CO 9500.0	2.000E+011	0.000
!REF:		
IC3H7O2+CH3CO3=>IC3H7O+CH3CO2+O2 1860.0	1.400E+016	-1.610
NC3H7O2+CH3CO3=>NC3H7O+CH3CO2+O2 1860.0	1.400E+016	-1.610
IC3H7O2+C2H5O2=>IC3H7O+C2H5O+O2 1860.0	1.400E+016	-1.610

NC3H7O2+C2H5O2=>NC3H7O+C2H5O+O2 1860.0	1.400E+016	-1.610
IC3H7O2+IC3H7O2=>O2+IC3H7O+IC3H7O 1860.0	1.400E+016	-1.610
NC3H7O2+NC3H7O2=>O2+NC3H7O+NC3H7O 1860.0	1.400E+016	-1.610
IC3H7O2+NC3H7O2=>IC3H7O+NC3H7O+O2 1860.0	1.400E+016	-1.610
IC3H7O2+CH3<=>IC3H7O+CH3O -1000.0	7.000E+012	0.000
IC3H7O2+C2H5<=>IC3H7O+C2H5O -1000.0	7.000E+012	0.000
IC3H7O2+IC3H7<=>IC3H7O+IC3H7O -1000.0	7.000E+012	0.000
IC3H7O2+NC3H7<=>IC3H7O+NC3H7O -1000.0	7.000E+012	0.000
IC3H7O2+C3H5-A<=>IC3H7O+C3H5O -1000.0	7.000E+012	0.000
NC3H7O2+CH3<=>NC3H7O+CH3O -1000.0	7.000E+012	0.000
NC3H7O2+C2H5<=>NC3H7O+C2H5O -1000.0	7.000E+012	0.000
NC3H7O2+IC3H7<=>NC3H7O+IC3H7O -1000.0	7.000E+012	0.000
NC3H7O2+NC3H7<=>NC3H7O+NC3H7O -1000.0	7.000E+012	0.000
NC3H7O2+C3H5-A<=>NC3H7O+C3H5O -1000.0	7.000E+012	0.000
NC3H7O2H<=>NC3H7O+OH 42500.0	1.500E+016	0.000
!REF:PITZ ESTIMATE		
IC3H7O+OH<=>IC3H7O2H 0.0	1.000E+015	-0.800
!REF:		
C2H5+CH2O<=>NC3H7O 3496.0	1.000E+011	0.000
C2H5CHO+H<=>NC3H7O 6260.0	4.000E+012	0.000
CH3+CH3CHO<=>IC3H7O 9256.0	1.000E+011	0.000
CH3COCH3+H<=>IC3H7O 7270.0	2.000E+012	0.000
!REF:BALLA ET AL., CHEM. PHYSICS, 99, 323 (1985)		
IC3H7O+O2<=>CH3COCH3+HO2 390.0	9.090E+009	0.000
!REF:		
NC3H7O2<=>C3H6OOH1-2 26850.0	6.000E+011	0.000
NC3H7O2<=>C3H6OOH1-3 24400.0	1.125E+011	0.000
IC3H7O2<=>C3H6OOH2-1 29400.0	1.800E+012	0.000
!REF:BOZZELLI, J. AND DEAN, A, 1992		

IC3H7O2<=>C3H6OOH2-2 48880.0	1.230E+035	-6.960
!REF:		
C3H6OOH1-2<=>C3H6O1-2+OH 22000.0	6.000E+011	0.000
C3H6OOH1-3<=>C3H6O1-3+OH 15250.0	7.500E+010	0.000
!REF:		
C3H6+HO2<=>C3H6OOH1-2 11000.0	1.000E+011	0.000
C3H6OOH1-3=>OH+CH2O+C2H4 27400.0	3.035E+015	-0.790
!REF:BOZZELLI AND PITZ, 1995		
C3H6OOH2-1<=>C2H3OOH+CH3 38320.0	6.540E+027	-5.140
C3H6OOH1-2=>C2H4+CH2O+OH 48120.0	1.310E+033	-7.010
!REF:ESTIMATE		
C3H6OOH2-2<=>CH3COCH3+OH 1500.0	9.000E+014	0.000
C3H6OOH1-2+O2<=>C3H6OOH1-2O2 0.0	5.000E+012	0.000
C3H6OOH1-3+O2<=>C3H6OOH1-3O2 0.0	4.520E+012	0.000
C3H6OOH2-1+O2<=>C3H6OOH2-1O2 0.0	4.520E+012	0.000
!REF:		
C3H6OOH1-2O2<=>C3KET12+OH 26400.0	6.000E+011	0.000
C3H6OOH1-3O2<=>C3KET13+OH 21400.0	7.500E+010	0.000
C3H6OOH2-1O2<=>C3KET21+OH 23850.0	3.000E+011	0.000
C3H6OOH2-1O2<=>C3H51-2-3OOH 24400.0	1.125E+011	0.000
C3H6OOH1-2O2<=>C3H51-2-3OOH 29400.0	9.000E+011	0.000
!REF: BOZZELLI AND PITZ, 1993.		
C3H51-2-3OOH<=>AC3H5OOH+HO2 17770.0	2.560E+013	-0.490
!REF:		
C3H6OOH1-3O2<=>C3H52-1-3OOH 26850.0	6.000E+011	0.000
!REF:BOZZELLI AND PITZ, 1993.		
C3H52-1-3OOH<=>AC3H5OOH+HO2 17250.0	1.150E+014	-0.630
!REF:		
C3KET12=>CH3CHO+HCO+OH 43000.0	9.450E+015	0.000

C3KET13=>CH2O+CH2CHO+OH 43000.0	1.000E+016	0.000
C3KET21=>CH2O+CH3CO+OH 43000.0	1.000E+016	0.000
!REF:ESTIMATE		
!REF:		
!REF:ACETALDEHYDE ANALOG		
C3H5O+O2<=>C*CCHO+HO2 6000.0	1.000E+012	0.000
!REF:PITZ ESTIMATE		
C2H3OOH<=>CH2CHO+OH 43000.0	8.400E+014	0.000
!REF:!FLOWERS, M. C., J. CHEM. SOC. FAR. TRANS. I 73, 1927 (1977)		
C3H6O1-2<=>C2H4+CH2O 60000.0	6.000E+014	0.000
!		
!REF:WESTBROOK ESTIMATE		
C3H6O1-2+OH=>CH2O+C2H3+H2O 0.0	5.000E+012	0.000
C3H6O1-2+H=>CH2O+C2H3+H2 5000.0	2.630E+007	2.000
C3H6O1-2+O=>CH2O+C2H3+OH 5200.0	8.430E+013	0.000
C3H6O1-2+HO2=>CH2O+C2H3+H2O2 15000.0	1.000E+013	0.000
C3H6O1-2+CH3O2=>CH2O+C2H3+CH3O2H 19000.0	1.000E+013	0.000
C3H6O1-2+CH3=>CH2O+C2H3+CH4 10000.0	2.000E+011	0.000
!REF:WESTBROOK AND PITZ ESTIMATE (1983)		
C3H6O1-3<=>C2H4+CH2O 60000.0	6.000E+014	0.000
!REF:PITZ ESTIMATE		
C3H6O1-3+OH=>CH2O+C2H3+H2O 0.0	5.000E+012	0.000
C3H6O1-3+O=>CH2O+C2H3+OH 5200.0	8.430E+013	0.000
C3H6O1-3+H=>CH2O+C2H3+H2 5000.0	2.630E+007	2.000
C3H6O1-3+CH3O2=>CH2O+C2H3+CH3O2H 19000.0	1.000E+013	0.000
C3H6O1-3+HO2=>CH2O+C2H3+H2O2 15000.0	1.000E+013	0.000
C3H6O1-3+CH3=>CH2O+C2H3+CH4 10000.0	2.000E+011	0.000
!REF:		
NC3H7O2<=>C3H6+HO2 39510.0	4.308E+036	-7.500

!REF:NEW TROE FIT FROM TIBOR NAGY

!REF:BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253  
C4H10 (+M) <=> C2H5 + C2H5 (+M) 1.355E+037 -6.036  
92929.0  
LOW/ 4.720E+018 0.000  
49578.0/  
TROE/ 7.998E-002 1.000E-020 3.243E+004 4.858E+003/

!REF:NEW TROE FIT FROM TIBOR NAGY

!REF:BASED ON OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253  
C4H10 (+M) <=> NC3H7 + CH3 (+M) 6.600E+052 -10.626  
100330.0  
LOW/ 5.340E+017 0.000  
42959.0/  
TROE/ 9.502E-002 1.000E-020 5.348E+003 4.326E+003/

!REF:

PC4H9+H <=> C4H10 3.610E+013 0.000  
0.0  
SC4H9+H <=> C4H10 3.610E+013 0.000  
0.0  
C4H10+O2 <=> PC4H9+HO2 6.000E+013 0.000  
52340.0  
C4H10+O2 <=> SC4H9+HO2 4.000E+013 0.000  
49800.0

!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)

C4H10+C3H5-A <=> PC4H9+C3H6 7.940E+011 0.000  
20500.0  
C4H10+C3H5-A <=> SC4H9+C3H6 3.160E+011 0.000  
16400.0  
C4H10+C2H5 <=> PC4H9+C2H6 1.580E+011 0.000  
12300.0  
C4H10+C2H5 <=> SC4H9+C2H6 1.000E+011 0.000  
10400.0

!REF:SUNDARAM, K. M. AND FROMENT, G. F., I. AND E. C. FUNDAMENTALS 17,  
174 (1978)

C4H10+C2H3 <=> PC4H9+C2H4 1.000E+012 0.000  
18000.0  
C4H10+C2H3 <=> SC4H9+C2H4 8.000E+011 0.000  
16800.0

!REF:

C4H10+CH3 <=> PC4H9+CH4 9.040E-001 3.650  
7154.0  
C4H10+CH3 <=> SC4H9+CH4 3.020E+000 3.460  
5481.0  
C4H10+H <=> PC4H9+H2 3.490E+005 2.690  
6450.0  
C4H10+H <=> SC4H9+H2 2.600E+006 2.400  
4471.0  
C4H10+OH <=> PC4H9+H2O 1.054E+010 0.970  
1586.0  
C4H10+OH <=> SC4H9+H2O 9.340E+007 1.610  
-35.0



!REF:MICHAEL, KEIL AND KLEM, INT. J. CHEM. KIN. 15, 705 (1983)		
C4H10+O<=>PC4H9+OH	1.130E+014	0.000
7850.0		
C4H10+O<=>SC4H9+OH	5.620E+013	0.000
5200.0		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C4H10+HO2<=>PC4H9+H2O2	4.080E+001	3.590
17160.0		
C4H10+HO2<=>SC4H9+H2O2	1.264E+002	3.370
13720.0		
!REF:DRYER ESTIMATE		
C4H10+CH3O<=>PC4H9+CH3OH	3.000E+011	0.000
7000.0		
C4H10+CH3O<=>SC4H9+CH3OH	6.000E+011	0.000
7000.0		
!REF:ANALOGY TO CH3O		
C4H10+C2H5O<=>PC4H9+C2H5OH	3.000E+011	0.000
7000.0		
C4H10+C2H5O<=>SC4H9+C2H5OH	6.000E+011	0.000
7000.0		
!REF:!WESTBROOK AND PITZ ESTIMATE (1983)		
C4H10+PC4H9<=>SC4H9+C4H10	1.000E+011	0.000
10400.0		
!REF:ANALOGY TO C2H6+HO2		
C4H10+CH3CO3<=>PC4H9+CH3CO3H	1.700E+013	0.000
20460.0		
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION		
!REF:SEATTLE, AUGUST, 1988		
C4H10+CH3CO3<=>SC4H9+CH3CO3H	1.120E+013	0.000
17700.0		
!REF:ANALOGY WITH RH+RO2 --> R+RO2H		
C4H10+O2CHO<=>PC4H9+HO2CHO	1.680E+013	0.000
20440.0		
C4H10+O2CHO<=>SC4H9+HO2CHO	1.120E+013	0.000
17690.0		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
!REF:SCALED AS PER CARSTENSEN ET AL		
CH3O2+C4H10<=>CH3O2H+PC4H9	1.386E+000	3.970
18280.0		
CH3O2+C4H10<=>CH3O2H+SC4H9	2.037E+001	3.580
14810.0		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
C2H5O2+C4H10<=>C2H5O2H+PC4H9	4.080E+001	3.590
17160.0		

C2H5O2+C4H10<=>C2H5O2H+SC4H9 13720.0	1.264E+002	3.370
!REF:ANALOGY TO C2H6+HO2 NC3H7O2+C4H10<=>NC3H7O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988 NC3H7O2+C4H10<=>NC3H7O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:ANALOGY TO C2H6+HO2 IC3H7O2+C4H10<=>IC3H7O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988 IC3H7O2+C4H10<=>IC3H7O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:ANALOGY TO C2H6+HO2 PC4H9O2+C3H8<=>PC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975 PC4H9O2+C3H8<=>PC4H9O2H+IC3H7 17000.0	2.000E+012	0.000
!REF:ANALOGY TO C2H6+HO2 PC4H9O2+C4H10<=>PC4H9O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988 PC4H9O2+C4H10<=>PC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:ANALOGY TO C2H6+HO2 SC4H9O2+C3H8<=>SC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
!REF:WALKER, R. W., REACTION KINETICS, VOL. 1, S. P. R. CHEMICAL SOCIETY, 1975 SC4H9O2+C3H8<=>SC4H9O2H+IC3H7 17000.0 SC4H9O2+C4H10<=>SC4H9O2H+PC4H9 20460.0	2.000E+012 1.700E+013	0.000 0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION !REF:SEATTLE, AUGUST, 1988 SC4H9O2+C4H10<=>SC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:D.M. MATHEU, W.H. GREEN JR., J.M. GREYDA, INT. J. CHEM. KINET. 35 (2003) 95-119.		

PC4H9<=>SC4H9 37300.0 DUP	3.560E+010	0.880
PC4H9<=>SC4H9 36600.0 DUP	3.800E+010	0.670
!REF:		
C2H5+C2H4<=>PC4H9 6130.0	1.320E+004	2.480
C3H6+CH3<=>SC4H9 6130.0	1.760E+004	2.480
C4H8-1+H<=>PC4H9 2620.0	2.500E+011	0.510
C4H8-2+H<=>SC4H9 2620.0	2.500E+011	0.510
C4H8-1+H<=>SC4H9 1230.0	4.240E+011	0.510
!REF:BASED ON KLIPPENSTEIN ET AL. N, IC3H7+O2		
PC4H9+O2<=>C4H8-1+HO2 11960.0	8.370E-001	3.590
SC4H9+O2<=>C4H8-1+HO2 9322.0	5.350E-001	3.710
SC4H9+O2<=>C4H8-2+HO2 9322.0	1.070E+000	3.710
!REF:WESTBROOK AND PITZ ESTIMATE (1983).		
C2H3+C2H5<=>C4H8-1 0.0	9.000E+012	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C3H5-A+CH3 (+M) <=>C4H8-1 (+M) -262.3	1.000E+014	-0.320
LOW/ 6250.0/ TROE/ 1.040E-001 1.606E+003 6.000E+004 6.118E+003/ H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/ 0.70/	3.910E+060	-12.810
!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)		
H+C4H71-3<=>C4H8-1 0.0	5.000E+013	0.000
!REF:ESTIMATE		
C4H8-1+O2<=>C4H71-3+HO2 37190.0	2.000E+013	0.000
!REF:		
C4H8-1+O<=>C4H71-3+OH 5884.0	1.750E+011	0.700
C4H8-2+O<=>C4H71-3+OH 7550.0	2.190E+011	0.810
!REF:TSANG '91		
C4H8-1+H<=>C4H71-3+H2 2492.0	1.730E+005	2.500

!REF:ESTIMATE		
C4H8-1+H<=>C4H71-4+H2 6756.0	6.651E+005	2.540
C4H8-1+OH<=>C4H71-1+H2O 1637.9	9.010E-001	3.941
C4H8-1+OH<=>C4H71-2+H2O 478.1	1.430E+001	3.534
C4H8-1+OH<=>C4H71-3+H2O -2802.5	6.690E+001	3.475
C4H8-1+OH<=>C4H71-4+H2O -767.0	4.280E+001	3.374
!REF:BASED ON 0.5 * C2H4+OH<=>C2H3+H2O		
!REF:ESTIMATE		
!REF:TSANG '91		
!REF:TSANG '91		
C4H8-1+CH3<=>C4H71-3+CH4 5675.0	2.210E+000	3.500
C4H8-1+CH3<=>C4H71-4+CH4 7154.0	4.520E-001	3.650
!REF:TSANG '91		
C4H8-1+HO2<=>C4H71-3+H2O2 5884.0	2.700E+004	0.700
C4H8-1+HO2<=>C4H71-4+H2O2 16490.0	2.380E+003	2.550
!REF:TSANG '91		
C4H8-1+CH3O2<=>C4H71-3+CH3O2H 5884.0	2.700E+004	0.700
C4H8-1+CH3O2<=>C4H71-4+CH3O2H 16490.0	2.380E+003	2.550
C4H8-1+CH3O<=>C4H71-3+CH3OH 8609.0	4.000E+001	2.900
C4H8-1+CH3O<=>C4H71-4+CH3OH 6458.0	2.170E+011	0.000
!REF:DECHAUX, J.C., OXID. COMM. 2, 95 (1981)		
C4H8-1+CH3CO3<=>C4H71-3+CH3CO3H 8000.0	1.000E+011	0.000
C4H8-1+C3H5-A<=>C4H71-3+C3H6 12400.0	7.900E+010	0.000
!REF:ALLARA, D. L. AND EDELSON, D., INT. J. CHEM. KINET. 7, 479 (1975).		
C4H71-3+C4H71-3<=>C4H8-1+C4H6 0.0	1.600E+012	0.000
C4H8-1+C2H5O2<=>C4H71-3+C2H5O2H 14900.0	1.400E+012	0.000
C4H8-1+NC3H7O2<=>C4H71-3+NC3H7O2H 14900.0	1.400E+012	0.000
C4H8-1+IC3H7O2<=>C4H71-3+IC3H7O2H 14900.0	1.400E+012	0.000
C4H8-1+PC4H9O2<=>C4H71-3+PC4H9O2H 14900.0	1.400E+012	0.000
C4H8-1+SC4H9O2<=>C4H71-3+SC4H9O2H 14900.0	1.400E+012	0.000
C4H8-1+CH3O2<=>C4H8O1-2+CH3O 14340.0	1.000E+012	0.000

!REF:ALLARA AND SHAW, 1980, PARALLEL  
H+C4H71-3<=>C4H8-2 5.000E+013 0.000  
0.0  
C4H8-2+O2<=>C4H71-3+HO2 4.000E+013 0.000  
39390.0

!REF:TSANG '91

!REF:PLUS DIFFERENCE BETWEEN 10 AND 20 IN ALKANE  
C4H8-2+H<=>C4H71-3+H2 4.440E+004 2.810  
4414.0  
C4H8-2+OH<=>C4H71-3+H2O 5.100E+008 1.400  
1250.0  
C4H8-2+CH3<=>C4H71-3+CH4 7.140E+000 3.570  
7642.0  
C4H8-2+HO2<=>C4H71-3+H2O2 5.940E+004 2.570  
16140.0  
C4H8-2+CH3O2<=>C4H71-3+CH3O2H 5.940E+004 2.570  
16140.0

!REF:ESTIMATE

C4H8-2+CH3O<=>C4H71-3+CH3OH 1.800E+001 2.950  
11990.0

!REF:!TWICE RATE OF C3H6+HO2

C4H8-2+C2H5O2<=>C4H71-3+C2H5O2H 3.200E+012 0.000  
14900.0  
C4H8-2+NC3H7O2<=>C4H71-3+NC3H7O2H 3.200E+012 0.000  
14900.0  
C4H8-2+IC3H7O2<=>C4H71-3+IC3H7O2H 3.200E+012 0.000  
14900.0  
C4H8-2+PC4H9O2<=>C4H71-3+PC4H9O2H 3.200E+012 0.000  
14900.0  
C4H8-2+SC4H9O2<=>C4H71-3+SC4H9O2H 3.200E+012 0.000  
14900.0

!REF:ANALOGY TO C3H6+HO2

C4H8-1+HO2<=>C4H8O1-2+OH 1.000E+012 0.000  
14340.0

!REF:!WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION

!REF:SEATTLE, AUGUST, 1988

C4H8-2+HO2<=>C4H8O2-3+OH 5.620E+011 0.000  
12310.0  
C4H8-2+CH3O2<=>C4H8O2-3+CH3O 5.620E+011 0.000  
12310.0

!REF:TULLY, PRIVATE COMMUNICATION, 1986.

C4H8-1+OH<=>PC4H8OH 4.750E+012 0.000  
-782.0  
C4H8-2+OH<=>SC4H8OH 4.750E+012 0.000  
-782.0  
PC4H8OH+O2<=>C4H8OH-1O2 2.000E+012 0.000  
0.0  
SC4H8OH+O2<=>C4H8OH-2O2 2.000E+012 0.000  
0.0

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!REF:ANALOGY TO PROPENE
C4H8OH-1O2=>C2H5CHO+CH2O+OH          1.000E+016    0.000
25000.0
C4H8OH-2O2=>OH+CH3CHO+CH3CHO          1.000E+016    0.000
25000.0
C2H2+C2H5<=>C4H71-1                    2.000E+011    0.000
7800.0
C3H4-A+CH3<=>C4H71-2                    2.000E+011    0.000
7800.0
C2H4+C2H3<=>C4H71-4                    2.000E+011    0.000
7800.0
C3H4-P+CH3<=>C4H72-2                    1.000E+011    0.000
7800.0

!REF:!ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)
C4H6+H<=>C4H71-3                        4.000E+013    0.000
1300.0

!REF:ESTIMATE
C4H71-3+C2H5<=>C4H8-1+C2H4              2.590E+012    0.000
-131.0
C4H71-3+CH3O<=>C4H8-1+CH2O             2.410E+013    0.000
0.0
C4H71-3+O<=>C*CCHO+CH3                  6.030E+013    0.000
0.0
C4H71-3+HO2<=>C4H7O+OH                  9.640E+012    0.000
0.0
C4H71-3+CH3O2<=>C4H7O+CH3O             9.640E+012    0.000
0.0

!REF:EDELSON AND ALLARA, 1980
C3H5-A+C4H71-3<=>C3H6+C4H6              6.310E+012    0.000
0.0

!REF:BALDWIN, BENNETT, AND WALKER, JCS FARADAY I, 76, 2396 (1980)
!C4H71-3+O2<=>C4H6+HO2                  1.000E+009    0.000
0.0
!
C4H6+HO2=C4H71-3+O2                      8.870E+022    -3.090
26586.0!Burke 2014 propene
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/
!

!REF:ALLARA, D. L. AND SHAW, R., J. PHYS. CHEM. REF. DATA 9, 523 (1980)
H+C4H71-3<=>C4H6+H2                      3.160E+013    0.000
0.0

!REF:EDELSON AND ALLARA, 1980
C2H5+C4H71-3<=>C4H6+C2H6                3.980E+012    0.000
0.0
C2H3+C4H71-3<=>C2H4+C4H6                3.980E+012    0.000
0.0

!REF:ANALOGY TO CH3O2+CH3

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C4H71-3+C2H5O2<=>C4H7O+C2H5O -1200.0	3.800E+012	0.000
IC3H7O2+C4H71-3<=>IC3H7O+C4H7O -1200.0	3.800E+012	0.000
NC3H7O2+C4H71-3<=>NC3H7O+C4H7O -1200.0	3.800E+012	0.000

!REF:ANALOGY TO BATT'S RATE FOR S-BUTOXY DECOMPOSITION

C4H7O<=>CH3CHO+C2H3 19000.0	7.940E+014	0.000
C4H7O<=>C*CCHO+CH3 19000.0	7.940E+014	0.000

!REF:LASKIN ET AL. IJCK 32 589-614 2000

C4H6<=>C4H5-I+H 112353.0	5.700E+036	-6.270
C4H6<=>C4H5-N+H 123608.0	5.300E+044	-8.620
C4H6<=>C4H4+H2 94700.0	2.500E+015	0.000
C4H6+H<=>C4H5-N+H2 12240.0	1.330E+006	2.530
C4H6+H<=>C4H5-I+H2 9240.0	6.650E+005	2.530
C4H6+H<=>C2H4+C2H3 21647.0	1.460E+030	-4.340
PLOG/ 1.0000 1.460E+030 -4.340 21647.0/		
PLOG/ 10.0000 5.450E+030 -4.510 21877.0/		
C4H6+H<=>C3H4-P+CH3 7000.0	2.000E+012	0.000
C4H6+H<=>C3H4-A+CH3 7000.0	2.000E+012	0.000
C4H6+O<=>C4H5-N+OH 3740.0	7.500E+006	1.900
C4H6+O<=>C4H5-I+OH 3740.0	7.500E+006	1.900

!REF:WKM

!REF:ADDED TO REDUCE EARLY CO2 PRODUCTION IN C4H6 FLOW REACTOR DUE TO UPDATE

!REF:IN HCCO+O2. BASED ON THE ANALYSIS FOUND IN LASKIN ET AL.

C4H6+O<=>C2H2+C2H4O1-2 -860.0	1.000E+008	1.450
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!!Curran

!C4H6+OH=C2H5+CH2CO 0.0 !CURRAN	1.000E+12	0.00
!C4H6+OH=CH2O+C3H5-A 0.0 !CURRAN	1.000E+12	0.00
!C4H6+OH=C2H3+CH3CHO 0.0 !CURRAN	1.000E+12	0.00
!		
C4H6+OH=C2H5+CH2CO -1040.0 !Heyberger	5.480E+12	0.0
C4H6+OH=CH2O+C3H5-A -1040.0 !Heyberger	5.480E+12	0.0

C4H6+OH=C2H3+CH3CHO				5.480E+12	0.0
-1040.0 !Heyberger					
!					
C4H6+O=C2H4+CH2CO				1.000E+12	0.00
0.0 !CURRAN					
C4H6+O=CH2O+C3H4-A				1.000E+12	0.00
0.0 !CURRAN					
C4H6+OH=HOC4H6				1.840E+12	0.0
-1170.0 !NIST					
DUP					
C4H6+OH=HOC4H6				5.700E+12	0.0
-570.0 !NIST					
DUP					
HOC4H6+O2=C*CCHO+CH2O+OH				1.000E+09	0.00
30.0 !STARK ET AL.,					
!REF:REDUCED THE CH3CHCHCO CHANNEL TO KEEP THE TOTAL K THE SAME.					
C4H6+O<=>CH3CHCHCO+H				5.000E+007	1.450
-860.0					
C4H6+O<=>CH2CHCHCHO+H				4.500E+008	1.450
-860.0					
C4H6+OH<=>C4H5-N+H2O				6.200E+006	2.000
3430.0					
C4H6+OH<=>C4H5-I+H2O				3.100E+006	2.000
430.0					
C4H6+HO2<=>C4H6O25+OH				1.200E+012	0.000
14000.0					
C4H6+HO2<=>C2H3CHOCH2+OH				4.800E+012	0.000
14000.0					
C4H6+CH3<=>C4H5-N+CH4				2.000E+014	0.000
22800.0					
C4H6+CH3<=>C4H5-I+CH4				1.000E+014	0.000
19800.0					
C4H6+C2H3<=>C4H5-N+C2H4				5.000E+013	0.000
22800.0					
C4H6+C2H3<=>C4H5-I+C2H4				2.500E+013	0.000
19800.0					
C4H6+C3H3<=>C4H5-N+C3H4-A				1.000E+013	0.000
22500.0					
C4H6+C3H3<=>C4H5-I+C3H4-A				5.000E+012	0.000
19500.0					
C4H6+C3H5-A<=>C4H5-N+C3H6				1.000E+013	0.000
22500.0					
C4H6+C3H5-A<=>C4H5-I+C3H6				5.000E+012	0.000
19500.0					
C4H71-4<=>C4H6+H				2.480E+053	-12.300
52000.0					
PLOG/	1.0000	2.480E+053	-12.300	52000.0/	
PLOG/	10.0000	1.850E+048	-10.500	51770.0/	
C2H3+C2H2<=>C4H4+H				7.200E+013	-0.480
6100.0					
PLOG/	0.0132	7.200E+013	-0.480	6100.0/	
PLOG/	0.0263	5.000E+014	-0.710	6700.0/	
PLOG/	0.1200	4.600E+016	-1.250	8400.0/	
PLOG/	1.0000	2.000E+018	-1.680	10600.0/	
PLOG/	10.0000	4.900E+016	-1.130	11800.0/	



C2H3+C2H2<=>C4H5-N				1.100E+031	-7.140
5600.0					
PLOG/	0.0132	1.100E+031	-7.140	5600.0/	
PLOG/	0.0263	1.100E+032	-7.330	6200.0/	
PLOG/	0.1200	2.400E+031	-6.950	5600.0/	
PLOG/	1.0000	9.300E+038	-8.760	12000.0/	
PLOG/	10.0000	8.100E+037	-8.090	13400.0/	
C2H3+C2H2<=>C4H5-I				5.000E+034	-8.420
7900.0					
PLOG/	0.0132	5.000E+034	-8.420	7900.0/	
PLOG/	0.0263	2.100E+036	-8.780	9100.0/	
PLOG/	0.1200	1.000E+037	-8.770	9800.0/	
PLOG/	1.0000	1.600E+046	-10.980	18600.0/	
PLOG/	10.0000	5.100E+053	-12.640	28800.0/	
C2H3+C2H3<=>C4H6				7.000E+057	-13.820
17629.0					
PLOG/	0.0263	7.000E+057	-13.820	17629.0/	
PLOG/	0.1200	1.500E+052	-11.970	16056.0/	
PLOG/	1.0000	1.500E+042	-8.840	12483.0/	
C2H3+C2H3<=>C4H5-I+H				1.500E+030	-4.950
12958.0					
PLOG/	0.0263	1.500E+030	-4.950	12958.0/	
PLOG/	0.1200	7.200E+028	-4.490	14273.0/	
PLOG/	1.0000	1.200E+022	-2.440	13654.0/	
C2H3+C2H3<=>C4H5-N+H				1.100E+024	-3.280
12395.0					
PLOG/	0.0263	1.100E+024	-3.280	12395.0/	
PLOG/	0.1200	4.600E+024	-3.380	14650.0/	
PLOG/	1.0000	2.400E+020	-2.040	15361.0/	
C4H5-N<=>C4H5-I				2.400E+060	-16.080
47500.0					
PLOG/	0.0132	2.400E+060	-16.080	47500.0/	
PLOG/	0.0263	1.300E+062	-16.380	49600.0/	
PLOG/	0.1200	4.900E+066	-17.260	55400.0/	
PLOG/	1.0000	1.500E+067	-16.890	59100.0/	
PLOG/	10.0000	2.000E+060	-14.460	58600.0/	
C4H5-N+H<=>C4H5-I+H				3.100E+026	-3.350
17423.0					
C4H5-N+H<=>C4H4+H2				1.500E+013	0.000
0.0					
C4H5-N+OH<=>C4H4+H2O				2.000E+012	0.000
0.0					
C4H5-N+HCO<=>C4H6+CO				5.000E+012	0.000
0.0					
C4H5-N+HO2=>C2H3+CH2CO+OH				6.600E+012	0.000
0.0					
C4H5-N+H2O2<=>C4H6+HO2				1.210E+010	0.000
-596.0					
C4H5-N+HO2<=>C4H6+O2				6.000E+011	0.000
0.0					
C4H5-N+O2<=>CH2CHCHCHO+O				3.000E+011	0.290
11.0					
C4H5-N+O2<=>HCO+C*CCHO				9.200E+016	-1.390
1010.0					
C4H5-I+H<=>C4H4+H2				3.000E+013	0.000
0.0					
C4H5-I+H<=>C3H3+CH3				2.000E+013	0.000
2000.0					

C4H5-I+OH<=>C4H4+H2O 0.0	4.000E+012	0.000
C4H5-I+HCO<=>C4H6+CO 0.0	5.000E+012	0.000
C4H5-I+HO2<=>C4H6+O2 0.0	6.000E+011	0.000
C4H5-I+HO2=>C2H3+CH2CO+OH 0.0	6.600E+012	0.000
C4H5-I+H2O2<=>C4H6+HO2 -596.0	1.210E+010	0.000
C4H5-I+O2<=>CH2CO+CH2CHO 2500.0	2.160E+010	0.000
C4H5-2<=>C4H5-I 59100.0	1.500E+067	-16.890
C4H5-2+H<=>C4H5-I+H 17423.0	3.100E+026	-3.350
C4H5-2+HO2=>OH+C2H2+CH3CO 0.0	8.000E+011	0.000
C4H5-2+O2<=>CH3CO+CH2CO 2500.0	2.160E+010	0.000
C4H612<=>C4H5-I+H 92600.0	4.200E+015	0.000
C4H612+H<=>C4H6+H 4000.0	2.000E+013	0.000
C4H612+H<=>C4H5-I+H2 2490.0	1.700E+005	2.500
C4H612+H<=>C3H4-A+CH3 2000.0	2.000E+013	0.000
C4H612+H<=>C3H4-P+CH3 2000.0	2.000E+013	0.000
C4H612+CH3<=>C4H5-I+CH4 18500.0	7.000E+013	0.000
C4H612+O<=>CH2CO+C2H4 327.0	1.200E+008	1.650
C4H612+O<=>C4H5-I+OH 5880.0	1.800E+011	0.700
C4H612+OH<=>C4H5-I+H2O -298.0	3.100E+006	2.000
C4H612<=>C4H6 65000.0	3.000E+013	0.000
C4H6-2<=>C4H6 65000.0	3.000E+013	0.000
C4H6-2<=>C4H612 67000.0	3.000E+013	0.000
C4H6-2+H<=>C4H612+H 4000.0	2.000E+013	0.000
C4H6-2+H<=>C4H5-2+H2 2490.0	3.400E+005	2.500
C4H6-2+H<=>CH3+C3H4-P 1000.0	2.600E+005	2.500
C4H6-2<=>H+C4H5-2 87300.0	5.000E+015	0.000
C4H6-2+CH3<=>C4H5-2+CH4 18500.0	1.400E+014	0.000
C2H3CHOCH2<=>C4H6O23 50600.0	2.000E+014	0.000
C4H6O23<=>SC3H5CHO 49400.0	1.950E+013	0.000

C4H6O23<=>C2H4+CH2CO				5.750E+015	0.000
69300.0					
C4H6O23<=>C2H2+C2H4O1-2				1.000E+016	0.000
75800.0					
C4H6O25<=>C4H4O+H2				5.300E+012	0.000
48500.0					
C4H4O<=>CO+C3H4-P				1.780E+015	0.000
77500.0					
C4H4O<=>C2H2+CH2CO				5.010E+014	0.000
77500.0					
!SC3H5CHO<=>C3H6+CO				3.900E+014	0.000
69000.0!in THF submech					
!SC3H5CHO+H<=>CH2CHCHCHO+H2				1.700E+005	2.500
2490.0!in THF submech					
!SC3H5CHO+H<=>CH3CHCHCO+H2				1.000E+005	2.500
2490.0!in THF submech					
!SC3H5CHO+H<=>CH3+C*CCO				4.000E+021	-2.390
11180.0!in THF submech					
!SC3H5CHO+H<=>C3H6+HCO				4.000E+021	-2.390
11180.0!in THF submech					
!SC3H5CHO+CH3<=>CH2CHCHCHO+CH4				2.100E+000	3.500
5675.0!in THF submech					
!SC3H5CHO+CH3<=>CH3CHCHCO+CH4				1.100E+000	3.500
5675.0!in THF submech					
SC3H5CHO+C2H3<=>CH2CHCHCHO+C2H4				2.210E+000	3.500
4682.0					
SC3H5CHO+C2H3<=>CH3CHCHCO+C2H4				1.110E+000	3.500
4682.0					
CH3CHCHCO<=>C3H5-S+CO				1.000E+014	0.000
30000.0					
CH3CHCHCO+H<=>SC3H5CHO				1.000E+014	0.000
0.0					
!CH2CHCHCHO<=>C3H5-A+CO				1.000E+014	0.000
25000.0!in THF submech					
CH2CHCHCHO+H<=>SC3H5CHO				1.000E+014	0.000
0.0					
C4H4+H<=>C4H5-N				1.200E+051	-12.570
12300.0					
PLOG/	0.0132	1.200E+051	-12.570	12300.0/	
PLOG/	0.0263	4.200E+050	-12.340	12500.0/	
PLOG/	0.1200	1.100E+050	-11.940	13400.0/	
PLOG/	1.0000	1.300E+051	-11.920	16500.0/	
PLOG/	10.0000	6.200E+045	-10.080	15800.0/	
C4H4+H<=>C4H5-I				6.100E+053	-13.190
14200.0					
PLOG/	0.0132	6.100E+053	-13.190	14200.0/	
PLOG/	0.0263	9.600E+052	-12.850	14300.0/	
PLOG/	0.1200	2.100E+052	-12.440	15500.0/	
PLOG/	1.0000	4.900E+051	-11.920	17700.0/	
PLOG/	10.0000	1.500E+048	-10.580	18800.0/	
C4H4+H<=>C4H3-N+H2				6.650E+005	2.530
12240.0					
C4H4+H<=>C4H3-I+H2				3.330E+005	2.530
9240.0					
C4H4+OH<=>C4H3-N+H2O				3.100E+007	2.000
3430.0					
C4H4+OH<=>C4H3-I+H2O				1.550E+007	2.000
430.0					

C4H4+O<=>C3H3+HCO	6.000E+008	1.450
-860.0		
C3H3+HCCO<=>C4H4+CO	2.500E+013	0.000
0.0		
C3H3+CH<=>C4H3-I+H	5.000E+013	0.000
0.0		
C3H3+CH2<=>C4H4+H	5.000E+013	0.000
0.0		
C3H3+CH3 (+M) <=>C4H612 (+M)	1.500E+012	0.000
0.0		
LOW/	2.600E+057	-11.940
9770.0/		
TROE/ 1.750E-001 1.341E+003 6.000E+004 9.770E+003/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ AR/		
0.70/		
C2H2+C2H (+M) <=>C4H3-N (+M)	8.300E+010	0.899
-363.0		
LOW/	1.240E+031	-4.718
1871.0/		
TROE/ 1.000E+000 1.000E+002 5.613E+003 1.339E+004/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/		
2.50/ C2H4/ 2.50/		
C4H3-N<=>C4H3-I	4.100E+043	-9.490
53000.0		
C4H3-N+H<=>C4H3-I+H	2.500E+020	-1.670
10800.0		
C4H3-N+H<=>C2H2+H2CC	6.300E+025	-3.340
10014.0		
C4H3-N+H<=>C4H4	2.000E+047	-10.260
13070.0		
C4H3-N+H<=>C4H2+H2	3.000E+013	0.000
0.0		
C4H3-N+OH<=>C4H2+H2O	2.000E+012	0.000
0.0		
C2H2+C2H (+M) <=>C4H3-I (+M)	8.300E+010	0.899
-363.0		
LOW/	1.240E+031	-4.718
1871.0/		
TROE/ 1.000E+000 1.000E+002 5.613E+003 1.339E+004/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/		
2.50/ C2H4/ 2.50/		
C4H3-I+H<=>C2H2+H2CC	2.800E+023	-2.550
10780.0		
C4H3-I+H<=>C4H4	3.400E+043	-9.010
12120.0		
C4H3-I+H<=>C4H2+H2	6.000E+013	0.000
0.0		
C4H3-I+OH<=>C4H2+H2O	4.000E+012	0.000
0.0		
C4H3-I+O2<=>HCCO+CH2CO	7.860E+016	-1.800
0.0		
!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)		
C4H3-I+CH2<=>C3H4-A+C2H	2.000E+013	0.000
0.0		

!REF:LASKIN ET AL. IJCK 32 589-614 2000

C2H2+C2H<=>C4H2+H 0.0	9.600E+013	0.000
C4H2+H<=>C4H3-N 15300.0	1.100E+042	-8.720
C4H2+H<=>C4H3-I 10800.0	1.100E+030	-4.920
C4H2+OH<=>H2C4O+H -410.0	6.600E+012	0.000
H2C4O+H<=>C2H2+HCCO 3000.0	5.000E+013	0.000
H2C4O+OH<=>CH2CO+HCCO 2000.0	1.000E+007	2.000
H2CC+C2H2 (+M) <=>C4H4 (+M) -2400.0	3.500E+005	2.055
LOW/ 7417.0/	1.400E+060	-12.599
TROE/ 9.800E-001 5.600E+001 5.800E+002 4.164E+003/		
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/ C2H6/ 3.00/ C2H2/ 3.00/ C2H4/ 3.00/		
H2CC+C2H4<=>C4H6 0.0	1.000E+012	0.000
!REF:WESTBROOK ESTIMATE		
C4H8O1-2+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
C4H8O1-2+H=>CH2O+C3H5-A+H2 0.0	5.000E+012	0.000
C4H8O1-2+O=>CH2O+C3H5-A+OH 0.0	5.000E+012	0.000
C4H8O1-2+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O1-2+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
C4H8O1-2+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
C4H8O1-3+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
C4H8O1-3+H=>CH2O+C3H5-A+H2 0.0	5.000E+012	0.000
C4H8O1-3+O=>CH2O+C3H5-A+OH 0.0	5.000E+012	0.000
C4H8O1-3+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O1-3+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
C4H8O1-3+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
C4H8O1-4+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
C4H8O1-4+H=>CH2O+C3H5-A+H2 0.0	5.000E+012	0.000
C4H8O1-4+O=>CH2O+C3H5-A+OH 0.0	5.000E+012	0.000
C4H8O1-4+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O1-4+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000

C4H8O1-4+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
C4H8O2-3+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
C4H8O2-3+H=>CH2O+C3H5-A+H2 0.0	5.000E+012	0.000
C4H8O2-3+O=>CH2O+C3H5-A+OH 0.0	5.000E+012	0.000
C4H8O2-3+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
C4H8O2-3+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
C4H8O2-3+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
!REF:ESTIMATE		
PC4H9+O2<=>PC4H9O2 0.0	4.520E+012	0.000
SC4H9+O2<=>SC4H9O2 0.0	7.540E+012	0.000
!REF:ANALOGY TO CH2O+HO2		
SC4H9O2+CH2O<=>SC4H9O2H+HCO 13600.0	5.600E+012	0.000
SC4H9O2+CH3CHO<=>SC4H9O2H+CH3CO 13600.0	2.800E+012	0.000
!REF:ESTIMATE		
SC4H9O2+HO2<=>SC4H9O2H+O2 -3275.0	1.750E+010	0.000
IC3H7O2+PC4H9<=>IC3H7O+PC4H9O -1000.0	7.000E+012	0.000
IC3H7O2+SC4H9<=>IC3H7O+SC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+PC4H9<=>NC3H7O+PC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+SC4H9<=>NC3H7O+SC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+SC4H9O2=>O2+SC4H9O+SC4H9O 1860.0	1.400E+016	-1.610
SC4H9O2+NC3H7O2=>SC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+IC3H7O2=>SC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+C2H5O2=>SC4H9O+C2H5O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+CH3O2=>SC4H9O+CH3O+O2 1860.0	1.400E+016	-1.610
SC4H9O2+CH3CO3=>SC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
H2+PC4H9O2<=>H+PC4H9O2H 26030.0	3.010E+013	0.000
H2+SC4H9O2<=>H+SC4H9O2H 26030.0	3.010E+013	0.000

!REF:WESTBROOK ESTIMATE

C2H6+PC4H9O2<=>C2H5+PC4H9O2H 20460.0	1.700E+013	0.000
C2H6+SC4H9O2<=>C2H5+SC4H9O2H 20460.0	1.700E+013	0.000
PC4H9O2+C2H5CHO<=>PC4H9O2H+C2H5CO 9500.0	2.000E+011	0.000
SC4H9O2+C2H5CHO<=>SC4H9O2H+C2H5CO 9500.0	2.000E+011	0.000
!REF:ESTIMATE		
SC4H9O2+CH3<=>SC4H9O+CH3O -1000.0	7.000E+012	0.000
SC4H9O2+C2H5<=>SC4H9O+C2H5O -1000.0	7.000E+012	0.000
SC4H9O2+IC3H7<=>SC4H9O+IC3H7O -1000.0	7.000E+012	0.000
SC4H9O2+NC3H7<=>SC4H9O+NC3H7O -1000.0	7.000E+012	0.000
SC4H9O2+PC4H9<=>SC4H9O+PC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+SC4H9<=>SC4H9O+SC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+C3H5-A<=>SC4H9O+C3H5O -1000.0	7.000E+012	0.000
!REF:ANALOGY TO CH2O+HO2		
PC4H9O2+CH2O<=>PC4H9O2H+HCO 13600.0	5.600E+012	0.000
!REF:HALF OF CH2O+HO2		
PC4H9O2+CH3CHO<=>PC4H9O2H+CH3CO 13600.0	2.800E+012	0.000
!REF:TSANG, JPC REF. DATA, 16:471 (1987)		
PC4H9O2+HO2<=>PC4H9O2H+O2 -3275.0	1.750E+010	0.000
!REF:ANALOGY TO C3H6+HO2		
C3H6+PC4H9O2<=>C3H5-A+PC4H9O2H 13288.1	5.350E-002	4.207
C3H6+SC4H9O2<=>C3H5-A+SC4H9O2H 13288.1	5.350E-002	4.207
!REF:ANALOGY TO C2H4+HO2		
C2H4+PC4H9O2<=>C2H3+PC4H9O2H 30430.0	1.130E+013	0.000
C2H4+SC4H9O2<=>C2H3+SC4H9O2H 30430.0	1.130E+013	0.000
!REF:ANALOGY TO CH3OH+HO2		
CH3OH+PC4H9O2<=>CH2OH+PC4H9O2H 19360.0	6.300E+012	0.000
CH3OH+SC4H9O2<=>CH2OH+SC4H9O2H 19360.0	6.300E+012	0.000
!REF:HALF OF CH2O+HO2		
C*CCHO+PC4H9O2<=>C2H3CO+PC4H9O2H 13600.0	2.800E+012	0.000

C*CCHO+SC4H9O2<=>C2H3CO+SC4H9O2H 13600.0	2.800E+012	0.000
!REF:ANALOGY TO CH4+HO2		
CH4+PC4H9O2<=>CH3+PC4H9O2H 24640.0	1.120E+013	0.000
CH4+SC4H9O2<=>CH3+SC4H9O2H 24640.0	1.120E+013	0.000
!REF:ESTIMATE		
C4H71-3+PC4H9O2<=>C4H7O+PC4H9O -1000.0	7.000E+012	0.000
C4H71-3+SC4H9O2<=>C4H7O+SC4H9O -1000.0	7.000E+012	0.000
!REF:ANALOGY TO H2O2+CH3O2<=>HO2+CH3O2H		
H2O2+PC4H9O2<=>HO2+PC4H9O2H 10000.0	2.400E+012	0.000
H2O2+SC4H9O2<=>HO2+SC4H9O2H 10000.0	2.400E+012	0.000
!REF:		
PC4H9O2+PC4H9O2=>O2+PC4H9O+PC4H9O 1860.0	1.400E+016	-1.610
PC4H9O2+SC4H9O2=>PC4H9O+SC4H9O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+NC3H7O2=>PC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+IC3H7O2=>PC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+C2H5O2=>PC4H9O+C2H5O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+CH3O2=>PC4H9O+CH3O+O2 1860.0	1.400E+016	-1.610
PC4H9O2+CH3CO3=>PC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
!REF:ESTIMATE		
PC4H9O2+CH3<=>PC4H9O+CH3O -1000.0	7.000E+012	0.000
PC4H9O2+C2H5<=>PC4H9O+C2H5O -1000.0	7.000E+012	0.000
PC4H9O2+IC3H7<=>PC4H9O+IC3H7O -1000.0	7.000E+012	0.000
PC4H9O2+NC3H7<=>PC4H9O+NC3H7O -1000.0	7.000E+012	0.000
PC4H9O2+PC4H9<=>PC4H9O+PC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+SC4H9<=>PC4H9O+SC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+C3H5-A<=>PC4H9O+C3H5O -1000.0	7.000E+012	0.000
PC4H9+HO2<=>PC4H9O+OH -1000.0	7.000E+012	0.000
SC4H9+HO2<=>SC4H9O+OH -1000.0	7.000E+012	0.000
CH3O2+PC4H9<=>CH3O+PC4H9O -1000.0	7.000E+012	0.000



CH3O2+SC4H9<=>CH3O+SC4H9O -1000.0	7.000E+012	0.000
!REF:		
PC4H9O2H<=>PC4H9O+OH 42500.0	1.500E+016	0.000
!REF:PITZ ESTIMATE		
SC4H9O+OH<=>SC4H9O2H 0.0	1.000E+015	-0.800
!REF:		
NC3H7+CH2O<=>PC4H9O 3457.0	5.000E+010	0.000
CH3+C2H5CHO<=>SC4H9O 9043.0	5.000E+010	0.000
C2H5+CH3CHO<=>SC4H9O 6397.0	3.330E+010	0.000
!REF:		
PC4H9O2<=>C4H8OOH1-2 31850.0	2.000E+011	0.000
PC4H9O2<=>C4H8OOH1-3 20850.0	2.500E+010	0.000
PC4H9O2<=>C4H8OOH1-4 22350.0	4.688E+009	0.000
SC4H9O2<=>C4H8OOH2-1 34500.0	3.000E+011	0.000
SC4H9O2<=>C4H8OOH2-3 31850.0	2.000E+011	0.000
SC4H9O2<=>C4H8OOH2-4 24400.0	3.750E+010	0.000
PC4H9O2<=>C4H8-1+HO2 39510.0	4.308E+036	-7.500
SC4H9O2<=>C4H8-1+HO2 41530.0	5.980E+042	-9.430
SC4H9O2<=>C4H8-2+HO2 39510.0	4.308E+036	-7.500
!REF:		
C4H8-1+HO2<=>C4H8OOH1-2 11000.0	1.000E+011	0.000
C4H8-1+HO2<=>C4H8OOH2-1 11750.0	1.000E+011	0.000
C4H8-2+HO2<=>C4H8OOH2-3 11750.0	1.000E+011	0.000
!REF:GREEN 2003		
C4H8OOH1-2<=>C4H8O1-2+OH 15900.0	1.380E+012	0.000
C4H8OOH1-3<=>C4H8O1-3+OH 19500.0	2.040E+011	0.000
C4H8OOH1-4<=>C4H8O1-4+OH 14800.0	5.130E+010	0.000
C4H8OOH2-1<=>C4H8O1-2+OH 17000.0	3.980E+012	0.000
C4H8OOH2-3<=>C4H8O2-3+OH 15900.0	1.380E+012	0.000

C4H8OOH2-4<=>C4H8O1-3+OH 4.470E+011 0.000  
21900.0

!REF:ESTIMATE

C4H8OOH1-1<=>NC3H7CHO+OH 9.000E+014 0.000  
1500.0

C4H8OOH2-2<=>C2H5COCH3+OH 9.000E+014 0.000  
1500.0

!REF:GREEN 2003

C4H8OOH1-3=>OH+CH2O+C3H6 6.635E+013 -0.160  
29900.0

C4H8OOH2-4=>OH+CH3CHO+C2H4 1.945E+018 -1.630  
26790.0

!REF:ESTIMATE?

C4H8OOH1-2+O2<=>C4H8OOH1-2O2 7.540E+012 0.000  
0.0

C4H8OOH1-3+O2<=>C4H8OOH1-3O2 7.540E+012 0.000  
0.0

C4H8OOH1-4+O2<=>C4H8OOH1-4O2 4.520E+012 0.000  
0.0

C4H8OOH2-1+O2<=>C4H8OOH2-1O2 4.520E+012 0.000  
0.0

C4H8OOH2-3+O2<=>C4H8OOH2-3O2 7.540E+012 0.000  
0.0

C4H8OOH2-4+O2<=>C4H8OOH2-4O2 4.520E+012 0.000  
0.0

!REF:

C4H8OOH1-2O2<=>NC4KET12+OH 2.000E+011 0.000  
31500.0

C4H8OOH1-3O2<=>NC4KET13+OH 2.500E+010 0.000  
21400.0

C4H8OOH1-4O2<=>NC4KET14+OH 3.125E+009 0.000  
19350.0

C4H8OOH2-1O2<=>NC4KET21+OH 1.000E+011 0.000  
28850.0

C4H8OOH2-3O2<=>NC4KET23+OH 1.000E+011 0.000  
28850.0

C4H8OOH2-4O2<=>NC4KET24+OH 1.250E+010 0.000  
17850.0

!REF:

NC4KET12=>C2H5CHO+HCO+OH 1.050E+016 0.000  
41600.0

NC4KET13=>CH3CHO+CH2CHO+OH 1.050E+016 0.000  
41600.0

NC4KET14=>CH2CH2CHO+CH2O+OH 1.500E+016 0.000  
42000.0

NC4KET21=>CH2O+C2H5CO+OH 1.500E+016 0.000  
42000.0

NC4KET23=>CH3CHO+CH3CO+OH 1.050E+016 0.000  
41600.0

NC4KET24=>CH2O+CH3COCH2+OH 1.500E+016 0.000  
42000.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995

C2H5COCH3+OH<=>CH2CH2COCH3+H2O 1586.0	7.550E+009	0.970
!REF:ANALOGY TO C2H5COC2H5+OH<=>PRODUCTS; CURRAN 1995		
C2H5COCH3+OH<=>CH3CHCOCH3+H2O -228.0	8.450E+011	0.000
!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+OH<=>C2H5COCH2+H2O 1192.0	5.100E+011	0.000
!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995		
C2H5COCH3+HO2<=>CH2CH2COCH3+H2O2 16490.0	2.380E+004	2.550
!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+HO2<=>CH3CHCOCH3+H2O2 8698.0	2.000E+011	0.000
C2H5COCH3+HO2<=>C2H5COCH2+H2O2 14690.0	2.380E+004	2.550
!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+O<=>CH2CH2COCH3+OH 7700.0	2.250E+013	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+O<=>CH3CHCOCH3+OH 3400.0	3.070E+013	0.000
!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+O<=>C2H5COCH2+OH 5962.0	5.000E+012	0.000
!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+H<=>CH2CH2COCH3+H2 7700.0	9.160E+006	2.000
!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+H<=>CH3CHCOCH3+H2 3200.0	4.460E+006	2.000
!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995		
C2H5COCH3+H<=>C2H5COCH2+H2 6357.0	9.300E+012	0.000
!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995		
C2H5COCH3+O2<=>CH2CH2COCH3+HO2 51310.0	2.050E+013	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995		
C2H5COCH3+O2<=>CH3CHCOCH3+HO2 41970.0	1.550E+013	0.000

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);  
CURRAN 1995  
C2H5COCH3+O2<=>C2H5COCH2+HO2 2.050E+013 0.000  
49150.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995  
C2H5COCH3+CH3<=>CH2CH2COCH3+CH4 3.190E+001 3.170  
7172.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);  
CURRAN 1995  
C2H5COCH3+CH3<=>CH3CHCOCH3+CH4 1.740E+000 3.460  
3680.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995  
C2H5COCH3+CH3<=>C2H5COCH2+CH4 1.620E+011 0.000  
9630.0

!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995  
C2H5COCH3+CH3O<=>CH2CH2COCH3+CH3OH 2.170E+011 0.000  
6460.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL  
(C<=>O); CURRAN 1995  
C2H5COCH3+CH3O<=>CH3CHCOCH3+CH3OH 1.450E+011 0.000  
2771.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL  
(C<=>O); CURRAN 1995  
C2H5COCH3+CH3O<=>C2H5COCH2+CH3OH 2.170E+011 0.000  
4660.0

!REF:ANALOGY TO C3H8+X<=>PC3H7+HX X 0.5 TSANG 88; CURRAN 1995  
C2H5COCH3+CH3O2<=>CH2CH2COCH3+CH3O2H 3.010E+012 0.000  
19380.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL  
(C<=>O); CURRAN 1995  
C2H5COCH3+CH3O2<=>CH3CHCOCH3+CH3O2H 2.000E+012 0.000  
15250.0

!REF:ANALOGY TO C3H8+X<=>C3H7+HX TSANG 88 EA - (6 X 0.3) KCAL/ MOL  
(C<=>O); CURRAN 1995  
C2H5COCH3+CH3O2<=>C2H5COCH2+CH3O2H 3.010E+012 0.000  
17580.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995  
C2H5COCH3+C2H3<=>CH2CH2COCH3+C2H4 5.000E+011 0.000  
10400.0

!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O);  
CURRAN 1995  
C2H5COCH3+C2H3<=>CH3CHCOCH3+C2H4 3.000E+011 0.000  
3400.0

!REF:ANALOGY TO CH3COCH3+X<=>CH2COCH3+HX X 0.5; CURRAN 1995  
C2H5COCH3+C2H3<=>C2H5COCH2+C2H4 6.150E+010 0.000  
4278.0

!REF:ANALOGY TO C2H5OH+X<=>PC2H4OH+HX; CURRAN 1995 C2H5COCH3+C2H5<=>CH2CH2COCH3+C2H6 13400.0	5.000E+010	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995 C2H5COCH3+C2H5<=>CH3CHCOCH3+C2H6 8600.0	3.000E+010	0.000
!REF:ANALOGY TO C2H5OH+X<=>SC2H4OH+HX EA - (6 X 0.3) KCAL/ MOL (C<=>O); CURRAN 1995 C2H5COCH3+C2H5<=>C2H5COCH2+C2H6 11600.0	5.000E+010	0.000
!REF: CURRAN AND GAFFURI, 1995 CH3CHCOCH3+O2<=>CH3CHOOOCOCH3 0.0 CH3CHOOOCOCH3<=>CH2CHOOHCOCH3 29700.0 C2H3COCH3+HO2<=>CH2CHOOHCOCH3 7800.0	1.000E+011  8.900E+012  7.000E+010	0.000  0.000  0.000
!REF: CH2CH2COCH3<=>C2H4+CH3CO 18000.0	1.000E+014	0.000
!REF: WKM 19/ 04/ 2010 C2H5COCH2<=>CH2CO+C2H5 35000.0	1.000E+014	0.000
!REF:ANALOGY WITH IC3H6CHO+X --> PRODUCTS C2H3COCH3+H<=>CH3CHCOCH3 1200.0	5.000E+012	0.000
!REF:ANALOGY WITH IC3H6CHO+X --> PRODUCTS !CH3CHCO+CH3<=>CH3CHCOCH3 7800.0!in THF submech	1.230E+011	0.000
!REF:ANALOGY WITH ACETALDEHYDE NC3H7CHO+O2<=>NC3H7CO+HO2 37560.0 NC3H7CHO+OH<=>NC3H7CO+H2O -1300.0 NC3H7CHO+H<=>NC3H7CO+H2 2320.0 NC3H7CHO+O<=>NC3H7CO+OH 1868.0	1.200E+005  2.000E+006  4.140E+009  5.940E+012	2.500  1.800  1.120  0.000
!REF:HALF OF CH2O+HO2 NC3H7CHO+HO2<=>NC3H7CO+H2O2 10200.0	4.090E+004	2.500
!REF:ANALOGY WITH ACETALDEHYDE NC3H7CHO+CH3<=>NC3H7CO+CH4 3210.0 NC3H7CHO+CH3O<=>NC3H7CO+CH3OH 3300.0	2.890E-003  1.000E+012	4.620  0.000

!REF:PITZ ESTIMATE		
NC3H7CHO+CH3O2<=>NC3H7CO+CH3O2H 10200.0	4.090E+004	2.500
!REF:CURRAN ESTIMATE		
NC3H7CHO+OH<=>C3H6CHO-1+H2O 1586.0	5.280E+009	0.970
NC3H7CHO+OH<=>C3H6CHO-2+H2O -35.0	4.680E+007	1.610
NC3H7CHO+OH<=>C3H6CHO-3+H2O -1176.0	5.520E+002	3.120
NC3H7CHO+HO2<=>C3H6CHO-1+H2O2 16490.0	2.379E+004	2.550
NC3H7CHO+HO2<=>C3H6CHO-2+H2O2 13910.0	9.640E+003	2.600
NC3H7CHO+HO2<=>C3H6CHO-3+H2O2 17880.0	3.440E+012	0.050
!REF:CURRAN ESTIMATE		
NC3H7CHO+CH3O2<=>C3H6CHO-1+CH3O2H 16490.0	2.379E+004	2.550
NC3H7CHO+CH3O2<=>C3H6CHO-2+CH3O2H 13910.0	9.640E+003	2.600
NC3H7CHO+CH3O2<=>C3H6CHO-3+CH3O2H 17880.0	3.440E+012	0.050
NC3H7CO<=>NC3H7+CO 9600.0	1.000E+011	0.000
!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95.		
!*!C3H6CHO-1<=>C2H4+CH2CHO 21970.0!déjà calculé par VER2015	7.400E+011	0.000
!REF:CURRAN ESTIMATE		
C2H5CHCO+H<=>C3H6CHO-3 1200.0	5.000E+012	0.000
C*CCHO+CH3<=>C3H6CHO-3 7800.0	1.230E+011	0.000
SC3H5CHO+H<=>C3H6CHO-2 2900.0	5.000E+012	0.000
C3H6+HCO<=>C3H6CHO-2 6000.0	1.000E+011	0.000
C2H5CHCO+OH<=>NC3H7+CO2 -1010.0	3.730E+012	0.000
C2H5CHCO+H<=>NC3H7+CO 1459.0	4.400E+012	0.000
C2H5CHCO+O<=>C3H6+CO2 -437.0	3.200E+012	0.000
!REF:ANALOGY WITH ACETALDEHYDE		
SC3H5CHO+OH<=>SC3H5CO+H2O -340.0	2.690E+010	0.760
!REF:PITZ ESTIMATE		
C3H5-S+CO<=>SC3H5CO 8000.0	5.000E+012	0.000
!REF:ANALOGY WITH IC3H5CHO+X --> IC3H5CO+HX		

SC3H5CHO+HO2<=>SC3H5CO+H2O2 11920.0	1.000E+012	0.000
SC3H5CHO+CH3<=>SC3H5CO+CH4 8700.0	3.980E+012	0.000
SC3H5CHO+O<=>SC3H5CO+OH 1389.0	7.180E+012	0.000
SC3H5CHO+O2<=>SC3H5CO+HO2 37600.0	4.000E+013	0.000
SC3H5CHO+H<=>SC3H5CO+H2 2600.0	2.600E+012	0.000

!REF:CURRAN ESTIMATE

C2H3COCH3+OH<=>CH3CHO+CH3CO 0.0	1.000E+011	0.000
C2H3COCH3+OH=>CH2CO+C2H3+H2O 1192.0	5.100E+011	0.000
C2H3COCH3+HO2=>CH2CHO+CH3CO+OH 7949.0	6.030E+009	0.000
C2H3COCH3+HO2=>CH2CO+C2H3+H2O2 20460.0	8.500E+012	0.000
C2H3COCH3+CH3O2=>CH2CHO+CH3CO+CH3O 17050.0	3.970E+011	0.000
C2H3COCH3+CH3O2=>CH2CO+C2H3+CH3O2H 17580.0	3.010E+012	0.000

!REF:NEW FIT FROM TIBOR NAGY BASED ON:

!REF:OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253

IC4H10 (+M) <=> CH3+IC3H7 (+M) 91495.0	2.520E+031	-4.102
LOW/ 52576.0/ TROE/ 3.662E-001 8.153E+002 6.079E+001 1.000E+020/	2.410E+019	0.000

!REF:OEHLSCHLAEGER ET AL. J. PHYS. CHEM. A 2004, 108:4247-4253.

IC4H10<=>TC4H9+H 145300.0	2.510E+098	-23.810
IC4H10<=>IC4H9+H 147600.0	9.850E+095	-23.110

!REF:TSANG, J. PHYS. CHEM. REF. DATA 19, 1-68 (1990)

IC4H10+H<=>TC4H9+H2 2583.0	6.020E+005	2.400
IC4H10+H<=>IC4H9+H2 6756.0	1.810E+006	2.540
IC4H10+CH3<=>TC4H9+CH4 4598.0	9.040E-001	3.460
IC4H10+CH3<=>IC4H9+CH4 7154.0	1.360E+000	3.650

!REF:JOE MICHAELS SYMP. PAPER 2008.

IC4H10+OH<=>TC4H9+H2O -1659.0	2.925E+004	2.531
IC4H10+OH<=>IC4H9+H2O -168.9	6.654E+004	2.665

!REF:ALLARA AND SHAW ANALOG

IC4H10+C2H5<=>IC4H9+C2H6 10400.0	1.510E+012	0.000
!REF:FROM ISOBUTYL RATE		
IC4H10+C2H5<=>TC4H9+C2H6 7900.0	1.000E+011	0.000
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
IC4H10+HO2<=>IC4H9+H2O2 17160.0	6.120E+001	3.590
!REF: X0.666		
IC4H10+HO2<=>TC4H9+H2O2 12090.0	4.332E+002	3.010
!REF:FIT TO TSANG 90 AND COHEN DATA		
!REF:NIST STANDARD REFERENCE DATABASE 17 -2Q98		
IC4H10+O<=>TC4H9+OH 1150.0	1.968E+005	2.402
IC4H10+O<=>IC4H9+OH 5136.0	4.046E+007	2.034
!REF:ANALOGY TO C3H8+CH3O		
IC4H10+CH3O<=>IC4H9+CH3OH 7000.0	4.800E+011	0.000
!REF:TAMURA ESTIMATE		
IC4H10+CH3O<=>TC4H9+CH3OH 2800.0	1.900E+010	0.000
!REF:		
IC4H10+O2<=>IC4H9+HO2 52290.0	9.000E+013	0.000
IC4H10+O2<=>TC4H9+HO2 48200.0	1.000E+013	0.000
!REF:BASED ON (SCALED AS PER CARSTENSEN)		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047-7054.		
IC4H10+CH3O2<=>IC4H9+CH3O2H 18280.0	2.079E+000	3.970
!REF:SCOTT AND WALKER C&F 129(4) 365--377 2002 (*1.5)		
IC4H10+C2H5O2<=>IC4H9+C2H5O2H 20460.0	2.550E+013	0.000
!REF:ANALOGY TO C2H6+HO2		
IC4H10+CH3CO3<=>IC4H9+CH3CO3H 20460.0	2.550E+013	0.000
IC4H10+NC3H7O2<=>IC4H9+NC3H7O2H 20460.0	2.550E+013	0.000
IC4H10+IC3H7O2<=>IC4H9+IC3H7O2H 20460.0	2.550E+013	0.000
IC4H10+IC4H9O2<=>IC4H9+IC4H9O2H 20460.0	2.550E+013	0.000



IC4H10+TC4H9O2<=>IC4H9+TC4H9O2H 20460.0	2.550E+013	0.000
!REF:ANALOGY WITH RH+RO2 --> R+RO2H		
IC4H10+O2CHO<=>IC4H9+HO2CHO 20440.0	2.520E+013	0.000
IC4H10+O2CHO<=>TC4H9+HO2CHO 16010.0	2.800E+012	0.000
!REF:WESTBROOK ESTIMATE		
IC4H10+SC4H9O2<=>IC4H9+SC4H9O2H 20460.0	2.250E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+SC4H9O2<=>TC4H9+SC4H9O2H 16000.0	2.800E+012	0.000
!REF:WESTBROOK ESTIMATE		
IC4H10+PC4H9O2<=>IC4H9+PC4H9O2H 20460.0	2.250E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+PC4H9O2<=>TC4H9+PC4H9O2H 16000.0	2.800E+012	0.000
!REF:BASED ON (SCALED AS PER CARSTENSEN		
!REF:J. AGUILERA-IPARRAGUIRRE ET AL. J PHYS CHEM A (2008) 112(30): 7047- 7054.		
IC4H10+CH3O2<=>TC4H9+CH3O2H 13190.0	1.366E+002	3.120
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION SEATTLE, AUGUST, 1988		
IC4H10+C2H5O2<=>TC4H9+C2H5O2H 16000.0	2.800E+012	0.000
IC4H10+CH3CO3<=>TC4H9+CH3CO3H 16000.0	2.800E+012	0.000
IC4H10+NC3H7O2<=>TC4H9+NC3H7O2H 16000.0	2.800E+012	0.000
IC4H10+IC3H7O2<=>TC4H9+IC3H7O2H 16000.0	2.800E+012	0.000
IC4H10+IC4H9O2<=>TC4H9+IC4H9O2H 16000.0	2.800E+012	0.000
IC4H10+TC4H9O2<=>TC4H9+TC4H9O2H 16000.0	2.800E+012	0.000
!REF:WESTBROOK AND PITZ ESTIMATE (1983)		
IC4H10+IC4H9<=>TC4H9+IC4H10 7900.0	2.500E+010	0.000
!REF:ESTIMATE		
IC4H9+HO2<=>IC4H9O+OH -1000.0	7.000E+012	0.000
TC4H9+HO2<=>TC4H9O+OH -1000.0	7.000E+012	0.000

CH3O2+IC4H9<=>CH3O+IC4H9O -1000.0	7.000E+012	0.000
CH3O2+TC4H9<=>CH3O+TC4H9O -1000.0	7.000E+012	0.000
!REF:		
IC4H9<=>TC4H9 34600.0	3.560E+010	0.880
!REF:CURRAN INT J CHEM KINET 38:250-275, 2006		
IC4H8+H<=>IC4H9 2620.0	6.250E+011	0.510
C3H6+CH3<=>IC4H9 6850.0	1.890E+003	2.670
H+IC4H8<=>TC4H9 1230.0	1.060E+012	0.510
!REF:		
TC4H9+O2<=>IC4H8+HO2 11960.0	8.370E-001	3.590
IC4H9+O2<=>IC4H8+HO2 9322.0	1.070E+000	3.710
NC3H7O2+IC4H9<=>NC3H7O+IC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+TC4H9<=>NC3H7O+TC4H9O -1000.0	7.000E+012	0.000
NC3H7O2+IC4H7<=>NC3H7O+IC4H7O -1000.0	7.000E+012	0.000
SC4H9O2+IC4H9<=>SC4H9O+IC4H9O -1000.0	7.000E+012	0.000
SC4H9O2+TC4H9<=>SC4H9O+TC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+IC4H9<=>PC4H9O+IC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+TC4H9<=>PC4H9O+TC4H9O -1000.0	7.000E+012	0.000
PC4H9O2+IC4H7<=>PC4H9O+IC4H7O -1000.0	7.000E+012	0.000
SC4H9O2+IC4H7<=>SC4H9O+IC4H7O -1000.0	7.000E+012	0.000
!REF:		
IC4H9+O2<=>IC4H9O2 0.0	2.260E+012	0.000
TC4H9+O2<=>TC4H9O2 0.0	1.410E+013	0.000
!REF:WALKER, R. W., 22ND SYMPOSIUM (INTERNATIONAL) ON COMBUSTION, SEATTLE, AUGUST, 1988.		
IC4H9O2+C4H10<=>IC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
TC4H9O2+C4H10<=>TC4H9O2H+SC4H9 17700.0	1.120E+013	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+C4H10<=>IC4H9O2H+PC4H9 20460.0	1.700E+013	0.000

TC4H9O2+C4H10<=>TC4H9O2H+PC4H9 20460.0	1.700E+013	0.000
!REF:ESTIMATE		
IC3H7O2+IC4H9<=>IC3H7O+IC4H9O -1000.0	7.000E+012	0.000
IC3H7O2+TC4H9<=>IC3H7O+TC4H9O -1000.0	7.000E+012	0.000
IC3H7O2+IC4H7<=>IC3H7O+IC4H7O -1000.0	7.000E+012	0.000
!REF:ANALOGY TO C3H6+HO2.		
IC4H9O2+C3H6<=>IC4H9O2H+C3H5-A 13288.1	5.350E-002	4.207
TC4H9O2+C3H6<=>TC4H9O2H+C3H5-A 13288.1	5.350E-002	4.207
!REF:WESTBROOK ESTIMATE		
IC4H9O2+IC4H8<=>IC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
TC4H9O2+IC4H8<=>TC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
PC4H9O2+IC4H8<=>PC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
SC4H9O2+IC4H8<=>SC4H9O2H+IC4H7 14900.0	1.400E+012	0.000
IC3H7O2+IC4H8<=>IC3H7O2H+IC4H7 14900.0	1.400E+012	0.000
NC3H7O2+IC4H8<=>NC3H7O2H+IC4H7 14900.0	1.400E+012	0.000
IC4H9O2+C4H8-1<=>IC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
TC4H9O2+C4H8-1<=>TC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
IC4H9O2+C4H8-2<=>IC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
TC4H9O2+C4H8-2<=>TC4H9O2H+C4H71-3 14900.0	1.400E+012	0.000
CC4H8O+OH=>CH2O+C3H5-A+H2O 0.0	5.000E+012	0.000
CC4H8O+H=>CH2O+C3H5-A+H2 5000.0	3.510E+007	2.000
CC4H8O+O=>CH2O+C3H5-A+OH 5200.0	1.124E+014	0.000
CC4H8O+HO2=>CH2O+C3H5-A+H2O2 15000.0	1.000E+013	0.000
CC4H8O+CH3O2=>CH2O+C3H5-A+CH3O2H 19000.0	1.000E+013	0.000
CC4H8O+CH3=>CH2O+C3H5-A+CH4 10000.0	2.000E+011	0.000
!REF:PITZ ESTIMATE		
C2H4+TC4H9O2<=>C2H3+TC4H9O2H 27132.0	8.590E+000	3.754
!REF:WESTBROOK ESTIMATE		
TC4H9O2+CH4<=>TC4H9O2H+CH3 20460.0	1.130E+013	0.000

!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986  
H2+TC4H9O2<=>H+TC4H9O2H 3.010E+013 0.000  
26030.0

!REF:WESTBROOK ESTIMATE  
TC4H9O2+C2H6<=>TC4H9O2H+C2H5 1.700E+013 0.000  
20460.0  
TC4H9O2+C3H8<=>TC4H9O2H+IC3H7 2.000E+012 0.000  
17000.0  
TC4H9O2+C3H8<=>TC4H9O2H+NC3H7 1.700E+013 0.000  
20460.0  
TC4H9O2+CH3OH<=>TC4H9O2H+CH2OH 6.300E+012 0.000  
19360.0  
TC4H9O2+C2H5OH<=>TC4H9O2H+PC2H4OH 6.300E+012 0.000  
19360.0  
TC4H9O2+C2H5OH<=>TC4H9O2H+SC2H4OH 4.200E+012 0.000  
15000.0

!REF:HALF OF CH2O+HO2  
IC4H9O2+CH3CHO<=>IC4H9O2H+CH3CO 2.800E+012 0.000  
13600.0  
TC4H9O2+CH3CHO<=>TC4H9O2H+CH3CO 2.800E+012 0.000  
13600.0  
IC4H9O2+C\*CCHO<=>IC4H9O2H+C2H3CO 2.800E+012 0.000  
13600.0  
TC4H9O2+C\*CCHO<=>TC4H9O2H+C2H3CO 2.800E+012 0.000  
13600.0  
IC4H9O2+C2H5CHO<=>IC4H9O2H+C2H5CO 2.800E+012 0.000  
13600.0  
TC4H9O2+C2H5CHO<=>TC4H9O2H+C2H5CO 2.800E+012 0.000  
13600.0

!REF:ESTIMATE?  
IC4H9O2+HO2<=>IC4H9O2H+O2 1.750E+010 0.000  
-3275.0  
TC4H9O2+HO2<=>TC4H9O2H+O2 1.750E+010 0.000  
-3275.0

!REF:WESTBROOK ESTIMATE  
IC4H9O2+H2O2<=>IC4H9O2H+HO2 2.400E+012 0.000  
10000.0  
TC4H9O2+H2O2<=>TC4H9O2H+HO2 2.400E+012 0.000  
10000.0  
IC4H9O2+CH2O<=>IC4H9O2H+HCO 1.300E+011 0.000  
9000.0  
TC4H9O2+CH2O<=>TC4H9O2H+HCO 1.300E+011 0.000  
9000.0

!REF:  
IC4H9O2+CH3O2=>IC4H9O+CH3O+O2 1.400E+016 -1.610  
1860.0  
TC4H9O2+CH3O2=>TC4H9O+CH3O+O2 1.400E+016 -1.610  
1860.0  
IC4H9O2+C2H5O2=>IC4H9O+C2H5O+O2 1.400E+016 -1.610  
1860.0  
TC4H9O2+C2H5O2=>TC4H9O+C2H5O+O2 1.400E+016 -1.610  
1860.0

IC4H9O2+CH3CO3=>IC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
TC4H9O2+CH3CO3=>TC4H9O+CH3CO2+O2 1860.0	1.400E+016	-1.610
IC4H9O2+IC4H9O2=>O2+IC4H9O+IC4H9O 1860.0	1.400E+016	-1.610
IC4H9O2+TC4H9O2=>IC4H9O+TC4H9O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+TC4H9O2=>O2+TC4H9O+TC4H9O 1860.0	1.400E+016	-1.610
IC4H9O2+PC4H9O2=>IC4H9O+PC4H9O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+PC4H9O2=>TC4H9O+PC4H9O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+SC4H9O2=>IC4H9O+SC4H9O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+SC4H9O2=>TC4H9O+SC4H9O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+NC3H7O2=>IC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+NC3H7O2=>TC4H9O+NC3H7O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+IC3H7O2=>IC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
TC4H9O2+IC3H7O2=>TC4H9O+IC3H7O+O2 1860.0	1.400E+016	-1.610
IC4H9O2+HO2=>IC4H9O+OH+O2 1860.0	1.400E+016	-1.610
TC4H9O2+HO2=>TC4H9O+OH+O2 1860.0	1.400E+016	-1.610

!REF:ESTIMATE

IC4H9O2+CH3<=>IC4H9O+CH3O -1000.0	7.000E+012	0.000
IC4H9O2+C2H5<=>IC4H9O+C2H5O -1000.0	7.000E+012	0.000
IC4H9O2+IC3H7<=>IC4H9O+IC3H7O -1000.0	7.000E+012	0.000
IC4H9O2+NC3H7<=>IC4H9O+NC3H7O -1000.0	7.000E+012	0.000
IC4H9O2+PC4H9<=>IC4H9O+PC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+SC4H9<=>IC4H9O+SC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+IC4H9<=>IC4H9O+IC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+TC4H9<=>IC4H9O+TC4H9O -1000.0	7.000E+012	0.000
IC4H9O2+C3H5-A<=>IC4H9O+C3H5O -1000.0	7.000E+012	0.000
IC4H9O2+C4H71-3<=>IC4H9O+C4H7O -1000.0	7.000E+012	0.000
IC4H9O2+IC4H7<=>IC4H9O+IC4H7O -1000.0	7.000E+012	0.000
TC4H9O2+CH3<=>TC4H9O+CH3O -1000.0	7.000E+012	0.000
TC4H9O2+C2H5<=>TC4H9O+C2H5O -1000.0	7.000E+012	0.000

TC4H9O2+IC3H7<=>TC4H9O+IC3H7O -1000.0	7.000E+012	0.000
TC4H9O2+NC3H7<=>TC4H9O+NC3H7O -1000.0	7.000E+012	0.000
TC4H9O2+PC4H9<=>TC4H9O+PC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+SC4H9<=>TC4H9O+SC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+IC4H9<=>TC4H9O+IC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+TC4H9<=>TC4H9O+TC4H9O -1000.0	7.000E+012	0.000
TC4H9O2+C3H5-A<=>TC4H9O+C3H5O -1000.0	7.000E+012	0.000
TC4H9O2+C4H71-3<=>TC4H9O+C4H7O -1000.0	7.000E+012	0.000
TC4H9O2+IC4H7<=>TC4H9O+IC4H7O -1000.0	7.000E+012	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+C2H4<=>IC4H9O2H+C2H3 6000.0	2.000E+011	0.000
IC4H9O2+CH4<=>IC4H9O2H+CH3 20460.0	1.130E+013	0.000
!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
H2+IC4H9O2<=>H+IC4H9O2H 26030.0	3.010E+013	0.000
!REF:WESTBROOK ESTIMATE		
IC4H9O2+C2H6<=>IC4H9O2H+C2H5 20460.0	1.700E+013	0.000
IC4H9O2+C3H8<=>IC4H9O2H+IC3H7 17000.0	2.000E+012	0.000
IC4H9O2+C3H8<=>IC4H9O2H+NC3H7 20460.0	1.700E+013	0.000
IC4H9O2+CH3OH<=>IC4H9O2H+CH2OH 19360.0	6.300E+012	0.000
IC4H9O2+C2H5OH<=>IC4H9O2H+PC2H4OH 19360.0	6.300E+012	0.000
IC4H9O2+C2H5OH<=>IC4H9O2H+SC2H4OH 15000.0	4.200E+012	0.000
!REF:		
IC4H9O2H<=>IC4H9O+OH 42500.0	1.500E+016	0.000
TC4H9O2H<=>TC4H9O+OH 42540.0	5.950E+015	0.000
!REF:ANALOGY CH3O+X --> CH2O+HX TSANG/ HAMPSON 86		
IC4H9O+HO2<=>IC3H7CHO+H2O2 0.0	1.000E+012	0.000
IC4H9O+OH<=>IC3H7CHO+H2O 0.0	1.810E+013	0.000
IC4H9O+CH3<=>IC3H7CHO+CH4 0.0	2.400E+013	0.000
IC4H9O+O<=>IC3H7CHO+OH 0.0	6.000E+012	0.000

IC4H9O+H<=>IC3H7CHO+H2 0.0	1.990E+013	0.000
!REF:CURRAN INC. INT J CHEM KINET 38: 250-275, 2006		
IC3H7CHO+H<=>IC4H9O 5860.0	1.000E+012	0.000
CH2O+IC3H7<=>IC4H9O 2330.0	5.000E+010	0.000
CH3COCH3+CH3<=>TC4H9O 11900.0	1.500E+011	0.000
!REF:ZABARNICK, S. AND HEICKLEN, J., IJCK, 17, 503 (1985).		
IC4H9O+O2<=>IC3H7CHO+HO2 1660.0	1.930E+011	0.000
!REF:PITZ ESTIMATE		
TC4H9O+O2<=>IC4H8O+HO2 4700.0	8.100E+011	0.000
!REF:FLOWERS, M.C.; PARKER, R.M. INTL. J. CHEM. KINET. 443-452, 1971.		
!REF: X 2.0		
IC4H8O<=>IC3H7CHO 52720.0	4.180E+013	0.000
!REF:		
IC4H8O+OH<=>IC3H6CHO+H2O 0.0	1.250E+012	0.000
IC4H8O+H<=>IC3H6CHO+H2 0.0	1.250E+012	0.000
IC4H8O+HO2<=>IC3H6CHO+H2O2 15000.0	2.500E+012	0.000
IC4H8O+CH3O2<=>IC3H6CHO+CH3O2H 19000.0	2.500E+012	0.000
IC4H8O+CH3<=>IC3H6CHO+CH4 10000.0	5.000E+010	0.000
IC4H8O+O<=>IC3H6CHO+OH 0.0	1.250E+012	0.000
!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES		
TC3H6CHO+H<=>IC3H7CHO 0.0	2.000E+014	0.000
!REF:TSANG J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
IC3H7+HCO<=>IC3H7CHO 0.0	1.810E+013	0.000
!REF:		
IC3H7CHO+HO2<=>IC3H7CO+H2O2 11920.0	3.000E+012	0.000
!REF:BALDWIN, R.R.; WALKER, R.W.		
!REF:SYMP. INTL. COMB. PROC. 1979, 17, 525.		
IC3H7CHO+HO2<=>TC3H6CHO+H2O2 11920.0	8.000E+010	0.000
!REF:BIRRELL, R.N.; TROTMAN-DICKENSON, A.F. J. CHEM. SOC. 1960, 2059		

IC3H7CHO+CH3<=>IC3H7CO+CH4 8700.0	3.980E+012	0.000
!REF:SINGLETON, D.L. ET AL. CAN. J. CHEM. 1977, 55, 3321.		
IC3H7CHO+O<=>IC3H7CO+OH 1389.0	7.180E+012	0.000
!REF:!BALDWIN, R.R. ET AL. J. CHEM. SOC. FAR. TRANS. 1979, 75, 1433		
IC3H7CHO+O2<=>IC3H7CO+HO2 37600.0	4.000E+013	0.000
!REF:SEMMES ET AL. INTL. J. CHEM. KINET. 1985, 17, 303.		
IC3H7CHO+OH<=>IC3H7CO+H2O -340.0	2.690E+010	0.760
IC3H7CHO+OH<=>TC3H6CHO+H2O -781.0	1.684E+012	0.000
!REF: CURRAN ESTIMATE		
IC3H7CHO+H<=>IC3H7CO+H2 2600.0	2.600E+012	0.000
IC3H7CHO+OH<=>IC3H6CHO+H2O -298.0	3.120E+006	2.000
IC3H7CHO+HO2<=>IC3H6CHO+H2O2 15500.0	2.740E+004	2.550
IC3H7CHO+CH3O2<=>IC3H6CHO+CH3O2H 16490.0	4.760E+004	2.550
!REF:NAROZNIK, M; NIEDZIELSKI, J. J. PHOTOCHEM. 1986, 32, 281		
IC3H7+CO<=>IC3H7CO 4810.0	1.500E+011	0.000
!REF:CURRAN ESTIMATE		
C3H6+HCO<=>IC3H6CHO 7800.0	1.000E+011	0.000
C*CCHO+CH3<=>IC3H6CHO 7800.0	1.000E+011	0.000
!REF:		
IC4H8+OH<=>IC4H8OH -960.0	9.930E+011	0.000
IC4H8OH+O2<=>IO2C4H8OH -1100.0	1.200E+011	0.000
IO2C4H8OH=>CH3COCH3+CH2O+OH 18900.0	1.250E+010	0.000
IC4H9O2<=>IC4H8O2H-I 24400.0	7.500E+010	0.000
TC4H9O2<=>TC4H8O2H-I 34500.0	9.000E+011	0.000
IC4H9O2<=>IC4H8O2H-T 29200.0	1.000E+011	0.000
IC4H9O2<=>IC4H8+HO2 39490.0	2.265E+035	-7.220
TC4H9O2<=>IC4H8+HO2 41490.0	7.612E+042	-9.410
!REF:		
IC4H8O2H-I+O2<=>IC4H8OOH-IO2 0.0	2.260E+012	0.000



TC4H8O2H-I+O2<=>TC4H8OOH-IO2 0.0	2.260E+012	0.000
IC4H8O2H-T+O2<=>IC4H8OOH-TO2 0.0	1.410E+013	0.000
!REF:		
IC4H8OOH-IO2<=>IC4KETII+OH 21400.0	5.000E+010	0.000
IC4H8OOH-TO2<=>IC4KETIT+OH 31500.0	4.000E+011	0.000
TC4H8OOH-IO2<=>TIC4H7Q2-I 24400.0	7.500E+010	0.000
!REF:CURRAN ESTIMATE		
IC4H7OOH+HO2<=>TIC4H7Q2-I 10600.0	1.000E+011	0.000
!REF:		
IC4H8OOH-IO2<=>IIC4H7Q2-I 24400.0	3.750E+010	0.000
IC4H8OOH-IO2<=>IIC4H7Q2-T 29200.0	1.000E+011	0.000
IC4H8OOH-TO2<=>TIC4H7Q2-I 34500.0	6.000E+011	0.000
!REF:CURRAN ESTIMATE		
AC3H5OOH+CH2O2H<=>IIC4H7Q2-I 10600.0	8.500E+010	0.000
IC4H7OOH+HO2<=>IIC4H7Q2-T 7800.0	1.000E+011	0.000
CH2O2H<=>CH2O+OH 1500.0	9.000E+014	0.000
IC4KETII=>CH2O+C2H5CO+OH 42000.0	1.500E+016	0.000
IC4KETIT=>CH3COCH3+HCO+OH 42540.0	9.500E+015	0.000
!REF:		
IC4H8+HO2<=>TC4H8O2H-I 12620.0	3.970E+011	0.000
IC4H8+HO2<=>IC4H8O2H-T 12620.0	3.970E+011	0.000
!REF:GREEN 2003		
IC4H8O2H-I<=>CC4H8O+OH 21900.0	4.470E+011	0.000
IC4H8O2H-T<=>IC4H8O+OH 13400.0	3.090E+012	0.000
TC4H8O2H-I<=>IC4H8O+OH 17000.0	3.980E+012	0.000
!REF:		
IC4H8O2H-I=>OH+CH2O+C3H6 29170.0	8.451E+015	-0.680
IC4H8<=>C3H5-T+CH3 128100.0	1.920E+066	-14.220
IC4H8<=>IC4H7+H 114300.0	3.070E+055	-11.490

IC4H8+H<=>C3H6+CH3 5.680E+033 -5.720  
20000.0

!REF:ANALOGY WITH TSANG '92: C3H6+R<=>PRODUCTS  
IC4H8+H<=>IC4H7+H2 3.400E+005 2.500  
2492.0

!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS  
IC4H8+O=>CH2CO+CH3+CH3 3.330E+007 1.760  
76.0

!REF:  
IC4H8+O=>IC3H6CO+H+H 1.660E+007 1.760  
76.0

!REF:ANALOGY WITH TSANG '91: C3H6+R<=>PRODUCTS  
IC4H8+O<=>IC4H7+OH 1.206E+011 0.700  
7633.0

!REF:  
IC4H8+CH3<=>IC4H7+CH4 4.420E+000 3.500  
5675.0  
IC4H8+HO2<=>IC4H7+H2O2 1.928E+004 2.600  
13910.0

!REF:ANALOGY WITH RH+RO2 --> R+RO2H  
IC4H8+O2CHO<=>IC4H7+HO2CHO 1.928E+004 2.600  
13910.0

!REF:  
IC4H8+O2<=>IC4H7+HO2 6.000E+012 0.000  
39900.0

!REF:WESTBROOK AND PITZ ESTIMATE 1983  
IC4H8+C3H5-A<=>IC4H7+C3H6 7.940E+011 0.000  
20500.0  
IC4H8+C3H5-S<=>IC4H7+C3H6 7.940E+011 0.000  
20500.0  
IC4H8+C3H5-T<=>IC4H7+C3H6 7.940E+011 0.000  
20500.0  
IC4H8+OH<=>IC4H7+H2O 5.200E+006 2.000  
-298.0  
IC4H8+O<=>IC3H7+HCO 1.580E+007 1.760  
-1216.0

!REF:  
IC4H8+CH3O2<=>IC4H7+CH3O2H 1.928E+004 2.600  
13910.0

!REF:BALDWIN, R. R., DEAN, C. E., AND WALKER, R. W., JCS FARADAY 2, 82,  
1445 (1986)  
IC4H8+HO2<=>IC4H8O+OH 1.290E+012 0.000  
13340.0

!REF:ANOLOGY WITH BOZZELLI C3H5-A+O2 @ 10 ATM  
IC4H7+O2<=>IC3H5CHO+OH 2.470E+013 -0.450  
23020.0

IC4H7+O2<=>CH3COCH2+CH2O 21050.0	7.140E+015	-1.210
IC4H7+O2=>C3H4-A+CH2O+OH 21450.0	7.290E+029	-5.710
!REF:		
IC4H7+O<=>IC3H5CHO+H 0.0	6.030E+013	0.000
IC4H7<=>C3H4-A+CH3 74260.0	1.230E+047	-9.740
CH3O2+IC4H7<=>CH3O+IC4H7O -1000.0	7.000E+012	0.000
IC4H7+HO2<=>IC4H7O+OH -1000.0	7.000E+012	0.000
C3H5-T+CH2O<=>IC4H7O 12600.0	1.000E+011	0.000
!REF:EA<=>8.6+7 (RING STRAIN+EABS OF PRIMARY H BY RO)		
IC4H7O<=>IC4H6OH 15600.0	1.391E+011	0.000
IC4H7O<=>IC3H5CHO+H 29100.0	5.000E+013	0.000
!REF:ANALOGY C3H5-A+X --> PRODUCTS		
IC4H6OH+H2<=>IC4H7OH+H 18990.0	2.160E+004	2.380
!REF:		
IC4H7OH+O2<=>IC4H6OH+HO2 39900.0	6.000E+013	0.000
!REF:RATE CONSTANT ANALOGY TO C3H5-A+CH2O (X 5)		
IC4H6OH+CH2O<=>IC4H7OH+HCO 18190.0	6.300E+008	1.900
!REF:CURRAN ESTIMATE		
IC4H6OH+IC4H8<=>IC4H7OH+IC4H7 19840.0	4.700E+002	3.300
IC4H6OH+H<=>IC4H7OH 0.0	1.000E+014	0.000
IC4H6OH+H2O2<=>IC4H7OH+HO2 13580.0	7.830E+005	2.050
C3H4-A+CH2OH<=>IC4H6OH 9200.0	1.000E+011	0.000
!REF:FROM BAULCH ET AL. J. PHYS. CHEM. REF. DATA, 21, 411--429, 1992		
IC4H7O+O2<=>IC3H5CHO+HO2 1649.0	3.000E+010	0.000
!REF:TSANG & HAMPSON, METHANE, J. PHYS. CHEM. REF. DATA, VOL 15, 1986		
!REF:ANALOGY CH3O+X --> CH2O+HX		
IC4H7O+HO2<=>IC3H5CHO+H2O2 0.0	3.000E+011	0.000
IC4H7O+CH3<=>IC3H5CHO+CH4 0.0	2.400E+013	0.000
IC4H7O+O<=>IC3H5CHO+OH 0.0	6.000E+012	0.000

IC4H7O+OH<=>IC3H5CHO+H2O 0.0	1.810E+013	0.000
IC4H7O+H<=>IC3H5CHO+H2 0.0	1.990E+013	0.000
!REF:CURRAN ESTIMATE		
IC3H5CHO+OH<=>IC3H5CO+H2O -340.0	2.690E+010	0.760
!REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
IC3H5CHO+HO2<=>IC3H5CO+H2O2 11920.0	1.000E+012	0.000
IC3H5CHO+CH3<=>IC3H5CO+CH4 8700.0	3.980E+012	0.000
IC3H5CHO+O<=>IC3H5CO+OH 1389.0	7.180E+012	0.000
!REF:		
IC3H5CHO+O2<=>IC3H5CO+HO2 40700.0	2.000E+013	0.000
!REF:ANALOGOUS TO ISOBUTERALDEHYDE+X		
IC3H5CHO+H<=>IC3H5CO+H2 2600.0	2.600E+012	0.000
IC3H5CO<=>C3H5-T+CO 34460.0	1.278E+020	-1.890
!REF:ANALOGY WITH C3H5-A+CH3 --> 1-C4H8 TSANG 91 (PROPENE).		
TC3H6OCHO+OH<=>TC3H6CHO+HO2 21010.0	2.018E+017	-1.200
!REF:CURRAN AND GAFFURI, 1995.		
TC3H6OCHO<=>CH3COCH3+HCO 9700.0	3.980E+013	0.000
!REF:		
IC3H5CHO+H<=>TC3H6CHO 1200.0	1.300E+013	0.000
IC3H6CO+H<=>TC3H6CHO 4800.0	1.300E+013	0.000
!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES		
TC3H6CHO+H2<=>IC3H7CHO+H 18990.0	2.160E+005	2.380
IC4H7O+OH<=>IC4H7OOH 0.0	1.000E+011	0.000
IC4H7O+H<=>IC4H7OH 0.0	4.000E+013	0.000
!REF:ANALOGY WITH IC4H9 --> IC4H8+H		
IC4H7OH+H<=>IC4H8OH 1200.0	1.000E+013	0.000
!REF:ANALOGY WITH HCO+H2 --> CH2O+H		
!REF:(TSANG/ HAMPSON 86) X 5		
IC4H7O+H2<=>IC4H7OH+H 17830.0	9.050E+006	2.000

!REF:CURRAN ESTIMATE		
IC4H7+OH<=>IC4H7OH	3.000E+013	0.000
0.0		
IC4H7OH+HCO<=>IC4H7O+CH2O	3.020E+011	0.000
18160.0		
!REF:ANALOGY WITH C3H5-A+X --> PRODUCTS. LITERATURE VALUES		
TC3H6CHO+CH2O<=>IC3H7CHO+HCO	2.520E+008	1.900
18190.0		
TC3H6CHO+IC4H8<=>IC3H7CHO+IC4H7	4.700E+002	3.300
19840.0		
!REF:ANALOGY TO 1C4H8+OH		
IC3H6CO+OH<=>IC3H7+CO2	1.730E+012	0.000
-1010.0		
!REF:CURRAN ESTIMATE		
TC3H6CHO+OH<=>TC3H6OHCHO	5.000E+013	0.000
0.0		
!REF:!TSANG, W. J. PHYS. CHEM. REF. DATA 17, 887 (1988)		
C3H6OH2-1+HCO<=>TC3H6OHCHO	1.810E+013	0.000
0.0		
!REF:ANALOGY WITH CH3CHOH --> CH3CHO+H.		
!REF:NATARAJAN & BHASKARAN SYMP. INTL. SHOCK 13		
CH3COCH3+H<=>C3H6OH2-1	8.000E+012	0.000
9500.0		
C2H5CHO+H<=>C3H6OH1-2	8.000E+012	0.000
9500.0		
!REF:BASED ON IC4H8+H<=>IC4H9		
IC3H5OH+H<=>C3H6OH2-1	6.250E+011	0.510
4020.0		
!REF:REVERSE BY ANALOGY HCO+OH --> PRODUCTS		
C3H5-T+OH<=>IC3H5OH	5.000E+013	0.000
0.0		
!REF:		
TC3H6CHO+O2<=>TC3H6O2CHO	1.990E+017	-2.100
0.0		
TC3H6O2CHO<=>IC3H5O2HCHO	6.000E+011	0.000
29880.0		
TC3H6O2CHO<=>TC3H6O2HCO	1.000E+011	0.000
25750.0		
!REF:REVERSE ANALOGY IC4H8+CH3 --> NEOC5H11.		
!REF:SLAGLE ET AL. J. PHYS. CHEM. 1991, 95		
IC3H5CHO+HO2<=>IC3H5O2HCHO	2.230E+011	0.000
10600.0		
!REF:		
TC3H6O2HCO=>CH3COCH3+CO+OH	4.244E+018	-1.430
4800.0		

!REF:!MIYOSHI, A; MATSUI, H; WASHIDA, N.; J. PHYS. CHEM. 1990, 94, 3016  
 C3H6OH2-1+O2<=>CH3COCH3+HO2 1.500E+012 0.000  
 5000.0  
 C3H6OH1-2+O2<=>C2H5CHO+HO2 1.500E+012 0.000  
 5000.0  
 !C3H6OH1-2+O2<=>C2H5CHO+HO2 3.780E+20 -2.429 3090.  
 ! PLOG / 0.001 5.260E+17 -1.637 838. /  
 ! PLOG / 0.01 5.260E+17 -1.637 838. /  
 ! PLOG / 0.1 5.260E+17 -1.637 838. /  
 ! PLOG / 1.0 5.280E+17 -1.638 839. /  
 ! PLOG / 10.0 1.540E+18 -1.771 1120. /  
 ! PLOG / 100.0 3.780E+20 -2.429 3090. /

!REF:CURRAN ESTIMATE  
 IC3H6CO+OH<=>C3H6OH2-1+CO 2.000E+012 0.000  
 -1010.0

!REF:!LOHDI, Z.H.; WALKER, R.W.; J. CHEM. SOC. FARAD. 1991 87, 2361  
 (C3H5-A+HO2) (X 0.5)  
 TC3H6CHO+HO2<=>IC3H7CHO+O2 3.675E+012 0.000  
 1310.0

!REF:CURRAN ESTIMATE  
 TC3H6CHO+CH3<=>IC3H5CHO+CH4 3.010E+012 -0.320  
 -131.0

!REF:REVERSE ADDN. ACROSS DOUBLE BOND. FORWARD FROM THERMRXN. CURRAN 95  
 TC4H8CHO<=>IC3H5CHO+CH3 1.000E+013 0.000  
 26290.0  
 TC4H8CHO<=>IC4H8+HCO 8.520E+012 0.000  
 20090.0

!REF:CURRAN ESTIMATE  
 TC4H8CHO+O2<=>O2C4H8CHO 2.000E+012 0.000  
 0.0  
 O2C4H8CHO<=>O2HC4H8CO 2.160E+011 0.000  
 15360.0  
 IC4H8O2H-T+CO<=>O2HC4H8CO 1.500E+011 0.000  
 4809.0

!REF:PITZ ESTIMATE  
 IC4H7O+IC4H8<=>IC4H7OH+IC4H7 2.700E+011 0.000  
 4000.0

!REF:  
 IC4H6OH+HO2=>CH2CCH2OH+CH2O+OH 1.446E+013 0.000  
 0.0

!REF:CURRAN ESTIMATE  
 IC4H8+CH2CCH2OH<=>IC4H7+C3H5OH 7.940E+011 0.000  
 20500.0  
 CH2CCH2OH+H2O2<=>C3H5OH+HO2 3.010E+009 0.000  
 2583.0  
 C3H5OH+OH<=>CH2CCH2OH+H2O 5.060E+012 0.000  
 5960.0  
 C3H5OH+H<=>CH2CCH2OH+H2 3.900E+005 2.500  
 5821.0

C3H5OH+O2<=>CH2CCH2OH+HO2 60690.0	4.000E+013	0.000
C3H5OH+CH3<=>CH2CCH2OH+CH4 8030.0	2.400E+011	0.000
!REF:CURRAN ESTIMATE		
CH2CCH2OH+CH3<=>IC4H7OH 0.0	3.000E+013	0.000
CH2CCH2OH+H<=>C3H5OH 0.0	1.000E+014	0.000
CH2CCH2OH+O2=>CH2OH+CO+CH2O 0.0	4.335E+012	0.000
CH2CCH2OH<=>C2H2+CH2OH 45110.0	2.163E+040	-8.310
C3H5-A+C2H2<=>C*CC*CCJ 6883.4	1.000E+012	0.000
C3H5-A+C2H3=>C5H6+H+H 61137.7	1.600E+035	-14.000
C3H4-A+C3H3<=>C6H6+H 9990.4	1.400E+012	0.000
!REF:LASKIN ET AL. IJCK 32 589-614 2000		
C4H6+C2H3=>C6H6+H2+H 3240.0	5.620E+011	0.000
C4H5-N+C2H2<=>C6H6+H 5400.0	1.600E+016	-1.330
C4H5-N+C2H3<=>C6H6+H2 -3611.0	1.840E-013	7.070
C4H5-2+C2H2<=>C6H6+H 25000.0	5.000E+014	0.000
C4H5-2+C2H4<=>C5H6+CH3 25000.0	5.000E+014	0.000
C6H2+H<=>C6H3 10800.0	1.100E+030	-4.920
C6H3+H<=>C4H2+C2H2 10780.0	2.800E+023	-2.550
C6H3+H<=>L-C6H4 12120.0	3.400E+043	-9.010
C6H3+H<=>C6H2+H2 0.0	3.000E+013	0.000
C6H3+OH<=>C6H2+H2O 0.0	4.000E+012	0.000
L-C6H4+H<=>C6H5 31400.0	1.700E+078	-19.720
L-C6H4+H<=>C-C6H4+H 34500.0	1.400E+054	-11.700
L-C6H4+H<=>C6H3+H2 9240.0	1.330E+006	2.530
L-C6H4+OH<=>C6H3+H2O 430.0	3.100E+006	2.000
C-C6H4+H<=>C6H5 29500.0	2.400E+060	-13.660
C4H3-N+C2H2<=>L-C6H4+H 10600.0	2.500E+014	-0.560
C4H3-N+C2H2<=>C6H5 31300.0	9.600E+070	-17.770
C4H3-N+C2H2<=>C-C6H4+H 30100.0	6.900E+046	-10.010

!REF:ZIEGLER ET AL. J. ANAL.APPLY.PYROLYSIS 73 212-230 (2005)  
C4H3-I+CH3<=>C5H6 1.000E+012 0.000  
0.0

!REF:LASKIN ET AL. IJCK 32 589-614 2000  
C4H2+C2H<=>C6H2+H 9.600E+013 0.000  
0.0  
C4H2+C2H<=>C6H3 4.500E+037 -7.680  
7100.0  
C4H4+C2H<=>L-C6H4+H 1.200E+013 0.000  
0.0

!REF:WANG ET AL. C&F, 110: 173. 1994  
C6H5+H(+M)<=>C6H6(+M) 1.000E+014 0.000  
0.0  
LOW/ 6.600E+075 -16.300  
7000.0/  
TROE/ 1.000E+000 1.000E-001 5.849E+002 6.113E+003/  
H2/ 2.00/ H2O/ 6.00/ CH4/ 2.00/ CO/ 1.50/ CO2/ 2.00/

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161  
C6H6+O2<=>C6H5+HO2 6.300E+013 0.000  
60000.0

!REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)  
C6H6+O<=>C6H5O+H 2.200E+013 0.000  
4530.0

!REF:ALZUETA ET AL. IJCK 32: 498-522 (2000)  
C6H6+O<=>C6H5+OH 2.000E+013 0.000  
14700.0

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161  
C6H6+H<=>C6H5+H2 2.500E+014 0.000  
16000.0

!REF:ESTIMATED  
C6H6+CH3<=>C6H5+CH4 7.320E+012 0.000  
18920.0

!REF:ESTIMATED  
C6H6+HO2<=>C6H5+H2O2 5.500E+012 0.000  
28900.0

!REF:CHEN&BOZ J. PHYS. CHEM. A 108: 4632 - 4652 2004  
C6H6+OH<=>C6H5+H2O 1.200E+000 4.100  
-301.0

!REF:TAKAMASA SETA, MASAKAZU NAKAJIMA, AND AKIRA MIYOSHI J. PHYS. CHEM.  
A, 2006, 110 (15), 5081-5090  
C6H6+OH<=>C6H5OH+H 1.320E+002 3.250  
5590.0

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)  
2007  
C6H5=>H+C4H2+C2H2 4.300E+012 0.620  
77294.0



!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)  
 2007  
 C6H5+CH2O<=>C6H6+HCO 8.550E+004 2.190  
 38.0

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

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)  
 2007  
 C6H5+HCO<=>C6H6+CO 8.550E+004 2.190  
 38.0

!REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003  
 C6H5+HO2<=>C6H5O+OH 5.000E+012 0.000  
 0.0

!REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833.  
 C6H5+O2<=>C6H5O+O 2.600E+013 0.000  
 6120.0

!REF:FRANK ET AL. SYMP (INT) COMBUST, [PROC] 1994, 25, 833.  
 C6H5+O2<=>O-C6H4O2+H 3.000E+013 0.000  
 8980.0

!REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575  
 C6H5+O2<=>C6H5OO 1.860E+013 -0.220  
 -711.0

!REF:DA SILVA AND BOZZELLI J PHYS CHEM 112: 3566-3575  
 C6H5OO<=>C6H5O+O 1.270E+015 -0.246  
 38536.0

!REF:WKM ESTIMATED  
 C6H5O+OH<=>C6H5OOH 2.000E+013 0.000  
 0.0

!REF:CHAOS ET AL. PAPER E26 5TH US COMBUSTION MEETING (WESTERN STATES)  
 2007  
 C6H5OO+C6H5OH<=>C6H5OOH+C6H5O 1.330E+011 0.000  
 14000.0

!REF:DA COSTA ET AL. INT J CHEM KINET 35: 503-524, 2003  
 C6H5OH+O2<=>C6H5O+HO2 1.000E+013 0.000  
 38800.0  
 C6H5OH+O<=>OC6H4OH+H 1.600E+013 0.000  
 3400.0  
 C6H5OH+H<=>C6H5O+H2 1.200E+014 0.000  
 12400.0  
 C6H5OH+O<=>C6H5O+OH 1.300E+013 0.000  
 2900.0  
 C6H5OH+OH<=>C6H5O+H2O 1.400E+008 1.400  
 -960.0  
 C6H5OH+HO2<=>C6H5O+H2O2 1.000E+012 0.000  
 10000.0  
 C6H5OH+CH3<=>C6H5O+CH4 1.800E+011 0.000  
 7700.0

C6H5OH+C6H5<=>C6H5O+C6H6	4.900E+012	0.000
4400.0		
C6H5OH+C3H5-A<=>C6H5O+C3H6	4.900E+011	0.000
9400.0		
C6H5OH+C4H5-I<=>C6H5O+C4H6	4.900E+011	0.000
9400.0		
C6H5OH+H<=>C6H4OH+H2	1.700E+014	0.000
16000.0		
C6H5OH+O<=>C6H4OH+OH	2.000E+013	0.000
14700.0		
C6H5OH+OH<=>C6H4OH+H2O	1.400E+013	0.000
4600.0		
C6H5OH+HO2<=>C6H4OH+H2O2	4.000E+011	0.000
28900.0		
C6H5OH+CH3<=>C6H4OH+CH4	2.000E+012	0.000
15000.0		
C6H4OH+O2<=>OC6H4OH+O	2.100E+013	0.000
6100.0		
C6H4OH+H<=>C6H5OH	1.000E+014	0.000
0.0		
OC6H4OH<=>C5H4OH+CO	7.400E+011	0.000
43800.0		

!REF:WKM REDUCED FROM 2.5E+14

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161

C6H5O+H(+M)<=>C6H5OH(+M)	2.000E+014	0.000
0.0		
LOW/	1.000E+094	-21.840
13880.0/		
TROE/ 4.300E-002 3.042E+002 6.000E+004 5.896E+003/		

!REF:XU AND LIN J PHYS CHEM 110 1672-1677 2006

!REF:WKM A FACTOR \*0.5 TO FIT PYROLYSIS DATA

C6H5OH<=>C5H6+CO	4.310E+015	-0.610
74115.0		

!REF:BAULCH AND COBOS

!REF:EVALUATED KINETIC DATA FOR COMBUSTION MODELLING J. PHYS. CHEM. REF. DATA 21, 411-429 (1992)

!REF:WKM A FACTOR REDUCED FROM 2.5E+11 TO 2.0E+11 TO FIT DATA BENZENE FLOW REACTOR DATA (LOVELL)

C6H5O<=>CO+C5H5	2.000E+011	0.000
43900.0		

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

C6H5O+H<=>CO+C5H6	1.000E+013	0.000
0.0		
C6H5O+O<=>C5H5+CO2	1.000E+013	0.000
0.0		
C6H5O+O<=>OC6H4OH	2.600E+010	0.470
800.0		

!REF:WKM

!REF:ESTIMATED TO IMPROVE AGREEMENT WITH

!REF:TOLUENE FLOW REACTOR DATA. PATHWAY TO FORM  
!REF:PARABENZOQUINONE REMOVED AS IT CAUSED IT TO BUILD

!REF:UP AND IT IS NOT SEEN IN THE EXPERIMENT

C6H5O+HO2<=>O-OC6H5OJ+OH 2.000E+012 0.000  
0.0

!REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38:  
250-275, 2006

P-C6H4O2+H<=>P-OC6H5OJ 4.000E+012 0.000  
9740.0

!REF: WKM ESTIMATED FROM METHODS DESCRIBED IN CURRAN INT J CHEM KINET 38:  
250-275, 2006

O-C6H4O2+H<=>O-OC6H5OJ 4.000E+012 0.000  
6960.0

!REF:ALZUETA ET AL. INT J CHEM KINET: 30: 683-697, 1998

C6H5O+O<=>P-C6H4O2+H 4.250E+013 0.000  
0.0

C6H5O+O<=>O-C6H4O2+H 8.500E+013 0.000  
0.0

O-C6H4O2<=>C5H4O+CO 1.000E+012 0.000  
40000.0

P-C6H4O2<=>C5H4O+CO 3.700E+011 0.000  
59000.0

P-C6H4O2+H<=>C5H5O+CO 2.500E+013 0.000  
4700.0

P-C6H4O2+H<=>P-C6H3O2+H2 2.000E+012 0.000  
8100.0

P-C6H4O2+O<=>P-C6H3O2+OH 1.400E+013 0.000  
14700.0

P-C6H4O2+OH<=>P-C6H3O2+H2O 1.000E+006 2.000  
4000.0

P-C6H3O2+H<=>P-C6H4O2 1.000E+014 0.000  
0.0

P-C6H3O2+H<=>2C2H2+2CO 1.000E+014 0.000  
0.0

P-C6H3O2+O=>C2H2+HCCO+2CO 1.000E+014 0.000  
0.0

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

P-C6H4O2+O=>2CO+C2H2+CH2CO 3.000E+013 0.000  
5000.0

C5H5+H(+M)<=>C5H6(+M) 2.600E+014 0.000  
0.0

LOW/ 4.400E+080 -18.280  
12994.0/

TROE/ 6.800E-002 4.007E+002 4.136E+003 5.502E+003/  
CO/ 1.50/ CO2/ 2.00/ H2O/ 6.00/ H2/ 2.00/ CH4/ 2.00/

!REF:MACKIE ET AL. PHYS CHEM CHEM PHYS 3 2467 2001

!REF:TROE FIT ADDED BY WKM (CHEMDIS)

C5H6(+M)<=>C3H4-A+C2H2(+M) 3.800E+017 0.000  
104000.0

LOW/ 126321.5/ TROE/ 1.441E-001 5.358E+000 3.284E+003 6.710E+009/ CO/ 1.50/ CO2/ 2.00/ H2O/ 6.00/ H2/ 2.00/ CH4/ 2.00/	1.000E+098	-22.250
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998 C5H6+O2<=>C5H5+HO2 37150.0 C5H6+HO2<=>C5H5+H2O2 12900.0 C5H6+OH<=>C5H5+H2O 0.0	4.000E+013 1.100E+004 3.080E+006	0.000 2.600 2.000
!REF:ROY AND FRANK, 21ST INTERNATIONAL SYMPOSIUM ON SHOCKWAVES, 1997 PPER 1560 C5H6+H<=>C5H5+H2 3500.0	7.200E+013	0.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998 C5H6+H<=>C2H2+C3H5-A 32890.0 C5H6+O<=>C5H5+OH 1100.0 C5H6+C2H3<=>C5H5+C2H4 0.0	1.548E+037 4.800E+004 1.200E-001	-6.180 2.710 4.000
!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161 C5H6+C6H5O<=>C5H5+C6H5OH 8000.0	3.160E+011	0.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998 C5H6+CH3<=>C5H5+CH4 0.0	1.800E-001	4.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998 C5H6+C6H5<=>C5H5+C6H6 0.0	1.000E-001	4.000
!REF:ON OTHER CONDITIONS. C5H6+C5H5<=>C6H6+C4H5-N 0.0	5.000E+009	0.000
!REF:LIN J COMPUT CHEM 21 415-425 2000 C5H5<=>C3H3+C2H2 124900.0	1.980E+068	-15.000
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998 C5H5+O<=>C4H5-N+CO 440.0 C5H5+O<=>C5H4O+H 20.0 C5H5+OH<=>C5H5OH -2730.0 DUP C5H5+OH<=>C5H5OH 18730.0 DUP	3.200E+013 5.800E+013 6.500E+014 1.100E+043	-0.170 -0.020 -0.850 -8.760

C5H5+OH<=>C5H5OH 33450.0 DUP	1.100E+059	-13.080
C5H5+OH<=>C5H4OH+H 48350.0	3.500E+057	-12.180
!REF:RISTORI ET AL. COMBUST. SCI. AND TECH 2001. VOL. 167. PP. 223-256		
C5H5+OH<=>C4H6+CO 4500.0	4.000E+014	0.000
C5H5+HO2<=>C5H5O+OH 11650.0	6.300E+029	-4.690
!REF:WKM REDUCED BY 50% TO PROVIDE		
!REF:AGREEMENT WITH C5H6 SHOCK TUBE DATA		
!REF:ZHONG & BOZZELI J PHYS CHEM A 102: 3537 1998		
C5H5+O2<=>C4H4O+HCO 10970.0	6.000E+018	-2.480
!REF:ALZUETA ET AL. INT J CHEM KINET: 32: 498-522, 2000		
C4H4O+H<=>C3H5-A+CO 2740.0 DUP	6.600E+013	-0.020
C4H4O+H<=>C3H5-A+CO 1300.0 DUP	5.900E+006	2.000
C4H4O+O<=>CH2CHO+HCCO -860.0	3.000E+008	1.450
C4H4O+OH<=>C3H5-A+CO2 0.0	3.000E+012	0.000
!REF:LIN J COMPUT CHEM 21 415-425 2000		
C3H3+C2H2<=>CTCC*CCJ 45400.0	4.110E+072	-18.200
CTCC*CCJ<=>C5H5 34058.3	8.000E+013	0.000
CTCC*CCJ+H<=>C5H6 0.0	1.000E+014	0.000
!REF:LINDSTEDT C&F 99:551-561 (1994)		
CTCC*CCJ+H<=>C5H6-L 0.0	1.000E+010	0.000
C5H6-L+O<=>CTCC*CCJ+OH 0.0	1.000E+010	0.000
C5H6-L+OH<=>CTCC*CCJ+H2O 0.0	1.000E+010	0.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.		
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)		
C5H5OH+H<=>C5H4OH+H2 0.0	3.200E+012	0.000
C5H5OH+H<=>C5H5O+H2 6094.0	4.000E+013	0.000
C5H5OH+OH<=>C5H4OH+H2O 1731.0	5.500E+012	0.000

C5H5OH+OH<=>C5H5O+H2O 1697.0	1.000E+013	0.000
C5H5OH+O<=>C5H4OH+OH 0.0	4.700E+011	0.000
C5H5OH+O<=>C5H5O+OH 4683.0	1.000E+013	0.000
C5H5OH+HO2<=>C5H4OH+H2O2 10531.0	3.600E+003	2.550
C5H5OH+HO2<=>C5H5O+H2O2 15800.0	1.000E+013	0.000
C5H5O<=>C5H4O+H 21220.0	2.900E+032	-6.500
C5H5O<=>C4H5-N+CO 66250.0	1.100E+079	-19.620
C5H5O<=>CJ*CC*CC*O 14338.0	2.000E+013	0.000

!REF:ESTIMATED FROM METHODS DESCRIBED IN CURRAN'S N-HEPTANE C&F 114: 149-177 (1998)

CJ*CC*CC*O<=>C*CC*CCJ*O 4118.0	4.300E+011	-1.050
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!REF:WKM ANALOGY TO C2H5+CO<=>C2H5CO

C4H5-N+CO<=>C*CC*CCJ*O 4810.0	1.510E+011	0.000
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!REF:SAKAI ET AL PROCEEDINGS OF THE COMBUSTION INSTITUTE 32 (2009) 411-418

CJ*CC*CC*O<=>C2H2+CJ*CC*O 43710.0	3.000E+013	0.000
CJ*CC*O<=>C2H3CO 32100.0	1.400E+009	0.980
C2H2+HCO<=>CJ*CC*O 7755.0	7.770E+006	1.410

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

C5H4OH+H<=>C5H5OH 0.0	1.000E+014	0.000
C5H4OH+H<=>C5H4O+H2 54000.0	2.100E+013	0.000
C5H4OH+O2<=>C5H4O+HO2 5000.0	3.000E+013	0.000

!REF:WANG AND BREZINSKY J PHYS CHEM A 102: 1530 1998

C5H4O=>CO+C2H2+C2H2 68500.0 DUP	5.700E+032	-6.760
C5H4O=>CO+C2H2+C2H2 98700.0 DUP	6.200E+041	-7.870

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

C5H4O+H<=>C4H5-N+CO 40810.0	2.100E+061	-13.270
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!REF:ALZUETA & GLARBORG IJCK 30: 683, 1998.

C5H4O+O<=>C4H4+CO2 2000.0	1.000E+013	0.000
C5H4O+H<=>C5H3O+H2 8100.0	2.000E+012	0.000
C5H4O+O<=>C5H3O+OH 1470.0	1.400E+013	0.000
C5H4O+OH<=>C5H3O+H2O 1450.0	1.100E+008	1.420
C5H3O+H<=>C5H4O 0.0	1.000E+014	0.000

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

C5H3O+O2=>CO2+C2H2+HCCO 38180.0	9.700E+058	-13.470
C5H3O=>C2H2+CO+C2H 51000.0	2.000E+013	0.000

!REF:ARENDS ET AL. J PHYS CHEM 97: 7914 1993

C5H7<=>C*CCJC*C 39500.0	3.200E+015	0.000
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!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

C5H7+H<=>C5H6+H2 0.0	3.600E+012	0.000
C5H7+O<=>C5H6+OH 0.0	1.000E+013	0.000

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)

C5H7+OH<=>C5H6+H2O 0.0	2.400E+013	0.000
C5H7+O2<=>OC5H7O 20000.0	8.900E+024	-3.800

!REF:ZHONG & BOZZELLI J PHYS CHEM A 102: 3537 1998

C5H6+H<=>C5H7 31500.0	2.400E+073	-17.850
C5H6+H<=>C*CCJC*C 3100.0	1.100E+014	-0.160
C5H6+O<=>C5H5O+H 590.0 DUP	8.900E+012	-0.150
C5H6+O<=>C5H5O+H 200.0 DUP	5.600E+012	-0.060
C5H6+OH<=>C*CCJC*COH 870.0	1.100E+013	-0.070
C5H6+HO2<=>C5H7+O2 9530.0	1.300E+015	-1.070
C5H6+HCO<=>C5H5+CH2O 16000.0	1.080E+008	1.900
C5H6+C2H3<=>C6H6+CH3 42460.0	2.100E+067	-16.080

!REF:EMDEE ET AL. J. PHYS. CHEM. 1992, 96, 2151-2161

C5H6+C4H5-I<=>C5H5+C4H6 6.000E+012 0.000  
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)  
C\*CCJC\*C<=>C\*CC\*CCJ 5.400E+011 -0.700  
60.0  
C\*CC\*CCJ+H<=>C\*CC\*CC 2.300E+020 -1.600  
3020.0  
C\*CC\*CC+H<=>C4H6+CH3 5.200E+071 -16.380  
51000.0

!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996

C\*CC\*CC+H<=>C\*CC\*CCJ+H2 7.000E+006 2.000  
5000.0  
C\*CC\*CC+OH<=>C\*CC\*CCJ+H2O 7.000E+006 2.000  
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)  
C\*CCJC\*C+O2<=>C\*CCHO+CH2CHO 1.200E+036 -7.250  
33600.0  
C\*CC\*CCJ+H<=>C4H5-N+CH3 2.900E+026 -2.180  
36770.0

!REF:MARINOV ET AL. COMBUST SCI TECH 116:211 1996

C\*CCJC\*C+O<=>C\*CCHO+C2H3 2.000E+014 0.000  
0.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)  
C\*CC\*CCJ+OH<=>C\*CC\*CCOH 1.500E+013 0.000  
0.0  
C\*CC\*CCJ+O2<=>C\*CCJC\*O+CH2O 8.200E+010 0.180  
9140.0  
C\*CC\*CCOH+H<=>C4H6+CH2OH 2.500E+034 -6.120  
16250.0

!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.

!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)  
OC5H7O+O2<=>OC4H6O+HOCO 6.300E+005 -7.250  
33600.0  
C\*CCJC\*COH+O2<=>HOC\*CC\*O+CH2CHO 1.200E+036 -7.250  
33600.0  
HOC\*CC\*O+OH<=>HOC\*CCJ\*O+H2O 2.690E+010 0.760  
-340.0  
HOC\*CC\*O+HO2<=>HOC\*CCJ\*O+H2O2 1.000E+012 0.000  
11920.0  
HOC\*CC\*O+CH3<=>HOC\*CCJ\*O+CH4 3.980E+012 0.000  
8700.0  
HOC\*CC\*O+O<=>HOC\*CCJ\*O+OH 7.180E+012 0.000  
1389.0  
HOC\*CC\*O+O2<=>HOC\*CCJ\*O+HO2 2.000E+013 0.000  
40700.0



HOC*CC*O+H<=>HOC*CCJ*O+H2 2600.0				2.600E+012	0.000
!REF:WKM ANALOGY TO C2H5+CO<=>C2H5CO					
C2H2OH+CO<=>HOC*CCJ*O 4810.0				1.510E+011	0.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.					
!REF:PRIVATE COMMUNICATION WITH BOZZELLI (ZHONG'S THESIS)					
OC4H6O+H<=>OC4H5O+H2 3279.0				2.300E+010	1.050
OC4H6O+OH<=>OC4H5O+H2O -447.0				3.500E+009	1.180
OC4H5O+O2<=>O2CCHOOJ+C2H4 20670.0				1.600E+045	-9.920
O2CCHOOJ<=>HOCO+CO2 4000.0				3.000E+013	0.000
!REF:ALZUETA & GLARBORG IJCK 32: 498-522, 2000.					
C*CCJC*O<=>C3H5-A+CO -1120.0				6.100E+005	0.920
C*CCJC*O+O2<=>C*CCHO+HOCO 33600.0				1.200E+036	-7.250
!REF: JOHN R. BARKER CALCULATION 7/ 3/ 2013					
HOCO<=>CO+OH 32470.0				6.300E+032	-5.960
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 34240.0				1.897E+038	-8.047
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/	
!C6H10+H<=>C6H9-A+H2 207.0				6.752E+005	2.360

!C6H10+CH3<=>C6H9-A+CH4				7.380E+000	3.310
4002.0					
!C6H10+O<=>C6H9-A+OH				1.320E+006	2.430
1210.0					
!C6H10+OH<=>C6H9-A+H2O				5.528E+004	2.640
-1919.0					
!C4H6+C2H3<=>C6H9-A				8.800E+005	2.500
6130.0					
!					
!!REF: Lynch et al. J. Phys. Chem. A, 2013, 117, 4750-4761 DECREASE 30%					
!C6H10<=>C3H5-A+C3H5-A				4.900E+022	-2.060
63355.5					
!PLOG/	1.0000	5.070E+047	-9.700	72680.0/	
!PLOG/	4.0000	4.220E+039	-7.300	69390.0/	
!PLOG/	10.0000	2.120E+035	-6.000	67620.0/	
!C3H5-A+C3H5-A<=>C3H4-A+C3H6				9.550E+040	-9.300
12470.0					
!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/	
!C6H10+O2<=>C6H9-A+HO2				4.000E+014	0.000
38890.0					
!C6H10+H=>C3H4-A+C3H5-A+H2				1.000E+012	0.000
0.0					
!C6H10+H<=>C3H5-A+C3H6				1.000E+013	0.000
0.0					
END					