

**Механизмы окисления топливных смесей н-гептан/толуол,  
метилгексаноат/н-гептан/толуол и этилпентаноат/н-гептан/толуол**

**Механизм окисления смеси н-гептан/толуол**

ELEMENTS  
H O C N AR  
END  
SPECIES

! Biradicals :

B10  
B2C0  
B3C  
B4CH  
B5CH2  
B6CH2

! Primary molecules :

! Reactants:

C7H16-1  
C8H18-1  
H2  
H2O  
O2  
H2O2  
CH4  
HCHO  
CH3OH  
CO2  
CH3OOH  
C2H2  
C2H4Z  
C2H6  
CH2COZ  
CH3CHO  
C2H5OH  
C2H3OH  
C2H5OOH  
CH3COOOH  
C3H6Y  
C3H8  
C4H8Y  
C4H10  
C2H5CHO  
C3H7OH  
C2H6CO  
C3H8CO  
C4H6Z2  
C2H3CHOZ  
C7H16  
C8H18  
C5H10Z  
C7H14Z

C6H12Z  
C7H14Y  
C8H16Y  
C8H16Z  
C5H10Y  
C4H100L  
C4H1002P  
C3H802P  
C5H12  
C5H100A  
C4H80A  
C5H120L  
C6H14

! Secondary molecules :

C6H120A  
C7H140A  
C9H18Z  
C10H20Z  
C13H26Z  
C12H24Z  
C11H22Z  
C14H28Z  
C8H160A  
C9H180A  
C12H240A  
C11H220A  
C10H200A  
C13H260A  
C3H60LY  
C3H602PY  
C4H60AY  
C4H80LY  
C6H10Y2  
C7H12Y2  
C10H18Y2  
C11H20Y2  
C8H14Y2  
C4H802PY  
C5H80AY  
C5H100LY  
C12H22Y2  
C9H16Y2  
C7H140LY  
C7H1402PY  
C8H140AY  
C8H160LY  
C14H26Y2  
C15H28Y2  
C8H1602PY  
C9H160AY  
C9H180LY  
C16H30Y2  
C13H24Y2

C5H1002PY  
C6H100AY  
C6H120LY  
C4H60KZ  
C5H80KZ  
C6H100KZ  
C7H120KZ

! Cyclic primary molecules :  
C2H40E#3

! Cyclic secondary molecules :  
C3H60E#3  
C4H80E#3  
C5H100E#3  
C7H140E#3  
C6H120E#3  
C8H160E#3  
C9H180E#3  
C10H200E#3  
C13H260E#3  
C12H240E#3  
C11H220E#3  
C14H280E#3

! Benzenic primary molecules :

! Free radicals :  
R1H ! .h  
R2OH ! .oh  
R3OOH ! .o/oh  
R4CH3 ! .ch3  
R5CHO ! .ch//o  
R6CH2OH ! .ch2/oh  
R7CH3O ! .o/ch3  
R8CH3OO ! .o/o/ch3  
R9C2H ! .c///ch  
R10C2H3V ! .ch//ch2  
R11C2H5 ! .ch2/ch3  
R12CHCOZ ! .ch//c//o  
R13CH2CHO ! .ch2/ch//o  
R14CH3CO ! .c(//o)/ch3  
R15C2H5O ! .o/ch2/ch3  
R16C2H4OOH ! .ch2/ch2/o/oh  
R17C2H5OO ! .o/o/ch2/ch3  
R18CH3COOO ! .o/o/c(//o)/ch3  
R19C3H7 ! .ch2/ch2/ch3  
R20C4H9 ! .ch2/ch2/ch2/ch3  
R21CH3OCO ! .c(//o)/o/ch3  
!R22CO2H ! .c(//o)/oh  
!R23C2H3O2B ! .ch2/c(//o)/oh  
!R24C2H4OH ! .ch2/ch2/oh  
!R25C2H4OH ! .ch(/oh)/ch3  
R23C2H4OH ! c.h2-ch2-oh

R24C2H40H ! ch3-c.h-oh  
R25C2H5C0 ! ch3-ch2-c.o  
  
R26C7H15 ! .ch(/ch2/ch2/ch3)2  
R27C7H15 ! .ch2/ch2/ch2/ch2/ch2/ch2/ch3  
R28C7H15 ! .ch(/ch3)/ch2/ch2/ch2/ch2/ch3  
R29C7H15 ! .ch(/ch2/ch3)/ch2/ch2/ch2/ch3  
R30C8H17 ! .ch2/c(/ch3)2/ch2/ch(/ch3)2  
R31C8H17 ! .ch2/ch(/ch3)/ch2/c(/ch3)3  
R32C8H17 ! .c(/ch3)2/ch2/c(/ch3)3  
R33C8H17 ! .ch(/ch(/ch3)2)/c(/ch3)3  
R34C4H9 ! .ch(/ch3)/ch2/ch3  
R35C5H11 ! .ch2/ch2/ch2/ch2/ch3  
R36C4H9 ! .ch2/ch(/ch3)2  
R37C5H11 ! .ch2/c(/ch3)3  
R38C4H9 ! .c(/ch3)3  
R39C5H11 ! .ch(/ch2/ch3)2  
R40C5H11 ! .ch(/ch3)/ch2/ch2/ch3  
R41C6H13 ! .ch2/ch2/ch2/ch2/ch2/ch3  
R42C7H15 ! .c(/ch3)2/ch2/ch(/ch3)2  
R43C3H7 ! .ch(/ch3)2  
R44C7H15 ! .ch(/ch3)/ch2/c(/ch3)3

!Cyclic free radicals:

!Benzenic free radicals:

! lumped Free radicals :

RC3H5Y  
RC4H7Y  
RC3H50  
RC7H13Y  
RC8H15Y  
RC5H9Y  
RC5H90  
RC4H70  
RC3H503  
RC6H110  
RC7H130  
RC5H903  
RC4H703  
RC6H1103  
RC7H1303  
RC8H150  
RC9H170  
RC12H230  
RC11H210  
RC10H190  
RC13H250  
RC8H1503  
RC9H1703  
RC11H23  
RC12H2303  
RC10H21  
RC11H2103  
RC9H19

RC10H1903  
RC12H25  
RC13H2503  
RC6H11Y

! lumped Cyclic free radicals :

N2  
AR

!!!!!!!!!!!!Especies rajoutées pour le мйса toluине

aC3H4	!ch2//ch//ch2	propadiene = allene
pC3H4	!ch///c/ch3	propyne
C4H2	!ch///c/c///ch	butadiyne = diacetylene
C4H4	!ch2//ch/c///ch	1-buten-3-yne ou vinyl
acetylene		
C4H6-12	!ch2//c//ch/ch3	1,2-butadiene ou
мйthyl allине		
C4H6-1	!ch///c/ch2/ch3	1-butyne
C4H6-2	!ch3/c///c/ch3	2-butyne
iC4H8	!ch2//c(ch3)/ch3	2methyl-propene
C5H8	!ex ch2//ch/ch2/ch//ch2	pentadiene
iC5H8	!ex ch3/c(ch3)//c//ch2	
!iC5H10	!ex ch3/ch(ch3)/ch//ch2	
!C5H10	!ex ch2//ch/ch2/ch2/ch3	pentene
C5H8#	!c(#1)h2/ch2/ch//ch/ch2/1	cyclopentene
C5H6#	!c(#1)h//ch/ch//ch/ch2/1	cyclopentadiene
C6H6#	!c(#1)h&ch&ch&ch&ch&1	benzene
toluene	!c(#1)h&ch&ch&ch&ch&1(/ch3)	
MCP	!c(#1)h2/ch2/ch//ch/ch(/ch3)/1	methylcyclopentene
MCPD	!c(#1)h//ch/ch//ch/ch(/ch3)/1	methylcyclopentadiene
C5H4O#	!o//c(#1)/ch//ch/ch//ch/1	
C3H2	!.ch//c//c(.)h	
C2H4O#3	!c(#1)h2/o/ch2/1	
C2H3CHO	!ch(/o)/ch//ch2	2-propenal
cC3H4	!c(#1)h2/ch//ch/1	cyclopropene
cC3H6	!c(#1)h2/ch2/ch2/1	cyclopropane
tC4H4	!ch2//c//c//ch2	1,2,3 butatriene
C6H2	!ch///c/c///c/c///ch	hexatriyne
cC4H6	!c(#1)h2/ch//ch/ch2/1	cyclobutene
lC6H4	!ch///c/ch//ch/c///ch	
!lC6H6	!ch2//ch/c///c/ch//ch2	!MF car n'intervient plus (une
rйaction)		
lC6H8	!ch2//ch/ch//ch/ch//ch2	
C6H8#	!c(#1)h2/ch//ch/ch2/ch//ch/1	cyclohexadiene
C6H10#	!c(#1)h2/ch//ch/ch2/ch2/1	cyclohexene
C8H10#	!c(#1)h2/ch//ch/ch//ch/ch//ch/ch2/1	cyclooctatriene
!Especies excitees		
OHE		
CHE		
iC3H7	!.ch(/ch3)2	
C3H3	!ch///c/ch2(.)	
C3H5Y	!.ch2/ch//ch2	
tC3H5	!ch2//c(.) /ch3	

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sC3H5      !.ch//ch/ch3
nC4H3      !.ch//ch/c///ch
iC4H3      !ch2//c(./c///ch
nC4H5      !.ch//ch/ch//ch2
iC4H5      !ch2//c(./ch//ch2
C4H5-1s    !ch///c/ch(./ch3
C4H5-1p    !.ch2/ch2/c///ch
C4H5-2     !.ch2/c///c/ch3
1C6H5      !ch///c/ch//ch/ch//ch(.)
1C6H7      !ex .ch//ch/ch//ch/ch//ch2
!1C6H9     !ex .ch//ch/ch//ch/ch2/ch3 !MF car n'intervient plus (une
rñaction)
C6H4#      !.c(#1)&ch&ch&ch&c(.)&1
C6H5#      !.c(#1)&ch&ch&ch&ch&1
C6H7#      !.c(#1)h/ch//ch/ch2/ch//ch/1
C6H9Z#     !.c(#1)h/ch//ch/ch2/ch2/ch2/1
C4H7-1     !.ch2/ch2/ch//ch2
C4H7-2     !ch3/c(./)/ch/ch3
C4H7Y      !ch3/c(./)h/ch//ch2
C4H7T      !ch2//c(./)/ch2/ch3
iC4H7      !.ch//c(/ch3)2
C4H7V      !.c(/ch3)//ch/ch3
!C5H7Y     !ch2//ch/ch//ch/c(.)h2
!iC5H7Y    !ch2//c(/c(.)h2)/ch//ch2
C5H9Y      !ch2//ch/c(./)h/ch2/ch3
iC5H9      !.ch2/ch(/ch3)/ch//ch2
!iC5H9Y    !ch3/c(./)(/ch3)/ch//ch2
CH2CHCO    !.ch2/ch//c//o
cC3H3      !.c(#1)h/ch//ch/1
! MECHANISM OF BENZENE
! Molecules
C4H4O      !ch2//ch/ch//c//o          vinylketene
!1C5H6     !ch///c/ch//ch/ch3          !MF car
n'intervient plus (une rñaction)
C5H5OH#    !c(#1)h//ch/ch//ch/ch(/oh)/1    cyclopentadienol
C6H5OH#    !c(#1)h&ch&ch&ch&c(/oh)&1      phñnol
OC6H4O     !o//c(#1)/ch//ch/ch//ch/c(/o)/1  orthobenzoquinone
C6H5#C2H   !ch///c/c(#1)&ch&ch&ch&ch/&1      phenylacetylene
etC6H5     !c(#1)h&ch&ch&ch&c(/ch2/ch3)&1    ethylbenzene
styrene    !c(#1)h&ch&ch&ch&c(/ch//ch2)&1
!C6H5C3H3 !c(#1)h&ch&ch&ch&c(/ch//c//ch2)&1 !MF car n'intervient plus
(une rñaction)
C10H10#    !c(#1)h(c(#1)h/ch//ch/ch//ch/1)/ch//ch/ch//ch/1 !
bicyclopentadienyl
C6H5CHO    !c(#1)h&ch&ch&ch&c(/ch//o)&1      benzaldehyde
biphenyl   !c(#1)h&ch&ch&ch&c(/c(#2)h&ch&ch&ch&c&2)&1
C6H5OOH

! Radicals
C5H5#      !c(#1)(.)h/ch//ch/ch//ch/1
1C5H5      !.c///c/ch//ch/ch3
C5H30#     !.c(#1)//ch/ch//ch/c(/o)&1
C5H50#     !c(#1)h//ch/ch//ch/ch(/o.)&1
C5H40H#    !.c(#1)//ch/ch//ch/ch(/oh)&1

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C6H50# !c(#1)h&ch&ch&ch&c(/o(.))&1  
 C6H502 !.c(#1)&ch&ch&ch&ch&c(/o/o(.))&1  
 C6H40H# !.c(#1)&ch&ch&ch&ch&c(/oh)&1  
 OC6H40H !c(#1)h&ch&ch&ch&ch(/o(.))&c(/oh)&1

!MECHANISM OF TOLUENE

HOC6H4CH3 !oh/c(#1)&ch&ch&ch&ch&c(/ch3)&1 cresol  
 C6H40HCHO !oh/c(#1)&ch&ch&ch&ch&c(/ch//o)&1  
 C6H5CH2OH !c(#1)h&ch&ch&ch&ch&c(/ch2/oh)&1  
 C6H5CH2OOH !c(#1)h&ch&ch&ch&ch&c(/ch2/o/oh)&1  
 bibenzyl !ok  
 stilbene !ok  
 benzyl !c(#1)h&ch&ch&ch&ch&c(/c(.)h2)&1  
 C6H4CH3 !c(#1)h&ch&ch&ch&ch&c(/ch3)&1  
 C6H40HCO !oh/c(#1)&ch&ch&ch&ch&c(/c(.)//o)&1  
 HOC6H4CH200 !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o/o(.))&1  
 OC6H4CH3 !o(.)/c(#1)&ch&ch&ch&ch&c(/ch3)&1  
 HOC6H4CH2 !oh/c(#1)&ch&ch&ch&ch&c(/c(.)h2)&1  
 C6H5CO !c(#1)h&ch&ch&ch&ch&c(/o(.))&1  
 C6H5CHOH !c(#1)h&ch&ch&ch&ch&c(/c(.)h/oh)&1  
 C6H5CH2O !c(#1)h&ch&ch&ch&ch&c(/ch2/o(.))&1  
 HOC6H4CH2O !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o(.))&1  
 C6H5CH2OO !c(#1)h&ch&ch&ch&ch&c(/ch2/o/o(.))&1  
 C8H9# !c(#1)h&ch&ch&ch&ch&c(/c(.)h2/ch2)&1  
 C8H9#-1 !c(#1)h&ch&ch&ch&ch&c(/ch2/c(.)h2)&1  
 C6H5C2H2 !c(#1)h&ch&ch&ch&ch&c(/ch//c(.)h)&1  
 C14H13# !bibenzyl -H

!MECHANISM OF CYCLOPENTENE!

!C5H8-12 !ch2//c//ch/ch2/ch3  
 !C5H7# !.c(#1)h/ch2/ch//ch/ch2/1  
 !C5H7#Y !c(#1)h2/c(.)h/ch//ch/ch2/1  
 !C5H7#V !c(#1)h2/ch2/c(.)//ch/ch2/1  
 !C5H7-1s !ch(.)//ch/ch2/ch//ch2  
 !C5H7-2t !ch2//ch/ch2/c(.)//ch2  
 !C5H7-4t !ch3/c(.)//ch/ch//ch2  
 !C5H7-3t !ch3/ch//c(.)/ch//ch2  
 !C5H7-5p !ch2(.)/ch2/ch2/c//ch  
 !C5H7-12-5p !ch2(.)/ch2/ch//c//ch2  
 !C5H9# !.c(#1)h/ch2/ch2/ch2/ch2/1  
 !C5H9 !(.)ch2/ch2/ch2/ch//ch2  
 !RMCP1 !c(#1)h(.)/ch2/ch//ch/ch(/ch3)/1  
 !RMCP2 !c(#1)h2/ch2/ch//ch/ch(/ch2(.))/1  
 !RMCPY1 !c(#1)h2/ch(.)/ch//ch/ch(/ch3)/1  
 !RMCPY2 !c(#1)h2/ch2/ch//ch/c(.)(/ch3)/1  
 !RMCPD !c(#1)h//ch/ch//ch/ch(/ch2(.))/1  
 !RMCPDY !c(#1)h//ch/ch//ch/c(.)(/ch3)/1

!\*Especies ajoutées\*!

!mfC5H5C2H2 !c(#1)h//ch/ch//ch/c(/ch//c(.)h)&1  
 !C5H4CCH2 !c(#1)h//ch/ch//ch/c(/c//ch2)/1

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!C5H5CCH !c(#1)h//ch/ch//ch/ch(/c//ch)/1
!C6H5COCH3 !C6H5x/CO/CH3
C8H9#00H !C6H5#ch(/ooh)/ch3 ! c(#1)h&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1
C8H9#0 !C6H5#ch(/o(.))/ch3 !
c(#1)h&ch&ch&ch&c(/ch(/o(.))/ch3)&1
00C6H4CH3 !o(.)/o/c(#1)&ch&ch&ch&c(/ch3)&1
!C6H5OCH2C6H5 !c(#1)h&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&2)&1
!To10CH2C6H5 !ch3/c(#1)&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&2)&1
!PhenolCH2bz !h/o/c(#1)&ch&ch&ch&c(/ch2/c(#2)&ch&ch&ch&ch&2)&1
!PhenolC2H4bz !h/o/c(#1)&ch&ch&ch&c(/ch2/ch2/c(#2)&ch&ch&ch&ch&2)&1
CH3bz0HCH2bz !h/o/c(#1)&ch&ch&c(/ch3)&ch&c(/ch2/c(#2)&ch&ch&ch&ch&2)&1
!Benzaldtol !
c(#1)h&ch&ch&ch&c(/c(/o)/o/c(#2)&ch&ch&c(/ch3)&ch&ch&2)&1
!HOC6H4CHO !h/o/c(#1)&ch&ch&ch&c(/ch//o)&ch&1
!C6H5C4H7 !c(#1)h&ch&ch&ch&c(/ch2/ch2/ch//ch2)&1
naphthalene
!benzofuran
C8H80# ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch2/2
C8H70# ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch(/.)/ch2/2
C8H70#-1 ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch(/.)/2
naphthyl
indenyl
indene
!cumene
!CH3styre
C9H11#-1
C2H3C6H4CH2
!phenanthrene
!C6H5CH2CHO
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
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END

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REACTIONS

!(k = A T\*\*b exp(-E/RT)) A units: mole-cm-sec-K, E units cal/mole)

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! -----
! PRIMARY REACTIONS
! -----
! molecular elimination :
! unimolecular initiations :
C7H16-1=>R19C3H7+R20C4H9 2.0E+0017 0.000 85750.3 ! UI 1 KB
C7H16-1=>R11C2H5+R35C5H11 1.6E+0017 0.000 85815.5 ! UI 2 KB
C7H16-1=>R4CH3+R41C6H13 3.2E+0017 0.000 87654.8 ! UI 3 KB
C8H18-1=>R4CH3+R42C7H15 1.2E+0018 0.000 81845.9 ! UI 4 KB
C8H18-1=>R36C4H9+R38C4H9 2.4E+0017 0.000 78804.1 ! UI 5 KB
C8H18-1=>R43C3H7+R37C5H11 4.6E+0017 0.000 83562.0 ! UI 6 KB
C8H18-1=>R4CH3+R44C7H15 8.0E+0017 0.000 87665.1 ! UI 7 KB

! bimolecular initiations :
C7H16-1+O2=>R300H+R26C7H15 1.4E+0013 0.000 50652.5 ! BI 8 CN
C7H16-1+O2=>R300H+R27C7H15 4.2E+0013 0.000 53033.1 ! BI 9 CN
C7H16-1+O2=>R300H+R28C7H15 2.8E+0013 0.000 50588.2 ! BI 10 CN

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C7H16-1+O2=>R300H+R29C7H15	2.8E+0013	0.000	50652.5	!	BI	11	CN
C8H18-1+O2=>R300H+R30C8H17	6.3E+0013	0.000	53033.0	!	BI	12	CN
C8H18-1+O2=>R300H+R31C8H17	4.2E+0013	0.000	52333.1	!	BI	13	CN
C8H18-1+O2=>R300H+R32C8H17	7.0E+0012	0.000	47243.3	!	BI	14	CN
C8H18-1+O2=>R300H+R33C8H17	1.4E+0013	0.000	50652.7	!	BI	15	CN

! additions :

! additions with oxygen:

! isomerisations :

R20C4H9=R34C4H9	3.3E+0009	1.000	37000.0	!	IS	16	KB
R26C7H15=R28C7H15	6.7E+0009	1.000	37000.0	!	IS	17	KB
R26C7H15=R27C7H15	1.7E+0009	1.000	19800.0	!	IS	18	KB
R27C7H15=R29C7H15	9.9E+0007	1.000	37000.0	!	IS	19	KB
R27C7H15=R28C7H15	1.7E+0007	1.000	17400.0	!	IS	20	KB
R28C7H15=R29C7H15	5.7E+0008	1.000	17300.0	!	IS	21	KB
R30C8H17=R33C8H17	3.3E+0009	1.000	37000.0	!	IS	22	KB
R30C8H17=R32C8H17	2.9E+0008	1.000	15300.0	!	IS	23	KB
R30C8H17=R31C8H17	3.0E+0008	1.000	14500.0	!	IS	24	KB
R31C8H17=R33C8H17	3.3E+0009	1.000	37000.0	!	IS	25	KB
R35C5H11=R39C5H11	3.3E+0009	1.000	37000.0	!	IS	26	KB
R35C5H11=R40C5H11	5.7E+0008	1.000	17300.0	!	IS	27	KB

! Decomposition of 00Q00H into branching agents:

! beta-scissions :

R19C3H7=>R4CH3+C2H4Z	2.0E+0013	0.000	31000.0	!	DE	28	CN
R19C3H7=>R1H+C3H6Y	3.0E+0013	0.000	38000.0	!	DE	29	CN
R20C4H9=>R11C2H5+C2H4Z	2.0E+0013	0.000	28700.0	!	DE	30	CW
R20C4H9=>R1H+C4H8Y	3.0E+0013	0.000	38000.0	!	DE	31	CN
R26C7H15=>R11C2H5+C5H10Z	4.0E+0013	0.000	28700.0	!	DE	32	CW
R26C7H15=>R1H+C7H14Z	6.0E+0013	0.000	38000.0	!	DE	33	CN
R27C7H15=>R35C5H11+C2H4Z	2.0E+0013	0.000	28700.0	!	DE	34	CW
R27C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	35	CN
R28C7H15=>R20C4H9+C3H6Y	2.0E+0013	0.000	28700.0	!	DE	36	CW
R28C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	37	CN
DUPLICATE							
R28C7H15=>R1H+C7H14Z	3.0E+0013	0.000	39000.0	!	DE	38	CN
DUPLICATE							
R29C7H15=>R19C3H7+C4H8Y	2.0E+0013	0.000	28700.0	!	DE	39	CW
R29C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	40	CN
DUPLICATE							
R29C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	41	CN
DUPLICATE							
R29C7H15=>R4CH3+C6H12Z	2.0E+0013	0.000	31000.0	!	DE	42	CN
R30C8H17=>R36C4H9+C4H8Y	2.0E+0013	0.000	28700.0	!	DE	43	CW
R30C8H17=>R4CH3+C7H14Y	4.0E+0013	0.000	31000.0	!	DE	44	CN
R31C8H17=>R37C5H11+C3H6Y	2.0E+0013	0.000	28700.0	!	DE	45	CW
R31C8H17=>R4CH3+C7H14Z	2.0E+0013	0.000	31000.0	!	DE	46	CN
R31C8H17=>R1H+C8H16Y	1.5E+0013	0.000	37500.0	!	DE	47	CN
R32C8H17=>R38C4H9+C4H8Y	2.0E+0013	0.000	26700.0	!	DE	48	
R32C8H17=>R1H+C8H16Y	6.0E+0013	0.000	39000.0	!	DE	49	CN
R32C8H17=>R1H+C8H16Z	3.0E+0013	0.000	38000.0	!	DE	50	CN

R33C8H17=>R4CH3+C7H14Z	4.0E+0013	0.000	31000.0	!	DE 51	CN
R33C8H17=>R4CH3+C7H14Y	6.0E+0013	0.000	31000.0	!	DE 52	CN
R33C8H17=>R1H+C8H16Z	3.0E+0013	0.000	37500.0	!	DE 53	CN
R34C4H9=>R4CH3+C3H6Y	2.0E+0013	0.000	31000.0	!	DE 54	CN
R34C4H9=>R1H+C4H8Y	3.0E+0013	0.000	38000.0	!	DE 55	CN
DUPLICATE						
R34C4H9=>R1H+C4H8Y	3.0E+0013	0.000	39000.0	!	DE 56	CN
DUPLICATE						
R35C5H11=>R19C3H7+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 57	CW
R35C5H11=>R1H+C5H10Z	3.0E+0013	0.000	38000.0	!	DE 58	CN
R36C4H9=>R4CH3+C3H6Y	4.0E+0013	0.000	31000.0	!	DE 59	CN
R36C4H9=>R1H+C4H8Y	3.0E+0013	0.000	37500.0	!	DE 60	CN
R37C5H11=>R4CH3+C4H8Y	6.0E+0013	0.000	31000.0	!	DE 61	CN
R38C4H9=>R1H+C4H8Y	9.0E+0013	0.000	39000.0	!	DE 62	CN
R39C5H11=>R4CH3+C4H8Y	4.0E+0013	0.000	31000.0	!	DE 63	CN
R39C5H11=>R1H+C5H10Y	6.0E+0013	0.000	38000.0	!	DE 64	CN
R40C5H11=>R11C2H5+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 65	CW
R40C5H11=>R1H+C5H10Z	3.0E+0013	0.000	39000.0	!	DE 66	CN
R40C5H11=>R1H+C5H10Y	3.0E+0013	0.000	38000.0	!	DE 67	CN
R41C6H13=>R20C4H9+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 68	CW
R41C6H13=>R1H+C6H12Z	3.0E+0013	0.000	38000.0	!	DE 69	CN
R42C7H15=>R43C3H7+C4H8Y	2.0E+0013	0.000	27700.0	!	DE 70	
R42C7H15=>R1H+C7H14Y	3.0E+0013	0.000	38000.0	!	DE 71	CN
DUPLICATE						
R42C7H15=>R1H+C7H14Y	6.0E+0013	0.000	39000.0	!	DE 72	CN
DUPLICATE						
R43C3H7=>R1H+C3H6Y	6.0E+0013	0.000	39000.0	!	DE 73	CN
R44C7H15=>R38C4H9+C3H6Y	2.0E+0013	0.000	26700.0	!	DE 74	
R44C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE 75	CN
DUPLICATE						
R44C7H15=>R1H+C7H14Z	3.0E+0013	0.000	39000.0	!	DE 76	CN
DUPLICATE						

! decomposition of R(.)CO free radicals

! decomposition to o-rings :

! oxidations :

R26C7H15+O2=>C7H14Z+R300H	3.9E+0012	0.000	5000.0	!	OX 77	CN
R27C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 78	CN
R28C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 79	CN
DUPLICATE						
R28C7H15+O2=>C7H14Z+R300H	8.1E+0011	0.000	5000.0	!	OX 80	CN
DUPLICATE						
R29C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 81	CN
DUPLICATE						
R29C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 82	CN
DUPLICATE						
R31C8H17+O2=>C8H16Y+R300H	6.4E+0011	0.000	5000.0	!	OX 83	CN
R32C8H17+O2=>C8H16Y+R300H	1.6E+0012	0.000	5000.0	!	OX 84	CN
R32C8H17+O2=>C8H16Z+R300H	1.9E+0012	0.000	5000.0	!	OX 85	CN
R33C8H17+O2=>C8H16Z+R300H	6.4E+0011	0.000	5000.0	!	OX 86	CN
R38C4H9+O2=>C4H8Y+R300H	1.6E+0012	0.000	5000.0	!	OX 87	CW
R43C3H7+O2=>C3H6Y+R300H	2.3E+0012	0.000	5000.0	!	OX 88	CW

! oxidations of R(.) (OH) radicals:

! metathesis :

B10+C7H16-1=>R20H+R26C7H15	2.6E+0013	0.000	5200.0	! ME 89 CW
B10+C7H16-1=>R20H+R27C7H15	1.0E+0014	0.000	7850.0	! ME 90 CW
B10+C7H16-1=>R20H+R28C7H15	5.2E+0013	0.000	5200.0	! ME 91 CW
B10+C7H16-1=>R20H+R29C7H15	5.2E+0013	0.000	5200.0	! ME 92 CW
B10+C8H18-1=>R20H+R30C8H17	1.5E+0014	0.000	7850.0	! ME 93 CW
B10+C8H18-1=>R20H+R31C8H17	1.0E+0014	0.000	7850.0	! ME 94 CW
B10+C8H18-1=>R20H+R32C8H17	1.0E+0013	0.000	3280.0	! ME 95 CW
B10+C8H18-1=>R20H+R33C8H17	2.6E+0013	0.000	5200.0	! ME 96 CW
C7H16-1+R1H=>H2+R26C7H15	9.0E+0006	2.000	5000.0	! ME 97 CW
C7H16-1+R1H=>H2+R27C7H15	5.7E+0007	2.000	7700.0	! ME 98 CW
C7H16-1+R1H=>H2+R28C7H15	1.8E+0007	2.000	5000.0	! ME 99 CW
C7H16-1+R1H=>H2+R29C7H15	1.8E+0007	2.000	5000.0	! ME 100 CW
C8H18-1+R1H=>H2+R30C8H17	8.6E+0007	2.000	7700.0	! ME 101 CW
C8H18-1+R1H=>H2+R31C8H17	5.7E+0007	2.000	7700.0	! ME 102 CW
C8H18-1+R1H=>H2+R32C8H17	4.2E+0006	2.000	2400.0	! ME 103 CN
C8H18-1+R1H=>H2+R33C8H17	9.0E+0006	2.000	5000.0	! ME 104 CW
C7H16-1+R20H=>H20+R26C7H15	2.6E+0006	2.000	-765.0	! ME 105 CW
C7H16-1+R20H=>H20+R27C7H15	5.4E+0006	2.000	450.0	! ME 106 CW
C7H16-1+R20H=>H20+R28C7H15	5.2E+0006	2.000	-765.0	! ME 107 CW
C7H16-1+R20H=>H20+R29C7H15	5.2E+0006	2.000	-765.0	! ME 108 CW
C8H18-1+R20H=>H20+R30C8H17	8.1E+0006	2.000	450.0	! ME 109 CW
C8H18-1+R20H=>H20+R31C8H17	5.4E+0006	2.000	450.0	! ME 110 CW
C8H18-1+R20H=>H20+R32C8H17	1.1E+0006	2.000	-1865.0	! ME 111 CW
C8H18-1+R20H=>H20+R33C8H17	2.6E+0006	2.000	-765.0	! ME 112 CW
C7H16-1+R300H=>H202+R26C7H15	4.0E+0011	0.000	15500.0	! ME 113 CN
C7H16-1+R300H=>H202+R27C7H15	1.2E+0012	0.000	17000.0	! ME 114 CN
C7H16-1+R300H=>H202+R28C7H15	8.0E+0011	0.000	15500.0	! ME 115 CN
C7H16-1+R300H=>H202+R29C7H15	8.0E+0011	0.000	15500.0	! ME 116 CN
C8H18-1+R300H=>H202+R30C8H17	1.8E+0012	0.000	17000.0	! ME 117 CN
C8H18-1+R300H=>H202+R31C8H17	1.2E+0012	0.000	17000.0	! ME 118 CN
C8H18-1+R300H=>H202+R32C8H17	2.0E+0011	0.000	14000.0	! ME 119 CN
C8H18-1+R300H=>H202+R33C8H17	4.0E+0011	0.000	15500.0	! ME 120 CN
C7H16-1+R4CH3=>CH4+R26C7H15	2.0E+0011	0.000	9600.0	! ME 121 CN
C7H16-1+R4CH3=>CH4+R27C7H15	6.0E-0001	4.000	8200.0	! ME 122 CN
C7H16-1+R4CH3=>CH4+R28C7H15	4.0E+0011	0.000	9600.0	! ME 123 CN
C7H16-1+R4CH3=>CH4+R29C7H15	4.0E+0011	0.000	9600.0	! ME 124 CN
C8H18-1+R4CH3=>CH4+R30C8H17	9.0E-0001	4.000	8200.0	! ME 125 CN
C8H18-1+R4CH3=>CH4+R31C8H17	6.0E-0001	4.000	8200.0	! ME 126 CN
C8H18-1+R4CH3=>CH4+R32C8H17	1.0E+0011	0.000	7900.0	! ME 127 CW
C8H18-1+R4CH3=>CH4+R33C8H17	2.0E+0011	0.000	9600.0	! ME 128 CN
C7H16-1+R5CHO=>HCHO+R26C7H15	1.0E+0007	1.900	17000.0	! ME 129 CN
C7H16-1+R5CHO=>HCHO+R27C7H15	2.0E+0005	2.500	18500.0	! ME 130 CN
C7H16-1+R5CHO=>HCHO+R28C7H15	2.2E+0007	1.900	17000.0	! ME 131 CN
C7H16-1+R5CHO=>HCHO+R29C7H15	2.2E+0007	1.900	17000.0	! ME 132 CN
C8H18-1+R5CHO=>HCHO+R30C8H17	3.1E+0005	2.500	18500.0	! ME 133 CN
C8H18-1+R5CHO=>HCHO+R31C8H17	2.0E+0005	2.500	18500.0	! ME 134 CN
C8H18-1+R5CHO=>HCHO+R32C8H17	3.4E+0004	2.500	13500.0	! ME 135 CN
C8H18-1+R5CHO=>HCHO+R33C8H17	1.0E+0007	1.900	17000.0	! ME 136 CN
C7H16-1+R6CH2OH=>CH3OH+R26C7H15	6.0E+0001	2.950	12000.0	! ME 137 CN
C7H16-1+R6CH2OH=>CH3OH+R27C7H15	2.0E+0002	2.950	14000.0	! ME 138 CN
C7H16-1+R6CH2OH=>CH3OH+R28C7H15	1.2E+0002	2.950	12000.0	! ME 139 CN

C7H16-1+R6CH20H=>CH30H+R29C7H15	1.2E+0002	2.950	12000.0	! ME 140 CN
C8H18-1+R6CH20H=>CH30H+R30C8H17	3.0E+0002	2.950	14000.0	! ME 141 CN
C8H18-1+R6CH20H=>CH30H+R31C8H17	2.0E+0002	2.950	14000.0	! ME 142 CN
C8H18-1+R6CH20H=>CH30H+R32C8H17	1.2E+0002	2.760	10800.0	! ME 143 CN
C8H18-1+R6CH20H=>CH30H+R33C8H17	6.0E+0001	2.950	12000.0	! ME 144 CN
C7H16-1+R7CH30=>CH30H+R26C7H15	1.5E+0011	0.000	4500.0	! ME 145 CN
C7H16-1+R7CH30=>CH30H+R27C7H15	3.2E+0011	0.000	7300.0	! ME 146 CN
C7H16-1+R7CH30=>CH30H+R28C7H15	2.9E+0011	0.000	4500.0	! ME 147 CN
C7H16-1+R7CH30=>CH30H+R29C7H15	2.9E+0011	0.000	4500.0	! ME 148 CN
C8H18-1+R7CH30=>CH30H+R30C8H17	4.9E+0011	0.000	7300.0	! ME 149 CN
C8H18-1+R7CH30=>CH30H+R31C8H17	3.2E+0011	0.000	7300.0	! ME 150 CN
C8H18-1+R7CH30=>CH30H+R32C8H17	2.3E+0010	0.000	2900.0	! ME 151 CN
C8H18-1+R7CH30=>CH30H+R33C8H17	1.5E+0011	0.000	4500.0	! ME 152 CN
C7H16-1+R8CH300=>CH300H+R26C7H15	3.0E+0012	0.000	17500.0	! ME 153
CN				
C7H16-1+R8CH300=>CH300H+R27C7H15	1.2E+0013	0.000	20000.0	! ME 154
CN				
C7H16-1+R8CH300=>CH300H+R28C7H15	6.0E+0012	0.000	17500.0	! ME 155
CN				
C7H16-1+R8CH300=>CH300H+R29C7H15	6.0E+0012	0.000	17500.0	! ME 156
CN				
C8H18-1+R8CH300=>CH300H+R30C8H17	1.8E+0013	0.000	20000.0	! ME 157
CN				
C8H18-1+R8CH300=>CH300H+R31C8H17	1.2E+0013	0.000	20000.0	! ME 158
CN				
C8H18-1+R8CH300=>CH300H+R32C8H17	1.5E+0012	0.000	15000.0	! ME 159
CN				
C8H18-1+R8CH300=>CH300H+R33C8H17	3.0E+0012	0.000	17500.0	! ME 160
CN				
C7H16-1+R11C2H5=>C2H6+R26C7H15	2.0E+0011	0.000	11000.0	! ME 161 CN
C7H16-1+R11C2H5=>C2H6+R27C7H15	6.0E+0011	0.000	13500.0	! ME 162 CR
C7H16-1+R11C2H5=>C2H6+R28C7H15	4.0E+0011	0.000	11000.0	! ME 163 CN
C7H16-1+R11C2H5=>C2H6+R29C7H15	4.0E+0011	0.000	11000.0	! ME 164 CN
C8H18-1+R11C2H5=>C2H6+R30C8H17	9.0E+0011	0.000	13500.0	! ME 165 CR
C8H18-1+R11C2H5=>C2H6+R31C8H17	6.0E+0011	0.000	13500.0	! ME 166 CR
C8H18-1+R11C2H5=>C2H6+R32C8H17	1.0E+0011	0.000	9200.0	! ME 167 CN
C8H18-1+R11C2H5=>C2H6+R33C8H17	2.0E+0011	0.000	11000.0	! ME 168 CN
C7H16-1+R38C4H9=>C4H10+R26C7H15	1.0E+0011	0.000	12700.0	! ME 169 CR
C7H16-1+R38C4H9=>C4H10+R27C7H15	3.0E+0011	0.000	15000.0	! ME 170 CR
C7H16-1+R38C4H9=>C4H10+R28C7H15	2.0E+0011	0.000	12700.0	! ME 171 CR
C7H16-1+R38C4H9=>C4H10+R29C7H15	2.0E+0011	0.000	12700.0	! ME 172 CR
C8H18-1+R38C4H9=>C4H10+R30C8H17	4.5E+0011	0.000	15000.0	! ME 173 CR
C8H18-1+R38C4H9=>C4H10+R31C8H17	3.0E+0011	0.000	15000.0	! ME 174 CR
C8H18-1+R38C4H9=>C4H10+R32C8H17	5.0E+0010	0.000	11100.0	! ME 175 CR
C8H18-1+R38C4H9=>C4H10+R33C8H17	1.0E+0011	0.000	12700.0	! ME 176 CR

! combinations :

R1H+R38C4H9=>C4H10	8.3E+0012	0.000	0.0	! CO 177 KB
R1H+R43C3H7=>C3H8	8.3E+0012	0.000	0.0	! CO 178 KB
R20H+R38C4H9=>C4H100L	5.7E+0012	0.000	0.0	! CO 179 KB
R20H+R43C3H7=>C3H70H	5.9E+0012	0.000	0.0	! CO 180 KB
R300H+R38C4H9=>C4H1002P	4.5E+0012	0.000	0.0	! CO 181 KB
R300H+R43C3H7=>C3H802P	4.8E+0012	0.000	0.0	! CO 182 KB
R4CH3+R38C4H9=>C5H12	1.5E+0013	0.000	0.0	! CO 183 KB

R4CH3+R43C3H7=>C4H10	1.5E+0013	0.000	0.0	!	CO	184	KB
R5CH0+R38C4H9=>C5H100A	4.9E+0012	0.000	0.0	!	CO	185	KB
R5CH0+R43C3H7=>C4H80A	5.2E+0012	0.000	0.0	!	CO	186	KB
R6CH20H+R38C4H9=>C5H120L	4.8E+0012	0.000	0.0	!	CO	187	KB
R6CH20H+R43C3H7=>C4H100L	5.1E+0012	0.000	0.0	!	CO	188	KB
R11C2H5+R38C4H9=>C6H14	4.9E+0012	0.000	0.0	!	CO	189	KB
R11C2H5+R43C3H7=>C5H12	5.2E+0012	0.000	0.0	!	CO	190	KB
R38C4H9+R38C4H9=>C8H18	2.0E+0012	0.000	0.0	!	CO	191	KB
R38C4H9+R43C3H7=>C7H16	4.3E+0012	0.000	0.0	!	CO	192	KB
R43C3H7+R43C3H7=>C6H14	2.3E+0012	0.000	0.0	!	CO	193	KB

! dismutations :

! -----  
! SECONDARY MECHANISM  
! -----

! Peroxide decomposition

! Hydroperoxide decomposition

C4H1002P=>R20H+R11C2H5+CH3CHO	1.5E+0016	0.000	43000.0	!	DHP	194
C3H802P=>R20H+R11C2H5+HCHO	1.5E+0016	0.000	43000.0	!	DHP	195
C3H602PY=>R20H+R1H+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP	196
C4H802PY=>R20H+R4CH3+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP	197
C7H1402PY=>R20H+R20C4H9+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP	198
C8H1602PY=>R20H+R35C5H11+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP	199
C5H1002PY=>R20H+R11C2H5+C2H3CHOZ	1.5E+0016	0.000	43000.0	!	DHP	200

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

! Aldohydroperoxide decomposition

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions

C3H8+R1H=>H2+R19C3H7	5.7E+0007	2.000	7700.0	!	MH	201
DUPLICATE						
C3H8+R1H=>H2+R19C3H7	9.0E+0006	2.000	5000.0	!	MH	202
DUPLICATE						
C3H8+R20H=>H20+R19C3H7	5.4E+0006	2.000	450.0	!	MH	203
DUPLICATE						
C3H8+R20H=>H20+R19C3H7	2.6E+0006	2.000	-765.0	!	MH	204
DUPLICATE						
C3H8+R300H=>H202+R19C3H7	1.2E+0012	0.000	17000.0	!	MH	205
DUPLICATE						
C3H8+R300H=>H202+R19C3H7	4.0E+0011	0.000	15500.0	!	MH	206
DUPLICATE						
C3H8+R4CH3=>CH4+R19C3H7	6.0E-0001	4.000	8200.0	!	MH	207

DUPLICATE					
C3H8+R4CH3=>CH4+R19C3H7	2.0E+0011	0.000	9600.0	!	MH 208
DUPLICATE					
C3H8+R8CH300=>CH300H+R19C3H7	1.2E+0013	0.000	20000.0	!	MH 209
DUPLICATE					
C3H8+R8CH300=>CH300H+R19C3H7	3.0E+0012	0.000	17500.0	!	MH 210
DUPLICATE					
C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	!	MH 211
DUPLICATE					
C3H8+R11C2H5=>C2H6+R19C3H7	2.0E+0011	0.000	11000.0	!	MH 212
DUPLICATE					
C4H10+R1H=>H2+R20C4H9	5.7E+0007	2.000	7700.0	!	MH 213
DUPLICATE					
C4H10+R1H=>H2+R20C4H9	1.8E+0007	2.000	5000.0	!	MH 214
DUPLICATE					
C4H10+R20H=>H20+R20C4H9	5.4E+0006	2.000	450.0	!	MH 215
DUPLICATE					
C4H10+R20H=>H20+R20C4H9	5.2E+0006	2.000	-765.0	!	MH 216
DUPLICATE					
C4H10+R300H=>H202+R20C4H9	1.2E+0012	0.000	17000.0	!	MH 217
DUPLICATE					
C4H10+R300H=>H202+R20C4H9	8.0E+0011	0.000	15500.0	!	MH 218
DUPLICATE					
C4H10+R4CH3=>CH4+R20C4H9	6.0E-0001	4.000	8200.0	!	MH 219
DUPLICATE					
C4H10+R4CH3=>CH4+R20C4H9	4.0E+0011	0.000	9600.0	!	MH 220
DUPLICATE					
C4H10+R8CH300=>CH300H+R20C4H9	1.2E+0013	0.000	20000.0	!	MH 221
DUPLICATE					
C4H10+R8CH300=>CH300H+R20C4H9	6.0E+0012	0.000	17500.0	!	MH 222
DUPLICATE					
C4H10+R11C2H5=>C2H6+R20C4H9	6.0E+0011	0.000	13500.0	!	MH 223
DUPLICATE					
C4H10+R11C2H5=>C2H6+R20C4H9	4.0E+0011	0.000	11000.0	!	MH 224
DUPLICATE					
C5H12+R1H=>H2+R35C5H11	5.7E+0007	2.000	7700.0	!	MH 225
DUPLICATE					
C5H12+R1H=>H2+R35C5H11	2.7E+0007	2.000	5000.0	!	MH 226
DUPLICATE					
C5H12+R20H=>H20+R35C5H11	5.4E+0006	2.000	450.0	!	MH 227
DUPLICATE					
C5H12+R20H=>H20+R35C5H11	7.8E+0006	2.000	-765.0	!	MH 228
DUPLICATE					
C5H12+R300H=>H202+R35C5H11	1.2E+0012	0.000	17000.0	!	MH 229
DUPLICATE					
C5H12+R300H=>H202+R35C5H11	1.2E+0012	0.000	15500.0	!	MH 230
DUPLICATE					
C5H12+R4CH3=>CH4+R35C5H11	6.0E-0001	4.000	8200.0	!	MH 231
DUPLICATE					
C5H12+R4CH3=>CH4+R35C5H11	6.0E+0011	0.000	9600.0	!	MH 232
DUPLICATE					
C5H12+R8CH300=>CH300H+R35C5H11	1.2E+0013	0.000	20000.0	!	MH 233
DUPLICATE					
C5H12+R8CH300=>CH300H+R35C5H11	9.0E+0012	0.000	17500.0	!	MH 234

DUPLICATE					
C5H12+R11C2H5=>C2H6+R35C5H11	6.0E+0011	0.000	13500.0	!	MH 235
DUPLICATE					
C5H12+R11C2H5=>C2H6+R35C5H11	6.0E+0011	0.000	11000.0	!	MH 236
DUPLICATE					
C6H14+R1H=>H2+R41C6H13	5.7E+0007	2.000	7700.0	!	MH 237
DUPLICATE					
C6H14+R1H=>H2+R41C6H13	3.6E+0007	2.000	5000.0	!	MH 238
DUPLICATE					
C6H14+R20H=>H20+R41C6H13	5.4E+0006	2.000	450.0	!	MH 239
DUPLICATE					
C6H14+R20H=>H20+R41C6H13	1.0E+0007	2.000	-765.0	!	MH 240
DUPLICATE					
C6H14+R300H=>H202+R41C6H13	1.2E+0012	0.000	17000.0	!	MH 241
DUPLICATE					
C6H14+R300H=>H202+R41C6H13	1.6E+0012	0.000	15500.0	!	MH 242
DUPLICATE					
C6H14+R4CH3=>CH4+R41C6H13	6.0E-0001	4.000	8200.0	!	MH 243
DUPLICATE					
C6H14+R4CH3=>CH4+R41C6H13	8.0E+0011	0.000	9600.0	!	MH 244
DUPLICATE					
C6H14+R8CH300=>CH300H+R41C6H13	1.2E+0013	0.000	20000.0	!	MH 245
DUPLICATE					
C6H14+R8CH300=>CH300H+R41C6H13	1.2E+0013	0.000	17500.0	!	MH 246
DUPLICATE					
C6H14+R11C2H5=>C2H6+R41C6H13	6.0E+0011	0.000	13500.0	!	MH 247
DUPLICATE					
C6H14+R11C2H5=>C2H6+R41C6H13	8.0E+0011	0.000	11000.0	!	MH 248
DUPLICATE					
! 0-ring decomposition					
C3H60E#3+R1H=>H2+R4CH3+CH2COZ	2.9E+0007	2.000	7700.0	!	DE# 249
DUPLICATE					
C3H60E#3+R1H=>H2+R4CH3+CH2COZ	1.3E+0007	2.000	5000.0	!	DE# 250
DUPLICATE					
C3H60E#3+R20H=>H20+R4CH3+CH2COZ	2.7E+0006	2.000	450.0	!	DE# 251
DUPLICATE					
C3H60E#3+R20H=>H20+R4CH3+CH2COZ	3.9E+0006	2.000	-765.0	!	DE# 252
DUPLICATE					
C3H60E#3+R300H=>H202+R4CH3+CH2COZ	6.0E+0011	0.000	17000.0	!	DE# 253
DUPLICATE					
C3H60E#3+R300H=>H202+R4CH3+CH2COZ	6.0E+0011	0.000	15500.0	!	DE# 254
DUPLICATE					
C3H60E#3+R4CH3=>CH4+R4CH3+CH2COZ	3.0E-0001	4.000	8200.0	!	DE# 255
DUPLICATE					
C3H60E#3+R4CH3=>CH4+R4CH3+CH2COZ	3.0E+0011	0.000	9600.0	!	DE# 256
DUPLICATE					
C3H60E#3+R8CH300=>CH300H+R4CH3+CH2COZ	6.0E+0012	0.000	20000.0	!	DE# 257
DUPLICATE					
C3H60E#3+R8CH300=>CH300H+R4CH3+CH2COZ	4.5E+0012	0.000	17500.0	!	DE# 258
DUPLICATE					

C3H60E#3+R11C2H5=>C2H6+R4CH3+CH2COZ	3.0E+0011	0.000	13500.0	! DE#
259				
DUPLICATE				
C3H60E#3+R11C2H5=>C2H6+R4CH3+CH2COZ	3.0E+0011	0.000	11000.0	! DE#
260				
DUPLICATE				
C4H80E#3+R1H=>H2+R11C2H5+CH2COZ	2.9E+0007	2.000	7700.0	! DE# 261
DUPLICATE				
C4H80E#3+R1H=>H2+R11C2H5+CH2COZ	2.3E+0007	2.000	5000.0	! DE# 262
DUPLICATE				
C4H80E#3+R20H=>H2O+R11C2H5+CH2COZ	2.7E+0006	2.000	450.0	! DE# 263
DUPLICATE				
C4H80E#3+R20H=>H2O+R11C2H5+CH2COZ	6.5E+0006	2.000	-765.0	! DE# 264
DUPLICATE				
C4H80E#3+R300H=>H2O2+R11C2H5+CH2COZ	6.0E+0011	0.000	17000.0	! DE#
265				
DUPLICATE				
C4H80E#3+R300H=>H2O2+R11C2H5+CH2COZ	1.0E+0012	0.000	15500.0	! DE#
266				
DUPLICATE				
C4H80E#3+R4CH3=>CH4+R11C2H5+CH2COZ	3.0E-0001	4.000	8200.0	! DE# 267
DUPLICATE				
C4H80E#3+R4CH3=>CH4+R11C2H5+CH2COZ	5.0E+0011	0.000	9600.0	! DE# 268
DUPLICATE				
C4H80E#3+R8CH300=>CH300H+R11C2H5+CH2COZ	6.0E+0012	0.000	20000.0	!
DE# 269				
DUPLICATE				
C4H80E#3+R8CH300=>CH300H+R11C2H5+CH2COZ	7.5E+0012	0.000	17500.0	!
DE# 270				
DUPLICATE				
C4H80E#3+R11C2H5=>C2H6+R11C2H5+CH2COZ	3.0E+0011	0.000	13500.0	! DE#
271				
DUPLICATE				
C4H80E#3+R11C2H5=>C2H6+R11C2H5+CH2COZ	5.0E+0011	0.000	11000.0	! DE#
272				
DUPLICATE				
C5H100E#3+R1H=>H2+R19C3H7+CH2COZ	2.9E+0007	2.000	7700.0	! DE# 273
DUPLICATE				
C5H100E#3+R1H=>H2+R19C3H7+CH2COZ	3.2E+0007	2.000	5000.0	! DE# 274
DUPLICATE				
C5H100E#3+R20H=>H2O+R19C3H7+CH2COZ	2.7E+0006	2.000	450.0	! DE# 275
DUPLICATE				
C5H100E#3+R20H=>H2O+R19C3H7+CH2COZ	9.1E+0006	2.000	-765.0	! DE# 276
DUPLICATE				
C5H100E#3+R300H=>H2O2+R19C3H7+CH2COZ	6.0E+0011	0.000	17000.0	! DE#
277				
DUPLICATE				
C5H100E#3+R300H=>H2O2+R19C3H7+CH2COZ	1.4E+0012	0.000	15500.0	! DE#
278				
DUPLICATE				
C5H100E#3+R4CH3=>CH4+R19C3H7+CH2COZ	3.0E-0001	4.000	8200.0	! DE#
279				
DUPLICATE				



C5H100E#3+R4CH3=>CH4+R19C3H7+CH2COZ	7.0E+0011	0.000	9600.0	! DE#
280				
DUPLICATE				
C5H100E#3+R8CH300=>CH300H+R19C3H7+CH2COZ	6.0E+0012	0.000	20000.0	!
DE# 281				
DUPLICATE				
C5H100E#3+R8CH300=>CH300H+R19C3H7+CH2COZ	1.0E+0013	0.000	17500.0	!
DE# 282				
DUPLICATE				
C5H100E#3+R11C2H5=>C2H6+R19C3H7+CH2COZ	3.0E+0011	0.000	13500.0	!
DE# 283				
DUPLICATE				
C5H100E#3+R11C2H5=>C2H6+R19C3H7+CH2COZ	7.0E+0011	0.000	11000.0	!
DE# 284				
DUPLICATE				
C7H140E#3+R1H=>H2+R20C4H9+C2H3CHOZ	2.9E+0007	2.000	7700.0	! DE# 285
DUPLICATE				
C7H140E#3+R1H=>H2+R20C4H9+C2H3CHOZ	5.0E+0007	2.000	5000.0	! DE# 286
DUPLICATE				
C7H140E#3+R20H=>H20+R20C4H9+C2H3CHOZ	2.7E+0006	2.000	450.0	! DE#
287				
DUPLICATE				
C7H140E#3+R20H=>H20+R20C4H9+C2H3CHOZ	1.4E+0007	2.000	-765.0	! DE#
288				
DUPLICATE				
C7H140E#3+R300H=>H202+R20C4H9+C2H3CHOZ	6.0E+0011	0.000	17000.0	!
DE# 289				
DUPLICATE				
C7H140E#3+R300H=>H202+R20C4H9+C2H3CHOZ	2.2E+0012	0.000	15500.0	!
DE# 290				
DUPLICATE				
C7H140E#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ	3.0E-0001	4.000	8200.0	! DE#
291				
DUPLICATE				
C7H140E#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ	1.1E+0012	0.000	9600.0	! DE#
292				
DUPLICATE				
C7H140E#3+R8CH300=>CH300H+R20C4H9+C2H3CHOZ	6.0E+0012	0.000		
20000.0 ! DE# 293				
DUPLICATE				
C7H140E#3+R8CH300=>CH300H+R20C4H9+C2H3CHOZ	1.7E+0013	0.000		
17500.0 ! DE# 294				
DUPLICATE				
C7H140E#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ	3.0E+0011	0.000	13500.0	!
DE# 295				
DUPLICATE				
C7H140E#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ	1.1E+0012	0.000	11000.0	!
DE# 296				
DUPLICATE				
C6H120E#3+R1H=>H2+R19C3H7+C2H3CHOZ	2.9E+0007	2.000	7700.0	! DE# 297
DUPLICATE				
C6H120E#3+R1H=>H2+R19C3H7+C2H3CHOZ	4.1E+0007	2.000	5000.0	! DE# 298
DUPLICATE				

C6H120E#3+R20H=>H20+R19C3H7+C2H3CHOZ 299	2.7E+0006	2.000	450.0	! DE#
DUPLICATE				
C6H120E#3+R20H=>H20+R19C3H7+C2H3CHOZ 300	1.1E+0007	2.000	-765.0	! DE#
DUPLICATE				
C6H120E#3+R300H=>H202+R19C3H7+C2H3CHOZ DE# 301	6.0E+0011	0.000	17000.0	!
DUPLICATE				
C6H120E#3+R300H=>H202+R19C3H7+C2H3CHOZ DE# 302	1.8E+0012	0.000	15500.0	!
DUPLICATE				
C6H120E#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 303	3.0E-0001	4.000	8200.0	! DE#
DUPLICATE				
C6H120E#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 304	9.0E+0011	0.000	9600.0	! DE#
DUPLICATE				
C6H120E#3+R8CH300=>CH300H+R19C3H7+C2H3CHOZ 20000.0 ! DE# 305	6.0E+0012	0.000		
DUPLICATE				
C6H120E#3+R8CH300=>CH300H+R19C3H7+C2H3CHOZ 17500.0 ! DE# 306	1.3E+0013	0.000		
DUPLICATE				
C6H120E#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ DE# 307	3.0E+0011	0.000	13500.0	!
DUPLICATE				
C6H120E#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ DE# 308	9.0E+0011	0.000	11000.0	!
DUPLICATE				
C8H160E#3+R1H=>H2+R20C4H9+C4H60KZ DUPLICATE	2.9E+0007	2.000	7700.0	! DE# 309
C8H160E#3+R1H=>H2+R20C4H9+C4H60KZ DUPLICATE	5.9E+0007	2.000	5000.0	! DE# 310
C8H160E#3+R20H=>H20+R20C4H9+C4H60KZ DUPLICATE	2.7E+0006	2.000	450.0	! DE# 311
C8H160E#3+R20H=>H20+R20C4H9+C4H60KZ 312	1.7E+0007	2.000	-765.0	! DE#
DUPLICATE				
C8H160E#3+R300H=>H202+R20C4H9+C4H60KZ 313	6.0E+0011	0.000	17000.0	! DE#
DUPLICATE				
C8H160E#3+R300H=>H202+R20C4H9+C4H60KZ 314	2.6E+0012	0.000	15500.0	! DE#
DUPLICATE				
C8H160E#3+R4CH3=>CH4+R20C4H9+C4H60KZ 315	3.0E-0001	4.000	8200.0	! DE#
DUPLICATE				
C8H160E#3+R4CH3=>CH4+R20C4H9+C4H60KZ 316	1.3E+0012	0.000	9600.0	! DE#
DUPLICATE				
C8H160E#3+R8CH300=>CH300H+R20C4H9+C4H60KZ DE# 317	6.0E+0012	0.000	20000.0	!
DUPLICATE				

C8H160E#3+R8CH300=>CH300H+R20C4H9+C4H60KZ	2.0E+0013	0.000	17500.0	!
DE# 318				
DUPLICATE				
C8H160E#3+R11C2H5=>C2H6+R20C4H9+C4H60KZ	3.0E+0011	0.000	13500.0	!
DE# 319				
DUPLICATE				
C8H160E#3+R11C2H5=>C2H6+R20C4H9+C4H60KZ	1.3E+0012	0.000	11000.0	!
DE# 320				
DUPLICATE				
C9H180E#3+R1H=>H2+R35C5H11+C4H60KZ	2.9E+0007	2.000	7700.0	! DE# 321
DUPLICATE				
C9H180E#3+R1H=>H2+R35C5H11+C4H60KZ	6.8E+0007	2.000	5000.0	! DE# 322
DUPLICATE				
C9H180E#3+R20H=>H20+R35C5H11+C4H60KZ	2.7E+0006	2.000	450.0	! DE#
323				
DUPLICATE				
C9H180E#3+R20H=>H20+R35C5H11+C4H60KZ	2.0E+0007	2.000	-765.0	! DE#
324				
DUPLICATE				
C9H180E#3+R300H=>H202+R35C5H11+C4H60KZ	6.0E+0011	0.000	17000.0	!
DE# 325				
DUPLICATE				
C9H180E#3+R300H=>H202+R35C5H11+C4H60KZ	3.0E+0012	0.000	15500.0	!
DE# 326				
DUPLICATE				
C9H180E#3+R4CH3=>CH4+R35C5H11+C4H60KZ	3.0E-0001	4.000	8200.0	! DE#
327				
DUPLICATE				
C9H180E#3+R4CH3=>CH4+R35C5H11+C4H60KZ	1.5E+0012	0.000	9600.0	! DE#
328				
DUPLICATE				
C9H180E#3+R8CH300=>CH300H+R35C5H11+C4H60KZ	6.0E+0012	0.000		
20000.0 ! DE# 329				
DUPLICATE				
C9H180E#3+R8CH300=>CH300H+R35C5H11+C4H60KZ	2.3E+0013	0.000		
17500.0 ! DE# 330				
DUPLICATE				
C9H180E#3+R11C2H5=>C2H6+R35C5H11+C4H60KZ	3.0E+0011	0.000	13500.0	!
DE# 331				
DUPLICATE				
C9H180E#3+R11C2H5=>C2H6+R35C5H11+C4H60KZ	1.5E+0012	0.000	11000.0	!
DE# 332				
DUPLICATE				
C10H200E#3+R1H=>H2+R35C5H11+C5H80KZ	2.9E+0007	2.000	7700.0	! DE#
333				
DUPLICATE				
C10H200E#3+R1H=>H2+R35C5H11+C5H80KZ	7.7E+0007	2.000	5000.0	! DE#
334				
DUPLICATE				
C10H200E#3+R20H=>H20+R35C5H11+C5H80KZ	2.7E+0006	2.000	450.0	! DE#
335				
DUPLICATE				
C10H200E#3+R20H=>H20+R35C5H11+C5H80KZ	2.2E+0007	2.000	-765.0	! DE#
336				

DUPLICATE					
C10H200E#3+R300H=>H2O2+R35C5H11+C5H80KZ	6.0E+0011	0.000	17000.0	!	
DE# 337					
DUPLICATE					
C10H200E#3+R300H=>H2O2+R35C5H11+C5H80KZ	3.4E+0012	0.000	15500.0	!	
DE# 338					
DUPLICATE					
C10H200E#3+R4CH3=>CH4+R35C5H11+C5H80KZ	3.0E-0001	4.000	8200.0	!	DE#
339					
DUPLICATE					
C10H200E#3+R4CH3=>CH4+R35C5H11+C5H80KZ	1.7E+0012	0.000	9600.0	!	DE#
340					
DUPLICATE					
C10H200E#3+R8CH300=>CH300H+R35C5H11+C5H80KZ	6.0E+0012	0.000	20000.0		
! DE# 341					
DUPLICATE					
C10H200E#3+R8CH300=>CH300H+R35C5H11+C5H80KZ	2.6E+0013	0.000	17500.0		
! DE# 342					
DUPLICATE					
C10H200E#3+R11C2H5=>C2H6+R35C5H11+C5H80KZ	3.0E+0011	0.000	13500.0	!	
DE# 343					
DUPLICATE					
C10H200E#3+R11C2H5=>C2H6+R35C5H11+C5H80KZ	1.7E+0012	0.000	11000.0	!	
DE# 344					
DUPLICATE					
C13H260E#3+R1H=>H2+R26C7H15+C6H100KZ	2.9E+0007	2.000	7700.0	!	DE#
345					
DUPLICATE					
C13H260E#3+R1H=>H2+R26C7H15+C6H100KZ	1.0E+0008	2.000	5000.0	!	DE#
346					
DUPLICATE					
C13H260E#3+R20H=>H2O+R26C7H15+C6H100KZ	2.7E+0006	2.000	450.0	!	DE#
347					
DUPLICATE					
C13H260E#3+R20H=>H2O+R26C7H15+C6H100KZ	3.0E+0007	2.000	-765.0	!	DE#
348					
DUPLICATE					
C13H260E#3+R300H=>H2O2+R26C7H15+C6H100KZ	6.0E+0011	0.000	17000.0	!	
DE# 349					
DUPLICATE					
C13H260E#3+R300H=>H2O2+R26C7H15+C6H100KZ	4.6E+0012	0.000	15500.0	!	
DE# 350					
DUPLICATE					
C13H260E#3+R4CH3=>CH4+R26C7H15+C6H100KZ	3.0E-0001	4.000	8200.0	!	
DE# 351					
DUPLICATE					
C13H260E#3+R4CH3=>CH4+R26C7H15+C6H100KZ	2.3E+0012	0.000	9600.0	!	
DE# 352					
DUPLICATE					
C13H260E#3+R8CH300=>CH300H+R26C7H15+C6H100KZ	6.0E+0012	0.000	20000.0		
! DE# 353					
DUPLICATE					
C13H260E#3+R8CH300=>CH300H+R26C7H15+C6H100KZ	3.5E+0013	0.000	17500.0		
! DE# 354					

DUPLICATE  
 C13H260E#3+R11C2H5=>C2H6+R26C7H15+C6H100KZ 3.0E+0011 0.000  
 13500.0 ! DE# 355  
 DUPLICATE  
 C13H260E#3+R11C2H5=>C2H6+R26C7H15+C6H100KZ 2.3E+0012 0.000  
 11000.0 ! DE# 356  
 DUPLICATE  
 C12H240E#3+R1H=>H2+R41C6H13+C6H100KZ 2.9E+0007 2.000 7700.0 ! DE#  
 357  
 DUPLICATE  
 C12H240E#3+R1H=>H2+R41C6H13+C6H100KZ 9.5E+0007 2.000 5000.0 ! DE#  
 358  
 DUPLICATE  
 C12H240E#3+R20H=>H2O+R41C6H13+C6H100KZ 2.7E+0006 2.000 450.0 ! DE#  
 359  
 DUPLICATE  
 C12H240E#3+R20H=>H2O+R41C6H13+C6H100KZ 2.7E+0007 2.000 -765.0 ! DE#  
 360  
 DUPLICATE  
 C12H240E#3+R300H=>H2O2+R41C6H13+C6H100KZ 6.0E+0011 0.000 17000.0 !  
 DE# 361  
 DUPLICATE  
 C12H240E#3+R300H=>H2O2+R41C6H13+C6H100KZ 4.2E+0012 0.000 15500.0 !  
 DE# 362  
 DUPLICATE  
 C12H240E#3+R4CH3=>CH4+R41C6H13+C6H100KZ 3.0E-0001 4.000 8200.0 !  
 DE# 363  
 DUPLICATE  
 C12H240E#3+R4CH3=>CH4+R41C6H13+C6H100KZ 2.1E+0012 0.000 9600.0 !  
 DE# 364  
 DUPLICATE  
 C12H240E#3+R8CH300=>CH300H+R41C6H13+C6H100KZ 6.0E+0012 0.000 20000.0  
 ! DE# 365  
 DUPLICATE  
 C12H240E#3+R8CH300=>CH300H+R41C6H13+C6H100KZ 3.2E+0013 0.000 17500.0  
 ! DE# 366  
 DUPLICATE  
 C12H240E#3+R11C2H5=>C2H6+R41C6H13+C6H100KZ 3.0E+0011 0.000  
 13500.0 ! DE# 367  
 DUPLICATE  
 C12H240E#3+R11C2H5=>C2H6+R41C6H13+C6H100KZ 2.1E+0012 0.000  
 11000.0 ! DE# 368  
 DUPLICATE  
 C11H220E#3+R1H=>H2+R41C6H13+C5H80KZ 2.9E+0007 2.000 7700.0 ! DE#  
 369  
 DUPLICATE  
 C11H220E#3+R1H=>H2+R41C6H13+C5H80KZ 8.6E+0007 2.000 5000.0 ! DE#  
 370  
 DUPLICATE  
 C11H220E#3+R20H=>H2O+R41C6H13+C5H80KZ 2.7E+0006 2.000 450.0 ! DE#  
 371  
 DUPLICATE  
 C11H220E#3+R20H=>H2O+R41C6H13+C5H80KZ 2.5E+0007 2.000 -765.0 ! DE#  
 372

DUPLICATE					
C11H220E#3+R300H=>H2O2+R41C6H13+C5H80KZ	6.0E+0011	0.000	17000.0	!	
DE# 373					
DUPLICATE					
C11H220E#3+R300H=>H2O2+R41C6H13+C5H80KZ	3.8E+0012	0.000	15500.0	!	
DE# 374					
DUPLICATE					
C11H220E#3+R4CH3=>CH4+R41C6H13+C5H80KZ	3.0E-0001	4.000	8200.0	!	DE#
375					
DUPLICATE					
C11H220E#3+R4CH3=>CH4+R41C6H13+C5H80KZ	1.9E+0012	0.000	9600.0	!	DE#
376					
DUPLICATE					
C11H220E#3+R8CH300=>CH300H+R41C6H13+C5H80KZ	6.0E+0012	0.000	20000.0		
! DE# 377					
DUPLICATE					
C11H220E#3+R8CH300=>CH300H+R41C6H13+C5H80KZ	2.9E+0013	0.000	17500.0		
! DE# 378					
DUPLICATE					
C11H220E#3+R11C2H5=>C2H6+R41C6H13+C5H80KZ	3.0E+0011	0.000	13500.0	!	
DE# 379					
DUPLICATE					
C11H220E#3+R11C2H5=>C2H6+R41C6H13+C5H80KZ	1.9E+0012	0.000	11000.0	!	
DE# 380					
DUPLICATE					
C14H280E#3+R1H=>H2+R26C7H15+C7H120KZ	2.9E+0007	2.000	7700.0	!	DE#
381					
DUPLICATE					
C14H280E#3+R1H=>H2+R26C7H15+C7H120KZ	1.1E+0008	2.000	5000.0	!	DE#
382					
DUPLICATE					
C14H280E#3+R20H=>H2O+R26C7H15+C7H120KZ	2.7E+0006	2.000	450.0	!	DE#
383					
DUPLICATE					
C14H280E#3+R20H=>H2O+R26C7H15+C7H120KZ	3.3E+0007	2.000	-765.0	!	DE#
384					
DUPLICATE					
C14H280E#3+R300H=>H2O2+R26C7H15+C7H120KZ	6.0E+0011	0.000	17000.0	!	
DE# 385					
DUPLICATE					
C14H280E#3+R300H=>H2O2+R26C7H15+C7H120KZ	5.0E+0012	0.000	15500.0	!	
DE# 386					
DUPLICATE					
C14H280E#3+R4CH3=>CH4+R26C7H15+C7H120KZ	3.0E-0001	4.000	8200.0	!	
DE# 387					
DUPLICATE					
C14H280E#3+R4CH3=>CH4+R26C7H15+C7H120KZ	2.5E+0012	0.000	9600.0	!	
DE# 388					
DUPLICATE					
C14H280E#3+R8CH300=>CH300H+R26C7H15+C7H120KZ	6.0E+0012	0.000	20000.0		
! DE# 389					
DUPLICATE					
C14H280E#3+R8CH300=>CH300H+R26C7H15+C7H120KZ	3.8E+0013	0.000	17500.0		
! DE# 390					

DUPLICATE  
C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H120KZ 3.0E+0011 0.000  
13500.0 ! DE# 391

DUPLICATE  
C14H28OE#3+R11C2H5=>C2H6+R26C7H15+C7H120KZ 2.5E+0012 0.000  
11000.0 ! DE# 392

DUPLICATE

! Metatheses of oxetanes, furanes and pyranes

! decompositions of cyclo-ether radicals

! Addition of oxygen on cyclo-ether radicals

! O2 elimination

! Isomerization

! Cylo-ether keto-hydroperoxide ester formation

! Decomposition of cylo-ether keto-hydroperoxide ester

! Isomerization of peroxy-radicals

! Addition of oxygen on cyclo-peroxy radicals

! Formation of cyclo-ether ketohydroperoxydes

! Decomposition of cyclo-ether ketohydroperoxydes

! Olefin reactions

! addition of H and CH3 on olefins

C3H6Y+R1H=>R19C3H7 1.3E+0013 0.000 1560.0 ! ADZ 393

DUPLICATE

C3H6Y+R1H=>R19C3H7 1.3E+0013 0.000 3260.0 ! ADZ 394

DUPLICATE

C4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 1560.0 ! ADZ 395

DUPLICATE

C4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 3260.0 ! ADZ 396

DUPLICATE

C4H8Y+R4CH3=>C3H6Y+R11C2H5 9.6E+0010 0.000 8000.0 ! ADZ 397

C5H10Z+R1H=>R35C5H11 1.3E+0013 0.000 1560.0 ! ADZ 398

DUPLICATE

C5H10Z+R1H=>R35C5H11 1.3E+0013 0.000 3260.0 ! ADZ 399

DUPLICATE

C5H10Z+R4CH3=>C4H8Y+R11C2H5 1.7E+0011 0.000 7400.0 ! ADZ 400

C5H10Z+R4CH3=>C3H6Y+R19C3H7 9.6E+0010 0.000 8000.0 ! ADZ 401

C7H14Z+R1H=>R26C7H15 1.3E+0013 0.000 1560.0 ! ADZ 402

DUPLICATE

C7H14Z+R1H=>R26C7H15 1.3E+0013 0.000 3260.0 ! ADZ 403

DUPLICATE

C7H14Z+R4CH3=>C4H8Y+R20C4H9 1.7E+0011 0.000 7400.0 ! ADZ 404

C7H14Z+R4CH3=>C3H6Y+R35C5H11 9.6E+0010 0.000 8000.0 ! ADZ 405

C6H12Z+R1H=>R41C6H13 1.3E+0013 0.000 1560.0 ! ADZ 406

DUPLICATE

C6H12Z+R1H=>R41C6H13 1.3E+0013 0.000 3260.0 ! ADZ 407

DUPLICATE

C6H12Z+R4CH3=>C4H8Y+R19C3H7	1.7E+0011	0.000	7400.0	! ADZ 408
C6H12Z+R4CH3=>C3H6Y+R20C4H9	9.6E+0010	0.000	8000.0	! ADZ 409
C7H14Y+R1H=>R26C7H15	1.3E+0013	0.000	1560.0	! ADZ 410
DUPLICATE				
C7H14Y+R1H=>R26C7H15	1.3E+0013	0.000	3260.0	! ADZ 411
DUPLICATE				
C7H14Y+R4CH3=>C4H8Y+R20C4H9	1.7E+0011	0.000	7400.0	! ADZ 412
C7H14Y+R4CH3=>C3H6Y+R35C5H11	9.6E+0010	0.000	8000.0	! ADZ 413
C8H16Y+R1H=>R30C8H17	1.3E+0013	0.000	1560.0	! ADZ 414
DUPLICATE				
C8H16Y+R1H=>R30C8H17	1.3E+0013	0.000	3260.0	! ADZ 415
DUPLICATE				
C8H16Y+R4CH3=>C4H8Y+R35C5H11	1.7E+0011	0.000	7400.0	! ADZ 416
C8H16Y+R4CH3=>C3H6Y+R41C6H13	9.6E+0010	0.000	8000.0	! ADZ 417
C8H16Z+R1H=>R30C8H17	1.3E+0013	0.000	1560.0	! ADZ 418
DUPLICATE				
C8H16Z+R1H=>R30C8H17	1.3E+0013	0.000	3260.0	! ADZ 419
DUPLICATE				
C8H16Z+R4CH3=>C4H8Y+R35C5H11	1.7E+0011	0.000	7400.0	! ADZ 420
C8H16Z+R4CH3=>C3H6Y+R41C6H13	9.6E+0010	0.000	8000.0	! ADZ 421
C5H10Y+R1H=>R35C5H11	1.3E+0013	0.000	1560.0	! ADZ 422
DUPLICATE				
C5H10Y+R1H=>R35C5H11	1.3E+0013	0.000	3260.0	! ADZ 423
DUPLICATE				
C5H10Y+R4CH3=>C4H8Y+R11C2H5	1.7E+0011	0.000	7400.0	! ADZ 424
C5H10Y+R4CH3=>C3H6Y+R19C3H7	9.6E+0010	0.000	8000.0	! ADZ 425
C9H18Z+R4CH3=>C4H8Y+R41C6H13	1.7E+0011	0.000	7400.0	! ADZ 426
C9H18Z+R4CH3=>C3H6Y+R26C7H15	9.6E+0010	0.000	8000.0	! ADZ 427
C10H20Z+R4CH3=>C4H8Y+R26C7H15	1.7E+0011	0.000	7400.0	! ADZ 428
C10H20Z+R4CH3=>C3H6Y+R30C8H17	9.6E+0010	0.000	8000.0	! ADZ 429
C11H22Z+R4CH3=>C4H8Y+R30C8H17	1.7E+0011	0.000	7400.0	! ADZ 430
C9H18Z+R1H=>4C2H4Z+R4CH3	9.6E+0010	0.000	8000.0	! ADZ 431
C10H20Z+R1H=>4C2H4Z+R11C2H5	9.6E+0010	0.000	8000.0	! ADZ 432
C13H26Z+R1H=>6C2H4Z+R4CH3	9.6E+0010	0.000	8000.0	! ADZ 433
C12H24Z+R1H=>5C2H4Z+R11C2H5	9.6E+0010	0.000	8000.0	! ADZ 434
C11H22Z+R1H=>5C2H4Z+R4CH3	9.6E+0010	0.000	8000.0	! ADZ 435
C14H28Z+R1H=>6C2H4Z+R11C2H5	9.6E+0010	0.000	8000.0	! ADZ 436
! addition of OH on olefins				
C3H6Y+R20H=>R4CH3+CH3CHO	1.4E+0012	0.000	-1040.0	! ADZ 437
C3H6Y+R20H=>R11C2H5+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 438
C4H8Y+R20H=>R4CH3+C2H5CHO	1.4E+0012	0.000	-1040.0	! ADZ 439
C4H8Y+R20H=>R19C3H7+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 440
C5H10Z+R20H=>R4CH3+C4H8OA	1.4E+0012	0.000	-1040.0	! ADZ 441
C5H10Z+R20H=>R20C4H9+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 442
C7H14Z+R20H=>R4CH3+C6H12OA	1.4E+0012	0.000	-1040.0	! ADZ 443
C7H14Z+R20H=>R41C6H13+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 444
C6H12Z+R20H=>R4CH3+C5H10OA	1.4E+0012	0.000	-1040.0	! ADZ 445
C6H12Z+R20H=>R35C5H11+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 446
C7H14Y+R20H=>R4CH3+C6H12OA	1.4E+0012	0.000	-1040.0	! ADZ 447
C7H14Y+R20H=>R41C6H13+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 448
C8H16Y+R20H=>R4CH3+C7H14OA	1.4E+0012	0.000	-1040.0	! ADZ 449
C8H16Y+R20H=>R26C7H15+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 450
C8H16Z+R20H=>R4CH3+C7H14OA	1.4E+0012	0.000	-1040.0	! ADZ 451



C8H16Z+R20H=>R26C7H15+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 452  
 C5H10Y+R20H=>R4CH3+C4H8OA 1.4E+0012 0.000 -1040.0 ! ADZ 453  
 C5H10Y+R20H=>R20C4H9+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 454  
 C9H18Z+R20H=>R4CH3+C8H16OA 1.4E+0012 0.000 -1040.0 ! ADZ 455  
 C9H18Z+R20H=>R30C8H17+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 456  
 C10H20Z+R20H=>R4CH3+C9H18OA 1.4E+0012 0.000 -1040.0 ! ADZ 457  
 C13H26Z+R20H=>R4CH3+C12H24OA 1.4E+0012 0.000 -1040.0 ! ADZ 458  
 C12H24Z+R20H=>R4CH3+C11H22OA 1.4E+0012 0.000 -1040.0 ! ADZ 459  
 C11H22Z+R20H=>R4CH3+C10H20OA 1.4E+0012 0.000 -1040.0 ! ADZ 460  
 C14H28Z+R20H=>R4CH3+C13H26OA 1.4E+0012 0.000 -1040.0 ! ADZ 461

C10H20Z+R20H=>HCHO+R4CH3+4C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 462  
 C13H26Z+R20H=>HCHO+R11C2H5+5C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 463  
 C12H24Z+R20H=>HCHO+R4CH3+5C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 464  
 C11H22Z+R20H=>HCHO+R11C2H5+4C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 465  
 C14H28Z+R20H=>HCHO+R4CH3+6C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 466

! addition of 0 on olefins

C3H6Y+B10=>CH2COZ+R1H+R4CH3 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C4H8Y+B10=>CH2COZ+R1H+R11C2H5 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C5H10Z+B10=>CH2COZ+R1H+R19C3H7 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C7H14Z+B10=>CH2COZ+R1H+R35C5H11 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C6H12Z+B10=>CH2COZ+R1H+R20C4H9 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C7H14Y+B10=>CH2COZ+R1H+R35C5H11 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C8H16Y+B10=>CH2COZ+R1H+R41C6H13 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C8H16Z+B10=>CH2COZ+R1H+R41C6H13 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C5H10Y+B10=>CH2COZ+R1H+R19C3H7 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C9H18Z+B10=>CH2COZ+R1H+R26C7H15 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C10H20Z+B10=>CH2COZ+R1H+R30C8H17 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 !C13H26Z+B10=>CH2COZ+R4CH3+R1H+5C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ 467  
 !C12H24Z+B10=>CH2COZ+R11C2H5+R1H+4C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ 467  
 !C11H22Z+B10=>CH2COZ+R4CH3+R1H+4C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ 467  
 !C14H28Z+B10=>CH2COZ+R11C2H5+R1H+5C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ 467

! retroene reactions

C5H10Z=>C3H6Y+C2H4Z 8.0E+0012 0.000 56500.0 ! RTZ 467  
 C7H14Z=>C3H6Y+C4H8Y 8.0E+0012 0.000 56500.0 ! RTZ 468  
 C6H12Z=>C3H6Y+C3H6Y 8.0E+0012 0.000 56500.0 ! RTZ 469  
 C7H14Y=>C3H6Y+C4H8Y 8.0E+0012 0.000 56500.0 ! RTZ 470  
 C8H16Y=>C3H6Y+C5H10Z 8.0E+0012 0.000 56500.0 ! RTZ 471  
 C8H16Z=>C3H6Y+C5H10Z 8.0E+0012 0.000 56500.0 ! RTZ 472  
 C5H10Y=>C3H6Y+C2H4Z 8.0E+0012 0.000 56500.0 ! RTZ 473  
 C9H18Z=>C3H6Y+C6H12Z 8.0E+0012 0.000 56500.0 ! RTZ 474  
 C10H20Z=>C3H6Y+C7H14Z 8.0E+0012 0.000 56500.0 ! RTZ 475  
 C13H26Z=>C3H6Y+C10H20Z 8.0E+0012 0.000 56500.0 ! RTZ 476  
 C12H24Z=>C3H6Y+C9H18Z 8.0E+0012 0.000 56500.0 ! RTZ 477  
 C11H22Z=>C3H6Y+C8H16Z 8.0E+0012 0.000 56500.0 ! RTZ 478  
 C14H28Z=>C3H6Y+C11H22Z 8.0E+0012 0.000 56500.0 ! RTZ 479

! addition of OOH on olefins

C3H6Y+R300H=>R20H+C3H60E#3	1.0E+0012	0.000	14200.0	! ADZ 480
C4H8Y+R300H=>R20H+C4H80E#3	1.0E+0012	0.000	14200.0	! ADZ 481
C5H10Z+R300H=>R20H+C5H100E#3	1.0E+0012	0.000	14200.0	! ADZ 482
C7H14Z+R300H=>R20H+C7H140E#3	1.0E+0012	0.000	14200.0	! ADZ 483
C6H12Z+R300H=>R20H+C6H120E#3	1.0E+0012	0.000	14200.0	! ADZ 484
C7H14Y+R300H=>R20H+C7H140E#3	1.0E+0012	0.000	14200.0	! ADZ 485
C8H16Y+R300H=>R20H+C8H160E#3	1.0E+0012	0.000	14200.0	! ADZ 486
C8H16Z+R300H=>R20H+C8H160E#3	1.0E+0012	0.000	14200.0	! ADZ 487
C5H10Y+R300H=>R20H+C5H100E#3	1.0E+0012	0.000	14200.0	! ADZ 488
C9H18Z+R300H=>R20H+C9H180E#3	1.0E+0012	0.000	14200.0	! ADZ 489
C10H20Z+R300H=>R20H+C10H200E#3	1.0E+0012	0.000	14200.0	! ADZ 490
C13H26Z+R300H=>R20H+C13H260E#3	1.0E+0012	0.000	14200.0	! ADZ 491
C12H24Z+R300H=>R20H+C12H240E#3	1.0E+0012	0.000	14200.0	! ADZ 492
C11H22Z+R300H=>R20H+C11H220E#3	1.0E+0012	0.000	14200.0	! ADZ 493
C14H28Z+R300H=>R20H+C14H280E#3	1.0E+0012	0.000	14200.0	! ADZ 494
! olefin to dienes				
C5H10Z+R1H=>H2+C4H6Z2+R4CH3	5.4E+0004	2.500	-1900.0	! MZ 495
DUPLICATE				
C5H10Z+R1H=>H2+C4H6Z2+R4CH3	2.9E+0007	2.000	7700.0	! MZ 496
DUPLICATE				
C5H10Z+R1H=>H2+C4H6Z2+R4CH3	9.0E+0006	2.000	5000.0	! MZ 497
DUPLICATE				
C5H10Z+R20H=>H20+C4H6Z2+R4CH3	3.0E+0006	2.000	-1520.0	! MZ 498
DUPLICATE				
C5H10Z+R20H=>H20+C4H6Z2+R4CH3	2.7E+0006	2.000	450.0	! MZ 499
DUPLICATE				
C5H10Z+R20H=>H20+C4H6Z2+R4CH3	2.6E+0006	2.000	-765.0	! MZ 500
DUPLICATE				
C5H10Z+R300H=>H202+C4H6Z2+R4CH3	6.4E+0003	2.600	12400.0	! MZ 501
DUPLICATE				
C5H10Z+R300H=>H202+C4H6Z2+R4CH3	6.0E+0011	0.000	17000.0	! MZ 502
DUPLICATE				
C5H10Z+R300H=>H202+C4H6Z2+R4CH3	4.0E+0011	0.000	15500.0	! MZ 503
DUPLICATE				
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	1.0E+0011	0.000	7300.0	! MZ 504
DUPLICATE				
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	3.0E-0001	4.000	8200.0	! MZ 505
DUPLICATE				
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	2.0E+0011	0.000	9600.0	! MZ 506
DUPLICATE				
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3	1.0E+0012	0.000	14550.0	! MZ 507
DUPLICATE				
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3	6.0E+0012	0.000	20000.0	! MZ 508
DUPLICATE				
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3	3.0E+0012	0.000	17500.0	! MZ 509
DUPLICATE				
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	1.5E+0000	3.500	4140.0	! MZ 510
DUPLICATE				
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	3.0E+0011	0.000	13500.0	! MZ 511
DUPLICATE				

C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3 DUPLICATE	2.0E+0011	0.000	11000.0	! MZ 512
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 513
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 514
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7 DUPLICATE	2.7E+0007	2.000	5000.0	! MZ 515
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 516
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 517
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7 DUPLICATE	7.8E+0006	2.000	-765.0	! MZ 518
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7 DUPLICATE	6.4E+0003	2.600	12400.0	! MZ 519
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 520
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7 DUPLICATE	1.2E+0012	0.000	15500.0	! MZ 521
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 522
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 523
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7 DUPLICATE	6.0E+0011	0.000	9600.0	! MZ 524
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7 525 DUPLICATE	1.0E+0012	0.000	14550.0	! MZ 525
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7 526 DUPLICATE	6.0E+0012	0.000	20000.0	! MZ 526
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7 527 DUPLICATE	9.0E+0012	0.000	17500.0	! MZ 527
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7 DUPLICATE	1.5E+0000	3.500	4140.0	! MZ 528
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7 529 DUPLICATE	3.0E+0011	0.000	13500.0	! MZ 529
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7 530 DUPLICATE	6.0E+0011	0.000	11000.0	! MZ 530
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 531
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 532
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5 DUPLICATE	1.8E+0007	2.000	5000.0	! MZ 533
C6H12Z+R20H=>H20+C4H6Z2+R11C2H5 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 534
C6H12Z+R20H=>H20+C4H6Z2+R11C2H5 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 535
C6H12Z+R20H=>H20+C4H6Z2+R11C2H5	5.2E+0006	2.000	-765.0	! MZ 536

DUPLICATE					
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5	6.4E+0003	2.600	12400.0	!	MZ 537
DUPLICATE					
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5	6.0E+0011	0.000	17000.0	!	MZ 538
DUPLICATE					
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5	8.0E+0011	0.000	15500.0	!	MZ 539
DUPLICATE					
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5	1.0E+0011	0.000	7300.0	!	MZ 540
DUPLICATE					
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5	3.0E-0001	4.000	8200.0	!	MZ 541
DUPLICATE					
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5	4.0E+0011	0.000	9600.0	!	MZ 542
DUPLICATE					
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5	1.0E+0012	0.000	14550.0	!	MZ 543
DUPLICATE					
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5	6.0E+0012	0.000	20000.0	!	MZ 544
DUPLICATE					
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5	6.0E+0012	0.000	17500.0	!	MZ 545
DUPLICATE					
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5	1.5E+0000	3.500	4140.0	!	MZ 546
DUPLICATE					
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5	3.0E+0011	0.000	13500.0	!	MZ 547
DUPLICATE					
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5	4.0E+0011	0.000	11000.0	!	MZ 548
DUPLICATE					
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	5.4E+0004	2.500	-1900.0	!	MZ 549
DUPLICATE					
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	2.9E+0007	2.000	7700.0	!	MZ 550
DUPLICATE					
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	3.6E+0007	2.000	5000.0	!	MZ 551
DUPLICATE					
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9	3.0E+0006	2.000	-1520.0	!	MZ 552
DUPLICATE					
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9	2.7E+0006	2.000	450.0	!	MZ 553
DUPLICATE					
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9	1.0E+0007	2.000	-765.0	!	MZ 554
DUPLICATE					
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9	6.4E+0003	2.600	12400.0	!	MZ 555
DUPLICATE					
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9	6.0E+0011	0.000	17000.0	!	MZ 556
DUPLICATE					
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9	1.6E+0012	0.000	15500.0	!	MZ 557
DUPLICATE					
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9	1.0E+0011	0.000	7300.0	!	MZ 558
DUPLICATE					
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9	3.0E-0001	4.000	8200.0	!	MZ 559
DUPLICATE					
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9	8.0E+0011	0.000	9600.0	!	MZ 560
DUPLICATE					

C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 561	1.0E+0012	0.000	14550.0	! MZ
DUPLICATE				
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 562	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 563	1.2E+0013	0.000	17500.0	! MZ
DUPLICATE				
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 564	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 565	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 566	8.0E+0011	0.000	11000.0	! MZ
DUPLICATE				
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11 567	5.4E+0004	2.500	-1900.0	! MZ
DUPLICATE				
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11 568	2.9E+0007	2.000	7700.0	! MZ
DUPLICATE				
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11 569	4.5E+0007	2.000	5000.0	! MZ
DUPLICATE				
C9H18Z+R20H=>H20+C4H6Z2+R35C5H11 570	3.0E+0006	2.000	-1520.0	! MZ
DUPLICATE				
C9H18Z+R20H=>H20+C4H6Z2+R35C5H11 571	2.7E+0006	2.000	450.0	! MZ
DUPLICATE				
C9H18Z+R20H=>H20+C4H6Z2+R35C5H11 572	1.3E+0007	2.000	-765.0	! MZ
DUPLICATE				
C9H18Z+R300H=>H202+C4H6Z2+R35C5H11 573	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
C9H18Z+R300H=>H202+C4H6Z2+R35C5H11 574	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
C9H18Z+R300H=>H202+C4H6Z2+R35C5H11 575	2.0E+0012	0.000	15500.0	! MZ
DUPLICATE				
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11 576	1.0E+0011	0.000	7300.0	! MZ
DUPLICATE				
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11 577	3.0E-0001	4.000	8200.0	! MZ
DUPLICATE				
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11 578	1.0E+0012	0.000	9600.0	! MZ
DUPLICATE				
C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 579	1.0E+0012	0.000	14550.0	! MZ
DUPLICATE				
C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 580	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 581	1.5E+0013	0.000	17500.0	! MZ
DUPLICATE				
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 582	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				

C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 583	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 584	1.0E+0012	0.000	11000.0	! MZ
DUPLICATE				
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 585	5.4E+0004	2.500	-1900.0	! MZ
DUPLICATE				
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 586	2.9E+0007	2.000	7700.0	! MZ
DUPLICATE				
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 587	5.4E+0007	2.000	5000.0	! MZ
DUPLICATE				
C10H20Z+R20H=>H20+C4H6Z2+R41C6H13 588	3.0E+0006	2.000	-1520.0	! MZ
DUPLICATE				
C10H20Z+R20H=>H20+C4H6Z2+R41C6H13 589	2.7E+0006	2.000	450.0	! MZ
DUPLICATE				
C10H20Z+R20H=>H20+C4H6Z2+R41C6H13 590	1.5E+0007	2.000	-765.0	! MZ
DUPLICATE				
C10H20Z+R300H=>H202+C4H6Z2+R41C6H13 591	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
C10H20Z+R300H=>H202+C4H6Z2+R41C6H13 592	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
C10H20Z+R300H=>H202+C4H6Z2+R41C6H13 593	2.4E+0012	0.000	15500.0	! MZ
DUPLICATE				
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 594	1.0E+0011	0.000	7300.0	! MZ
DUPLICATE				
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 595	3.0E-0001	4.000	8200.0	! MZ
DUPLICATE				
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 596	1.2E+0012	0.000	9600.0	! MZ
DUPLICATE				
C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 597	1.0E+0012	0.000	14550.0	!
DUPLICATE				
C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 598	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 599	1.8E+0013	0.000	17500.0	!
DUPLICATE				
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 600	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 601	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 602	1.2E+0012	0.000	11000.0	! MZ
DUPLICATE				
!C13H26Z+R1H=>H2+C4H6Z2+R4CH3+4C2H4Z 603	5.4E+0004	2.500	-1900.0	! MZ

!C13H26Z+R20H=>H20+C4H6Z2+R4CH3+4C2H4Z 604	3.0E+0006	2.000	-1520.0	! MZ
!C13H26Z+R300H=>H202+C4H6Z2+R4CH3+4C2H4Z MZ 605	6.4E+0003	2.600	12400.0	!
!C13H26Z+R4CH3=>CH4+C4H6Z2+R4CH3+4C2H4Z 606	1.0E+0011	0.000	7300.0	! MZ
!C13H26Z+R8CH300=>CH300H+C4H6Z2+R4CH3+4C2H4Z ! MZ 607	1.0E+0011	0.000	7300.0	!
!C13H26Z+R11C2H5=>C2H6+C4H6Z2+R4CH3+4C2H4Z MZ 608	1.5E+0000	3.500	4140.0	!
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 609
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 610
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17 DUPLICATE	7.2E+0007	2.000	5000.0	! MZ 611
C12H24Z+R20H=>H20+C4H6Z2+R30C8H17 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 612
C12H24Z+R20H=>H20+C4H6Z2+R30C8H17 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 613
C12H24Z+R20H=>H20+C4H6Z2+R30C8H17 DUPLICATE	2.1E+0007	2.000	-765.0	! MZ 614
C12H24Z+R300H=>H202+C4H6Z2+R30C8H17 615	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
C12H24Z+R300H=>H202+C4H6Z2+R30C8H17 616	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
C12H24Z+R300H=>H202+C4H6Z2+R30C8H17 617	3.2E+0012	0.000	15500.0	! MZ
DUPLICATE				
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 618
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 619
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17 DUPLICATE	1.6E+0012	0.000	9600.0	! MZ 620
C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17 MZ 621	1.0E+0012	0.000	14550.0	!
DUPLICATE				
C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17 MZ 622	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17 MZ 623	2.4E+0013	0.000	17500.0	!
DUPLICATE				
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 624	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 625	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 626	1.6E+0012	0.000	11000.0	! MZ

DUPLICATE					
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15	5.4E+0004	2.500	-1900.0	!	MZ 627
DUPLICATE					
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15	2.9E+0007	2.000	7700.0	!	MZ 628
DUPLICATE					
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15	6.3E+0007	2.000	5000.0	!	MZ 629
DUPLICATE					
C11H22Z+R20H=>H20+C4H6Z2+R26C7H15	3.0E+0006	2.000	-1520.0	!	MZ 630
DUPLICATE					
C11H22Z+R20H=>H20+C4H6Z2+R26C7H15	2.7E+0006	2.000	450.0	!	MZ 631
DUPLICATE					
C11H22Z+R20H=>H20+C4H6Z2+R26C7H15	1.8E+0007	2.000	-765.0	!	MZ 632
DUPLICATE					
C11H22Z+R300H=>H202+C4H6Z2+R26C7H15	6.4E+0003	2.600	12400.0	!	MZ 633
DUPLICATE					
C11H22Z+R300H=>H202+C4H6Z2+R26C7H15	6.0E+0011	0.000	17000.0	!	MZ 634
DUPLICATE					
C11H22Z+R300H=>H202+C4H6Z2+R26C7H15	2.8E+0012	0.000	15500.0	!	MZ 635
DUPLICATE					
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15	1.0E+0011	0.000	7300.0	!	MZ 636
DUPLICATE					
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15	3.0E-0001	4.000	8200.0	!	MZ 637
DUPLICATE					
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15	1.4E+0012	0.000	9600.0	!	MZ 638
DUPLICATE					
C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15	1.0E+0012	0.000	14550.0	!	MZ 639
DUPLICATE					
C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15	6.0E+0012	0.000	20000.0	!	MZ 640
DUPLICATE					
C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15	2.1E+0013	0.000	17500.0	!	MZ 641
DUPLICATE					
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15	1.5E+0000	3.500	4140.0	!	MZ 642
DUPLICATE					
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15	3.0E+0011	0.000	13500.0	!	MZ 643
DUPLICATE					
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15	1.4E+0012	0.000	11000.0	!	MZ 644
DUPLICATE					
!C14H28Z+R1H=>H2+C4H6Z2+R11C2H5+4C2H4Z	5.4E+0004	2.500	-1900.0	!	MZ 645
!C14H28Z+R20H=>H20+C4H6Z2+R11C2H5+4C2H4Z	3.0E+0006	2.000	-1520.0	!	MZ 646
!C14H28Z+R300H=>H202+C4H6Z2+R11C2H5+4C2H4Z	6.4E+0003	2.600	12400.0	!	MZ 647
!C14H28Z+R4CH3=>CH4+C4H6Z2+R11C2H5+4C2H4Z	1.0E+0011	0.000	7300.0	!	MZ 648



!C14H28Z+R8CH300=>CH300H+C4H6Z2+R11C2H5+4C2H4Z	1.0E+0011	0.000		
7300.0 ! MZ 649				
!C14H28Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5+4C2H4Z	1.5E+0000	3.500	4140.0	
! MZ 650				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	8.8E+0010	0.700	3250.0	! MZ 651
DUPLICATE				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	5.1E+0013	0.000	7850.0	! MZ 652
DUPLICATE				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	2.6E+0013	0.000	5200.0	! MZ 653
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	8.8E+0010	0.700	3250.0	! MZ 654
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	5.1E+0013	0.000	7850.0	! MZ 655
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	7.8E+0013	0.000	5200.0	! MZ 656
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	8.8E+0010	0.700	3250.0	! MZ 657
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	5.1E+0013	0.000	7850.0	! MZ 658
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	5.2E+0013	0.000	5200.0	! MZ 659
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	8.8E+0010	0.700	3250.0	! MZ 660
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	5.1E+0013	0.000	7850.0	! MZ 661
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	1.0E+0014	0.000	5200.0	! MZ 662
DUPLICATE				
C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	8.8E+0010	0.700	3250.0	! MZ 663
DUPLICATE				
C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	5.1E+0013	0.000	7850.0	! MZ 664
DUPLICATE				
C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	1.3E+0014	0.000	5200.0	! MZ 665
DUPLICATE				
C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	8.8E+0010	0.700	3250.0	! MZ 666
DUPLICATE				
C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	5.1E+0013	0.000	7850.0	! MZ 667
DUPLICATE				
C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	1.6E+0014	0.000	5200.0	! MZ 668
DUPLICATE				
C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	8.8E+0010	0.700	3250.0	! MZ 669
DUPLICATE				
C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	5.1E+0013	0.000	7850.0	! MZ 670
DUPLICATE				
C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	2.1E+0014	0.000	5200.0	! MZ 671
DUPLICATE				
C11H22Z+B10=>R20H+C4H6Z2+R26C7H15	8.8E+0010	0.700	3250.0	! MZ 672
DUPLICATE				
C11H22Z+B10=>R20H+C4H6Z2+R26C7H15	5.1E+0013	0.000	7850.0	! MZ 673
DUPLICATE				
C11H22Z+B10=>R20H+C4H6Z2+R26C7H15	1.8E+0014	0.000	5200.0	! MZ 674
DUPLICATE				

! Metathesis with YH

C3H6Y+R1H=>RC3H5Y+H2	1.7E+0005	2.500	2510.0	! MES 675
C3H6Y+R20H=>RC3H5Y+H20	3.0E+0006	2.000	-298.0	! MES 676
C3H6Y+R300H=>RC3H5Y+H202	9.6E+0003	2.600	13900.0	! MES 677
C3H6Y+R4CH3=>RC3H5Y+CH4	2.2E+0000	3.500	5670.0	! MES 678
C3H6Y+R8CH300=>RC3H5Y+CH300H	2.0E+0012	0.000	17050.0	! MES 679
C3H6Y+R11C2H5=>RC3H5Y+C2H6	2.2E+0000	3.500	6640.0	! MES 680
C4H8Y+R1H=>RC4H7Y+H2	5.4E+0004	2.500	-1900.0	! MES 681
DUPLICATE				
C4H8Y+R1H=>RC4H7Y+H2	2.9E+0007	2.000	7700.0	! MES 682
DUPLICATE				
C4H8Y+R20H=>RC4H7Y+H20	3.0E+0006	2.000	-1520.0	! MES 683
DUPLICATE				
C4H8Y+R20H=>RC4H7Y+H20	2.7E+0006	2.000	450.0	! MES 684
DUPLICATE				
C4H8Y+R300H=>RC4H7Y+H202	6.4E+0003	2.600	12400.0	! MES 685
DUPLICATE				
C4H8Y+R300H=>RC4H7Y+H202	6.0E+0011	0.000	17000.0	! MES 686
DUPLICATE				
C4H8Y+R4CH3=>RC4H7Y+CH4	1.0E+0011	0.000	7300.0	! MES 687
DUPLICATE				
C4H8Y+R4CH3=>RC4H7Y+CH4	3.0E-0001	4.000	8200.0	! MES 688
DUPLICATE				
C4H8Y+R8CH300=>RC4H7Y+CH300H	1.0E+0012	0.000	14550.0	! MES 689
DUPLICATE				
C4H8Y+R8CH300=>RC4H7Y+CH300H	6.0E+0012	0.000	20000.0	! MES 690
DUPLICATE				
C4H8Y+R11C2H5=>RC4H7Y+C2H6	1.5E+0000	3.500	4140.0	! MES 691
DUPLICATE				
C4H8Y+R11C2H5=>RC4H7Y+C2H6	3.0E+0011	0.000	13500.0	! MES 692
DUPLICATE				
C7H14Y+R1H=>RC7H13Y+H2	5.4E+0004	2.500	-1900.0	! MES 693
DUPLICATE				
C7H14Y+R1H=>RC7H13Y+H2	2.9E+0007	2.000	7700.0	! MES 694
DUPLICATE				
C7H14Y+R1H=>RC7H13Y+H2	2.7E+0007	2.000	5000.0	! MES 695
DUPLICATE				
C7H14Y+R20H=>RC7H13Y+H20	3.0E+0006	2.000	-1520.0	! MES 696
DUPLICATE				
C7H14Y+R20H=>RC7H13Y+H20	2.7E+0006	2.000	450.0	! MES 697
DUPLICATE				
C7H14Y+R20H=>RC7H13Y+H20	7.8E+0006	2.000	-765.0	! MES 698
DUPLICATE				
C7H14Y+R300H=>RC7H13Y+H202	6.4E+0003	2.600	12400.0	! MES 699
DUPLICATE				
C7H14Y+R300H=>RC7H13Y+H202	6.0E+0011	0.000	17000.0	! MES 700
DUPLICATE				
C7H14Y+R300H=>RC7H13Y+H202	1.2E+0012	0.000	15500.0	! MES 701
DUPLICATE				
C7H14Y+R4CH3=>RC7H13Y+CH4	1.0E+0011	0.000	7300.0	! MES 702
DUPLICATE				
C7H14Y+R4CH3=>RC7H13Y+CH4	3.0E-0001	4.000	8200.0	! MES 703
DUPLICATE				
C7H14Y+R4CH3=>RC7H13Y+CH4	6.0E+0011	0.000	9600.0	! MES 704
DUPLICATE				

C7H14Y+R8CH300=>RC7H13Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 705
C7H14Y+R8CH300=>RC7H13Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 706
C7H14Y+R8CH300=>RC7H13Y+CH300H DUPLICATE	9.0E+0012	0.000	17500.0	! MES 707
C7H14Y+R11C2H5=>RC7H13Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 708
C7H14Y+R11C2H5=>RC7H13Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 709
C7H14Y+R11C2H5=>RC7H13Y+C2H6 DUPLICATE	6.0E+0011	0.000	11000.0	! MES 710
C8H16Y+R1H=>RC8H15Y+H2 DUPLICATE	5.4E+0004	2.500	-1900.0	! MES 711
C8H16Y+R1H=>RC8H15Y+H2 DUPLICATE	2.9E+0007	2.000	7700.0	! MES 712
C8H16Y+R1H=>RC8H15Y+H2 DUPLICATE	3.6E+0007	2.000	5000.0	! MES 713
C8H16Y+R20H=>RC8H15Y+H20 DUPLICATE	3.0E+0006	2.000	-1520.0	! MES 714
C8H16Y+R20H=>RC8H15Y+H20 DUPLICATE	2.7E+0006	2.000	450.0	! MES 715
C8H16Y+R20H=>RC8H15Y+H20 DUPLICATE	1.0E+0007	2.000	-765.0	! MES 716
C8H16Y+R300H=>RC8H15Y+H202 DUPLICATE	6.4E+0003	2.600	12400.0	! MES 717
C8H16Y+R300H=>RC8H15Y+H202 DUPLICATE	6.0E+0011	0.000	17000.0	! MES 718
C8H16Y+R300H=>RC8H15Y+H202 DUPLICATE	1.6E+0012	0.000	15500.0	! MES 719
C8H16Y+R4CH3=>RC8H15Y+CH4 DUPLICATE	1.0E+0011	0.000	7300.0	! MES 720
C8H16Y+R4CH3=>RC8H15Y+CH4 DUPLICATE	3.0E-0001	4.000	8200.0	! MES 721
C8H16Y+R4CH3=>RC8H15Y+CH4 DUPLICATE	8.0E+0011	0.000	9600.0	! MES 722
C8H16Y+R8CH300=>RC8H15Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 723
C8H16Y+R8CH300=>RC8H15Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 724
C8H16Y+R8CH300=>RC8H15Y+CH300H DUPLICATE	1.2E+0013	0.000	17500.0	! MES 725
C8H16Y+R11C2H5=>RC8H15Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 726
C8H16Y+R11C2H5=>RC8H15Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 727
C8H16Y+R11C2H5=>RC8H15Y+C2H6 DUPLICATE	8.0E+0011	0.000	11000.0	! MES 728
C5H10Y+R1H=>RC5H9Y+H2 DUPLICATE	5.4E+0004	2.500	-1900.0	! MES 729
C5H10Y+R1H=>RC5H9Y+H2 DUPLICATE	2.9E+0007	2.000	7700.0	! MES 730
C5H10Y+R1H=>RC5H9Y+H2 DUPLICATE	9.0E+0006	2.000	5000.0	! MES 731

C5H10Y+R20H=>RC5H9Y+H20 DUPLICATE	3.0E+0006	2.000	-1520.0	! MES 732
C5H10Y+R20H=>RC5H9Y+H20 DUPLICATE	2.7E+0006	2.000	450.0	! MES 733
C5H10Y+R20H=>RC5H9Y+H20 DUPLICATE	2.6E+0006	2.000	-765.0	! MES 734
C5H10Y+R300H=>RC5H9Y+H202 DUPLICATE	6.4E+0003	2.600	12400.0	! MES 735
C5H10Y+R300H=>RC5H9Y+H202 DUPLICATE	6.0E+0011	0.000	17000.0	! MES 736
C5H10Y+R300H=>RC5H9Y+H202 DUPLICATE	4.0E+0011	0.000	15500.0	! MES 737
C5H10Y+R4CH3=>RC5H9Y+CH4 DUPLICATE	1.0E+0011	0.000	7300.0	! MES 738
C5H10Y+R4CH3=>RC5H9Y+CH4 DUPLICATE	3.0E-0001	4.000	8200.0	! MES 739
C5H10Y+R4CH3=>RC5H9Y+CH4 DUPLICATE	2.0E+0011	0.000	9600.0	! MES 740
C5H10Y+R8CH300=>RC5H9Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 741
C5H10Y+R8CH300=>RC5H9Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 742
C5H10Y+R8CH300=>RC5H9Y+CH300H DUPLICATE	3.0E+0012	0.000	17500.0	! MES 743
C5H10Y+R11C2H5=>RC5H9Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 744
C5H10Y+R11C2H5=>RC5H9Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 745
C5H10Y+R11C2H5=>RC5H9Y+C2H6 DUPLICATE	2.0E+0011	0.000	11000.0	! MES 746
C3H6Y+B10=>RC3H5Y+R20H	1.7E+0011	0.700	5900.0	! MES 747
C4H8Y+B10=>RC4H7Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 748
C4H8Y+B10=>RC4H7Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 749
C7H14Y+B10=>RC7H13Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 750
C7H14Y+B10=>RC7H13Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 751
C7H14Y+B10=>RC7H13Y+R20H DUPLICATE	7.8E+0013	0.000	5200.0	! MES 752
C8H16Y+B10=>RC8H15Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 753
C8H16Y+B10=>RC8H15Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 754
C8H16Y+B10=>RC8H15Y+R20H DUPLICATE	1.0E+0014	0.000	5200.0	! MES 755
C5H10Y+B10=>RC5H9Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 756
C5H10Y+B10=>RC5H9Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 757
C5H10Y+B10=>RC5H9Y+R20H DUPLICATE	2.6E+0013	0.000	5200.0	! MES 758

! Addition of .Y on YH

RC3H5Y+C5H10Y=>R10C2H3V+C6H12Z	6.0E+0009	0.000	11400.0	! ADY 759
RC3H5Y+C8H16Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 760
RC3H5Y+C7H14Y=>R10C2H3V+C8H16Z	6.0E+0009	0.000	11400.0	! ADY 761
RC3H5Y+C4H8Y=>R10C2H3V+C5H10Z	6.0E+0009	0.000	11400.0	! ADY 762
RC3H5Y+C3H6Y=>R10C2H3V+C4H8Y	6.0E+0009	0.000	11400.0	! ADY 763
RC4H7Y+C5H10Y=>R10C2H3V+C7H14Z	6.0E+0009	0.000	11400.0	! ADY 764
RC4H7Y+C8H16Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 765
RC4H7Y+C7H14Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 766
RC4H7Y+C4H8Y=>R10C2H3V+C6H12Z	6.0E+0009	0.000	11400.0	! ADY 767
RC4H7Y+C3H6Y=>R10C2H3V+C5H10Z	6.0E+0009	0.000	11400.0	! ADY 768
RC7H13Y+C5H10Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 769
RC7H13Y+C8H16Y=>R10C2H3V+C13H26Z	6.0E+0009	0.000	11400.0	! ADY 770
RC7H13Y+C7H14Y=>R10C2H3V+C12H24Z	6.0E+0009	0.000	11400.0	! ADY 771
RC7H13Y+C4H8Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 772
RC7H13Y+C3H6Y=>R10C2H3V+C8H16Z	6.0E+0009	0.000	11400.0	! ADY 773
RC8H15Y+C5H10Y=>R10C2H3V+C11H22Z	6.0E+0009	0.000	11400.0	! ADY 774
RC8H15Y+C8H16Y=>R10C2H3V+C14H28Z	6.0E+0009	0.000	11400.0	! ADY 775
RC8H15Y+C7H14Y=>R10C2H3V+C13H26Z	6.0E+0009	0.000	11400.0	! ADY 776
RC8H15Y+C4H8Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 777
RC8H15Y+C3H6Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 778
RC5H9Y+C5H10Y=>R10C2H3V+C8H16Z	6.0E+0009	0.000	11400.0	! ADY 779
RC5H9Y+C8H16Y=>R10C2H3V+C11H22Z	6.0E+0009	0.000	11400.0	! ADY 780
RC5H9Y+C7H14Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 781
RC5H9Y+C4H8Y=>R10C2H3V+C7H14Z	6.0E+0009	0.000	11400.0	! ADY 782
RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z	6.0E+0009	0.000	11400.0	! ADY 783

! Alcohol reactions

C3H7OH+R1H=>H2+R2OH+C3H6Y	2.9E+0007	2.000	7700.0	! MOL 784
DUPLICATE				
C3H7OH+R1H=>H2+R2OH+C3H6Y	1.8E+0007	2.000	5000.0	! MOL 785
DUPLICATE				
C3H7OH+R1H=>H2+R11C2H5+HCHO	2.4E+0006	2.000	6525.0	! MOL 786
C3H7OH+R2OH=>H2O+R2OH+C3H6Y	2.7E+0006	2.000	450.0	! MOL 787
DUPLICATE				
C3H7OH+R2OH=>H2O+R2OH+C3H6Y	5.2E+0006	2.000	-765.0	! MOL 788
DUPLICATE				
C3H7OH+R2OH=>H2O+R11C2H5+HCHO	4.0E+0005	2.000	-475.0	! MOL 789
C3H7OH+R300H=>H2O2+R2OH+C3H6Y	6.0E+0011	0.000	17000.0	! MOL 790
DUPLICATE				
C3H7OH+R300H=>H2O2+R2OH+C3H6Y	8.0E+0011	0.000	15500.0	! MOL 791
DUPLICATE				
C3H7OH+R300H=>H2O2+R11C2H5+HCHO	5.4E+0004	2.000	15025.0	! MOL 792
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y	3.0E-0001	4.000	8200.0	! MOL 793
DUPLICATE				
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y	4.0E+0011	0.000	9600.0	! MOL 794
DUPLICATE				
C3H7OH+R4CH3=>CH4+R11C2H5+HCHO	3.9E+0004	2.000	7525.0	! MOL 795
C3H7OH+R8CH300=>CH300H+R2OH+C3H6Y	1.6E+0011	0.000	7300.0	! MOL 796
DUPLICATE				
C3H7OH+R8CH300=>CH300H+R2OH+C3H6Y	2.9E+0011	0.000	4500.0	! MOL 797
DUPLICATE				
C3H7OH+R8CH300=>CH300H+R11C2H5+HCHO	0.0E+0000	0.000	0.0	! MOL 798
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y	3.0E+0011	0.000	13500.0	! MOL 799

DUPLICATE					
C3H7OH+R11C2H5=>C2H6+R2OH+C3H6Y	4.0E+0011	0.000	11000.0	!	MOL 800
DUPLICATE					
C3H7OH+R11C2H5=>C2H6+R11C2H5+HCHO	2.3E+0004	2.000	10525.0	!	MOL 801
C4H100L+R1H=>H2+R2OH+C4H8Y	2.9E+0007	2.000	7700.0	!	MOL 802
DUPLICATE					
C4H100L+R1H=>H2+R2OH+C4H8Y	2.7E+0007	2.000	5000.0	!	MOL 803
DUPLICATE					
C4H100L+R1H=>H2+R19C3H7+HCHO	2.4E+0006	2.000	6525.0	!	MOL 804
C4H100L+R2OH=>H2O+R2OH+C4H8Y	2.7E+0006	2.000	450.0	!	MOL 805
DUPLICATE					
C4H100L+R2OH=>H2O+R2OH+C4H8Y	7.8E+0006	2.000	-765.0	!	MOL 806
DUPLICATE					
C4H100L+R2OH=>H2O+R19C3H7+HCHO	4.0E+0005	2.000	-475.0	!	MOL 807
C4H100L+R300H=>H2O2+R2OH+C4H8Y	6.0E+0011	0.000	17000.0	!	MOL 808
DUPLICATE					
C4H100L+R300H=>H2O2+R2OH+C4H8Y	1.2E+0012	0.000	15500.0	!	MOL 809
DUPLICATE					
C4H100L+R300H=>H2O2+R19C3H7+HCHO	5.4E+0004	2.000	15025.0	!	MOL 810
C4H100L+R4CH3=>CH4+R2OH+C4H8Y	3.0E-0001	4.000	8200.0	!	MOL 811
DUPLICATE					
C4H100L+R4CH3=>CH4+R2OH+C4H8Y	6.0E+0011	0.000	9600.0	!	MOL 812
DUPLICATE					
C4H100L+R4CH3=>CH4+R19C3H7+HCHO	3.9E+0004	2.000	7525.0	!	MOL 813
C4H100L+R8CH300=>CH300H+R2OH+C4H8Y	1.6E+0011	0.000	7300.0	!	MOL 814
DUPLICATE					
C4H100L+R8CH300=>CH300H+R2OH+C4H8Y	4.4E+0011	0.000	4500.0	!	MOL 815
DUPLICATE					
C4H100L+R8CH300=>CH300H+R19C3H7+HCHO	0.0E+0000	0.000	0.0	!	MOL 816
C4H100L+R11C2H5=>C2H6+R2OH+C4H8Y	3.0E+0011	0.000	13500.0	!	MOL 817
DUPLICATE					
C4H100L+R11C2H5=>C2H6+R2OH+C4H8Y	6.0E+0011	0.000	11000.0	!	MOL 818
DUPLICATE					
C4H100L+R11C2H5=>C2H6+R19C3H7+HCHO	2.3E+0004	2.000	10525.0	!	MOL 819
C5H120L+R1H=>H2+R2OH+C5H10Z	2.9E+0007	2.000	7700.0	!	MOL 820
DUPLICATE					
C5H120L+R1H=>H2+R2OH+C5H10Z	3.6E+0007	2.000	5000.0	!	MOL 821
DUPLICATE					
C5H120L+R1H=>H2+R20C4H9+HCHO	2.4E+0006	2.000	6525.0	!	MOL 822
C5H120L+R2OH=>H2O+R2OH+C5H10Z	2.7E+0006	2.000	450.0	!	MOL 823
DUPLICATE					
C5H120L+R2OH=>H2O+R2OH+C5H10Z	1.0E+0007	2.000	-765.0	!	MOL 824
DUPLICATE					
C5H120L+R2OH=>H2O+R20C4H9+HCHO	4.0E+0005	2.000	-475.0	!	MOL 825
C5H120L+R300H=>H2O2+R2OH+C5H10Z	6.0E+0011	0.000	17000.0	!	MOL 826
DUPLICATE					
C5H120L+R300H=>H2O2+R2OH+C5H10Z	1.6E+0012	0.000	15500.0	!	MOL 827
DUPLICATE					
C5H120L+R300H=>H2O2+R20C4H9+HCHO	5.4E+0004	2.000	15025.0	!	MOL 828
C5H120L+R4CH3=>CH4+R2OH+C5H10Z	3.0E-0001	4.000	8200.0	!	MOL 829
DUPLICATE					
C5H120L+R4CH3=>CH4+R2OH+C5H10Z	8.0E+0011	0.000	9600.0	!	MOL 830
DUPLICATE					

C5H120L+R4CH3=>CH4+R20C4H9+HCHO 3.9E+0004 2.000 7525.0 ! MOL 831  
 C5H120L+R8CH300=>CH300H+R20H+C5H10Z 1.6E+0011 0.000 7300.0 ! MOL 832  
 DUPLICATE  
 C5H120L+R8CH300=>CH300H+R20H+C5H10Z 5.8E+0011 0.000 4500.0 ! MOL 833  
 DUPLICATE  
 C5H120L+R8CH300=>CH300H+R20C4H9+HCHO 0.0E+0000 0.000 0.0 ! MOL 834  
 C5H120L+R11C2H5=>C2H6+R20H+C5H10Z 3.0E+0011 0.000 13500.0 ! MOL 835  
 DUPLICATE  
 C5H120L+R11C2H5=>C2H6+R20H+C5H10Z 8.0E+0011 0.000 11000.0 ! MOL 836  
 DUPLICATE  
 C5H120L+R11C2H5=>C2H6+R20C4H9+HCHO 2.3E+0004 2.000 10525.0 ! MOL 837  
 C3H70H+B10=>R20H+R20H+C3H6Y 3.9E+0013 0.000 5200.0 ! MOL 838  
 DUPLICATE  
 C3H70H+B10=>R20H+R20H+C3H6Y 4.0E+0013 0.000 5200.0 ! MOL 839  
 DUPLICATE  
 C3H70H+B10=>R20H+R11C2H5+HCHO 1.3E+0006 2.000 5025.0 ! MOL 840  
 C4H100L+B10=>R20H+R20H+C4H8Y 3.9E+0013 0.000 5200.0 ! MOL 841  
 DUPLICATE  
 C4H100L+B10=>R20H+R20H+C4H8Y 6.0E+0013 0.000 5200.0 ! MOL 842  
 DUPLICATE  
 C4H100L+B10=>R20H+R19C3H7+HCHO 1.3E+0006 2.000 5025.0 ! MOL 843  
 C5H120L+B10=>R20H+R20H+C5H10Z 3.9E+0013 0.000 5200.0 ! MOL 844  
 DUPLICATE  
 C5H120L+B10=>R20H+R20H+C5H10Z 8.0E+0013 0.000 5200.0 ! MOL 845  
 DUPLICATE  
 C5H120L+B10=>R20H+R20C4H9+HCHO 1.3E+0006 2.000 5025.0 ! MOL 846

! Aldehydes metathesis

C2H5CHO+R1H=>H2+RC3H50 4.0E+0013 0.000 4200.0 ! ADZ 847  
 C2H5CHO+R20H=>H20+RC3H50 4.2E+0012 0.000 500.0 ! ADZ 848  
 C2H5CHO+R300H=>H202+RC3H50 1.0E+0012 0.000 10000.0 ! ADZ 849  
 C2H5CHO+R4CH3=>CH4+RC3H50 2.0E-0006 5.600 2500.0 ! ADZ 850  
 C2H5CHO+R11C2H5=>C2H6+RC3H50 1.3E+0012 0.000 8500.0 ! ADZ 851  
 C5H100A+R1H=>H2+RC5H90 4.0E+0013 0.000 4200.0 ! ADZ 852  
 C5H100A+R20H=>H20+RC5H90 4.2E+0012 0.000 500.0 ! ADZ 853  
 C5H100A+R300H=>H202+RC5H90 1.0E+0012 0.000 10000.0 ! ADZ 854  
 C5H100A+R4CH3=>CH4+RC5H90 2.0E-0006 5.600 2500.0 ! ADZ 855  
 C5H100A+R11C2H5=>C2H6+RC5H90 1.3E+0012 0.000 8500.0 ! ADZ 856  
 C4H80A+R1H=>H2+RC4H70 4.0E+0013 0.000 4200.0 ! ADZ 857  
 C4H80A+R20H=>H20+RC4H70 4.2E+0012 0.000 500.0 ! ADZ 858  
 C4H80A+R300H=>H202+RC4H70 1.0E+0012 0.000 10000.0 ! ADZ 859  
 C4H80A+R4CH3=>CH4+RC4H70 2.0E-0006 5.600 2500.0 ! ADZ 860  
 C4H80A+R11C2H5=>C2H6+RC4H70 1.3E+0012 0.000 8500.0 ! ADZ 861  
 C6H120A+R1H=>H2+RC6H110 4.0E+0013 0.000 4200.0 ! ADZ 862  
 C6H120A+R20H=>H20+RC6H110 4.2E+0012 0.000 500.0 ! ADZ 863  
 C6H120A+R300H=>H202+RC6H110 1.0E+0012 0.000 10000.0 ! ADZ 864  
 C6H120A+R4CH3=>CH4+RC6H110 2.0E-0006 5.600 2500.0 ! ADZ 865  
 C6H120A+R11C2H5=>C2H6+RC6H110 1.3E+0012 0.000 8500.0 ! ADZ 866  
 C7H140A+R1H=>H2+RC7H130 4.0E+0013 0.000 4200.0 ! ADZ 867  
 C7H140A+R20H=>H20+RC7H130 4.2E+0012 0.000 500.0 ! ADZ 868  
 C7H140A+R300H=>H202+RC7H130 1.0E+0012 0.000 10000.0 ! ADZ 869

C7H140A+R4CH3=>CH4+RC7H130 2.0E-0006 5.600 2500.0 ! ADZ 870  
C7H140A+R11C2H5=>C2H6+RC7H130 1.3E+0012 0.000 8500.0 ! ADZ 871  
C8H160A+R1H=>H2+RC8H150 4.0E+0013 0.000 4200.0 ! ADZ 872  
C8H160A+R20H=>H20+RC8H150 4.2E+0012 0.000 500.0 ! ADZ 873  
C8H160A+R300H=>H202+RC8H150 1.0E+0012 0.000 10000.0 ! ADZ 874  
C8H160A+R4CH3=>CH4+RC8H150 2.0E-0006 5.600 2500.0 ! ADZ 875  
C8H160A+R11C2H5=>C2H6+RC8H150 1.3E+0012 0.000 8500.0 ! ADZ 876  
C9H180A+R1H=>H2+RC9H170 4.0E+0013 0.000 4200.0 ! ADZ 877  
C9H180A+R20H=>H20+RC9H170 4.2E+0012 0.000 500.0 ! ADZ 878  
C9H180A+R300H=>H202+RC9H170 1.0E+0012 0.000 10000.0 ! ADZ 879  
C9H180A+R4CH3=>CH4+RC9H170 2.0E-0006 5.600 2500.0 ! ADZ 880  
C9H180A+R11C2H5=>C2H6+RC9H170 1.3E+0012 0.000 8500.0 ! ADZ 881  
C12H240A+R1H=>H2+RC12H230 4.0E+0013 0.000 4200.0 ! ADZ 882  
C12H240A+R20H=>H20+RC12H230 4.2E+0012 0.000 500.0 ! ADZ 883  
C12H240A+R300H=>H202+RC12H230 1.0E+0012 0.000 10000.0 ! ADZ 884  
C12H240A+R4CH3=>CH4+RC12H230 2.0E-0006 5.600 2500.0 ! ADZ 885  
C12H240A+R11C2H5=>C2H6+RC12H230 1.3E+0012 0.000 8500.0 ! ADZ 886  
C11H220A+R1H=>H2+RC11H210 4.0E+0013 0.000 4200.0 ! ADZ 887  
C11H220A+R20H=>H20+RC11H210 4.2E+0012 0.000 500.0 ! ADZ 888  
C11H220A+R300H=>H202+RC11H210 1.0E+0012 0.000 10000.0 ! ADZ 889  
C11H220A+R4CH3=>CH4+RC11H210 2.0E-0006 5.600 2500.0 ! ADZ 890  
C11H220A+R11C2H5=>C2H6+RC11H210 1.3E+0012 0.000 8500.0 ! ADZ 891  
C10H200A+R1H=>H2+RC10H190 4.0E+0013 0.000 4200.0 ! ADZ 892  
C10H200A+R20H=>H20+RC10H190 4.2E+0012 0.000 500.0 ! ADZ 893  
C10H200A+R300H=>H202+RC10H190 1.0E+0012 0.000 10000.0 ! ADZ 894  
C10H200A+R4CH3=>CH4+RC10H190 2.0E-0006 5.600 2500.0 ! ADZ 895  
C10H200A+R11C2H5=>C2H6+RC10H190 1.3E+0012 0.000 8500.0 ! ADZ 896  
C13H260A+R1H=>H2+RC13H250 4.0E+0013 0.000 4200.0 ! ADZ 897  
C13H260A+R20H=>H20+RC13H250 4.2E+0012 0.000 500.0 ! ADZ 898  
C13H260A+R300H=>H202+RC13H250 1.0E+0012 0.000 10000.0 ! ADZ 899  
C13H260A+R4CH3=>CH4+RC13H250 2.0E-0006 5.600 2500.0 ! ADZ 900  
C13H260A+R11C2H5=>C2H6+RC13H250 1.3E+0012 0.000 8500.0 ! ADZ 901  
  
C4H60AY+R1H=>H2+R10C2H3V+CH2COZ 4.0E+0013 0.000 4200.0 ! ADZ 902  
C4H60AY+R20H=>H20+R10C2H3V+CH2COZ 4.0E+0012 0.000 500.0 ! ADZ 903  
C4H60AY+R300H=>H202+R10C2H3V+CH2COZ 1.0E+0012 0.000 10000.0 ! ADZ  
904  
C4H60AY+R4CH3=>CH4+R10C2H3V+CH2COZ 2.0E-0006 0.000 2500.0 ! ADZ 905  
C4H60AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ 1.3E+0012 0.000 8500.0 ! ADZ  
906  
C5H80AY+R1H=>H2+RC3H5Y+CH2COZ 4.0E+0013 0.000 4200.0 ! ADZ 907  
C5H80AY+R20H=>H20+RC3H5Y+CH2COZ 4.0E+0012 0.000 500.0 ! ADZ 908  
C5H80AY+R300H=>H202+RC3H5Y+CH2COZ 1.0E+0012 0.000 10000.0 ! ADZ 909  
C5H80AY+R4CH3=>CH4+RC3H5Y+CH2COZ 2.0E-0006 0.000 2500.0 ! ADZ 910  
C5H80AY+R11C2H5=>C2H6+RC3H5Y+CH2COZ 1.3E+0012 0.000 8500.0 ! ADZ  
911  
!C8H140AY+R1H=>H2+R10C2H3V+CH2COZ+2C2H4Z 4.0E+0013 0.000 4200.0 !  
ADZ 912  
!C8H140AY+R20H=>H20+R10C2H3V+CH2COZ+2C2H4Z 4.0E+0012 0.000 500.0 !  
ADZ 913  
!C8H140AY+R300H=>H202+R10C2H3V+CH2COZ+2C2H4Z 1.0E+0012 0.000 10000.0  
! ADZ 914  
!C8H140AY+R4CH3=>CH4+R10C2H3V+CH2COZ+2C2H4Z 2.0E-0006 0.000  
2500.0 ! ADZ 915



!C8H140AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+2C2H4Z 1.3E+0012 0.000  
 8500.0 ! ADZ 916  
 !C9H160AY+R1H=>H2+RC3H5Y+CH2COZ+2C2H4Z 4.0E+0013 0.000 4200.0 ! ADZ  
 917  
 !C9H160AY+R20H=>H20+RC3H5Y+CH2COZ+2C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 918  
 !C9H160AY+R300H=>H202+RC3H5Y+CH2COZ+2C2H4Z 1.0E+0012 0.000  
 10000.0 ! ADZ 919  
 !C9H160AY+R4CH3=>CH4+RC3H5Y+CH2COZ+2C2H4Z 2.0E-0006 0.000 2500.0 !  
 ADZ 920  
 !C9H160AY+R11C2H5=>C2H6+RC3H5Y+CH2COZ+2C2H4Z 1.3E+0012 0.000 8500.0  
 ! ADZ 921  
 !C6H100AY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z 4.0E+0013 0.000 4200.0 !  
 ADZ 922  
 !C6H100AY+R20H=>H20+R10C2H3V+CH2COZ+C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 923  
 !C6H100AY+R300H=>H202+R10C2H3V+CH2COZ+C2H4Z 1.0E+0012 0.000 10000.0  
 ! ADZ 924  
 !C6H100AY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z 2.0E-0006 0.000 2500.0 !  
 ADZ 925  
 !C6H100AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z 1.3E+0012 0.000 8500.0  
 ! ADZ 926

! Keto radicals decomposition

RC3H50=>B2C0+R11C2H5 1.8E+0014 0.000 15600.0 ! COR 927  
 RC5H90=>B2C0+R20C4H9 1.8E+0014 0.000 15600.0 ! COR 928  
 RC4H70=>B2C0+R19C3H7 1.8E+0014 0.000 15600.0 ! COR 929  
 RC6H110=>B2C0+R35C5H11 1.8E+0014 0.000 15600.0 ! COR 930  
 RC7H130=>B2C0+R41C6H13 1.8E+0014 0.000 15600.0 ! COR 931  
 RC8H150=>B2C0+R26C7H15 1.8E+0014 0.000 15600.0 ! COR 932  
 RC9H170=>B2C0+R30C8H17 1.8E+0014 0.000 15600.0 ! COR 933  
 RC12H230=>B2C0+R4CH3+5C2H4Z 1.8E+0014 0.000 15600.0 ! COR 934  
 RC11H210=>B2C0+R11C2H5+4C2H4Z 1.8E+0014 0.000 15600.0 ! COR 935  
 RC10H190=>B2C0+R4CH3+4C2H4Z 1.8E+0014 0.000 15600.0 ! COR 936  
 RC13H250=>B2C0+R11C2H5+5C2H4Z 1.8E+0014 0.000 15600.0 ! COR 937

! keto radicals addition to O2

RC3H50+O2=>RC3H503 3.0E+0019 -2.500 0.0 ! COR 938  
 RC5H90+O2=>RC5H903 3.0E+0019 -2.500 0.0 ! COR 939  
 RC4H70+O2=>RC4H703 3.0E+0019 -2.500 0.0 ! COR 940  
 RC6H110+O2=>RC6H1103 3.0E+0019 -2.500 0.0 ! COR 941  
 RC7H130+O2=>RC7H1303 3.0E+0019 -2.500 0.0 ! COR 942  
 RC8H150+O2=>RC8H1503 3.0E+0019 -2.500 0.0 ! COR 943  
 RC9H170+O2=>RC9H1703 3.0E+0019 -2.500 0.0 ! COR 944  
 RC12H230+O2=>RC12H2303 3.0E+0019 -2.500 0.0 ! COR 945  
 RC11H210+O2=>RC11H2103 3.0E+0019 -2.500 0.0 ! COR 946  
 RC10H190+O2=>RC10H1903 3.0E+0019 -2.500 0.0 ! COR 947  
 RC13H250+O2=>RC13H2503 3.0E+0019 -2.500 0.0 ! COR 948

! Peroxide radical decomposition

RC3H503=>C2H4Z+R20H+C02 4.5E+0011 0.000 25000.0 ! PER 949  
 RC5H903=>C4H8Y+R20H+C02 4.5E+0011 0.000 25000.0 ! PER 950  
 RC4H703=>C3H6Y+R20H+C02 4.5E+0011 0.000 25000.0 ! PER 951

RC6H1103=>C5H10Y+R20H+C02	4.5E+0011	0.000	25000.0	! PER 952
RC7H1303=>C6H12Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 953
RC8H1503=>C7H14Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 954
RC9H1703=>C8H16Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 955
RC12H2303=>C11H22Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 956
RC11H2103=>C10H20Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 957
RC10H1903=>C9H18Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 958
RC13H2503=>C12H24Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 959

! Ketones reactions

!C2H6CO+R1H=>H2+CH2COZ+R4CH3	5.7E+0007	2.000	7700.0	! MK 960
!C2H6CO+R20H=>H2O+CH2COZ+R4CH3	5.4E+0006	2.000	450.0	! MK 961
!C2H6CO+R300H=>H2O2+CH2COZ+R4CH3	1.2E+0012	0.000	17000.0	! MK 962
!C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3	6.0E-0001	4.000	8200.0	! MK 963
!C2H6CO+R8CH300=>CH300H+CH2COZ+R4CH3	1.2E+0013	0.000	20000.0	! MK 964
!C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3	6.0E+0011	0.000	13500.0	! MK 965
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	5.7E+0007	2.000	7700.0	! MK 966
DUPLICATE				
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	9.0E+0006	2.000	5000.0	! MK 967
DUPLICATE				
C3H8CO+R20H=>H2O+CH2COZ+R11C2H5	5.4E+0006	2.000	450.0	! MK 968
DUPLICATE				
C3H8CO+R20H=>H2O+CH2COZ+R11C2H5	2.6E+0006	2.000	-765.0	! MK 969
DUPLICATE				
C3H8CO+R300H=>H2O2+CH2COZ+R11C2H5	1.2E+0012	0.000	17000.0	! MK 970
DUPLICATE				
C3H8CO+R300H=>H2O2+CH2COZ+R11C2H5	4.0E+0011	0.000	15500.0	! MK 971
DUPLICATE				
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	6.0E-0001	4.000	8200.0	! MK 972
DUPLICATE				
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	2.0E+0011	0.000	9600.0	! MK 973
DUPLICATE				
C3H8CO+R8CH300=>CH300H+CH2COZ+R11C2H5	1.2E+0013	0.000	20000.0	! MK 974
DUPLICATE				
C3H8CO+R8CH300=>CH300H+CH2COZ+R11C2H5	3.0E+0012	0.000	17500.0	! MK 975
DUPLICATE				
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	6.0E+0011	0.000	13500.0	! MK 976
DUPLICATE				
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	2.0E+0011	0.000	11000.0	! MK 977
DUPLICATE				

! Unsaturated ester reactions

! Esters metathesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis

! Addition on unsaturated esters

! Carboxylic acid reactions

! Carboxylic acid metathesis

! Carboxylic acid decomposition

! Alkohol ene to dienes

C3H60LY+R1H=>H2+HCHO+R10C2H3V	5.4E+0004	2.500	-1900.0	! ROH 978
C3H60LY+R20H=>H2O+HCHO+R10C2H3V	3.0E+0006	2.000	-1520.0	! ROH 979
C3H60LY+R300H=>H2O2+HCHO+R10C2H3V	6.4E+0003	2.600	12400.0	! ROH 980
C3H60LY+R4CH3=>CH4+HCHO+R10C2H3V	1.0E+0011	0.000	7300.0	! ROH 981
C3H60LY+R8CH300=>CH300H+HCHO+R10C2H3V	1.0E+0012	0.000	14550.0	! ROH 982
C3H60LY+R11C2H5=>C2H6+HCHO+R10C2H3V	1.5E+0000	3.500	4140.0	! ROH 983
C4H80LY+R1H=>H2+HCHO+RC3H5Y	5.4E+0004	2.500	-1900.0	! ROH 984
C4H80LY+R20H=>H2O+HCHO+RC3H5Y	3.0E+0006	2.000	-1520.0	! ROH 985
C4H80LY+R300H=>H2O2+HCHO+RC3H5Y	6.4E+0003	2.600	12400.0	! ROH 986
C4H80LY+R4CH3=>CH4+HCHO+RC3H5Y	1.0E+0011	0.000	7300.0	! ROH 987
C4H80LY+R8CH300=>CH300H+HCHO+RC3H5Y	1.0E+0012	0.000	14550.0	! ROH 988
C4H80LY+R11C2H5=>C2H6+HCHO+RC3H5Y	1.5E+0000	3.500	4140.0	! ROH 989
C5H100LY+R1H=>H2+HCHO+RC4H7Y	5.4E+0004	2.500	-1900.0	! ROH 990
C5H100LY+R20H=>H2O+HCHO+RC4H7Y	3.0E+0006	2.000	-1520.0	! ROH 991
C5H100LY+R300H=>H2O2+HCHO+RC4H7Y	6.4E+0003	2.600	12400.0	! ROH 992
C5H100LY+R4CH3=>CH4+HCHO+RC4H7Y	1.0E+0011	0.000	7300.0	! ROH 993
C5H100LY+R8CH300=>CH300H+HCHO+RC4H7Y	1.0E+0012	0.000	14550.0	! ROH 994
C5H100LY+R11C2H5=>C2H6+HCHO+RC4H7Y	1.5E+0000	3.500	4140.0	! ROH 995
C7H140LY+R1H=>H2+HCHO+RC6H11Y	5.4E+0004	2.500	-1900.0	! ROH 996
C7H140LY+R20H=>H2O+HCHO+RC6H11Y	3.0E+0006	2.000	-1520.0	! ROH 997
C7H140LY+R300H=>H2O2+HCHO+RC6H11Y	6.4E+0003	2.600	12400.0	! ROH 998
C7H140LY+R4CH3=>CH4+HCHO+RC6H11Y	1.0E+0011	0.000	7300.0	! ROH 999
C7H140LY+R8CH300=>CH300H+HCHO+RC6H11Y	1.0E+0012	0.000	14550.0	! ROH 1000
C7H140LY+R11C2H5=>C2H6+HCHO+RC6H11Y	1.5E+0000	3.500	4140.0	! ROH 1001
C8H160LY+R1H=>H2+HCHO+RC7H13Y	5.4E+0004	2.500	-1900.0	! ROH 1002
C8H160LY+R20H=>H2O+HCHO+RC7H13Y	3.0E+0006	2.000	-1520.0	! ROH 1003
C8H160LY+R300H=>H2O2+HCHO+RC7H13Y	6.4E+0003	2.600	12400.0	! ROH 1004
C8H160LY+R4CH3=>CH4+HCHO+RC7H13Y	1.0E+0011	0.000	7300.0	! ROH 1005
C8H160LY+R8CH300=>CH300H+HCHO+RC7H13Y	1.0E+0012	0.000	14550.0	! ROH 1006
C8H160LY+R11C2H5=>C2H6+HCHO+RC7H13Y	1.5E+0000	3.500	4140.0	! ROH 1007
C9H180LY+R1H=>H2+HCHO+RC8H15Y	5.4E+0004	2.500	-1900.0	! ROH 1008
C9H180LY+R20H=>H2O+HCHO+RC8H15Y	3.0E+0006	2.000	-1520.0	! ROH 1009
C9H180LY+R300H=>H2O2+HCHO+RC8H15Y	6.4E+0003	2.600	12400.0	! ROH 1010
C9H180LY+R4CH3=>CH4+HCHO+RC8H15Y	1.0E+0011	0.000	7300.0	! ROH 1011
C9H180LY+R8CH300=>CH300H+HCHO+RC8H15Y	1.0E+0012	0.000	14550.0	! ROH 1012

C9H180LY+R11C2H5=>C2H6+HCHO+RC8H15Y 1.5E+0000 3.500 4140.0 ! ROH  
 1013  
 C6H120LY+R1H=>H2+HCHO+RC5H9Y 5.4E+0004 2.500 -1900.0 ! ROH 1014  
 C6H120LY+R20H=>H2O+HCHO+RC5H9Y 3.0E+0006 2.000 -1520.0 ! ROH 1015  
 C6H120LY+R300H=>H2O2+HCHO+RC5H9Y 6.4E+0003 2.600 12400.0 ! ROH 1016  
 C6H120LY+R4CH3=>CH4+HCHO+RC5H9Y 1.0E+0011 0.000 7300.0 ! ROH 1017  
 C6H120LY+R8CH300=>CH300H+HCHO+RC5H9Y 1.0E+0012 0.000 14550.0 ! ROH  
 1018  
 C6H120LY+R11C2H5=>C2H6+HCHO+RC5H9Y 1.5E+0000 3.500 4140.0 ! ROH  
 1019

! Additions on dienes

C4H6Z2+R20H=>RC3H5Y+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1020!!!!!!ds  
 мйса toлуине

!

!C4H6Z2+R20H=>RC3H5Y+HCHO 3.0E+0012 0.000 -1040.0 !

!

C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V 1.0E+0005 2.500 -1900.0 ! AD 1021  
 C6H10Y2+R20H=>H2O+C4H6Z2+R10C2H3V 6.0E+0006 2.000 -1520.0 ! AD 1022  
 C6H10Y2+R300H=>H2O2+C4H6Z2+R10C2H3V 1.2E+0004 2.600 12400.0 ! AD  
 1023  
 C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD 1024  
 C6H10Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD  
 1025  
 C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V 3.0E+0000 3.500 4140.0 ! AD  
 1026  
 C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y 1.0E+0005 2.500 -1900.0 ! AD 1027  
 C7H12Y2+R20H=>H2O+C4H6Z2+RC3H5Y 6.0E+0006 2.000 -1520.0 ! AD 1028  
 C7H12Y2+R300H=>H2O2+C4H6Z2+RC3H5Y 1.2E+0004 2.600 12400.0 ! AD 1029  
 C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD 1030  
 C7H12Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD  
 1031  
 C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y 3.0E+0000 3.500 4140.0 ! AD  
 1032  
 !C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+2C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1033  
 !C10H18Y2+R20H=>H2O+C4H6Z2+R10C2H3V+2C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1034  
 !C10H18Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1035  
 !C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1036  
 !C10H18Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1037  
 !C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1038  
 !C11H20Y2+R1H=>H2+C4H6Z2+RC3H5Y+2C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1039  
 !C11H20Y2+R20H=>H2O+C4H6Z2+RC3H5Y+2C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1040  
 !C11H20Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+2C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1041  
 !C11H20Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+2C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1042

!C11H20Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1043  
 !C11H20Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+2C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1044  
 !C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1045  
 !C8H14Y2+R20H=>H2O+C4H6Z2+R10C2H3V+C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1046  
 !C8H14Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1047  
 !C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1048  
 !C8H14Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1049  
 !C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1050  
 !C12H22Y2+R1H=>H2+C4H6Z2+R10C2H3V+3C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1051  
 !C12H22Y2+R20H=>H2O+C4H6Z2+R10C2H3V+3C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1052  
 !C12H22Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+3C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1053  
 !C12H22Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1054  
 !C12H22Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1055  
 !C12H22Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+3C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1056  
 !C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1057  
 !C9H16Y2+R20H=>H2O+C4H6Z2+RC3H5Y+C2H4Z 6.0E+0006 2.000 -1520.0 ! AD  
 1058  
 !C9H16Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+C2H4Z 1.2E+0004 2.600 12400.0 !  
 AD 1059  
 !C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0 ! AD  
 1060  
 !C9H16Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0  
 ! AD 1061  
 !C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z 3.0E+0000 3.500 4140.0 !  
 AD 1062  
 !C14H26Y2+R1H=>H2+C4H6Z2+R10C2H3V+4C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1063  
 !C14H26Y2+R20H=>H2O+C4H6Z2+R10C2H3V+4C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1064  
 !C14H26Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+4C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1065  
 !C14H26Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+4C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1066  
 !C14H26Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+4C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1067  
 !C14H26Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+4C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1068  
 !C15H28Y2+R1H=>H2+C4H6Z2+RC3H5Y+4C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1069

!C15H28Y2+R20H=>H20+C4H6Z2+RC3H5Y+4C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1070  
 !C15H28Y2+R300H=>H202+C4H6Z2+RC3H5Y+4C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1071  
 !C15H28Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+4C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1072  
 !C15H28Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+4C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1073  
 !C15H28Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+4C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1074  
 !C16H30Y2+R1H=>H2+C4H6Z2+R10C2H3V+5C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1075  
 !C16H30Y2+R20H=>H20+C4H6Z2+R10C2H3V+5C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1076  
 !C16H30Y2+R300H=>H202+C4H6Z2+R10C2H3V+5C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1077  
 !C16H30Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+5C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1078  
 !C16H30Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+5C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1079  
 !C16H30Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+5C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1080  
 !C13H24Y2+R1H=>H2+C4H6Z2+RC3H5Y+3C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1081  
 !C13H24Y2+R20H=>H20+C4H6Z2+RC3H5Y+3C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1082  
 !C13H24Y2+R300H=>H202+C4H6Z2+RC3H5Y+3C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1083  
 !C13H24Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+3C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1084  
 !C13H24Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1085  
 !C13H24Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+3C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1086

! Diels Alder

! .Y termination

RC3H5Y+R1H=>C3H6Y 1.0E+0014 0.000 0.0 ! TER  
 1087 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliñ x10  
 RC3H5Y+R20H=>C3H60LY 1.0E+0013 0.000 0.0 ! TER 1088  
 RC3H5Y+R300H=>C3H602PY 5.0E+0012 0.000 0.0 ! TER 1089  
 RC3H5Y+R4CH3=>C4H8Y 1.0E+0013 0.000 0.0 ! TER 1090  
 RC3H5Y+R5CH0=>C4H60AY 1.0E+0013 0.000 0.0 ! TER 1091  
 RC3H5Y+R6CH20H=>C4H80LY 1.0E+0013 0.000 0.0 ! TER 1092  
 RC3H5Y+R8CH300=>HCH0+R7CH30+R10C2H3V 1.0E+0013 0.000 0.0 ! TER 1093  
 RC3H5Y+R11C2H5=>C5H10Y 1.0E+0013 0.000 0.0 ! TER 1094  
 RC4H7Y+R1H=>C4H8Y 1.0E+0014 0.000 0.0 ! TER  
 1095 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliñ x10  
 RC4H7Y+R20H=>C4H80LY 1.0E+0013 0.000 0.0 ! TER 1096  
 RC4H7Y+R300H=>C4H802PY 5.0E+0012 0.000 0.0 ! TER 1097  
 RC4H7Y+R4CH3=>C5H10Y 1.0E+0013 0.000 0.0 ! TER 1098  
 RC4H7Y+R5CH0=>C5H80AY 1.0E+0013 0.000 0.0 ! TER 1099  
 RC4H7Y+R6CH20H=>C5H100LY 1.0E+0013 0.000 0.0 ! TER 1100

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RC4H7Y+R8CH300=>HCH0+R7CH30+RC3H5Y    1.0E+0013  0.000  0.0  ! TER 1101
RC4H7Y+R11C2H5=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1102
RC7H13Y+R1H=>C7H14Y    1.0E+0014  0.000  0.0  ! TER
1103!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliъ x10
RC7H13Y+R20H=>C7H140LY    1.0E+0013  0.000  0.0  ! TER 1104
RC7H13Y+R300H=>C7H1402PY    5.0E+0012  0.000  0.0  ! TER 1105
RC7H13Y+R4CH3=>C8H16Y    1.0E+0013  0.000  0.0  ! TER 1106
RC7H13Y+R5CHO=>C8H140AY    1.0E+0013  0.000  0.0  ! TER 1107
RC7H13Y+R6CH20H=>C8H160LY    1.0E+0013  0.000  0.0  ! TER 1108
RC7H13Y+R8CH300=>HCH0+R7CH30+RC6H11Y    1.0E+0013  0.000  0.0  ! TER 1109
RC7H13Y+R11C2H5=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1110
RC8H15Y+R1H=>C8H16Y    1.0E+0014  0.000  0.0  ! TER
1111!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliъ x10
RC8H15Y+R20H=>C8H160LY    1.0E+0013  0.000  0.0  ! TER 1112
RC8H15Y+R300H=>C8H1602PY    5.0E+0012  0.000  0.0  ! TER 1113
RC8H15Y+R4CH3=>C9H18Z    1.0E+0013  0.000  0.0  ! TER 1114
RC8H15Y+R5CHO=>C9H160AY    1.0E+0013  0.000  0.0  ! TER 1115
RC8H15Y+R6CH20H=>C9H180LY    1.0E+0013  0.000  0.0  ! TER 1116
RC8H15Y+R8CH300=>HCH0+R7CH30+RC7H13Y    1.0E+0013  0.000  0.0  ! TER 1117
RC8H15Y+R11C2H5=>C10H20Z    1.0E+0013  0.000  0.0  ! TER 1118
RC5H9Y+R1H=>C5H10Y    1.0E+0014  0.000  0.0  ! TER
1119!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliъ x10
RC5H9Y+R20H=>C5H100LY    1.0E+0013  0.000  0.0  ! TER 1120
RC5H9Y+R300H=>C5H1002PY    5.0E+0012  0.000  0.0  ! TER 1121
RC5H9Y+R4CH3=>C6H12Z    1.0E+0013  0.000  0.0  ! TER 1122
RC5H9Y+R5CHO=>C6H100AY    1.0E+0013  0.000  0.0  ! TER 1123
RC5H9Y+R6CH20H=>C6H120LY    1.0E+0013  0.000  0.0  ! TER 1124
RC5H9Y+R8CH300=>HCH0+R7CH30+RC4H7Y    1.0E+0013  0.000  0.0  ! TER 1125
RC5H9Y+R11C2H5=>C7H14Y    1.0E+0013  0.000  0.0  ! TER 1126
RC3H5Y+RC3H5Y=>C6H10Y2    1.0E+0013  0.000  0.0  ! TER 1127
RC3H5Y+RC4H7Y=>C7H12Y2    1.0E+0013  0.000  0.0  ! TER 1128
RC3H5Y+RC7H13Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1129
RC3H5Y+RC8H15Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1130
RC3H5Y+RC5H9Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1131
RC4H7Y+RC4H7Y=>C8H14Y2    1.0E+0013  0.000  0.0  ! TER 1132
RC4H7Y+RC7H13Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1133
RC4H7Y+RC8H15Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1134
RC4H7Y+RC5H9Y=>C9H16Y2    1.0E+0013  0.000  0.0  ! TER 1135
RC7H13Y+RC7H13Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1136
RC7H13Y+RC8H15Y=>C15H28Y2    1.0E+0013  0.000  0.0  ! TER 1137
RC7H13Y+RC5H9Y=>C12H22Y2    1.0E+0013  0.000  0.0  ! TER 1138
RC8H15Y+RC8H15Y=>C16H30Y2    1.0E+0013  0.000  0.0  ! TER 1139
RC8H15Y+RC5H9Y=>C13H24Y2    1.0E+0013  0.000  0.0  ! TER 1140
RC8H15Y+RC6H11Y=>C14H26Y2    1.0E+0013  0.000  0.0  ! TER 1141
RC5H9Y+RC5H9Y=>C10H18Y2    1.0E+0013  0.000  0.0  ! TER 1142
RC5H9Y+RC6H11Y=>C11H20Y2    1.0E+0013  0.000  0.0  ! TER 1143

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!speces excitees!
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R1H+B10+M=0HE+M          6.0E14          0.0          6.94E3          !
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<HALL05>!
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B4CH+O2=B2CO+OHE <HALL05>!	4.0E13	0.0	0.0	!
OHE+AR=R20H+AR <HALL05>!	5.2E10	0.5	0.0	!
OHE+H2O=R20H+H2O <HALL05>!	8.6E12	0.5	0.0	!
OHE+H2=R20H+H2 <HALL05>!	1.5E12	0.5	0.0	!
OHE+R1H=R20H+R1H <HALL05>!	1.5E12	0.5	0.0	!
OHE+O2=R20H+O2 <HALL05>!	1.5E12	0.5	0.0	!
OHE+B10=R20H+B10 <HALL05>!	1.5E12	0.5	0.0	!
OHE+R20H=R20H+R20H <HALL05>!	1.5E12	0.5	0.0	!
OHE=>R20H <HALL05>!	1.4E6	0.0	0.0	!
OHE+CO2=R20H+CO2 <HALL05>!	2.75E12	0.5	-968.	!
OHE+B2CO=R20H+B2CO <HALL05>!	3.23E12	0.5	-787.	!
OHE+CH4=R20H+CH4 <HALL05>!	3.36E12	0.5	-635.	!
R9C2H+B10=B2CO+CHE <HALL05>!	6.2E12	0.0	0.0	!
R9C2H+O2=CO2+CHE <HALL05>!	2.17E10	0.0	0.0	!
CHE+AR=B4CH+AR <HALL05>!	4.0E10	0.5	0.0	!
CHE+O2=B4CH+O2 <HALL05>!	2.48E6	2.14	0.0	!
CHE+H2O=B4CH+H2O <HALL05>!	5.3E13	0.0	0.0	!
CHE+H2=B4CH+H2 <HALL05>!	1.47E14	0.0	1360.	!
CHE+CO2=B4CH+CO2 <HALL05>!	2.41E-1	4.3	-1694.	!
CHE+B2CO=B4CH+B2CO <HALL05>!	2.44E12	0.5	0.0	!
CHE+CH4=B4CH+CH4 <HALL05>!	1.73E13	0.0	167.	!
CHE=>B4CH <HALL05>!	1.86E6	0.0	0.0	!

! \*\*\*\*\*!  
! REACTIONS DE LA MATRICE O(0)C(y)H(z) !  
! \*\*\*\*\*!

! \*\*\*\*\* REACTIONS DE H2\*\*\*\*\*!

R1H+R1H+M=H2+M 1.87E18 -1.00 0.00  
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ H2/0.0/ C2H6/3.0/  
AR/0.35/



! N2/0.4/ HE/0.35/

!\*\*\*\*\* REACTIONS DE B4CH \*\*\*\*\*!

B4CH+R1H=B3C+H2 7.8E13 0. 0. !(2, -  
2)<PEETERS97>!

!\*\*\*\*\* REACTIONS DE B6CH2 \*\*\*\*\*!

B6CH2+M=B5CH2+M 1.51E13 0.0 0.0  
O2/.4/ B2CO/.75/ CO2/1.5/ H2O/6.5/ CH4/.48/ C2H4Z/1.6/  
AR/.24/  
B6CH2+R1H=B4CH+H2 3.0E13 0. 0. !(4, -  
4)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE B5CH2 \*\*\*\*\*!

B5CH2+R1H=B4CH+H2 6.0E12 0. -1.8E3 !(5, -  
5)<BAULCH94>!  
B5CH2+B3C=R9C2H+R1H 5.0E13 0. 0. !(6, -  
6)<RAnZI94>!  
B5CH2+B5CH2=>C2H2+R1H+R1H 1.2E14 0. 0.8E3 !  
(7)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE R4CH3 \*\*\*\*\*!

R4CH3+M=B5CH2+R1H+M 2.91E16 0.0 90.7E3  
O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
!  
N2/0.4/ HE/0.35/  
R4CH3+R1H=B6CH2+H2 6.0E13 0. 15.0E3 !  
(9, -9)<BAULCH94>!  
R4CH3+B4CH=R10C2H3V+R1H 3.0E13 0. 0. !(10, -  
10)<DAGAUT91>  
R4CH3+B6CH2=C2H4Z+R1H 1.8E13 0. 0. !(11, -  
11)<TSAnG86>!  
R4CH3+B5CH2=C2H4Z+R1H 4.2E13 0. 0. !(12, -  
12)<BAULCH94>!  
R4CH3+B3C=C2H2+R1H 5.0E13 0. 0. !(13, -  
13)<RAnZI94>!  
R4CH3+R4CH3(+M)=>C2H6(+M) 3.61E13 0. 0. !  
(14)<BAULCH94>!

O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
!  
N2/0.4/ HE/0.35/

LOW / 3.63E41 -7.0 2.76E3 /  
TROE / 0.62 73 1180 /  
C2H6(+M)=>R4CH3+R4CH3(+M) 1.8E21 -1.24 90.9E3 !(-  
14)<BAULCH94>!

O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
!  
N2/0.4/ HE/0.35/

LOW / 1.89E49 -8.24 93.7E3/  
TROE / 0.62 73 1180 /  
R4CH3+R4CH3=R11C2H5+R1H 3.0E13 0. 13.5E3 !(15, -  
15)<BAULCH94>!  
R4CH3+R4CH3=C2H4Z+H2 2.1E14 0. 19.3E3 !(16, -  
16)<FRAnK86nIST>!

!\*\*\*\*\* REACTIONS DE CH4 \*\*\*\*\*!

R1H+R4CH3(+M)=>CH4(+M) 1.67E14 0. 0. !  
(17)<BAULCH94>!  
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
LOW / 1.408E24 -1.8 0.0 /  
TROE / 0.37 3315 61 /  
CH4(+M)=>R4CH3+R1H(+M) 2.4E16 0. 105.0E3 !(-  
17)<BAULCH94>!  
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
LOW / 1.29E18 0.00 90.9E3 /  
TROE / 0 1350 1 7830 /  
CH4(+CH4)=>R4CH3+R1H(+CH4) 2.4E16 0. 105.0E3 !(-  
17')<BAULCH94>!  
LOW / 8.43E17 0.00 90.9E3 /  
TROE / 0.69 90 2210 /  
CH4+R1H=R4CH3+H2 1.3E04 3. 8.0E3 !(18, -  
18)<BAULCH94>!  
CH4+B4CH=C2H4Z+R1H 3.0E13 0. -0.4E3 !(19, -  
19)<DAGAUT91BAULCH94>!  
CH4+B6CH2=R4CH3+R4CH3 4.2E13 0. 0. !(20, -  
20)<TSAnG86>!  
!\*\*\*\*\* REACTIONS DE R9C2H \*\*\*\*\*!  
R9C2H+B6CH2=C2H2+B4CH 1.8E13 0. 0. !(21, -  
21)<TSAnG86>!  
R9C2H+B5CH2=C2H2+B4CH 1.8E13 0. 0. !(22, -  
22)<TSAnG86>!  
R9C2H+CH4=C2H2+R4CH3 1.2E12 0. 0. !(23, -  
23)<BAULCH94>!  
!\*\*\*\*\* REACTIONS DE C2H2 \*\*\*\*\*!  
C2H2+M=R9C2H+R1H+M 1.14E17 0. 107.0E3 !(24, -  
24)<BAULCH94>!  
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
C2H2+R1H=R9C2H+H2 6.6E13 0. 27.7E3 !(25, -  
25)<BAULCH94>!  
!\*\*\*\*\* REACTIONS DE R10C2H3V \*\*\*\*\*!  
R10C2H3V(+M)=C2H2+R1H(+M) 2.0E14 0. 39.8E3 !(26, -  
26)<BAULCH94>!  
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
LOW / 1.19E42 -7.50 45.55E3 /  
TROE /0.35 1.0 1.E8/  
R10C2H3V+R1H=C2H2+H2 1.2E13 0. 0. !(27, -  
27)<BAULCH94>!  
R10C2H3V+B6CH2=C2H2+R4CH3 1.8E13 0. 0. !(28, -  
28)<TSAnG86>!  
R10C2H3V+B5CH2=C2H2+R4CH3 1.8E13 0. 0. !(29, -  
29)<TSAnG86>!  
R10C2H3V+R4CH3=CH4+C2H2 3.9E11 0. 0. !(30, -  
30)<TSAnG86>!

R10C2H3V+R9C2H=2C2H2 9.6E11 0. 0. !(31, -  
 31)<TSAnG86>!  
 R10C2H3V+R10C2H3V=C2H4Z+C2H2 9.6E11 0. 0. !(32, -  
 32)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE C2H4Z \*\*\*\*\*!

C2H4Z+M=C2H2+H2+M 9.97E16 0. 71.6E3 !(33, -  
 33)<BAULCH94>!  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 C2H4Z+M=R10C2H3V+R1H+M 7.40E17 0. 96.7E3 !(34, -  
 34)<BAULCH94>!  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 !C2H4Z+R1H=R10C2H3V+H2 5.4E14 0. 14.8E3 !(35, -  
 35)<BAULCH94>!  
 C2H4Z+R1H=R10C2H3V+H2 5.0E7 1.93 13.0E3 !(35, -  
 35)SLAGLE96!  
 !C2H4Z+R4CH3=CH4+R10C2H3V 4.1E12 0. 11.1E3 !(36, -  
 36)<BAULCH94>!  
 C2H4Z+R4CH3=CH4+R10C2H3V 6.3E11 0. 16.0E3 !(36, -  
 36)BACK89!

!\*\*\*\*\* REACTIONS DE R11C2H5 \*\*\*\*\*!

!C2H4Z+R1H(+M)=>R11C2H5(+M) 3.97E09 1.28 1.3E3  
 ! 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 ! LOW / 1.35E19 0.00 0.76E3 /  
 ! TROE / 0.76 40 1025/  
 R11C2H5(+M)=C2H4Z+R1H(+M) 8.2E13 0. 40.0E3  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 ! LOW / 3.40E17 0.00 33.4E3 /  
 ! TROE / 0.75 97 1379/  
 R11C2H5+R1H=C2H4Z+H2 1.8E12 0. 0. !(38, -  
 38)<TSAnG86>!  
 R11C2H5+R1H=C2H6 3.6E13 0. 0. !(39, -  
 39)<TSAnG86>!  
 R11C2H5+B6CH2=C2H4Z+R4CH3 9.0E12 0. 0. !(40, -  
 40)<TSAnG86>!  
 R11C2H5+B5CH2=C2H4Z+R4CH3 1.8E13 0. 0. !(41, -  
 41)<TSAnG86>!  
 R11C2H5+R4CH3=C2H4Z+CH4 1.1E12 0. 0. !(42, -  
 42)<BAULCH94>!  
 R11C2H5+R9C2H=C2H2+C2H4Z 1.8E12 0. 0. !(43, -  
 43)<TSAnG86>!  
 R11C2H5+R10C2H3V=2C2H4Z 4.8E11 0. 0. !(44, -  
 44)<TSAnG86>!  
 R11C2H5+R10C2H3V=C2H2+C2H6 4.8E11 0. 0. !(45, -  
 45)<TSAnG86>!  
 R11C2H5+R11C2H5=C2H4Z+C2H6 1.4E12 0. 0. !(46, -  
 46)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE C2H6 \*\*\*\*\*!

C2H6+M=C2H4Z+H2+M 47)<SCHULTZ85nIST>!	2.3E17	0.	67.4E3	!(47, -
C2H6+R1H=R11C2H5+H2 48)<BAULCH94>!	1.4E9	1.5	7.4E3	!(48, -
C2H6+B6CH2=R4CH3+R11C2H5 49)<TSAnG86>!	1.1E14	0.	0.	!(49, -
C2H6+R4CH3=R11C2H5+CH4 50)<BAULCH94>!	1.5E-7	6.0	5.8E3	!(50, -
C2H6+R9C2H=C2H2+R11C2H5 51)<TSAnG86>!	3.6E12	0.	0.	!(51, -
C2H6+R10C2H3V=R11C2H5+C2H4Z 52)<TSAnG86>!	6.0E2	3.3	10.5E3	!(52, -

!  
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! \*\*\*\*\*!  
 ! REACTIONS DE LA MATRICE O(x)C(y)H(z) x>0 !  
 ! \*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE B10 \*\*\*\*\*!  

B10+H2=R20H+R1H 53)<BAULCH94>!	5.1E4	2.67	6.2E3	!(53, -
B10+B4CH=B2C0+R1H 54)<BAULCH94>!	3.9E13	0.	0.	!(54, -
B10+B4CH=B3C+R20H 55)<MUR86nIS>!	1.5E13	0.	4.7E3	!(55, -
B10+B6CH2=>B2C0+2R1H <TSAnG86>!	1.5E13	0.	0.	!(56)
B10+B6CH2=B2C0+H2 <TSAnG86>!	1.5E13	0.	0.	!(57, -57)
B10+B5CH2=>B2C0+2R1H <BAULCH94>!	7.2E13	0.	0.	!(58)
B10+B5CH2=B2C0+H2 59)<BAULCH94>!	4.8E13	0.	0.	!(59, -
B10+R4CH3=HCH0+R1H 60)<BAULCH94>!	8.4E13	0.	0.	!(60, -
B10+R4CH3=R7CH30 61)<DEAn87nIS>!	8.0E15	-2.12	0.6E3	!(61, -
B10+CH4=R4CH3+R20H 62)<BAULCH94>!	7.2E8	1.56	8.4E3	!(62, -
B10+R9C2H=B4CH+B2C0 63)<DAGAUT91>!	1.0E13	0.	0.	!(63, -
B10+C2H2=B5CH2+B2C0 64)<BAULCH LEEDS>!	2.17E06	2.1	1.6E3	!(64, -
B10+C2H2=R12CHCOZ+R1H 65)<BAULCH LEEDS>!	5.06E06	2.1	1.6E3	!(65, -

R20H+R9C2H=C2H2+B10	1.8E13	0.	0.	!(89, -
89)<TSANG86>! modif MF				
B10+R10C2H3V=R4CH3+B2CO	3.0E13	0.	0.	!(66, -
66)<DAGAUT91>!				
B10+R10C2H3V=CH2COZ+R1H	9.6E13	0.	0.	!(67, -
67)<TSAnG86>!				
B10+C2H4Z=R4CH3+R5CHO	8.1E6	1.88	0.2E3	!(68, -
68)<BAULCH94>!				
B10+C2H4Z=HCHO+B5CH2	4.00E5	1.88	0.2E3	!(69, -
69)<BAULCH94>!				
B10+C2H4Z=CH2COZ+H2	6.6E5	1.88	0.2E3	!(70, -
70)<BAULCH94>!				
B10+C2H4Z=R13CH2CHO+R1H	4.7E6	1.88	0.2E3	!(71, -
71)<BAULCH94>!				
B10+C2H4Z=R20H+R10C2H3V	1.5E7	1.91	3.7E3	!(72, -
72)<MAHMUD87nIST>!				
B10+R11C2H5=HCHO+R4CH3	1.1E13	0.	0.	!(73, -
73)<BAULCH94>!				
B10+R11C2H5=CH3CHO+R1H	5.5e13	0.	0.	!(74, -
74)<BAULCH94>!				
B10+R11C2H5=C2H4Z+R20H	3.0E13	0.	0.	!(75, -
75)<DAGAUT91>!				
B10+C2H6=R11C2H5+R20H	1.0E9	1.5	5.8E3	!(76, -
76)<BAULCH94>!				

!\*\*\*\*\* REACTIONS DE R20H \*\*\*\*\*!

R1H+B10+M=R20H+M	1.18E19	-1.0	0.0	
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
R1H+R20H+M=H2O+M	5.53E+22	-2.0	0.0	
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/				
! N2/0.4/ HE/0.35/				
R20H+H2=R1H+H2O	1.0E8	1.6	3.3E3	!(79, -
79)<BAULCH94>!				
R20H+B3C=B2CO+R1H	5.0E13	0.	0.	!(80, -
80)<RAnZI94>!				
R20H+B4CH=R5CHO+R1H	3.0E13	0.	0.	!(81, -
81)<DAGAUT91>!				
R20H+B6CH2=HCHO+R1H	3.0E13	0.	0.	!(82, -
82)<TSAnG86>!				
R20H+B5CH2=HCHO+R1H	1.8E13	0.	0.	!(83, -
83)<TSAnG86>!				
R20H+R4CH3=B6CH2+H2O	7.2E13	0.	2.7E3	!(84, -
84)<BAULCH94>!				
R20H+R4CH3(+M)=CH3OH(+M)	6.0E13	0.	0.	!(85, -
85)<BAULCH94>!				
LOW /1.4E44 -8.2 0./				
TROE /0.82 200. 1438./				
R20H+R4CH3=HCHO+H2	3.2E12	-0.53	10.8E3	!(86, -
86)<DAGAUT91>!				
R20H+R4CH3=R7CH30+R1H	5.7E12	-0.23	13.9E3	!(87, -
87)<DAGAUT91>!				
R20H+CH4=R4CH3+H2O	1.6E7	1.83	2.7E3	!(88, -
88)<BAULCH94>!				

!R20H+R9C2H=C2H2+B10 89)<TSAnG86>!	1.8E13	0.	0.	!(89, -
R20H+R9C2H=B5CH2+B2C0 90)<TSAnG86>!	1.8E13	0.	0.	!(90, -
R20H+R9C2H=R12CHCOZ+R1H 91)<DAGAUT91>!	2.0E13	0.	0.	!(91, -
R20H+C2H2=R9C2H+H20 92)<KONNOV00>!	3.385E+07	2.0	14000.0	!(92, -
R20H+C2H2=CH2COZ+R1H 93)<KONNOV00>!	1.100E+13	0.0	7170.0	!(93, -
R20H+C2H2=R4CH3+B2C0 94)<DAGAUT91>!	4.8E-4	4.	-2.0E3	!(94, -
R20H+R10C2H3V=C2H2+H20 95)<TSAnG86>!	3.0E13	0.	0.	!(95, -
R20H+R10C2H3V=CH3CHO 96)<TSAnG86>!	3.0E13	0.	0.	!(96, -
R20H+C2H4Z=R10C2H3V+H20 97)<BAULCH94>!	2.0E13	0.	5.9E3	!(97, -
R20H+C2H4Z=R4CH3+HCHO 98)<GLARBORG86>!	2.0E12	0.	0.9E3	!(98, -
R20H+R11C2H5=C2H4Z+H20 99)<TSAnG86>!	2.4E13	0.	0.	!(99, -
R20H+R11C2H5=>R4CH3+R1H+HCHO <TSAnG86>!	2.4E13	0.	0.	!(100)
R20H+C2H6=R11C2H5+H20 101)<BAULCH94>!	7.2E6	2.	0.9E3	!(101, -
R20H+R20H=H20+B10 102)<BAULCH94>!	1.5E9	1.14	0.1E3	!(102, -
!***** REACTIONS DE H2O *****!				
H20+B4CH=R6CH2OH 103)<BAULCH94>!	5.7E12	0.	-0.8E3	!(103, -
H20+B6CH2=CH3OH 104)<TSAnG86>!	1.8E13	0.	0.	!(104, -
!REACTIOnS DE B2C0!				
B2C0+R4CH3(+M)=R14CH3CO(+M) 105)<BAULCH94>!	5.0E11	0.	6.9E3	!(105, -
LOW /1.1E14	0.	3.8E3/		
TROE /0.5	1.0	1.0E8/		
B2C0+B10+M=C02+M 106)<TSAnG86>!	1.54E15	0.0	3.0E3	!(106, -
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
B2C0+R20H=C02+R1H 107)<BAULCH94>!	6.3E6	1.5	-0.5E3	!(107, -
!REACTIOnS DE R5CHO!				
R5CHO+M=R1H+B2C0+M 108)<WAnG97>!	1.9E17	-1.	17.0E3	!(108, -
H2/2.0/ B2C0/1.5/ C02/2.0/ H20/6.0/				
R5CHO+R1H=H2+B2C0 109)<BAULCH94>!	9.0E13	0.	0.	!(109, -

R5CHO+R1H=B10+B5CH2 110)<TSUB0I81nIST>!	4.0E13	0.	102.5E3	!(110, -
R5CHO+B6CH2=R4CH3+B2CO 111)<TSAnG86>!	1.8E13	0.	0.	!(111, -
R5CHO+B5CH2=R4CH3+B2CO 112)<TSAnG86>!	1.8E13	0.	0.	!(112, -
R5CHO+R4CH3=CH4+B2CO 113)<TSAnG86>!	1.2E14	0.	0.	!(113, -
R5CHO+R4CH3=CH3CHO 114)<TSAnG86>!	1.8E13	0.	0.	!(114, -
R4CH3+HCHO=R5CHO+CH4 115)<BAULCH94>!	7.7E-8	6.1	1.97E3	!(115, -
R5CHO+R9C2H=C2H2+B2CO 116)<TSAnG86>!	6.0E13	0.	0.	!(116, -
R5CHO+R10C2H3V=C2H4Z+B2CO 117)<TSAnG86>!	9.0E13	0.	0.	!(117, -
R10C2H3V+HCHO=R5CHO+C2H4Z 118)<TSAnG86>!	5.4E3	2.81	5.9E3	!(118, -
R5CHO+R11C2H5=C2H6+B2CO 119)<TSAnG86>!	1.2E14	0.	0.	!(119, -
R11C2H5+HCHO=R5CHO+C2H6 120)<TSAnG86>!	5.57E3	2.81	5.86E3	!(120, -
R5CHO+B10=R1H+C02 121)<BAULCH94>!	3.0E13	0.	0.	!(121, -
R5CHO+B10=R20H+B2CO 122)<BAULCH94>!	3.0E13	0.	0.	!(122, -
R5CHO+R20H=H2O+B2CO 123)<BAULCH94>!	1.1E14	0.	0.	!(123, -
R5CHO+R5CHO=HCHO+B2CO 124)<BAULCH94>!	3.0E13	0.	0.	!(124, -

!\*\*\*\*\* REACTIONS DE HCHO \*\*\*\*\*!

HCHO+M=R5CHO+R1H+M 125)<BAULCH94>!	1.40E36	-5.54	96.8E3	!(125, -
02/0.4/ B2CO/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/				
HCHO+M=H2+B2CO+M 126)<BAULCH94>!	3.26E36	-5.54	96.8E3	!(126, -
02/0.4/ B2CO/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/				
HCHO+R1H=R5CHO+H2 127)<BAULCH94>!	1.3E8	1.62	2.1E3	!(127, -
HCHO+B4CH=R13CH2CHO 128)<BAULCH94average>!	9.6E13	0.	-0.5E3	!(128, -
HCHO+B6CH2=R4CH3+R5CHO 129)<TSAnG86>!	1.2E12	0.	0.	!(129, -
HCHO+B10=R5CHO+R20H 130)<BAULCH94>!	4.1E11	0.57	2.7E3	!(130, -
HCHO+R20H=R5CHO+H2O Vasudevan Int. J. Chem. Kin. 37(2005)98-109	7.82E07	1.63	-1.06E3	!MF

!\*\*\*\*\* REACTIONS DE R7CH3O \*\*\*\*\*!

R7CH3O+M=HCHO+R1H+M	1.55E14	0.00	13.5E3	
02/0.4/ B2CO/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				

!	N2/0.4/ HE/0.35/				
R7CH30+R1H=HCHO+H2	1.8E13	0.	0.	!	(133, -
133)<BAULCH94>!					
R7CH30+B6CH2=R4CH3+HCHO	1.8E13	0.	0.	!	(134, -
134)<TSAnG86>!					
R7CH30+B5CH2=R4CH3+HCHO	1.8E13	0.	0.	!	(135, -
135)<TSAnG86>!					
R7CH30+R4CH3=HCHO+CH4	2.4E13	0.	0.	!	(136, -
136)<TSAnG86>!					
R7CH30+CH4=R4CH3+CH3OH	1.6E11	0.	8.8E3	!	(137, -
137)<TSAnG86>!					
R7CH30+R9C2H=HCHO+C2H2	2.4E13	0.	0.	!	(138, -
138)<TSAnG86>!					
R7CH30+R10C2H3V=HCHO+C2H4Z	2.4E13	0.	0.	!	(139, -
139)<TSAnG86>!					
R7CH30+C2H4Z=HCHO+R11C2H5	1.2E11	0.	6.7E3	!	(140, -
140)<TSAnG86>!					
R7CH30+R11C2H5=HCHO+C2H6	2.4E13	0.	0.	!	(141, -
141)<TSAnG86>!					
R7CH30+C2H6=R11C2H5+CH3OH	2.4E11	0.	7.0E3	!	(142, -
142)<TSAnG86>!					
R7CH30+B10=HCHO+R20H	1.8E12	0.	0.	!	(143, -
143)<BAULCH94>!					
R7CH30+R20H=HCHO+H2O	1.8E13	0.	0.	!	(144, -
144)<TSAnG86>!					
R7CH30+B2C0=R4CH3+C02	1.6E13	0.	11.7E3	!	(145, -
145)<TSAnG86>!					
R7CH30+R5CHO=CH3OH+B2C0	9.1E13	0.	0.	!	(146, -
146)<TSAnG86>!					
R7CH30+HCHO=CH3OH+R5CHO	1.0E11	0.	3.0E3	!	(147, -
147)<TSAnG86>!					
R7CH30+R7CH30=CH3OH+HCHO	6.0E13	0.	0.	!	(148, -
148)<TSAnG86>!					

!\*\*\*\*\* REACTIONS DE R6CH2OH \*\*\*\*\*!

R6CH2OH+M=HCHO+R1H+M	1.26E16	0.00	30.0E3	!	(149, -
149)<BAULCHLEEDS>!					
	02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
!	N2/0.4/ HE/0.35/				
R6CH2OH+R1H=R4CH3+R20H	9.6E13	0.	0.	!	(150, -
150)<TSAnG87>!					
R6CH2OH+R1H=HCHO+H2	6.0E12	0.	0.	!	(151, -
151)<TSAnG87>!					
R6CH2OH+H2=CH3OH+R1H	6.7E5	2.	13.4E3	!	(152, -
152)<TSAnG87>!					
R6CH2OH+B6CH2=CH3CHO+R1H	1.8E13	0.	0.	!	(153, -
153)<TSAnG87>!					
R6CH2OH+B5CH2=C2H4Z+R20H	2.4E13	0.	0.	!	(154, -
154)<TSAnG87>!					
R6CH2OH+B5CH2=R4CH3+HCHO	1.2E12	0.	0.	!	(155, -
155)<TSAnG87>!					
R6CH2OH+R4CH3=C2H5OH	1.2E13	0.	0.	!	(156, -
156)<TSAnG87>!					



R6CH2OH+R4CH3=CH4+HCHO	2.4E12	0.	0.	!(157, -
157)<TSAnG87>!				
R6CH2OH+CH4=CH3OH+R4CH3	21.7	3.1	16.2E3	!(158, -
158)<TSAnG87>!				
R6CH2OH+R9C2H=C2H2+HCHO	4.8E13	0.	0.	!(159, -
159)<TSAnG87>!				
!la constante de vitesse du processus 159 est globalisee!				
!R6CH2OH+R9C2H=C3H3+R2OH	1.2E13	0.	0.	!(159a, -
159a)<TSAnG87>!				
!R6CH2OH+R9C2H=C2H2+HCHO	3.6E13	0.	0.	!(159b, -
159b)<TSAnG87>!				
R6CH2OH+C2H2=R10C2H3V+HCHO	7.2E11	0.	9.0E3	!(160, -
160)<TSAnG87>!				
R6CH2OH+R10C2H3V=C2H4Z+HCHO	4.2E13	0.	0.	!(161, -
161)<TSAnG87>!				
!La constante de vitesse du processus 161 est globalisee!				
R6CH2OH+R11C2H5=C2H4Z+CH3OH	2.4E12	0.	0.	!(162, -
162)<TSAnG87>!				
R6CH2OH+R11C2H5=C2H6+HCHO	2.4E12	0.	0.	!(163, -
163)<TSAnG87>!				
R6CH2OH+C2H6=CH3OH+R11C2H5	199.	3.	14.0E3	!(164, -
164)<TSAnG87>!				
R6CH2OH+B10=HCHO+R2OH	4.2E13	0.	0.	!(165, -
165)<TSAnG87>!				
R6CH2OH+R2OH=H2O+HCHO	2.4E13	0.	0.	!(166, -
166)<TSAnG87>!				
!attention (167) metatheses dans les reactions de CH3OH!				
!R6CH2OH+H2O=CH3OH+R2OH	1.6E14	0.	26.3E3	!(167, -
167)<TSUBO181nIST>!				
R6CH2OH+R5CHO=CH3OH+B2CO	1.2E14	0.	0.	!(168, -
168)<TSAnG87>!				
R6CH2OH+R5CHO=HCHO+HCHO	1.8E14	0.	0.	!(169, -
169)<TSAnG87>!				
R6CH2OH+HCHO=CH3OH+R5CHO	5.5E3	2.8	5.9E3	!(170, -
170)<TSAnG87>!				
R6CH2OH+R7CH3O=CH3OH+HCHO	2.4E13	0.	0.	!(171, -
171)<TSAnG87>!				
R6CH2OH+R6CH2OH=CH3OH+HCHO	1.4E13	0.	0.	!(172, -
172)<TSAnG87>!				
!la constante de vitesse du processus 172 est globalisee!				
!R6CH2OH+R6CH2OH=CH3OH+HCHO	4.8E12	0.	0.	!(172a, -
172a)<TSAnG87>!				
!R6CH2OH+R6CH2OH=HOCH2CH2OH	9.6E12	0.	0.	!(172b, -
172b)<TSAnG87>!				
!***** REACTIONS DE CH3OH *****!				
CH3OH+R1H=R4CH3+H2O	2.0E14	0.	5.3E3	!(173, -
173)<HIDAKA89nIST>!				
CH3OH+R1H=R7CH3O+H2	4.2E6	2.1	4.9E3	!(174, -
174)<TSAnG87>!				
CH3OH+B6CH2=R6CH2OH+R4CH3	1.5E12	0.	0.	!(175, -
175)<TSAnG87>!				
CH3OH+B5CH2=R4CH3+R6CH2OH	31.9	3.2	7.2E3	!(176, -
176)<TSAnG87>!				

CH3OH+B5CH2=R4CH3+R7CH30 177)<TSAnG87>!	14.4	3.1	6.9E3	!(177, -
CH3OH+R9C2H=C2H2+R6CH2OH 178)<TSAnG87>!	6.0E12	0.	0.	!(178, -
CH3OH+R9C2H=C2H2+R7CH30 179)<TSAnG87>!	1.2E12	0.	0.	!(179, -
CH3OH+R10C2H3V=C2H4Z+R6CH2OH 180)<TSAnG87>!	31.9	3.2	7.2E3	!(180, -
CH3OH+R10C2H3V=C2H4Z+R7CH30 181)<TSAnG87>!	14.4	3.1	6.9E3	!(181, -
CH3OH+B10=R6CH2OH+R20H 182)<GROTHEER81nIST>!	3.4E13	0.	5.5E3	!(182, -
CH3OH+B10=R7CH30+R20H 183)<WARnATZ84>!	1.0E13	0.	4.7E3	!(183, -
!modification des metatheses avec OH!				
!CH3OH+R20H=R7CH30+H2O 184)<WARnATZ84>!	1.0E13	0.	1.7E3	!(184, -
CH3OH+R20H=R6CH2OH+H2O 184a)<Atkinson86>85%!	3.1E06	2.	-3.4E2	!(184a, -
CH3OH+R20H=R7CH30+H2O 184b)<Atkinson86>15%!	5.4E05	2.	-3.4E2	!(184b, -
CH3OH+R7CH30=CH3OH+R6CH2OH 185)<TSAnG87>!	3.0E11	0.	4.1E3	!(185, -
!***** REACTIONS DE R12CHCOD *****!				
R12CHCOZ+M=B4CH+B2CO+M 186)<DAGAUT91>!	6.0E15	0.	58.8E3	!(186, -
R12CHCOZ+R1H=B5CH2+B2CO 187a)<BAULCH94>!	1.5E14	0.	0.	!(187a, -
R12CHCOZ+R1H=B6CH2+B2CO 187b)<PEETERS97>!	1.3E14	0.	0.	!(187b, -
R12CHCOZ+B5CH2=R9C2H+HCHO 188)<DAGAUT91>!	1.0E13	0.	2.0E3	!(188, -
R12CHCOZ+B5CH2=R10C2H3V+B2CO 189)<DAGAUT91>!	3.0E13	0.	0.	!(189, -
R12CHCOZ+B10=>B2CO+B2CO+R1H (190)<BAULCH94>!	9.6E13	0.	0.	!
R12CHCOZ+R20H=>R5CHO+B2CO+R1H (191)<DAGAUT91>!	1.0E13	0.	0.	!
!***** REACTIONS DE CH2COD *****!				
CH2COZ+M=B6CH2+B2CO+M 192)<FRAnK86nIST>!	6.57E15	0.0	57.6E3	!(192, -
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
CH2COZ+M=R12CHCOZ+R1H+M 193)<FRAnK86nIST>!	2.7E17	0.	87.0E3	!(193, -
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
CH2COZ+R1H=R4CH3+B2CO 194)<BAULCH94>!	1.8E13	0.	3.4E3	!(194, -
CH2COZ+R1H=R12CHCOZ+H2 195)<DAGAUT91>!	5.0E13	0.	8.0E3	!(195, -

CH2COZ+B5CH2=C2H4Z+B2CO 196)<CAN0SA-MAS84nIST>!	1.3E14	0.	0.	!(196, -
CH2COZ+B10=B5CH2+C02 197)<DAGAUT91>!	1.8E12	0.	1.3E3	!(197, -
CH2COZ+B10=R12CHCOZ+R20H 198)<DAGAUT91>!	1.0E13	0.	8.0E3	!(198, -
CH2COZ+R20H=R12CHCOZ+H2O 199)<DAGAUT91>!	7.5E12	0.	2.0E3	!(199, -
!CH2COZ+R20H=R5CHO+HCHO 200)<VAnD00REn77nIST>!	2.8E13	0.	0.	!(200, -
CH2COZ+R20H=R4CH3+C02 200a)<BAULCH LEEDS>!	2.52E12	0.	0.	!(200a, -
CH2COZ+R20H=R6CH20H+B2CO 200b)<BAULCH LEEDS>!	4.68E12	0.	0.	!(200b, -

!\*\*\*\*\* REACTIONS DE R14CH3CO \*\*\*\*\*!

R14CH3CO+R1H=R4CH3+R5CHO 201)<TSAnG86>!	9.6E13	0.	0.	!(201, -
R14CH3CO+B6CH2=R4CH3+CH2COZ 202)<TSAnG86>!	1.8E13	0.	0.	!(202, -
R14CH3CO+B5CH2=R4CH3+CH2COZ 203)<TSAnG86>!	1.8E13	0.	0.	!(203, -
R14CH3CO+B10=R4CH3+C02 204)<TSAnG86>!	9.6E12	0.	0.	!(204, -
R14CH3CO+R20H=CH2COZ+H2O 205)<TSAnG86>!	1.2E13	0.	0.	!(205, -
R14CH3CO+R20H=>R4CH3+B2CO+R20H (206)<TSAnG86>!	3.0E13	0.	0.	!
R14CH3CO+R5CHO=CH3CHO+B2CO 207)<TSAnG86>!	9.0E12	0.	0.	!(207, -
R14CH3CO+HCHO=CH3CHO+R5CHO 208)<TSAnG86>!	1.8E11	0.	12.9E3	!(208, -
R14CH3CO+R7CH3O=CH3OH+CH2COZ 209)<TSAnG86>!	6.0E12	0.	0.	!(209, -
R14CH3CO+R7CH3O=HCHO+CH3CHO 210)<TSAnG86>!	6.0E12	0.	0.	!(210, -
R14CH3CO+CH3OH=CH3CHO+R6CH20H 211)<TSAnG87>!	4.85E3	3.	12.3E3	!(211, -
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 212)<TSAnG86>!	1.2E13	0.	0.	!(212, -

!\*\*\*\*\* REACTIONS DE R13CH2CHO \*\*\*\*\*!

!R13CH2CHO=R14CH3CO (213, -213)<COLKET75nIST>!	1.0E13	0.	47.0E3	!
!R13CH2CHO=R1H+CH2COZ (214, -214)<COLKET75nIST>!	1.6E13	0.	35.0E3	!
R13CH2CHO=R4CH3+B2CO infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.	2.93E12	0.29	40.3E3	!at
R13CH2CHO=R1H+CH2COZ infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.	1.43E15	-0.15	45.6E3	!at

!\*\*\*\*\* REACTIONS DE CH3CHO \*\*\*\*\*!

!CH3CHO+R1H=H2+R14CH3CO (215, -215)<WARnATZ84>!	4.0E13	0.	4.2E3	!
!CH3CHO+R4CH3=R14CH3CO+CH4 (216, -216)<BAULCH94>!	2.0E-6	5.6	2.5E3	!
!CH3CHO+R10C2H3V=C2H4Z+R14CH3CO (217, -217)<SCHERZER87>!	8.1E10	0.	3.7E3	!
!CH3CHO+R11C2H5=C2H6+R14CH3CO (218, -218)<HOHLEIn70>!	1.3E12	0.	8.5E3	!
!CH3CHO+B10=R14CH3CO+R20H (219, -219)<CAVAnAGH90>!	1.4E13	0.	2.3E3	!
!CH3CHO+R20H=R14CH3CO+H2O (220, -220)<CAVAnAGH90>!	4.2E12	0.	0.5E3	!
!CH3CHO+R7CH30=R14CH3CO+CH30H (221, -221)<CAVAnAGH90>!	2.4E11	0.	1.8E3	!
!CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO (222, -222)<SCHUCHMAnn70nIST>!	2.5E7	0.	0.	!

!\*\*\*\*\* REACTIONS DE C2H4O# \*\*\*\*\*!

C2H4O#3=CH4+B2CO 223)<LIFSHITZ83nIST>!	1.2E13	0.	57.2E3	!(223, -
C2H4O#3=CH3CHO 224)<LIFSHITZ83nIST>!	7.3E13	0.	57.2E3	!(224, -
C2H4O#3=R4CH3+R5CHO 225)<LIFSHITZ83nIST>!	3.6E13	0.	57.2E3	!(225, -
C2H4O#3+R1H=H2+R13CH2CHO 226)<LIFSHITZ83nIST*>!	2.0E13	0.	8.3E3	!(226, -
C2H4O#3+R1H=H2O+R10C2H3V 227)<LIFSHITZ83nIST>!	5.0E9	0.	5.0E3	!(227, -
C2H4O#3+R1H=C2H4Z+R20H 228)<LIFSHITZ83nIST>!	9.5E10	0.	5.0E3	!(228, -
C2H4O#3+R4CH3=CH4+R13CH2CHO 229)<BALDWIn84nIST*>!	1.1E12	0.	11.8E3	!(229, -
C2H4O#3+R4CH3=R11C2H5+HCHO 230)<RAnZI94>!	1.4E11	0.	7.6E3	!(230, -
C2H4O#3+R4CH3=C2H4Z+R7CH30 231)<RAnZI94>!	1.5E10	0.	7.6E3	!(231, -
C2H4O#3+R9C2H=C2H2+R13CH2CHO 232)<RAnZI94>!	1.2E12	0.	9.8E3	!(232, -
C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO 233)<RAnZI94>!	2.0E12	0.	9.3E3	!(233, -
C2H4O#3+R11C2H5=C2H6+R13CH2CHO 234)<RAnZI94>!	6.8E11	0.	11.4E3	!(234, -
C2H4O#3+B10=R20H+R13CH2CHO 235)<BOGAn78nIST>!	1.9E12	0.	5.2E3	!(235, -
C2H4O#3+R20H=H2O+R13CH2CHO 236)<BALDWIn84nIST*>!	1.8E13	0.	3.6E3	!(236, -
C2H4O#3+R5CHO=HCHO+R13CH2CHO 237)<RAnZI94>!	3.7E12	0.	15.8E3	!(237, -
C2H4O#3+R7CH30=CH30H+R13CH2CHO 238)<RAnZI94>!	1.3E12	0.	5.8E3	!(238, -
C2H4O#3+R6CH20H=CH30H+R13CH2CHO 239)<RAnZI94>!	8.4E11	0.	13.4E3	!(239, -
C2H4O#3+R14CH3CO=CH3CHO+R13CH2CHO 240)<RAnZI94>!	4.0E12	0.	17.5E3	!(240, -

C2H4O#3+R13CH2CHO=CH3CHO+R13CH2CHO 6.8E11 0. 15.4E3 !(241, -  
241)<RAnZI94>!

!\* assuming that C2H3O decompose rapidly to R13CH2CHO!

!\*\*\*\*\* REACTIONS DE R15C2H5O \*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C2H5OH \*\*\*\*\*!

!Voir Plus bas meca 10a Luc Sy Tran

!\*\*\*\*\* REACTIONS DE O2 \*\*\*\*\*!

B10+B10+M=O2+M 5.40E13 0. -1.79E3 !(244, -  
244)<BAULCH94>!

02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/

O2+R1H=R20H+B10 9.8E13 0. 14.8E3 !(245, -  
245)<BAULCH94>!

!O2+R1H+M=R300H+M 2.10E18 -0.8 0.00 !(246, -  
246)<baseLeeds>!

! 02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/  
! N2/0.4/ HE/0.35/

!O2+R1H+H2O=R300H+H2O 6.90E15 0.0 -2.10E3 !(246, -  
246bis)<base Leeds>!

O2+R1H(+M)=R300H(+M) 4.52E13 0. 0. !(246, -  
246)<COBOS85>!

LOW /1.8E18 -0.8 0.00/ !k0  
BAULCH94!

TROE /0.5 1.0 1.0E8/  
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/  
! N2/0.4/ HE/0.35/

!O2+R1H(+H2O)=R300H(+H2O) 1.63E14 0. 761. !(246b, -  
246b)<COBOS85>!

O2+R1H(+H2O)=R300H(+H2O) 4.52E13 0. 0. !(246b, -  
246b)<BAULCH94>!

LOW /6.9E15 0.0 -2080/  
TROE /0.45 1.0 1.0E8/

O2+B3C=B2CO+B10 1.2E14 0. 0. !(247, -  
247)<RAnZI94>!

O2+B4CH=R5CHO+B10 3.3E13 0. 0. !(248, -  
248)<DAGAUT91>!

O2+B4CH=B2CO+R20H 3.2E13 0. 0. !(249, -  
249)<PEETERS97>!

O2+B6CH2=>B2CO+R20H+R1H 3.1E12 0. 0. !  
(250)<BAULCH94>!

O2+B5CH2=R5CHO+R20H 4.3E10 0. -0.5E3 !(251, -  
251)<DAGAUT91>!

O2+B5CH2=C02+H2 6.9E11 0. 0.5E3 !(252, -  
252)<DAGAUT91>!

O2+B5CH2=>C02+R1H+R1H 1.6E12 0. 1.0E3 !  
(253)<DAGAUT91>!

O2+B5CH2=B2CO+H2O 1.9E10 0. -1.0E3 !(254, -  
254)<DAGAUT91>!

02+B5CH2=>B2CO+R20H+R1H (255)<DAGAUT91>!	8.6E10	0.	-0.5E3	!
02+B5CH2=HCHO+B10 256)<DAGAUT91>!	1.0E14	0.	4.5E3	!(256, -
02+R4CH3(+M)=R8CH300(+M) 257)<BAULCH94>!	7.8E8	1.2	0.	!(257, -
	LOW /5.6E25	-3.3	0./	
	TROE /0.36	1.0	1.0E8/	
02+R4CH3=R7CH30+B10 258)<BAULCH94>!	1.3E14	0.	31.3E3	!(258, -
!02+R4CH3=R7CH30+B10 258)<HWAnG&RABInOVITCH99>!	1.6E13	0.	31.4E3	!(258, -
02+R4CH3=HCHO+R20H 259)<DAGAUT91>!	3.0E30	-4.69	36.6E3	!(259, -
02+CH4=R4CH3+R300H 260)<BAULCH94>!	4.0E13	0.	56.7E3	!(260, -
02+R9C2H=B2CO+R5CHO 261)<TIESEMAAnn97/TSAnG86>!	3.8E13	-0.16	0.	!(261, -
02+R9C2H=R12CHCOZ+B10 262)<TIESEMAAnn97/TSAnG86>!	9.0E12	-0.16	0.	!(262, -
02+C2H2=R9C2H+R300H 263)<TSAnG86>!	1.2E13	0.	74.5E3	!(263, -
!02+C2H2=R12CHCOZ+R20H 264)<DAGAUT91>!	2.0E8	1.5	30.1E3	!(264, -
02+C2H2=R5CHO+R5CHO 264)<BEnS0n95>!	7.0E7	1.8	30.6E3	!(264, -
!02+R10C2H3V=C2H2+R300H 265)<TSAnG86>!	1.2E11	0.	0.	!(265, -
!02+R10C2H3V=C2H2+R300H 265)<WAnG97>! !at 760 Torr	1.6E14	-0.83	2.5E3	!(265, -
!02+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	8.6E21	-2.97	3.3E3	!(266a, -
!02+R10C2H3V=B10+R13CH2CHO 266b)<WAnG97>! !at 20-90 Torr	1.2E13	-0.12	1.7E3	!(266b, -
!02+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	1.6E21	-2.78	2.5E3	!(266a, -
!02+R10C2H3V=B10+R13CH2CHO 266b)<WAnG97>!	2.5E12	0.057	0.9E3	!(266b, -
02+R10C2H3V=C2H2+R300H 265)<MEBEL nIST>!	1.34E6	1.61	-0.4E3	!(265, -
02+R10C2H3V=HCHO+R5CHO 266a)<MEBEL nIST>!	4.5E16	-1.39	1.0E3	!(266a, -
02+R10C2H3V=B10+R13CH2CHO 266b)<MEBEL nIST>!	3.3E11	-0.29	10.	!(266b, -
02+C2H4Z=R10C2H3V+R300H 267)<TSAnG86>!	4.2E13	0.	57.4E3	!(267, -

02+R11C2H5=R17C2H500 268)<WAGnER90>!	2.2E10	0.77	-0.6E3	!(268, -
02+R11C2H5=C2H4Z+R300H 269)<TSAnG86>!	8.4E11	0.	3.9E3	!(269, -
02+R11C2H5=R15C2H50+B10 270)<BOZZELLI90nIST>!	1.2E13	-0.2	27.9E3	!(270, -
02+R11C2H5=CH3CHO+R20H 271)<TSAnG86>!	6.0E10	0.	6.9E3	!(271, -
02+C2H6=R11C2H5+R300H 272)<BAULCH94>!	6.0E13	0.	51.7E3	!(272, -
02+R20H=R300H+B10 273)<TSAnG86>!	2.2E13	0.	52.5E3	!(273, -
02+B2C0=C02+B10 274)<TSAnG86>!	2.5E12	0.	47.7E3	!(274, -
!02+R5CH0=B2C0+R300H 275)<TSAnG86>!	5.1E13	0.	1.7E3	!(275, -
02+R5CH0=B2C0+R300H 275)<TIM0nEn88>!	7.6E12	0.	0.41E3	!(275, -
02+HCHO=R5CH0+R300H 276)<TSAnG86>!	2.0E13	0.	38.8E3	!(276, -
02+R7CH30=HCHO+R300H 277)<BAULCH94>!	2.2E10	0.	1.7E3	!(277, -
02+R6CH20H=HCHO+R300H 278)<TSAnG87>!	1.2E12	0.	0.	!(278, -
02+CH30H=R6CH20H+R300H 279)<TSAnG87>!	2.0E13	0.	44.9E3	!(279, -
02+R12CHC0Z=>B2C0+B2C0+R20H <DAGAUT91>!	1.5E12	0.	2.5E3	!(280)
!02+CH2C0Z=HCHO+C02 281)<DAGAUT91>!bizarre	1.0E8	0.	0.	!(281, -
02+R14CH3C0=R18CH3C000 282)<COX90>!	2.4E12	0.	0.	!(282, -
02+R13CH2CHO=>HCHO+R20H+B2C0 <COX90>!	5.9E9	0.	-1.4E3	!(283)
02+R13CH2CHO=CH2C0Z+R300H 284)<COX90>!	1.0E10	0.	-1.4E3	!(284, -
02+CH3CHO=R14CH3C0+R300H 285)<COX90>!	5.0E13	0.	36.4E3	!(285, -
! ajout demande par Laetitia le 25 Avril 95				
02+CH3CHO=R13CH2CHO+R300H 285)<Ranzi94>!	1.0E13	0.5	46.0E3	!(285', -
02+C2H40#3=R300H+R13CH2CHO 286)<RAnZI94>!	5.0E13	0.	48.0E3	!(286, -
!02+R15C2H50=CH3CHO+R300H 287)<BAULCH94>!	6.0E10	0.	1.7E3	!(287, -
!***** REACTIONS DE R300H *****!				
R300H+R1H=H2+O2 288)<BAULCH94>!	4.3E13	0.	1.4E3	!(288, -
R300H+R1H=2R20H 289)<BAULCH94>!	1.7E14	0.	0.9E3	!(289, -
R300H+R1H=H2O+B10 290)<BAULCH94>!	3.0E13	0.	1.7E3	!(290, -

R300H+B6CH2=HCHO+R20H 291)<TSAnG86>!	3.0E13	0.	0.	!(291, -
R300H+B5CH2=HCHO+R20H 292)<TSAnG86>!	1.8E13	0.	0.	!(292, -
R300H+R4CH3=R7CH30+R20H 293)<BAULCH94>!	1.8E13	0.	0.	!(293, -
!R300H+R4CH3=R7CH30+R20H 293)<DAGAUT>	4.0E13	0.	5.0E3	!(293, -
R300H+CH4=R4CH3+H2O2 294)<BAULCH94>!	9.0E12	0.	24.6E3	!(294, -
R300H+R9C2H=R12CHCOZ+R20H 295)<TSAnG86>!	1.8E13	0.	0.	!(295, -
R300H+C2H2=CH2COZ+R20H 296)<TSAnG86>!	6.0E9	0.	8.0E3	!(296, -
!incertitude au moins un facteur 10				
R300H+R10C2H3V=>R20H+R4CH3+B2CO <TSAnG86>!	3.0E13	0.	0.	!(297)
R300H+C2H4Z=CH3CHO+R20H 298)<TSAnG86>!	6.0E9	0.	7.9E3	!(298, -
R300H+C2H4Z=C2H40#3+R20H 299)<BAULCH94>!	2.2E12	0.	17.2E3	!(299, -
R300H+R11C2H5=>R4CH3+HCHO+R20H <TSAnG86>!	2.4E13	0.	0.	!(300)
R300H+R11C2H5=C2H4Z+H2O2 301)<TSAnG86>!	3.0E11	0.	0.	!(301, -
R300H+C2H6=R11C2H5+H2O2 302)<BAULCH94>!	1.3E13	0.	20.4E3	!(302, -
R300H+R20H=H2O+O2 303)<BAULCH94>!	2.9E13	0.	-0.5E3	!(303, -
R300H+B2CO=CO2+R20H Phys. Chem. A 111(2007)4031 - 4042	1.57E05	2.18	17.9E3	!MF Wang, J.
R300H+R5CHO=>R20H+R1H+CO2 <TSAnG86>!	3.0E13	0.	0.	!(305)
R300H+HCHO=R5CHO+H2O2 306)<BAULCH94>!	3.0E12	0.	13.0E3	!(306, -
R300H+R7CH30=HCHO+H2O2 307)<TSAnG86>!	3.0E11	0.	0.	!(307, -
R300H+R6CH20H=HCHO+H2O2 308)<TSAnG87>!	1.2E13	0.	0.	!(308, -
R300H+CH30H=R6CH20H+H2O2 309)<TSAnG87>!	9.6E10	0.	12.6E3	!(309, -
R300H+R14CH3CO=>R4CH3+CO2+R20H (310)<TSAnG86>!	3.0E13	0.	0.	!
R300H+CH3CHO=R14CH3CO+H2O2 311)<CAVAnAGH90>!	1.0E12	0.	10.0E3	!(311, -
R300H+C2H40#3=H2O2+R13CH2CHO 312)<RAnZI94>	1.6E12	0.	15.0E3	!(312, -
R300H+R300H=H2O2+O2 313)<BAULCH 94>!	1.3E11	0.	-1.63E3	!(313, -
DUPLICATE				
R300H+R300H=H2O2+O2 313)<BAULCH 94>!	4.2E14	0.	11.98E3	!(313, -
DUPLICATE				



!\*\*\*\*\* REACTIONS DE H2O2 \*\*\*\*\*!

!R2OH+R2OH(+ M)=>H2O2 (+ M) 7.23E13 -0.37 0.00  
! 02/0.4/ B2C0/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
!! N2/0.4/ HE/0.35/  
! LOW /5.53E19 -0.76 0.00 /  
! TROE /0.5 1 1.E8/  
!H2O2(+M)=>R2OH+R2OH(+M) 3.00E14 0.00 48.5E3  
! 02/0.4/ B2C0/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
!! N2/0.4/ HE/0.35/  
! LOW /3.0E17 0.0 45.5E3/  
! TROE /0.5 1 1.E8/

! MF Troe, Comb.Flam. 158(2011)594-601

H2O2(+M)=R2OH+R2OH(+M) 1.99E12 0.9 4.8749E4 !<BAULCH94>!  
AR/0.68/ 02/0.79/ N2/1.00/ C02/1.06/ H2O/5.1/ H2O2/5.2/  
LOW /3.65e24 -2.3 4.8749E4/  
TROE /0.43 1 1.E8/

H2O2+R1H=H2+R300H 1.7E12 0. 3.7E3 !(315, -  
315)<BAULCH94>!  
H2O2+R1H=H2O+R20H 1.0E13 0. 3.6E3 !(316, -  
316)<BAULCH94>!  
H2O2+B6CH2=R7CH30+R20H 3.0E13 0. 0. !(317, -  
317)<TSAnG86>!  
H2O2+R10C2H3V=C2H4Z+R300H 1.2E10 0. -0.6E3 !(318, -  
318)<TSAnG86>!  
H2O2+B10=R20H+R300H 6.6E11 0. 4.0E3 !(319, -  
319)<BAULCH94>!  
H2O2+R20H=H2O+R300H 7.8E12 0. 1.3E3 !(320, -  
320)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE CO2 \*\*\*\*\*!

CO2+B5CH2=HCHO+B2C0 2.3E10 0. 0. !(321, -  
321)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE R8CH300 \*\*\*\*\*!

R8CH300=HCHO+R20H 1.5E13 0. 47.0E3 !(322, -  
322)<RAnZI94>!  
R8CH300+R1H=R7CH30+R20H 9.6E13 0. 0. !(323, -  
323)<TSAnG86>!  
R8CH300+H2=CH300H+R1H 3.0E13 0. 26.0E3 !(324, -  
324)<TSAnG86>!  
R8CH300+B6CH2=HCHO+R7CH30 1.8E13 0. 0. !(325, -  
325)<TSAnG86>!  
R8CH300+B5CH2=HCHO+R7CH30 1.8E13 0. 0. !(326, -  
326)<TSAnG86>!  
R8CH300+R4CH3=R7CH30+R7CH30 5.0E12 0. -1.4E3 !(327, -  
327)<CAVAnAGH90>!  
R8CH300+CH4=CH300H+R4CH3 1.8E11 0. 18.5E3 !(328, -  
328)<TSAnG86>!  
R8CH300+R9C2H=R7CH30+R12CHCOZ 2.4E13 0. 0. !(329, -  
329)<TSAnG86>!  
!R8CH300+C2H2=CH300H+R9C2H 5.6E11 0. 24.5E3 !(330, -  
330)<RAnZI94>! MF car i<<0

R8CH300+R10C2H3V=R7CH30+R13CH2CHO	2.4E13	0.	0.	!(331, -
331)<TSAnG86*>!				
!* assuming that C2H3O decompose rapidly to R13CH2CHO!				
R8CH300+C2H4Z=R7CH30+C2H4O#3	1.1E15	0.	20.0E3	!(332, -
332)<nIKISHA81/MOSHKInA80nIST>!				
R8CH300+C2H4Z=CH300H+R10C2H3V	3.9E12	0.	24.5E3	!(333, -
333)<RAnZI94>!				
R8CH300+R11C2H5=R7CH30+R15C2H5O	2.4E13	0.	0.	!(334, -
334)<TSAnG86>!				
R8CH300+C2H6=CH300H+R11C2H5	2.9E11	0.	14.9E3	!(335, -
335)<TSAnG86>!				
R8CH300+B10=R7CH30+O2	3.6E13	0.	0.	!(336, -
336)<TSAnG86>!				
R8CH300+R20H=CH30H+O2	6.0E13	0.	0.	!(337, -
337)<TSAnG86>!				
R8CH300+R20H=R7CH30+R300H	3.0E12	0.	0.	!(338, -
338)<RAnZI94>!				
R8CH300+B2CO=R7CH30+CO2	1.0E14	0.	24.0E3	!(339, -
339)<RAnZI94>!				
R8CH300+R5CHO=>R7CH30+R1H+CO2	3.0E13	0.	0.	!(340)
<TSAnG86>!				
R8CH300+HCHO=CH300H+R5CHO	1.0E12	0.	12.1E3	!(341, -
341)<CAVAnAGH90>!				
R8CH300+R7CH30=HCHO+CH300H	3.0E11	0.	0.	!(342, -
342)<TSAnG86>!				
R8CH300+R6CH2OH=>R7CH30+R20H+HCHO	1.2E13	0.	0.	!
(343)<TSAnG87>!				
R8CH300+CH30H=CH300H+R6CH2OH	1.8E12	0.	13.7E3	!(344, -
344)<TSAnG87>!				
R8CH300+CH30H=CH300H+R7CH30	2.8E11	0.	18.8E3	!(345, -
345)<RAnZI94>!				
R8CH300+CH2COZ=CH300H+R12CHCOZ	1.7E12	0.	27.0E3	!(346, -
346)<RAnZI94>!				
R8CH300+R14CH3CO=R4CH3+CO2+R7CH30	2.4E13	0.	0.	!(347, -
347)<TSAnG86>!				
R8CH300+CH3CHO=CH300H+R14CH3CO	1.0E12	0.	12.1E3	!(348, -
348)<CAVAnAGH90>!				
R8CH300+CH3CHO=CH300H+R13CH2CHO	1.7E12	0.	19.2E3	!(349, -
349)<RAnZI94>!				
R8CH300+C2H4O#3=CH300H+R13CH2CHO	2.2E12	0.	16.0E3	!(350, -
350)<RAnZI94>!				
R8CH300+R300H=CH300H+O2	2.5E11	0.	-1.6E3	!(351, -
351)<BAULCH94>!				
R8CH300+R300H=>O2+HCHO+H2O	5.0E10	0.	0.	!
(352)<RAnZI94>!				
R8CH300+H2O2=CH300H+R300H	2.4E12	0.	9.9E3	!(353, -
353)<TSAnG86>!				
R8CH300+R8CH300=CH30H+HCHO+O2	2.5E10	0.	-0.8E3	!(354, -
354)<BAULCH94>!				
R8CH300+R8CH300=R7CH30+R7CH30+O2	2.5E10	0.	-0.8E3	!(355, -
355)<BAULCH94>!				

!\*\*\*\*\* REACTIOns DE CH300H \*\*\*\*\*!

CH300H=R7CH30+R20H 356)<BAULCH94>!	6.0E14	0.	42.3E3 !(356, -
CH300H+B10=R8CH300+R20H 357)<BAULCH94average>!	2.0E13	0.	4.8E3 !(357, -
CH300H+R20H=H2O+R8CH300 358)<BAULCH94average>!	1.8E12	0.	-0.37E3 !(358, -
CH300H+R7CH30=>CH30H+R20H+HCHO (359)<RAnZI94>!	1.5E11	0.	6.5E3 !
!***** REACTIOnS DE R17C2H500 *****!			
R17C2H500=R16C2H400H 360)<HUGHES93>!	4.2E12	0.	36.9E3 !(360, -
R17C2H500+H2=C2H500H+R1H 361)<RAnZI94>!	7.9E12	0.	21.0E3 !(361, -
R17C2H500+R4CH3=R15C2H50+R7CH30 362)<RAnZI94>!	2.0E12	0.	-1.2E3 !(362, -
R17C2H500+CH4=C2H500H+R4CH3 363)<RAnZI94>!	3.9E12	0.	24.0E3 !(363, -
R17C2H500+C2H2=C2H500H+R9C2H 364)<RAnZI94>!	5.6E11	0.	24.4E3 !(364, -
R17C2H500+C2H4Z=C2H500H+R10C2H3V 365)<RAnZI94>!	3.9E12	0.	24.4E3 !(365, -
R17C2H500+C2H4Z=R15C2H50+C2H40#3 366)<MOSHKInA80nIST>!	2.3E16	0.	21.9E3 !(366, -
R17C2H500+C2H6=C2H500H+R11C2H5 367)<RAnZI94>!	5.1E12	0.	19.5E3 !(367, -
R17C2H500+H2O=C2H500H+R20H 368)<RAnZI94>!	5.6E12	0.	30.6E3 !(368, -
R17C2H500+B2C0=C02+R15C2H50 369)<RAnZI94>!	1.0E14	0.	24.0E3 !(369, -
R17C2H500+HCHO=C2H500H+R5CHO 370)<RAnZI94>!	4.5E12	0.	14.4E3 !(370, -
R17C2H500+CH30H=C2H500H+R7CH30 371)<RAnZI94>!	2.8E11	0.	18.4E3 !(371, -
R17C2H500+CH30H=C2H500H+R6CH20H 372)<RAnZI94>!	2.8E12	0.	19.5E3 !(372, -
R17C2H500+CH2COZ=C2H500H+R12CHCOZ 373)<RAnZI94>!	1.7E12	0.	24.4E3 !(373, -
R17C2H500+CH3CHO=C2H500H+R14CH3CO 374)<RAnZI94>!	3.9E12	0.	14.4E3 !(374, -
R17C2H500+CH3CHO=C2H500H+R13CH2CHO 375)<RAnZI94>!	1.7E12	0.	19.5E3 !(375, -
R17C2H500+C2H40#3=C2H500H+R13CH2CHO 376)<RAnZI94>!	2.2E12	0.	16.3E3 !(376, -
R17C2H500+R300H=O2+C2H500H 377)<BAULCH89>!	3.9E11	0.	-1.3E3 !(377, -
!Rate constant measured between 240 and 380K!			
R17C2H500+H2O2=C2H500H+R300H 378)<RAnZI94>!	4.5E11	0.	10.8E3 !(378, -
R17C2H500+R8CH300=>R15C2H50+R7CH30+O2 (379)<RAnZI94>!	2.0E11	0.	0. !
R17C2H500+CH300H=C2H500H+R8CH300 380)<RAnZI94>!	1.1E12	0.	16.3E3 !(380, -

R17C2H500+R17C2H500=2R15C2H50+02 4.1E10 0. 0.2E3 !(381, -  
 381)<LIGHTFOOT92>!  
 R17C2H500+R17C2H500=C2H50H+CH3CHO+02 1.8E10 0. 0.2E3 !(382, -  
 382)<LIGHTFOOT92>!

!\*\*\*\*\* REACTIONS DE R16C2H400H \*\*\*\*\*!

R16C2H400H=C2H40#3+R20H 1.5E11 0. 20.0E3 !(383, -  
 383)<RAnZI94>!  
 R16C2H400H=R6CH20H+HCHO 2.5E13 0. 27.5E3 !(384, -  
 384)<RAnZI94>!  
 R16C2H400H=C2H4Z+R300H 2.0E13 0. 23.5E3 !(385, -  
 385)<RAnZI94>!

!\*\*\*\*\* REACTIONS DE C2H500H \*\*\*\*\*!

C2H500H=R15C2H50+R20H 4.0E15 0. 42.9E3 !(386, -  
 386)<BAULCH94>!  
 C2H500H+R1H=>CH3CHO+R20H+H2 3.2E13 0. 7.7E3 !  
 (387)<RAnZI94>!  
 C2H500H+R4CH3=>CH3CHO+R20H+CH4 5.7E11 0. 8.7E3 !  
 (388)<RAnZI94>!  
 C2H500H+R9C2H=>CH3CHO+R20H+C2H2 6.0E11 0. 9.2E3 !  
 (389)<RAnZI94>!  
 C2H500H+R10C2H3V=>CH3CHO+R20H+C2H4Z 1.0E12 0. 8.7E3 !  
 (390)<RAnZI94>!  
 C2H500H+R11C2H5=>CH3CHO+R20H+C2H6 3.4E11 0. 11.4E3 !  
 (391)<RAnZI94>!  
 C2H500H+R20H=>CH3CHO+R20H+H2O 5.9E12 0. 0.9E3 !  
 (392)<RAnZI94>!  
 C2H500H+R5CHO=>CH3CHO+R20H+HCHO 1.8E12 0. 16.7E3 !  
 (393)<RAnZI94>!  
 C2H500H+R7CH3O=>CH3CHO+R20H+CH3OH 6.3E11 0. 5.5E3 !  
 (394)<RAnZI94>!  
 C2H500H+R6CH20H=>CH3CHO+R20H+CH3OH 4.2E11 0. 13.6E3 !  
 (395)<RAnZI94>!  
 C2H500H+R14CH3CO=>2CH3CHO+R20H 2.0E12 0. 18.5E3 !  
 (396)<RAnZI94>!  
 C2H500H+R13CH2CHO=>2CH3CHO+R20H 3.4E11 0. 15.7E3 !  
 (397)<RAnZI94>!  
 C2H500H+R300H=>CH3CHO+R20H+H2O2 8.0E11 0. 16.2E3 !  
 (398)<RAnZI94>!  
 C2H500H+R8CH300=>CH3CHO+R20H+CH300H 1.1E12 0. 16.7E3 !  
 (399)<RAnZI94>!  
 C2H500H+R17C2H500=>CH3CHO+R20H+C2H500H 1.1E12 0. 16.7E3 !  
 (400)<RAnZI94>!

!\*\*\*\*\* REACTIONS DE R18CH3C000 \*\*\*\*\*!

R18CH3C000+C2H40#3=CH3C000H+R13CH2CHO 1.0E12 0. 9.3E3 !  
 (401, -402)<RAnZI94>!  
 R18CH3C000+R300H=CH3C000H+02 5.5E10 0. -2.6E3 !  
 (402, -402)<COX90>!  
 R18CH3C000+C2H500H=CH3C000H+R17C2H500 5.0E11 0. 9.2E3 !  
 (403, -403)<RAnZI94>!  
 R18CH3C000+C2H500H=>CH3CHO+R20H+CH3C000H 5.0E11 0. 9.2E3 !  
 (404)<RAnZI94>!



C2H50H(+M)=R24C2H40H+R1H(+M) 7.54E+16 -0.275 94.05E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!  
 LOW /7.708E+96 -22.47 116.9E+3/  
 !T=500-1800K  
 !LOW /5.58E+82 -21.20 37824.5/  
 !T=1800-3000K

DUPLICATE

C2H50H(+M)=R15C2H50+R1H(+M) 2.70E+15 0.305 101.3E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011b!  
 LOW /2.794E+88 -19.76 121.0E+3/  
 !T=500-1800K;  
 !LOW /4.246E+91 -23.49 49435.8/  
 !T=1800-3000K,

DUPLICATE

!Bimolecular initiation

C2H50H+O2=R23C2H40H+R300H 2.100E+13 0.0 52400.0  
 C2H50H+O2=R24C2H40H+R300H 1.400E+13 0.0 46300.0  
 C2H50H+O2=R15C2H50+R300H 7.000E+12 0.0 55730.0

!Metatheses with abstraction of H-atom

!C2H50H+R20H=R23C2H40H+H2O 6.203E+03 2.68 -576.3  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!  
 C2H50H+R20H=R23C2H40H+H2O 3.60E+06 2.0 950.0  
 !Nancy, correlation Bozzelli 1999!

!C2H50H+R20H=R24C2H40H+H2O 1.307E+05 2.43 -1456.6  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!  
 C2H50H+R20H=R24C2H40H+H2O 2.40E+06 2.00 -2100.0  
 !Nancy, correlation Bozzelli 1999!

C2H50H+R20H=R15C2H50+H2O 2.812E+02 2.97 -580.3  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!

C2H50H+B10=R23C2H40H+R20H 9.69E+02 3.23 4658.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007

C2H50H+B10=R24C2H40H+R20H 1.45E+05 2.47 876.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H50H+B10=R15C2H50+R20H 1.46E-03 4.73 1727.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H50H+R1H=R23C2H40H+H2 1.88E+03 3.20 7150.0  
 !T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H50H+R1H=R24C2H40H+H2 1.79E+05 2.53 3420.0  
 !T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H50H+R1H=R15C2H50+H2 5.33E-23 10.58 -4459.0  
 !T=300-1000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

!C2H50H+R1H=R15C2H50+H2	5.36E+4	2.53	8753.6	
!T=1000-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).				
!C2H50H+R4CH3=R23C2H40H+CH4	6.99E-83	30.14	-15663.0	
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
C2H50H+R4CH3=R23C2H40H+CH4	3.30E+02	3.30	12291.0	
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
!C2H50H+R4CH3=R24C2H40H+CH4	1.02E-47	18.51	-9409.4	
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
C2H50H+R4CH3=R24C2H40H+CH4	1.99E+01	3.37	7635.0	
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)				
!C2H50H+R4CH3=R15C2H50+CH4	1.01E-51	19.68	-10323.5	
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
C2H50H+R4CH3=R15C2H50+CH4	2.035E+0	3.57	7722.0	
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)				
C2H50H+R300H=R23C2H40H+H2O2	4.2E+04	2.69	19080	
!correlation (Dean and Bozzelli 2000)				
C2H50H+R300H=R24C2H40H+H2O2	2.80E+04	2.69	15420	
!correlation (Dean and Bozzelli 2000)				
C2H50H+R300H=R15C2H50+H2O2	5.400E+04	2.0	15025.0	!
Grana et al.2010				
C2H50H+R11C2H5=R23C2H40H+C2H6	1.500E+12	0.0	11700.0	!
Konnov 2005!				
C2H50H+R11C2H5=R24C2H40H+C2H6	4.000E+13	0.0	10000.0	!
Konnov 2005!				
C2H50H+R11C2H5=R15C2H50+C2H6	2.300E+04	2.0	10525.0	!
Grana et al.2010!				
C2H50H+R6CH2OH=R24C2H40H+CH3OH	4.000E+11	0.0	9700.0	!
Konnov 2005!				
C2H50H+R7CH3O=R24C2H40H+CH3OH	2.000E+11	0.0	7000.0	!
Konnov 2005!				
C2H50H+R15C2H5O=C2H50H+R24C2H40H	2.000E+11	0.0	7000.0	!
Konnov 2005!				

!\*\*\*\*\*!  
!\* REACTIONs OF R23C2H40H \*!  
!\*\*\*\*\*!

R23C2H40H=C2H4Z+R2OH	3.52E-34	11.84	-18737.4	
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.				
!	1.35E+43	-10.29	28035.5	
!at 1 atm, T=300-1000K				

!		7.93E+2	1.51	15180.3
!at 1 Torr, T=300-3000K				
!		1.51E+33	-6.54	26960.4
!at 100 atm, T=300-1000K				
!		4.90E-24	9.44	-12183.6
!at 100 atm, T=1000-3000K				
R23C2H40H=R1H+C2H30H		3.33E+28	-5.26	35586.9
!at 1 atm, T=300-3000K.ref: Lin et al 2009, chemphyschem, 10(6),972-81.				
!		2.67E+15	-1.92	29386.8
!at 1 Torr, T=300-3000K.				
!		2.67E+27	-4.44	37208.5
!at 100 atm, T=300-3000K				
R23C2H40H=R24C2H40H		1.000E+11	0.0	39500.0
! A=Konnov 2005; Ea=Lin et al 2009, chemphyschem, 10(6),972-81				
R23C2H40H+O2=C2H30H+R300H		1.600E+12	0.0	5000.0
!*****!				
!* REACTIONs OF R24C2H40H *				
!*****!				
R24C2H40H=CH3CHO+R1H		8.34E+27	-5.19	35576.9
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.				
!!		8.96E+13	-1.61	28844.3
!at 1 Torr, T=300-3000K				
!!		5.47E+27	-4.67	37685.4
!at 100 atm, T=300-3000K				
R24C2H40H=R1H+C2H30H		2.00E+28	-5.08	39380.5
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81				
!!		4.44E+21	-3.23	36570.6
!at 1 Torr, T=300-3000K				
!!		1.22E+30	-5.17	41916.2
!at 100 atm, T=300-3000K				
R24C2H40H=R4CH3+HCHO		1.14E+22	-3.59	34662.9
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81				
!!		5.92E+11	-1.04	28739.0
!at 1 Torr, T=300-3000K				
!!		4.36E+23	-3.55	38679.0
!at 100 atm, T=300-3000K				
R24C2H40H+O2=CH3CHO+R300H		5.26E+17	-1.637	838.0
!at 0.1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.				
!!R24C2H40H+O2=CH3CHO+R300H		5.28E+17	-1.637	839.0
!at 1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.				
R24C2H40H+O2=C2H30H+R300H		5.33E+2	2.490	-402
!at 0.1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.				
!!R24C2H40H+O2=C2H30H+R300H		7.62E+2	2.446	-296
!at 1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.				



R24C2H40H+R1H=CH3CHO+H2	1.361E+09	1.29	2823.8
! T=100-2000K! ref: Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H=R6CH20H+R4CH3	8.67E+16	-0.891	2903.3
!Reaction (b2), Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H=C2H30H+H2	4.896E+08	1.70	588.2
!Reaction (b11), T=100-2000K! Ref: Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H(+M)=C2H50H(+M)	3.607E+13	0.06	437.2
!Reaction (b1), T=500-2000K!Ref: Lin et al 2011b, JphyschemA,115,3509-22,			
	LOW /2.767E+56	-15.72	
10.7E+03/			
Duplicate			
R24C2H40H+R20H=CH3CHO+H2O	1.500E+13	0.0	0.0
!Konnov 2005			
R24C2H40H+B10=CH3CHO+R20H	9.040E+13	0.0	0.0
!Konnov 2005			
!*****!			
!* REACTIOnS OF R15C2H50 *!			
!*****!			
R15C2H50=R4CH3+HCHO	4.4E-29	10.69	-16245.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.			
!!	1.03E+23	-3.82	19303.7
!at 1 atm, T=300-1000K,			
!!	2.71E+24	-4.50	21018.7
!at 1 Torr, T=300-1000K,			
!!	1.87E-28	10.39	-12910.9
!at 1 Torr, T=1000-3000K,			
!!	5.31E+21	-2.97	19560.1
!at 100 atm, T=300-1000K,			
!!	9.56E-17	7.66	-7408.3
!at 100 atm, T=1000-3000K,			
R15C2H50=R1H+CH3CHO	4.25E-32	11.49	-16541.5
!at 1 atm,T=1000-3000K ref: Lin et al 2009, chemphyschem, 10(6),972-81			
!!	1.33E+38	-8.61	25513.8
!at 1 atm,T=300-1000K			
!!	7.25E+31	-7.58	21370.4
!at 1 Torr,T=300-1000K			
!!	2.14E-34	11.63	-15651.2
!at 1 Torr,T=1000-3000K			
!!	2.61E+19	-2.15	21996.4
!at 100 atm,T=300-1000K			
!!	1.64E-27	10.5	-15315.4
!at 100 atm,T=1000-3000K			

R15C2H50+O2=CH3CHO+R300H 6.0E+10 0.0 1.7E+3  
!(287, -287)<BAULCH94>!

R15C2H50+R20H=CH3CHO+H2O 1.0E+13 0.0 0.0  
!Marinov 1998

R15C2H50+R1H=CH3CHO+H2 7.47E+09 1.15 673.7  
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22

R15C2H50+R1H(+M)=C2H5OH(+M) 3.08E+11 0.894 12.9  
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22  
LOW / 3.772E+51 -15.55  
11.1E+3/

DUPLICATE

R15C2H50+B10=CH3CHO+R20H 1.210E+14 0.0 0.0  
!Konnov 2005

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!\* Secondary mechanism of the  
oxidation of Ethanol \*!

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

!\* REACTIONS OF C2H3OH \*!

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

!C2H3OH+B10=R13CH2CHO+R20H 4.4E+10 0.7 3250.0  
!<PAG,Ulisier paras. des m̃tathises d'atome H allylique secondaire>!  
C2H3OH+B10=R13CH2CHO+R20H 1.4E+13 0.0 2.3E3  
!Ac̃tald̃hyde! (219, -219)<CAVAnAGH90>

!C2H3OH+R1H=R13CH2CHO+H2 2.700E+04 2.5  
-1900.0 !<PAG,Ulisier paras. des m̃tathises d'atome H allylique  
secondaire>!

!C2H3OH+R1H=R13CH2CHO+H2 1477.2 3.077  
7230 !T=300-3000!RAO 2011! J Phys Chem 2011,115  
! REV /1.41 3.721 24600/  
C2H3OH+R1H=R13CH2CHO+H2 1.31E+5 2.58 1220.0  
!Ac̃tald̃hyde! T=200-2500K!Klippenstein et al.2010. J Phys Chem  
A,114,755-764.

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!C2H3OH+R2OH=R13CH2CHO+H2O          1.500E+06      2.0
-1520.0      !<PAG,Ulisier paras. des m̃tathises d'atome H allylique
secondaire>!
C2H3OH+R2OH=R13CH2CHO+H2O          2.300E+10      0.73      -1100.0
!Ac̃tald̃hyde! Konnov 2005

!C2H3OH+R3OOH=R13CH2CHO+H2O2        3.200E+03      2.6
12400.0     !<PAG,Ulisier paras. des m̃tathises d'atome H allylique
secondaire>!
!C2H3OH+R3OOH=R13CH2CHO+H2O2        1.626E+12      0.0
16295.1     !Syn_CH2H3OH! ajout̃ le 20/10/2011 !Altarawneh et al 2011!
T=700-1300K!
C2H3OH+R3OOH=R13CH2CHO+H2O2        1.0E12          0.0          10.0E3
!Ac̃tald̃hyde! (311, -311)<CAVANAGH90>!

!C2H3OH+R4CH3=R13CH2CHO+CH4          5.000E+10      0.0
7300.0      !<PAG,Ulisier paras. des m̃tathises d'atome H allylique
secondaire>!
C2H3OH+R4CH3=R13CH2CHO+CH4          2.0E-6          5.6          2.5E+3
!Ac̃tald̃hyde! (216, -216)<BAULCH94>!Nancy! T=300-125

!C2H3OH+R11C2H5=R13CH2CHO+C2H6        0.740           3.5          4140.0
!<PAG,Ulisier paras. des m̃tathises d'atome H allylique secondaire>!
C2H3OH+R11C2H5=R13CH2CHO+C2H6        1.3E12          0.0          8.5E3
!Ac̃tald̃hyde! (218, -218)<HOHLEIn70>

C2H3OH=CH3CHO                          4.5E+06         1.8          5.1E+4
!Prof. Fournet
!!C2H3OH=CH3CHO                         8.590E+11       0.318        55900.00
! DaSilva 2006!
!!                                       REV/  1.050E+09     1.202
66300.00 /

!C2H3OH+R3OOH=CH3CHO+R3OOH           1.49E+05        1.67         6810.0
!P=1atm, T=300-2000K!Da silva 2009, Chem Phys Letters 483, 25-29
C2H3OH+R1H=CH3CHO+R1H                 1.00E+13        0.00         1506.0
!T=300-2000K!form observation in Huynh et al 2009, j phys chem A
113,3177-3185:

!"The rate of this reaction is close to that of the H addition to C2H4:
C2H4 + H=C2H5, ref: Warnatz 1984

C2H3OH+R2OH=R4CH3+C02+H2              1.40E+12        0.00         -1040.0
!Nancy, tableau A-I-5
!C2H3OH+R2OH=HCHO+R6CH2OH             1.40E+12        0.00         -1040.0
!Nancy, tableau A-I-5

!C2H4+OH<=>C2H3OH+H                   1.070E+04       2.600        4133.00
!Senosiain et al 2006
C2H4Z+R2OH=C2H3OH+R1H                 4.000E+12       0.000        4880.00
!Hippler et al 2000

!*****!
!*          REACTIONs OF CH3CHO          *!

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

CH3CHO+R20H=R14CH3CO+H2O 2.300E+10 0.73  
-1100.0 ! Konnov 2005!  
CH3CHO+R1H=H2+R14CH3CO 1.31E+5 2.58  
1220.0 !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-  
764.  
CH3CHO+R4CH3=R14CH3CO+CH4 2.0E-6 5.6  
2.5E+3 !(216, -216)<BAULCH94>! T=300-1250K  
CH3CHO+B10=R14CH3CO+R20H 1.4E+13 0.  
2.3E3 !(219, -219)<CAVAnAGH90>!  
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO 8.1E10 0.  
3.7E3 !(217, -217)<SCHERZER87>T=480-520K!NIST  
CH3CHO+R11C2H5=C2H6+R14CH3CO 1.3E12 0.  
8.5E3 !(218, -218)<HOHLEIn70>!  
CH3CHO+R7CH3O=R14CH3CO+CH3OH 5.000E+12 0.0  
0.0 !Konnov 2005!  
CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 3.000E+12 0.0  
11200.0 !Konnov 2005!

!CH3CHO+R20H=R13CH2CHO+H2O 1.600E+13 0.0  
2000.0 !T=1000-1700K, P=1.2-2.8 atm. ref: Yasunaga et al 2008, J  
Chem Kin 2008,40,73-102  
CH3CHO+R20H=R13CH2CHO+H2O 3.370e+11 0.0  
-619.98 !Mech Sandiego=ref:Juan Li's PhD thesis!  
!CH3CHO+R1H=R13CH2CHO+H2 4.40E+14 0.0  
10.0E+3 !NIST! 2008YAS/KUB73-102! T=1000-1700K, P=1.2-2.8 atm  
CH3CHO+R1H=R13CH2CHO+H2 2.72E+03 3.1  
5206.5 !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-  
764.  
!CH3CHO+R4CH3=R13CH2CHO+CH4 6.00E+12 0.0  
11000.0 !2008YAS/KUB73-102!T=1000-1700K, P=1.2-2.8 atm  
CH3CHO+R4CH3=R13CH2CHO+CH4 2.45E+1 3.15  
5727.0 !Marinov 1998  
CH3CHO+B10=R13CH2CHO+R20H 3.720E+13 -0.2  
3556.0 !Marinov 1998

!\*\*\*\*\* REACTIONS DE C2H5 \*\*\*\*\*!

R11C2H5+R10C2H3V=>C4H8Y 1.5E13 0. 0. !  
(61, -61)<TSAng86>!  
!R11C2H5+R11C2H5=>C4H10 1.1E13 0. 0. !  
(65, -65)<BAULCH94>!

!\*\*\*\*\* REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE \*\*\*\*\*!

C2H3CHO+R20H=CH2CHCO+H2O 1.0E13 0.0 0.0 !  
<MARInOV>!  
C2H3CHO+B10=CH2CHCO+R20H 7.2E12 0.0 2.0E3 !  
<MARInOV>!

C2H3CHO+B10=CH2COZ+R5CHO+R1H <MARInOV>!	5.0E7	1.76	0.08E3 !
C2H3CHO+R1H=CH2CHCO+H2 <MARInOV>!	4.0E13	0.0	4.2E3 !
C2H3CHO+R1H=C2H4Z+R5CHO <MARInOV>!	2.0E13	0.0	3.5E3 !
C2H3CHO+O2=CH2CHCO+R3OOH <MARInOV99>+ MF correlation Baptiste	3.0E13	0.0	38.5E3 !
CH2CHCO=R10C2H3V+B2CO <MARInOV>!	1.0E14	0.0	34.0E3 !
CH2CHCO+B10=R10C2H3V+CO2 <MARInOV>!	1.0E14	0.0	0.0 !
C3H5Y+R300H=>C2H3CHO+R1H+R20H <TSAng91>!	7.0E18	-2.0	0.0 !
C3H5Y+O2=C2H3CHO+R20H <BOZELLI93>!	1.8E13	-0.41	22.9E3 !
C3H5Y+B10=C2H3CHO+R1H <SLAGLE92>!	1.8E14	0.0	0.0 !

!\*\*\*\*\*!  
! REACTIONS DES ESPECES NON OXYGENNS EN C3 !  
!\*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C3H2 \*\*\*\*\* (CHCCH(..))\*\*\*\*\*!

B4CH+C2H2=C3H2+R1H <MILLER92/BAULCH94>!	2.1E14	0.0	-0.5E3 !
C3H2+B10=R9C2H+R1H+B2CO <PEETERS97>!	3.0E13	0.0	0.0 !
C3H2+R20H=C2H2+R5CHO <MILLER92>!	5.0E13	0.0	0.0 !
C3H2+O2=R12CHCOZ+B2CO+R1H <MILLER92>!	5.0E13	0.0	0.0 !

!\*\*\*\*\* REACTIONS DE C3H3 \*\*\*\*\* (CHCCH2(..)) Propargyl\*\*\*\*\*stabilise par resonance !

B6CH2+C2H2=C3H3+R1H <MILLER87/BAULCH94>!	1.8E14	0.0	0.0 !
C3H3+R1H=C3H2+H2 <MILLER92/BRAUn89>!	2.0E13	0.0	0.0 !
C3H3+B10=R9C2H+HCHO <MILLER92/SLAGUE91>!	1.4E14	0.0	0.0 !
C3H3+R20H=C3H2+H2O <MILLER92>!	2.0E13	0.0	0.0 !
C3H3+R20H=R10C2H3V+R5CHO <WAnG97>!	4.0E13	0.0	0.0 !
C2H2+R12CHCOZ=C3H3+B2CO <MILLER92>!	1.0E11	0.0	3.0E3 !
C3H3+O2=CH2COZ+R5CHO <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3 !
C3H2+R1H=C3H3 <est>!	1.0E14	0.0	0.0 !

C3H3+R300H=>R20H+R9C2H+HCHO <Heyberger>!	1.0E15	-0.8	0.0	!
C3H3+C3H3=C6H6# <STEIn90>shocktube!	1.0E12	0.0	0.0	!
C3H3+C3H3=C6H5#+R1H <STEIn90>flame!	1.0E12	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE pC3H4 \*\*\*\*\* (CH3CCH) Propyne \*\*\*\*\*!

!pC3H4=>aC3H4 !<HIDAKA89>!	2.1E12	0.0	60.0E3	
pC3H4+M=C3H3+R1H+M !<HIDAKA89>!	4.7E18	0.0	80.0E3	
C2H2+B5CH2=pC3H4 !<TSAnG86>!	3.5E12	0.0	0.0	
pC3H4=R9C2H+R4CH3 <KInGAS1500>!	4.2E15	0.0	125.0E3	!
pC3H4+O2=C3H3+R300H <est Ingham>!	2.1E12	0.0	40.8E3	!
pC3H4+R1H=C2H2+R4CH3 <hidaka89> !	1.3E5	2.5	1.00E3	!
pC3H4+R1H(+M)=tC3H5(+M) <WAGnER72>!	8.5E12	0.0	1.7E3	!
LOW /5.6E25	-7.27	6.58E3/		
!<Marinov97>!				
pC3H4+R1H(+M)=sC3H5(+M) <WAGnER72>!	5.8E12	0.0	3.1E3	!
LOW /3.8E25	-7.27	7.98E3/		
!<estimated>!				
pC3H4+R4CH3=C3H3+CH4 <asTSAnG91>!	2.2E0	3.5	5.7E3	!
pC3H4+R1H=C3H3+H2 <asTSAnG91>	1.7E5	2.5	2.5E3	!
pC3H4+R9C2H=C3H3+C2H2 !<asTSAnG91>!	3.6E12	0.0	0.0	
pC3H4+R10C2H3V=C3H3+C2H4Z <asTSAnG91>!	2.2E0	3.5	4.7E3	!
pC3H4+R11C2H5=C3H3+C2H6 <asTSAnG91>!	2.2E0	3.5	6.6E3	!
pC3H4+B10=R12CHCOZ+R4CH3 <WARnATZ84>!	1.5E13	0.0	2.1E3	!
pC3H4+B10=R20H+C3H3 <<ADUSEI, G.Y, 1996>>!	3.4E4	2.16	4.8E3	!
pC3H4+R20H=CH2COZ+R4CH3 <BOODAGHIANs87>!	4.3E11	0.0	-0.8E3	!
pC3H4+R20H=R1H+C2H3CHO <asBOODAGHIANs87>!	4.3E11	0.0	-0.8E3	!
pC3H4+R20H=C3H3+H2O <asTSAnG91>!	3.1E6	2.0	-0.3E3	!

pC3H4+R300H=C2H4Z+B2C0+R20H as296<TSAnG86>!	6.0E9	0.0	8.0E3	!
pC3H4+R300H=C3H3+H202 <asTSAnG91>!	9.6E3	2.6	13.9E3	!
pC3H4+R7CH30=CH30H+C3H3 <Heyberger>!	2.0E12	0.0	4.0E3	!

!\*\*\*\*\* REACTIONS DE aC3H4 \*\*\*\*\* (CH2CCH2) Allene \*\*\*\*\*!

aC3H4=pC3H4 <HIDAKA89>!	2.5E12	0.0	59.0E3	!
aC3H4+M=C3H3+R1H+M <HIDAKA89>!	2.0E18	0.0	80.0E3	!
aC3H4+O2=C3H3+R300H <Estimation Ingham>!	2.8E13	0.0	39.0E3	!
aC3H4+R1H(+M)=C3H5Y(+M) 2.7E3 !<WAGnER72>!		4.0E12	0.0	
LOW /5.6E33 -5.0 4.44E3/ !<Marinov97> !				
aC3H4+R1H(+M)=tC3H5(+M) <WAGnER72>!	8.5E12	0.0	2.0E3	!
LOW /1.1E34 -5.0 4.44E3/ !<Marinov97>!				
C2H4Z+B4CH=aC3H4+R1H <BAULCH94base>!	1.3E14	0.0	-0.3E3	!
R10C2H3V+B5CH2=aC3H4+R1H <MILLER92>!	3.0E13	0.0	0.0	!
iC4H3+B5CH2=aC3H4+R9C2H <MILLER92>!	2.0E13	0.0	0.0	!
aC3H4+B10=R1H+B2C0+R10C2H3V <Aleksandrev nist>!	6.6E12	0.0	3.0E3	!
aC3H4+R20H=CH2COZ+R4CH3 <LIU88>!	2.0E12	0.0	-0.2E3	!
aC3H4+R20H=HCHO+R10C2H3V <LIU88>!	2.0E12	0.0	-0.2E3	!
aC3H4+R1H=C3H3+H2 <est.butatiene>!	1.3E6	2.53	9.2E3	!
aC3H4+B10=C3H3+R20H <fromAleksandrev nist>!	6.2E12	0.0	1.9E3	!
!d'après leur vitesse de réaction total et d'addition !				
aC3H4+R20H=C3H3+H20 <est.butadiene>!	6.2E6	2.0	0.4E3	!
aC3H4+R4CH3=C3H3+CH4 <WU87>!	2.0E12	0.0	7.7E3	!
aC3H4+R9C2H=C3H3+C2H2 <WU87>!	1.0E13	0.0	0.0	!
aC3H4+C3H5Y=C3H3+C3H6Y <DAGAUT92>	2.0E12	0.0	7.7E3	!
aC3H4+R7CH30=CH30H+C3H3 9.6E3 !<correlations a partir de Heyberger>!		4.0E12	0.0	
aC3H4+R11C2H5=C2H6+C3H3 !<asbutadiene>!	5.0E14	0.0	19.8E3	

aC3H4+R10C2H3V=C2H4Z+C3H3 <asbutadiene>!	5.0E14	0.0	19.8E3	!
!aC3H4+R4CH3=C4H7T <Scherzer>!	5.7E10	0.0	6.8E3	!
!aC3H4+R4CH3=C4H7T !<Tsang91x2>!	3.4E11	0.0	7.4E3	
!aC3H4+R4CH3=iC4H7 !<Tsang73>!	1.6E11	0.0	5.0E3	
!aC3H4+R4CH3=C4H7T 7.4E3 !<Tsang91x2/4>!	0.8E11	0.0		
aC3H4+R4CH3=iC4H7 !<Tsang73/3>!	0.4E11	0.0	5.0E3	

!fort effet de fall off, environ un facteur 4 pour 6.7 kPa et 1100 K (Tsang91)!

!aC3H4+C3H3=C6H6#+R1H <HIDAKA89>!	1.4E12	0.0	10.0E3	!
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!\*\*\*\*\* REACTIONS DE cC3H4 \*\*\*\*\* cyclopropene \*\*\*\*\*!

cC3H4=aC3H4 <Karni>	1.5E14	0.0	50.5E3	!
cC3H4=pC3H4 <Karni>	7.1E13	0.0	47.8E3	!
cC3H4+R1H=cC3H3+H2 <Heyberger>!	5.4E4	2.5	-1.9E3	!
cC3H4+R20H=cC3H3+H2O <Heyberger>!	3.0E6	2.0	-1.5E3	!
cC3H4+R20H=C2H4Z+R5CHO <Heyberger>!	2.8E12	0.0	-1.0E3	!
cC3H3+R300H=R20H+C2H2+R5CHO <Heyberger>!	1.0E15	-0.8	0.0	!
cC3H3+R4CH3=cC4H6 <estimation>!	1.0E13	0.0	0.0	!
cC3H3+R1H=cC3H4 <estimation>!	1.0E14	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE C3H5Y \*\*\*\*\* (CH2CHCH2(.)) Allyl \*\*\*\*\*stabilise par resonance !

!C3H5Y+R1H=C3H6Y <TSAnG91>!	2.0E13	0.0	0.0	!
C3H5Y+R1H=aC3H4+H2 TSANG 91!* C3H5Y+R1H=C3H6Y <allara>!!	1.8E13	0.0	0.0	!
	1.0E14	0.0	0.0	!

!rñaction importante pour la formation de propine!

C3H5Y+R4CH3=aC3H4+CH4 <TSAnG91>!	3.0E12	-0.32	-0.1E3	!
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C3H5Y+R4CH3=C4H8Y <TSAnG91>!	1.0E14	-0.32	-0.1E3	!
C3H5Y+R20H=aC3H4+H2O Tsang 91! !peu d'effet de fall off!	6.03E12	0.0	0.0	!
C3H5Y+R10C2H3V=aC3H4+C2H4Z <TSAnG91>!	2.4E12	0.0	0.0	!
!C3H5Y+R11C2H5=aC3H4+C2H6 <TSAnG91>!	9.6E11	0.0	-0.1E3	!
C3H5Y+R11C2H5=aC3H4+C2H6 <TSAnG91>MODIF!!!!	2.0E13	0.0	-0.1E3	!
C3H5Y+B10=R10C2H3V+HCHO <SLAGLE90,LEUnG95>!	1.8E14	0.0	0.0	!
!processus non elementaire impliquant la formation-decomposition de l'hydroperoxyde				
!C3H5Y+C3H3=C6H6#+2R1H <MARInOV97>!	5.6E20	-2.535	1.7E3	!
C3H5Y+C3H5Y=aC3H4+C3H6Y <TSAnG91>!	8.4E10	0.0	-0.3E3	!

!\*\*\*\*\* REACTIONS DE sC3H5 \*\*\*\*\* (CH3CHCH(.)) 2-methyl vinyl \*\*\*\*\*!

sC3H5=C3H5Y <WEISSMAN89>!	5.0E13	0.0	37.0E3	!
R4CH3+C2H2=sC3H5 <BAULCH94>!	6.0E11	0.0	7.7E3	!

!\*\*\*\*\* REACTIONS DE tC3H5 \*\*\*\*\* (CH3C(.)CH2) 1-methyl vinyl \*\*\*\*\*!

tC3H5+R1H=aC3H4+H2 <DAGAUT90>!	3.3E12	0.0	0.0	!
tC3H5+R4CH3=aC3H4+CH4 <DAGAUT90>!	1.0E11	0.0	0.0	!
tC3H5+R10C2H3V=aC3H4+C2H4Z <LEUnG95>!	1.0E12	0.0	0.0	!
tC3H5+R11C2H5=aC3H4+C2H6 <LEUnG95>!	1.0E12	0.0	0.0	!
tC3H5+B10=CH2COZ+R4CH3 <LEUnG95>!	1.8E14	0.0	0.0	!
tC3H5+O2=R4CH3+B2CO+HCHO <DAGAUT90>!	4.3E12	0.0	0.0	!
tC3H5=C3H5Y <Weissman89>!	2.0E13	0.0	47.0E3	!

!\*\*\*\*\* REACTIONS DE C3H6Y \*\*\*\*\* (CH3CHCH2) propene \*\*\*\*\*!

C2H4Z+B6CH2=C3H6Y <BAULCH94>!	9.6E13	0.0	0.0	!
C2H4Z+B5CH2=C3H6Y <BAULCH94>!	3.2E12	0.0	5.1E3	!
!duplicate R10C2H3V+R4CH3=C3H6Y <TSAnG86>!	2.5E13	0.0	0.0	!

C2H4Z+R4CH3=C3H6Y+R1H <TSAnG86>!	6.6E11	0.0	15.9E3	!
R11C2H5+B6CH2=C3H6Y+R1H <TSAnG86>!	9.0E12	0.0	0.0	!
C2H6+B4CH=C3H6Y+R1H <BAULCH94>!	1.1E14	0.0	-0.3E3	!
C3H6Y+R1H=sC3H5+H2 <TSAnG92>!	7.83E5	2.5	12.28E3	!
C3H6Y+R1H=tC3H5+H2 <TSAnG92>!	3.9E5	2.5	5.82E3	!
C3H6Y+R1H=C3H5Y+H2 <TSAnG91>!	1.7E5	2.5	2.5E3	!
C3H6Y+R4CH3=C3H5Y+CH4 <TSAnG91>!	2.2E0	3.5	5.7E3	!
C3H6Y+R4CH3=sC3H5+CH4 <TSAnG91>!	8.4E-1	3.5	11.7E3	!
C3H6Y+R4CH3=tC3H5+CH4 <TSAnG91>!	1.3E0	3.5	12.9E3	!
C3H6Y+R11C2H5=C3H5Y+C2H6 <TSAnG91>!	2.2E0	3.5	6.6E3	!
!C3H6Y+B10=>CH2COZ+R1H+R4CH3 <TSAnG91>! MF!!ds мйса PRF	1.2E+5	2.56	-1130.0	!
C3H6Y+B10=C3H5Y+R20H <TSAnG91>!	1.7E11	0.7	5.9E3	!
!C3H6Y+R20H=HCHO+R11C2H5 <TSAnG91>! MF!!ds мйса PRF	1.45E12	0.0	-0.9E3	!
!C3H6Y+R20H=R4CH3+CH3CHO <TSAnG91>! MF!!ds мйса PRF	1.45E12	0.0	-0.9E3	!
C3H6Y+R20H=C3H5Y+H20 <TSAnG91>!	3.1E6	2.0	-0.3E3	!
C3H6Y+R20H=sC3H5+H20 <TSAnG91>!	1.1E6	2.0	1.45E3	!
C3H6Y+R20H=tC3H5+H20 <TSAnG91>!	2.1E6	2.0	2.8E3	!
C3H6Y+O2=C3H5Y+R300H <WALKER93>!	1.9E12	0.0	39.0E3	!
C3H6Y+R300H=C3H5Y+H202 <TSAnG91>!	9.6E3	2.6	13.9E3	!
C3H6Y+R9C2H=pC3H4+R10C2H3V 91 mehdi!	1.2E13	0.0	0.0	!TSANG

!\*\*\*\*\* REACTIONS DE cC3H6 \*\*\*\*\* cyclopropane \*\*\*\*\*!

cC3H6=C3H6Y <Hidaka87>!	4.6E14	0.0	62.6E3	!
cC3H6+R1H=C3H5Y+H2 <Marshall86>!	1.6E14	0.0	11.7E3	!
cC3H6+R20H=C3H5Y+H20 <Dobe82>!	7.0E7	1.5	1.0E3	!
cC3H6+R4CH3=C3H5Y+CH4 <Exgas>!	2.0E11	0.0	9.6E3	!

!\*\*\*\*\* REACTIONS DE R19C3H7 et iC3H7 \*\*\*\*\* CH3CH2CH2(.) et CH3CH(.)CH3  
 \*\*\*\*\* !

!R19C3H7 = R4CH3+C2H4Z	6.400E+12	0.00	31000.0!!
ds мйса PRF			
!R19C3H7 = R1H+C3H6Y	3.000E+13	0.00	38000.00!!
ds мйса PRF			
iC3H7 = R1H+C3H6Y	6.000E+13	0.00	39000.00
R19C3H7 = iC3H7	1.960E+10	1.00	38600.00
!R19C3H7+O2 =R300H+C3H6Y	1.600E+12	0.00	5000.00
R19C3H7+O2 =R300H+C3H6Y	3.7e16	-1.63	3420 !
2003DES/KLI4415-4427			
iC3H7+O2 = R300H+C3H6Y	1.400E+12	0.00	5000.00

!\*\*\*\*\* Propane (C3H8) chemistry \*\*\*\*\*!

R11C2H5+R4CH3=C3H8	3.4E13	0.	0.	!(59, -
59)<BAULCH94>!				
C3H8+O2=>R300H+iC3H7	1.4E+0013	0.000	50323.7	! BI 2 CN
C3H8+O2=>R300H+R19C3H7	4.2E+0013	0.000	53033.0	! BI 3 CN
B10+C3H8=>R20H+iC3H7	2.6E+0013	0.000	5200.0	! ME 15 CW
B10+C3H8=>R20H+R19C3H7	1.0E+0014	0.000	7850.0	! ME 16 CW
C3H8+R1H=>H2+iC3H7	9.0E+0006	2.000	5000.0	! ME 17 CW
!C3H8+R1H=>H2+R19C3H7	5.7E+0007	2.000	7700.0	! ME 18 CW!!ds
мйса PRF				
C3H8+R20H=>H2O+iC3H7	2.6E+0006	2.000	-765.0	! ME 19 CW
!C3H8+R20H=>H2O+R19C3H7	5.4E+0006	2.000	450.0	! ME 20 CW!!ds
мйса PRF				
C3H8+R300H=>H2O2+iC3H7	4.0E+0011	0.000	15500.0	! ME 21 CN
!C3H8+R300H=>H2O2+R19C3H7	1.2E+0012	0.000	17000.0	! ME 22 CN!!ds
мйса PRF				
C3H8+R4CH3=>CH4+iC3H7	2.0E+0011	0.000	9600.0	! ME 23 CN
!C3H8+R4CH3=>CH4+R19C3H7	6.0E-0001	4.000	8200.0	! ME 24 CN!!ds
мйса PRF				
C3H8+R5CH0=>HCHO+iC3H7	1.0E+0007	1.900	17000.0	! ME 25 CN
C3H8+R5CH0=>HCHO+R19C3H7	2.0E+0005	2.500	18500.0	! ME 26 CN
C3H8+R11C2H5=>C2H6+iC3H7	2.0E+0011	0.000	11000.0	! ME 33 CN
!C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	! ME 34 CR!!ds
мйса PRF				
C3H8+iC3H7=>C3H8+R19C3H7	8.4E-0003	4.200	8700.0	! ME 35 CN
R1H+iC3H7=>C3H8	8.3E+0012	0.000	0.0	! CO 36 K

!\*\*\*\*\*Reactions of Acetone\*\*\*\*\*!

!R14CH3CO+R4CH3=>C2H6CO	4.0E15	-0.8	0. !
(231, -231)<TSAnG86>!			
R14CH3CO+R4CH3=>C2H6CO	2.7E15	-0.8	0. !
(231, -231)<TSAnG86>! A/1.5 to improve the agreement simu/exp at low pressure.			
iC3H7+B10=>C2H6CO+R1H	1.0	0.0	0.0 !
Tsang88 (Nist)			
C2H6CO+O2=>R300H+CH2COZ+R4CH3	4.2E12	0.0	49.28E3 !
Kingas!			
C2H6CO+B10=>CH2COZ+R4CH3+R20H	1.02E14	0.0	7.85E3 !
Buda!			

C2H6CO+R1H=>CH2COZ+R4CH3+H2	5.70E07	2.0	7.70E3
C2H6CO+R20H=>CH2COZ+R4CH3+H2O	5.34E06	2.0	0.45E3
C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4	6.00E-1	4.0	8.20E3
C2H6CO+R300H=>CH2COZ+R4CH3+H2O2	1.20E12	0.0	17.0E3

!\*\*\*\*\*Reactions of Propanal\*\*\*\*\*!

!R5CHO+R11C2H5=>C2H5CHO	1.8E13	0.	0.
!(141, -141)<TSAng86>!			
!C2H5CHO=R5CHO+R11C2H5	1.07E+14	0.0	62600
!Decottignies et al.COMBT.FLAME 2002, 130, 225-240			
R5CHO+R11C2H5=C2H5CHO	3.4E+13	0.0	0.0
!= "CH3+C2H5=C3H8".			
!C2H5CHO=R5CHO+R11C2H5	2.45E+15	0.0	72864.5
!Lifshitz et al.J. Phys. Chem., 94 (1990)			
R13CH2CHO+R4CH3=C2H5CHO	3.4E+13	0.0	0.0
!= "CH3+C2H5=C3H8".			
!C2H5CHO=R4CH3+R13CH2CHO	7.00E+15	0	81703
!Baulch et al 1992, J. Phys.Chem.Ref.Data 21 411-429.			
B10+C3H6Y=>C2H5CHO	1.000E+12	0	5000.0
!Mech Franssoldati			
!C2H5CHO+R1H=H2+B2CO+R11C2H5	4.0E13	0.0	4.2E3
!<Heyberger>! ADZ 714			
!C2H5CHO+R20H=H2O+B2CO+R11C2H5	4.0E12	0.0	0.5E3
!<Heyberger>! ADZ 715			
!C2H5CHO=R4CH3+R13CH2CHO	2.00E+16	0	83800.
!Mech Franssoldati			
C2H5CHO+R1H=H2+R25C2H5CO	1.17E+11	0.0	6000
!Decottignies et al.2002.			
C2H5CHO+B10=R20H+R25C2H5CO	5.000e+12	0.0	
1.790e+03 !Curran et al. Fuel (2011) 90(1) 331-338.			
C2H5CHO+R20H=H2O+R25C2H5CO	2.690e+10	0.760	
-3.400e+02 !Curran et al. Fuel (2011) 90(1) 331-338.			
R25C2H5CO=B2CO+R11C2H5	2.95E+12	0.0	11100.0
!Decottignies et al.2002.			

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! REACTIONS DES ESPECES NON OXYGENES EN C4 !

!\*\*\*\*\* REACTIONS DE C4H2 \*\*\*\*\* (CH//CC//CH) diacetylene \*\*\*\*\* !

R9C2H+R9C2H=C4H2	1.8E13	0.0	0.0	!
<TSAng86>!				
2C2H2=C4H2+H2	1.5E13	0.0	42.7E3	!
<LEUnG95>!				

C2H2+R9C2H=C4H2+R1H BAULCH94!	9.0E13	0.0	0.0	!
!C4H2+R1H=C2H2+R9C2H <MEREDITH86>!	6.0E14	0.0	15.4E3	!
C4H2+R20H=>R5CHO+C3H2 <LEEDS-website>!	6.7E12	0.0	-0.4E3	!
C4H2+O2=R12CHCOZ+R12CHCOZ <HIDAKA02>!!!	9.6E12	0.0	31.1E3	!
C4H2+R9C2H=>C6H2+R1H <MEREDITH86>!	4.0E13	0.0	0.0	!
C6H2+R1H=>C4H2+R9C2H <MEREDITH86>!	9.3E14	0.0	15.1E3	!

!\*\*\*\*\* REACTIONS DE nC4H3 \*\*\*\*\* (ΓCH//CHC///CH) \*\*\*\*\*!

nC4H3(+M)=C4H2+R1H(+M) <MILLER92>!	1.0E14	0.0	36.0E3	!
LOW /1.0E14 0.0 30E3/ TROE / 1.0 1.0 1.0E8/				
C3H3+B4CH=nC4H3+R1H <MILLER92>!	7.0E13	0.0	0.0	!
!C3H3+B4CH=nC4H3+R1H <MILLER92>!	5.0E13	0.0	0.0	!
R9C2H+R10C2H3V=nC4H3+R1H <TSAng86>!	1.8E13	0.0	0.0	!
nC4H3+R1H=iC4H3+R1H <WAnG97>20Torr!	2.4E11	0.79	2.41E3	!
nC4H3+R1H=C4H2+H2 <0.5* la cst de la react(c2h3+h)>!	0.6E13	0.0	0.0	!
2C2H2=nC4H3+R1H <LEUnG95>!	1.0E12	0.0	64.1E3	!
nC4H3+R20H=C4H2+H2O <0.5* la cst de la react(c2h3+oh)>!	1.5E13	0.0	0.0	!
!***				
!nC4H3+C2H2=C6H4#+R1H <WESTMORELANd89, p=2.6kPa>!	1.64E9	0.73	12.2E3	!
nC4H3+C2H2=C6H4#+R1H <WESTMORELANd89, p=101kPa>!	3.0E-11	6.48	6.6E3	!
!***				
!nC4H3+C2H2=lC6H4+R1H <WESTMORELANd89, p=2.6kPa>!	29.6	3.33	9.6E3	!
nC4H3+C2H2=lC6H4+R1H <WESTMORELANd89, p=101kPa>!	2.77E-7	5.59	6.0E3	!
!***				
!nC4H3+C2H2=lC6H5 <WESTMORELANd89, p=2.6kPa>!	1.73E11	-0.41	4.0E3	!
nC4H3+C2H2=lC6H5 <WESTMORELANd89, p=101kPa>!	6.17E15	-1.51	4.8E3	!
!***				
!nC4H3+C2H2=C6H5# <WESTMORELANd89, p=2.6kPa>!	3.33E24	-3.89	9.2E3	!
nC4H3+C2H2=C6H5# <WESTMORELANd89, p=101kPa>!	7.0E14	-0.86	6.4E3	!
!***				

!\*\*\*\*\* REACTIONS DE iC4H3 \*\*\*\*\* (CH2//CΓC///CH) \*\*\*\*\*

iC4H3=nC4H3 <LEUnG95>!	1.5E13	0.0	67.8E3	!
iC4H3(+M)=C4H2+R1H(+M) <MILLER92>!	1.0E14	0.0	55.0E3	!
LOW /2.0E15 0.0 48E3/ TROE /1.0 1.0 1.0E8/				
C3H2+B5CH2=iC4H3+R1H as(7)<BAULCH94>!	1.2E14	0.0	0.8E3	!
iC4H3+R1H=2C2H2 <WAnG97>20Torr! !	2.40E19	-1.6	2800	!
C3H3+B4CH=iC4H3+R1H <MILLER92>!	7.0E13	0.0	0.0	!
iC4H3+R1H=C4H2+H2 <equiv a la cst de la react(c2h3+h)>!	1.2E13	0.0	0.0	!
iC4H3+B10=CH2COZ+R9C2H <MILLER92>!	2.0E13	0.0	0.0	!
iC4H3+R20H=C4H2+H2O equiv a la cst de la react(c2h3+oh)>!	3.0E13	0.0	0.0	!<
iC4H3+O2=CH2COZ+R12CHCOZ <MILLER92>!	1.0E12	0.0	0.0	!
*				
iC4H3+R10C2H3V=2C3H3 MILLER 92 !	4.0E12	0.0	0.0	!
iC4H3+R10C2H3V=>1C6H5+R1H MILLER 92!	6.0E12	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE C4H4 \*\*\*\*\* (CH2//CHC///CH) vinylacetylene \*\*\*\*\*!

C3H3+B5CH2=C4H4+R1H <MILLER92>!	4.0E13	0.0	0.0	!
R10C2H3V+C2H2=>C4H4+R1H (40, -40)<DOUTE95>!	2.0E13	0.0	25.1E3	!
C4H4+R1H=>R10C2H3V+C2H2 <DOUTE95>	2.0E13	0.0	12.4E3	!
C2H4Z+R9C2H=C4H4+R1H (50, -50)<TSAnG86>!	1.2E13	0.0	0.0	!
C4H4+R1H=nC4H3+H2 <Miller 92>!	2.0E7	2.0	15.E3	!
C4H4+R1H=iC4H3+H2 <Miller 92>!	3.0E7	2.0	5.E3	!
R9C2H+C4H4=>C2H2+iC4H3 <MEREDITH86>!	4.0E13	0.0	0.0	!
C2H2+iC4H3=>R9C2H+C4H4 <MEREDITH86>!	3.0E13	0.0	27.9E3	!
R10C2H3V+C4H4=>C2H4Z+nC4H3 <MEREDITH86>!	5.0E11	0.0	16.3E3	!
nC4H3+C2H4Z=>R10C2H3V+C4H4 <MEREDITH86>!	3.5E11	0.0	13.4E3	!
R10C2H3V+C4H4=>C2H4Z+iC4H3 <MEREDITH86>!	5.0E11	0.0	16.3E3	!

iC4H3+C2H4Z=>R10C2H3V+C4H4 <MEREDITH86>!	1.3E11	0.0	24.1E3 !
C4H4+C2H2=C6H5#+R1H BENSON !MF	1.0E09	0.0	30.02E3 !
C4H4+R10C2H3V=C6H6#+R1H <LInSTEDT96>!	1.9E12	0.0	2.5E3 !
C4H4+B10=aC3H4+B2C0 <LEUnG95>!	3.0E13	0.0	1.8E3 !
C4H4+B10=pC3H4+B2C0 <MILLER>!	2.7E13	0.0	1.8E3 !
C4H4+R20H=nC4H3+H20 <MILLER92>!	7.5E6	2.0	5.0E3 !
C4H4+R20H=iC4H3+H20 <MILLER92>!	1.0E7	2.0	2.0E3 !
aC3H4+aC3H4=C2H4Z+C4H4 <HIDAKA89>!	1.0E15	0.0	48.0E3 !

!\*\*\*\*\* REACTIONS DE tC4H4 \*\*\*\*\* (CH2//C//C//CH2) \*\*\*\*\*!

tC4H4+R20H=iC4H3+H20 <Marinov>!	2.0E7	2.0	2.0E3 !
tC4H4+R1H=iC4H3+H2 <Marinov>!	3.0E7	2.0	6.0E3 !

!\*\*\*\*\* REACTIONS DE nC4H5 \*\*\*\*\* (ΓCH//CHCH//CH2) \*\*\*\*\*

nC4H5(+M)=R1H+C4H4(+M) <MILLER92>!	1.0E14	0.0	37.0E3 !
LOW /1.00e+14 0.0 30000/			
nC4H5+R1H=C4H4+H2 <WAnG97>!	1.5E13	0.0	0.0 !
nC4H5+R1H=iC4H5+R1H <MILLER92>!	1.0E14	0.0	0.0 !
nC4H5+R4CH3=C5H8 <estimated> !	1.0E13	0.0	0.0 !
nC4H5=C2H2+R10C2H3V <HIDAKA96>!	1.0E14	0.0	43.9E3 !
!*** !MF car lC6H6 n'intervient qu'ici			
!nC4H5+C2H2=lC6H6+R1H <WESTMORELANd89, p=2.6kPa>!	1.17E-15	7.84	2.0E3 !
!nC4H5+C2H2=lC6H6+R1H <WESTMORELANd89, p=101kPa>!	3.47E-15	7.73	2.5E3 !
!*** !nC4H5+C2H2=C6H6#+R1H <WESTMORELANd89, p=2.6kPa>!	1.90E7	1.47	4.2E3 !
nC4H5+C2H2=C6H6#+R1H <WESTMORELANd89, p=101kPa>!	2.38E8	1.18	3.7E3 !
!*** !nC4H5+C2H2=lC6H7 <WESTMORELANd89, p=2.6kPa>!	8.74E12	-1.27	3.6E3 !

nC4H5+C2H2=1C6H7 <WESTMORELANd89, p=101kPa>! !***	7.24E14	-1.38	4.0E3 !
!nC4H5+C2H2=C6H7# <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=C6H7# <WESTMORELANd89, p=101kPa>! !***	1.96E19	-3.35	5.2E3 !
!R10C2H3V+nC4H5=1C6H7+R1H <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=1C6H7+R1H <WESTMORELANd89, p=101kPa>! !***	7.12E21	-3.64	6.3E3 !
!R10C2H3V+nC4H5=1C6H8 <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=1C6H8 <WESTMORELANd89, p=101kPa>! !***	8.28E-28	11.89	5.0E3 !
!R10C2H3V+nC4H5=C6H8# <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=C6H8# <WESTMORELANd89, p=101kPa>! !***	3.55E-43	16.16	-0.2E3 !
!R10C2H3V+nC4H5=C6H6#+H2 <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=C6H6#+H2 <WESTMORELANd89, p=101kPa>! !***	2.90E15	-0.78	1.0E3 !
nC4H5+R20H=C4H4+H20 <WAnG97>!	1.50E13	-0.075	0.1E3 !
!nC4H5+O2=R5CHO+C2H3CHO as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>	5.50E15	-1.67	1.5E3 !
nC4H5+O2=R5CHO+C2H3CHO	8.53E13	-1.11	0.8E3 !
nC4H5+O2=C2H4Z+B2CO+R5CHO	2.80E-7	5.63	-1.9E3 !
nC4H5+O2=C4H4+R300H MF as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>	1.84E-13	7.07	-3.6E3 !
!***** REACTIONS DE iC4H5 ***** (CH2//CHCΓ//CH2) *****stabililise par resonnance	2.5E12	0.0	0.0 !
iC4H5=nC4H5 <LEUnG95>!	1.7e29	-5.31	6.5E3 !MF
iC4H5(+M)=R1H+C4H4(+M) <MILLER92>!	5.67E28	-5.31	6.5E3 !MF
LOW /2.0E15 0.0 42000/	1.13e29	-5.31	6.5E3 !MF
iC4H5+R1H=C4H4+H2 <WAnG97>!	5.19E15	-1.26	3.31e3 !
iC4H5+R4CH3=iC5H8 <estimated> !			
2R10C2H3V=iC4H5+R1H <WAnG97>20Torr!	1.5E30	-4.95	13.0E3 !



!***2R10C2H3V=iC4H5+R1H <WAnG97>760Torr!	1.2E22	-2.44	13.7E3 !
iC4H5+R20H=C4H4+H2O <WAnG97>!	5.50E12	0.0	0.0 !
iC4H5+O2=HCHO+CH2CHCO estimй par{O2+C2H3=HCHO+CHO}!	4.5E16	-1.39	1.0E3 !
iC4H5+O2=C4H4+R300H estimй par {O2+C2H3=C2H2+O0H}!	1.34E6	1.61	-400 !

!\*\*\*\*\* REACTIONS DE C4H5-1s \*\*\*\*\* (CH3/CH<sup>Г</sup>/C///CH) \*\*\*\*\*stabililise par  
resonance

!C4H5-1s=R1H+C4H4 <HIDAKA96>!	3.0E13	0.0	45.0E3 !
C4H5-1s=R1H+C4H4 add inverse!	6.0E13	0.0	50.4E3 !
! Les rñactions suivantes sont deduites de celles de C3H3			
C4H5-1s+R1H=C4H4+H2 <MILLER92/BRAUn89>!	2.0E13	0.0	0.0 !
C4H5-1s+B10=R9C2H+CH3CHO <MILLER92/SLAGUE91>!	1.4E14	0.0	0.0 !
C4H5-1s+R20H=C4H4+H2O <MILLER92>!	2.0E13	0.0	0.0 !
C4H5-1s+R20H=R5CHO+sC3H5 <WAnG97>!	4.0E13	0.0	0.0 !
C4H5-1s+O2=R5CHO+B2CO+C2H4Z <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3 !
C4H5-1s+C4H5-1s=C8H10# <STEIn90>shocktube!	1.0E12	0.0	0.0 !

!\*\*\*\*\* REACTIONS DE C4H5-1p \*\*\*\*\* (CH2<sup>Г</sup>/CH2/C///CH) \*\*\*\*\*

!C4H5-1p=R1H+C4H4 <HIDAKA96>!	3.0E13	0.0	45.0E3 !
!C4H5-1p=R1H+C4H4 <HIDAKA96>!	4.0E13	0.0	38.8E3 !
C4H5-1p=R9C2H+C2H4Z <HIDAKA96>!	2.0E14	0.0	57.0E3 !
C4H5-1p+O2=C4H4+R300H PAG00!	1.6E12	0.0	5.0E3 !
C4H5-1p=C4H5-1s PAG00!	5.0E12	0.0	37.4E3 !

!\*\*\*\*\* REACTIONS DE C4H5-2 \*\*\*\*\* (CH3/C///C/CH2<sup>Г</sup>) \*\*\*\*\*stabililise par  
resonance

!C4H5-2=R1H+tC4H4 <fromHIDAKA96+5!>	3.0E13	0.0	50.0E3 !
C4H5-2=R1H+tC4H4 toto!	6.0E13	0.0	54.3E3 !
!C4H5-2=iC4H5 <fromHIDAKA96>!	3.0E13	0.0	50.0E3 !

C4H5-2=iC4H5 PAG00!	5.0E12	0.0	50.5E3 !
C4H5-2+C4H5-2=C8H10# <STEIn90>shocktube!	1.0E12	0.0	0.0 !

! Les rñactions suivantes sont deduities de celles de C3H3

C4H5-2+B10=C3H3+HCHO <MILLER92/SLAGUE91>!	1.4E14	0.0	0.0 !
C4H5-2+R20H=R10C2H3V+B2C0+R4CH3 <WAnG97>!	4.0E13	0.0	0.0 !
C4H5-2+O2=CH2COZ+B2C0+R4CH3 <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3 !

!\*\*\*\*\* REACTIONS DE C4H6Z2 \*\*\*\*\* 1,3 Butadiene (CH2CHCHCH2) \*\*\*\*\*!

!R10C2H3V+R10C2H3V=C4H6Z2 <TSAnG86 P=2.6KPa T=1500>!	6.8E12	0.0	0.0 !
R10C2H3V+R10C2H3V=C4H6Z2 <HIDAKA96shocktube>!	9.8E14	-0.5	0.0 !
!			
C4H6Z2=C4H4+H2 <HIDAKA96>	2.5E15	0.0	94.7E3 !
C4H6Z2=iC4H5+R1H <HIDAKA96>!	1.4E15	0.0	98.0E3 !
!			
C2H4Z+R10C2H3V=C4H6Z2+R1H <TSAnG86>!	5.0E11	0.0	7.3E3 !
!			
C4H6Z2+R1H=nC4H5+H2 <WAnG97>!	1.3E6	2.53	12.2E3 !
C4H6Z2+R1H=iC4H5+H2 <WAnG97>!	6.6E5	2.53	9.2E3 !
!			
!C4H6Z2+R1H=C4H7-1 ESTIMATED *2!	2.6E13	0	3.2E3 !
!C4H6Z2+R1H=C4H7Y ESTIMATED *2!	2.6E13	0	1.56E3 !
C4H6Z2+R1H=C4H7-1 ESTIMATED	1.3E13	0	3.2E3 !
C4H6Z2+R1H=C4H7Y ESTIMATED !	1.3E13	0	1.56E3 !
!			
C4H6Z2+R4CH3=nC4H5+CH4 <WU87>!	7.0E13	0.0	18.5E3 !
C4H6Z2+R4CH3=iC4H5+CH4 <WU87-3kcal>!	7.0E13	0.0	15.5E3 !
!C4H6Z2+R4CH3=C5H9Y 88 nist!	6.3E10	0.0	7.49E3 ! PERRIN
!C4H6Z2+R4CH3=iC5H9 Estimated*2!	1.8E11	0.0	8.0E3 !
C4H6Z2+R4CH3=C5H9Y PERRIN 88 nist!	6.31E10	0.0	7.49E3 !
C4H6Z2+R4CH3=iC5H9 Estimated!	9.64E10	0.0	8.0E3 !

!				
!C4H6Z2+R10C2H3V=nC4H5+C2H4Z	5.0E14	0.0	22.8E3	!
<HIDAKA96>!				
C4H6Z2+R10C2H3V=iC4H5+C2H4Z	5.0E14	0.0	19.8E3	!
<HIDAKA96-3kcal>!				
!				
C4H6Z2+B10=C3H5Y+R1H+B2C0	6.0E08	1.45	0.9E3	!
<LEUnG95, BREZInSKY84>!				
!				
R10C2H3V+C4H6Z2=C6H8#+R1H	7.4E014	-0.66	8.42E3	!
<frenklach >!				
!R10C2H3V+C4H6Z2=C6H8#+R1H	2.28E12	-0.24	9.9E3	!
<WESTMORELANd89, p=2.6kPa>!				
!R10C2H3V+C4H6Z2=C6H8#+R1H	4.15E-11	6.39	2.4E3	!
<WESTMORELANd89, p=101kPa>!				
!***				
!R10C2H3V+C4H6Z2=lC6H8+R1H	1.0E10	1.05	14.0E3	!
<WESTMORELANd89, p=2.6kPa>!				
!R10C2H3V+C4H6Z2=lC6H8+R1H	2.48E-15	8.20	6.3E3	!
<WESTMORELANd89, p=101kPa>!				
!***				
C4H6Z2+C2H2=C6H8#	2.3E12	0.0	35.0E3	!
<WESTMORELANd89>!				
!***				
!MF car lC6H9 n'intervient qu'ici				
!R10C2H3V+C4H6Z2=lC6H9	5.48E28	-5.31	9.3E3	!
<WESTMORELANd89, p=2.6kPa>!				
!R10C2H3V+C4H6Z2=lC6H9	1.48E12	-0.17	3.2E3	!
<WESTMORELANd89, p=101kPa>!				
!***				
R10C2H3V+C4H6Z2=C6H9Z#	1.64E29	-6.12	9.6E3	!
<WESTMORELANd89, p=2.6kPa>!				
!R10C2H3V+C4H6Z2=C6H9Z#	7.06E13	-1.35	4.0E3	!
<WESTMORELANd89, p=101kPa>!				
!***				
C4H6Z2+C2H4Z=C6H10#	2.3E10	0.0	27.0E3	!
<WESTMORELANd89>!				
C4H6Z2+R20H=nC4H5+H2O	6.2E6	2.0	3.4E3	!
<WAnG97>!				
C4H6Z2+R20H=iC4H5+H2O	3.1E6	2.0	0.4E3	!
<WAnG97>!				
C4H6Z2+R20H=C3H5Y+HCHO	2.8E12	0.0	-0.9E3	!
<LIInSTEDT96>!				
C4H6Z2+R20H=CH3CHO+R10C2H3V	5.6E12	0.0	-0.9E3	!
<fromLIInSTEDT96>!				
C4H6Z2+O2=iC4H5+R300H	4.0E13	0.0	57.9E3	!
<LEUnG95>!				
C4H6Z2+C3H3=nC4H5+aC3H4	1.0E13	0.0	22.5E3	!
<HIDAKA96>!				
C4H6Z2+C3H3=iC4H5+aC3H4	1.0E13	0.0	19.5E3	!
<HIDAKA96-3kcal>!				

!\*\*\*\*\* REACTIONS DE C4H6-12 \*\*\*\*\* (1,2) Butadiene (CH2CCHCH3) \*\*\*\*\*

!C4H6-12=C4H6Z2	3.0E13	0.0	65.0E3 !
<HIDAKA96>!			
!C4H6-12=iC4H5+R1H	4.2E15	0.0	92.6E3 !
<LEUnG95>!			
!C4H6-12+R1H=R10C2H3V+C2H4Z	4.0E11	0.0	0.0 !
<LEUnG95>!			
!C4H6-12=C3H3+R4CH3	7.3E14	0.0	75.4E3 !
<kingas1500K>!			
!C4H6-12+R1H=C4H7-2	1.3E13	0.0	1.6E3 !
<heyberger> !			
!C4H6-12+R1H=C4H7Y	1.2E11	0.69	3.0E3 !
<heyberger>!			
!C4H6-12+R1H=C4H7T	1.3E13	0.0	3.2E3 !
<heyberger> !			
!C4H6-12+R1H=iC4H5+H2	1.7E5	2.5	2.5E3 !
<asTSAnG91>!			
!C4H6-12+R4CH3=iC4H5+CH4	2.2E0	3.5	5.7E3 !
<asTSAnG91>!			
!C4H6-12+R11C2H5=iC4H5+C2H6	2.2E0	3.5	6.6E3 !
<asTSAnG91>!			
!C4H6-12+B10=iC4H5+R20H	1.7E11	0.7	5.9E3 !
<asTSAnG91>!			
!C4H6-12+R20H=iC4H5+H20	3.1E6	2.0	-0.3E3 !
<asTSAnG91>!			
!C4H6-12+R300H=iC4H5+H202	9.6E3	2.6	13.9E3 !
<asTSAnG91>!			

!\*\*\*\*\* REACTIONS DE (c-C4H6) \*\*\*\*\* methyl-cyclopropene \*\*\*\*\*

!B6CH2+pC3H4=cC4H6	1.8E14	0.0	0.0 !
<LEUnG95>!			
!cC4H6=C4H6Z2	3.0E13	0.0	42.3E3 !
<LEUnG95>!			
!cC4H6=C4H6-12	3.0E13	0.0	43.8E3 !
<LEUnG95>!			

!\*\*\*\*\* REACTIONS DE (C4H6-1) \*\*\*\*\* 1 Butyne \*\*\*\*\*

!C4H6-1=C4H6-12	2.5E13	0.0	65.0E3 !
<HIDAKA96>!			
!C4H6-1=C4H5-1s+R1H	7.7E14	0.0	87.9E3 !
Kinga&dH Melius!			
!C4H6-1=C4H5-1p+R1H	9.1E14	0.0	99.6E3 !
Kingas!			
!C4H6-1=>C3H3+R4CH3	3.0E15	0.0	75.8E3 !
<HIDAKA96>!			
!C4H6-1+R1H=R4CH3+aC3H4	1.3E5	2.5	1.0E3 !
<HIDAKA96>!			
!C4H6-1+R1H=R11C2H5+C2H2	6.5E4	2.5	1.0E3 !
<HIDAKA96>!			
!C4H6-1+R1H=R4CH3+aC3H4	3.2E12	0.0	1.7E3 !
<asWAGnER72>!			

!C4H6-1+R1H=R11C2H5+C2H2 <asWAGnER72>!	3.2E12	0.0	1.7E3 !
! Les rñactions suivantes sont deduities de celles de 1-C4H8 generes par EXGAS			
!C4H6-1+R1H=H2+C4H5-1s <EXGAS>!	5.4E4	2.5	-1.9E3 !
!C4H6-1+R4CH3=CH4+C4H5-1s <EXGAS>!	1.5E12	0.0	7.1E3 !
!C4H6-1+B10=R20H+C4H5-1s <EXGAS>!	8.8E10	0.7	3.2E3 !
!C4H6-1+R20H=H2O+C4H5-1s <EXGAS>!	3.0E6	2.0	-1.5E3 !
!C4H6-1+O2=>R300H+C4H5-1s <InGHAM95sec>!	1.4E12	0.0	36.0E3 !
!C4H6-1+O2=>R300H+C4H5-1s <InGHAM95sec>!	1.4E12	0.0	41.4E3 !
!C4H6-1+O2=>R300H+C4H5-1s <DAGAUT90sec>!	4.2E12	0.0	49.5E3 !
!C4H6-1+R300H=>H2O2+C4H5-1s <EXGAS>!	6.4E3	2.6	12.4E3 !
! Les rñactions suivantes sont deduities de celles generes par EXGAS pour H primaires			
!C4H6-1+R1H=H2+C4H5-1p <EXGAS>!	2.9E7	2.0	7.7E3 !
!C4H6-1+R4CH3=CH4+C4H5-1p <EXGAS>!MF	3.7	4.0	8.2E3 !
!C4H6-1+B10=R20H+C4H5-1p <EXGAS>!	5.1E13	0.0	7.8E3 !
!C4H6-1+R20H=>H2O+C4H5-1p <EXGAS>!	2.7E6	2.0	-0.4E3 !
!C4H6-1+O2=>R300H+C4H5-1p <EXGAS>!	1.2E13	0.0	49.0E3 !
!C4H6-1+R300H=>H2O2+C4H5-1p <EXGAS>!	6.0E11	0.0	17.0E3 !
! Les rñactions d'addition suivantes sont deduities de celles de pC3H4			
!C4H6-1+B10=R12CHCOZ+R11C2H5 <asWARnATZ84>!	1.5E13	0.0	2.1E3 !
!C4H6-1+R20H=CH2COZ+R11C2H5 <asB00DAGHIANs87>!	4.3E11	0.0	-0.8E3 !
!***** REACTIONS DE (C4H6-2)***** 2 Butyne *****			
!C4H6-2=C4H6Z2 <HIDAKA96>!	3.0E13	0.0	65.0E3 !
!C4H6-2=C4H6-12 <HIDAKA96>!	3.0E13	0.0	67.0E3 !
!C4H6-2=C4H5-2+R1H <HIDAKA96>!	2.0E14	0.0	87.3E3 !
!C4H6-2+R1H=R4CH3+pC3H4 <HIDAKA96>!	2.6E5	2.5	1.0E3 !
!C4H6-2+R1H=R4CH3+pC3H4 <asWAGnER72>	6.5E12	0.0	1.7E3 !

! Les rñactions suivantes sont deduities de celles de pC3H4

!C4H6-2+R1H=C4H5-2+H2	3.4E5	2.5	2.5E3 !
<asTSAnG91*2>!			
!C4H6-2+R4CH3=C4H5-2+CH4	4.4E0	3.5	5.7E3 !
<asTSAnG91*2>!			
!C4H6-2+B10=B2C0+R10C2H3V+R4CH3	1.5E13	0.0	2.1E3 !
<asWARnATZ84>!			
!C4H6-2+B10=R20H+C4H5-2	1.2E11	0.7	7.6E3 !
<asTSAnG91*2>!			
!C4H6-2+R20H=B2C0+C2H4Z+R4CH3	4.3E11	0.0	-0.8E3 !
<asB00DAGHIANs87>!			
!C4H6-2+R20H=C4H5-2+H20	6.2E6	2.0	-0.3E3 !
<asTSAnG91*2>!			
!C4H6-2+02=C4H5-2+R300H	4.2E12	0.0	44.0E3 !
<InGHAM95*2>+4!			
!C4H6-2+R300H=C4H5-2+H202	1.9E4	2.6	13.9E3 !
<asTSAnG91*2>!			

!\*\*\*\*\* Reactions de C4H7-1 (CH2=CH-CH2-CH2.)!

!C4H7-1=C4H7Y	3.34E09	1.0	39.1E3 !
ESTIMATED !			
!C4H7-1=C4H7V	3.3E9	1.0	20.7E3 !
Estimated!			
!C4H7-1=C2H4Z+R10C2H3V	2.0E13	0.0	35.5E3 !
Estimated!			
!C4H7-1+R4CH3=C5H10	2.0E13	0.0	0.0 !
Estimated !			
!C4H7-1+R1H=C4H8Y	1.0E14	0.0	0.0 !
Estimated!			

!\*\*\*\*\* Reactions de C4H7Y (CH3-CH.-CH=CH2)!\*\*\*\*\*stabililise par resonance

!C4H7Y+R1H=C4H8Y	2.0E13	0.0	0.0 !
asTSANG 91!!			
!C4H7Y+R1H=H2+C4H6Z2	0.9E13	0.0	0.0 !
asTSANG 91!!			
!C4H7Y+R1H=H2+C4H6-12	0.9E13	0.0	0.0 !
asTSANG 91!			
!C4H7Y+R300H=R20H+C2H3CHO+R4CH3	1.0E15	-0.8	0.0 !
<Heyberger>!			
!C4H7Y+R4CH3=iC5H10	0.5E13	0.0	0.0 !
Estimated !			

!\*\*\*\*\*Reactions de C4H7V (CH3-CH2-CH=CH.)\*\*\*\*\*!

!C4H7V=C4H7Y	1.9E10	1.0	36.3E3 !
Heyberger!			
!C4H7V=R11C2H5+C2H2	2.0E13	0.0	33.0E3 !
Heyberger!			

!\*\*\*\*\*Reactions de C4H7-2 (CH3-C.=CH-CH3)\*\*\*\*\*!

!C4H7-2=C4H7Y	2.9E10	1.0	37.8E3 !
ESTIMATED !			

!C4H7-2=R4CH3+pC3H4 2.0E13 0.0 31.5E3 !  
ESTIMATED !

!\*\*\*\*\*Reactions de C4H7T (CH2=C.-CH2-CH3)\*\*\*\*\*!

!C4H7T=C4H7-1 3.34E09 1.0 40.6E3 !  
ESTIMATED !  
!C4H7T=C4H7Y 2.0E13 0.0 47.0E3 !  
<Heyberger>!  
!C4H7T=R4CH3+aC3H4 2.0E13 0.0 32.5E3 !  
ESTIMATED !

!\*\*\*\*\*Reactions du 1-butene!

!C4H8Y+O2=C4H7Y+R300H 3.6E12 0.0 38.2E3 !  
<Heyberger>!  
!C4H8Y+R1H=C4H7Y+H2 5.4E4 2.5 -1.9E3 !  
<Heyberger>!  
!C4H8Y+R20H=>HCHO+R4CH3+C2H4Z 1.4E12 0.0 -1.0E3 !  
<Heyberger>!  
!C4H8Y+R20H=R4CH3+C2H5CHO 1.4E12 0.0 -1.0E3 !  
<Heyberger>!!ds мйса PRF  
!C4H8Y+R20H=C4H7Y+H2O 3.0E6 2.0 -1.52E3 !  
<Heyberger>!  
!C4H8Y+R4CH3=C4H7Y+CH4 1.0E11 0.0 7.3E3 !  
<Heyberger>!  
  
!C2H5CHO+R1H=H2+B2CO+R11C2H5 4.0E13 0.0 4.2E3 !  
<Heyberger>!  
!C2H5CHO+R20H=H2O+B2CO+R11C2H5 4.0E12 0.0 0.5E3 !  
<Heyberger>!

!\*\*\*\*\*reactions de iC4H8\*\*\*\*\*!

!iC4H8+R20H=iC3H7+HCHO 1.4E12 0.0 -1040.0 !  
(idem RF)  
!iC4H8+R1H=>iC4H7+H2 3.5E5 2.5 2510 !  
(idem RF)  
!iC4H8+R20H=>iC4H7+H2O 6.0D+06 2.000 -298.0 !  
MES 878<C.M.>!(idem RF)  
!iC4H7+R1H=iC4H8 1.0E14 0.0 0.0 !  
<estimation>!  
!iC4H7+R300H=>R20H+HCHO+tC3H5 1.0E15 -0.8 0.0 !  
<Heyberger>!

!  
\*\*\*\*\*

\*\*!

!  
\*\*\*\*\*

\*\*\*\*\*!

!\* MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE  
\*!

```

!*
*!
!*      efficiency coefficients for O2, CO, CO2, H2O, AR, C6H6#
*!
!
*****
*****!
!*          PRIMARY MECHANISM OF THE OXIDATION OF BENZENE
*!
!
*****
*****!

```

!REACTIONS OF BENZENE MOLECULES!

!\*\*\*Umimolecular inititiation!

C6H5#+R1H(+M)=C6H6#(+M)                    1.0E14            0.0            0.0            !  
<WANG97>!

LOW /6.6E75 -16.3 7.0E3/  
TROE /1.0 0.1 585 6113/

O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/

!\*\*\*Bimolecular inititiation!

C6H6#+O2=C6H5#+R300H                    6.0E13            0.0            63.4E3        !  
<ALZUETA00>!

!\*\*\*additions!

C6H6#+R1H=C6H7#                    3.2E13            0.0            3.2E3        !  
<MEBEL97>!

C6H6#+B10=C6H50#+R1H                    2.8E13            0.0            4.91E3        !  
<EMDEE92>!

C6H6#+R20H=C6H50H#+R1H                    1.3E13            0.0            10.6E3        !  
<BAULCH94>!

C6H6#+R9C2H=C6H5#C2H+R1H                    5.0E13            0.0            0.0            !  
<WANG97>!

C6H6#+R10C2H3V=styrene+R1H                    7.9E11            0.0            6.4E3        !  
<WANG97>!

!\*\*\*Metatheses!

!\*modif Zhenyu\*!

!C6H6#+R1H=C6H5#+H2                    6.0E8            1.8            16.8E3        !  
<MEBEL97>!

C6H6#+R1H=C6H5#+H2                    1.22E8            2.031            15.88E3        !  
calcul CBS-QB3 Fournet

C6H6#+B10=C6H5#+R20H                    2.0E13            0.0            14.7E3        !  
<LINDSTEDT94>!

!\*modif Zhenyu\*!

!C6H6#+R20H=C6H5#+H2O                    1.6E8            1.42            1.45E3        !  
<BAULCH92>!

C6H6#+R20H=C6H5#+H2O                    1.36E4            2.7            0.6196E3        !as  
toluene+R20H=C6H4CH3+H2O

!\*modif Zhenyu\*!



!C6H6#+R300H=C6H5#+H202 <BAULCH94>!	5.5E12	0.0	28.9E3	!
C6H6#+R300H=C6H5#+H202 toluene+R300H=C6H4CH3+H202	9.2E12	0.0	28.81E3	!as
!*modif Zhenyu*!				
!C6H6#+R4CH3=C6H5#+CH4 <ZHANG89>!	2.0E12	0.0	15.0E3	!
C6H6#+R4CH3=C6H5#+CH4 calcul CBS-QB3 Fournet	2.07E0	3.861	13.3E3	!
C6H6#+R11C2H5=C6H5#+C2H6 <ZHANG89>!	6.3E11	0.0	15.0E3	!
C6H5#+C3H6Y=C6H6#+C3H5Y <Heckmann, Hippler, Troe(1996)>	7.94E13	0.0	11.94E3	!MF
C6H6#+nC4H5=C6H5#+C4H6Z2 estimated!	6.3E11	0.0	15.0E3	!
C6H6#+iC4H5=C6H5#+C4H6Z2 estimated!	6.3E11	0.0	20.0E3	!
!REACTIONS OF C6H7# RADICALS!				
!***Isomerization!				
C6H7#=lC6H7 <WEISSMAN89!	2.5E14	0.7	41.8E3	!
!***Decomposition by beta-scission!				
!C6H7#=>C2H2+nC4H5 estimated!	2.0E13	0.0	50.0E3	!
!Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by HEYBERGER02!				
!***Oxidation!				
C6H7#+O2=C6H6#+R300H estimated!	7.9E11	0.0	9.9E3	!
!Oxidation of an allylic radical as proposed by HEYBERGER02!				
!combinations!				
C6H7#+R1H=C6H8# estimated!	1.0E14	0.0	0.0	!
!***Disproportionnations!				
C6H7#+R1H=C6H6#+H2 <RISTORI01>!	3.3E12	0.0	0.0	!
C6H7#+R20H=C6H6#+H2O estimated!	1.0E13	0.0	0.0	!
C6H7#+R4CH3=C6H6#+CH4 estimated!	3.0E12	-0.32	-0.1E3	!
C6H7#+C6H7#=C6H6#+C6H8# estimated!	8.4E10	0.0	-0.3E3	!
!analogy with the disproportionnations ofC3H5Y proposed by TSANG91!				
!REACTIONS OF C6H5# RADICALS!				
!***Isomerization!				
C6H5#=lC6H5 <BRAUN89>!	5.0E13	0.0	72.5E3	!
!lC6H5 = ch///c/ch//ch/ch//ch(.)!				

1C6H5=>2C2H2+R9C2H	2.0E13	0.0	51.0E3	!
estimated!				
!DH298 =44kcal/mol, Eadd=7 kcal/mol!				
1C6H5=1C6H4+R1H	2.0E12	0.0		
41.0E3 !estimated!				
!1C6H4 = ch///c/ch//ch/c///ch , DH298 =38kcal/mol, Eadd=3 kcal/mol!				
!from BRAUN89 at 1500 K!				
!***Reactions with O2!				
C6H5#+O2=C6H5O2	2.2E19	-2.5	0.0	!
estimated!				
C6H5#+O2=C6H5O#+B10	2.6E13	0.0	6.1E3	!
<FRANK94>!				
C6H5#+O2=OC6H4O+R1H	3.0E13	0.0	9.0E3	!
<FRANK94>!				
!as the addition of oxygen to alkyl radicals proposed by GLAUDE99!				
!***Additions!				
C6H5#+C2H2=C6H5#C2H+R1H	4.0E13	0.0	10.1E3	!
<MARINOV97>!				
C6H5#+C6H6#=biphenyl+R1H	5.6E12	-0.074	7.5E3	!
<WANG97>!				
!***Combinations!				
C6H5#+B10=C5H5#+B2C0	1.0E14	0.0	0.0	!
<FRANK94>!				
C6H5#+R20H=C6H5OH#	1.0E13	0.0	0.0	
!calculated!				
!toluene=C6H5#+R4CH3	1.0E16	0.0	97.0E3	
!<COLKET94>!				
!calculation by KINGAS!				
C6H5#+R5CHO=C6H5CHO	5.0E12	0.0	0.0	!
estimated!				
C6H5#+R10C2H3V=styrene	5.0E12	0.0	0.0	!
estimated!				
C6H5#+R11C2H5=etC6H5	5.0E12	0.0	0.0	!
estimated!				
C6H5#+R300H=C6H5O#+R20H	5.0E12	0.0	0.0	!
estimated!				
!C6H5C3H3 n'intervient qu'ici				
!C6H5#+C3H3=C6H5C3H3	3.0E12	0.0	0.0	!
<D'ANNA98>!				
C6H5#+C6H5#=biphenyl	3.8E31	-5.75	7.9E3	!
<WANG97>!				
!***disproportionations!				
C6H5#+R20H=C6H5O#+R1H	5.0E13	0.0	0.0	!
<ALZUETA00>!				
C6H5#+C6H7#=C6H6#+C6H6#	1.0E12	0.0	0.0	!
<SHANDROSS96>!				
!REACTIONS OF PHENYLPEROXY RADICALS!				
!***Decomposition by beta-scission!				
!mfC6H5O2=OC6H4O+R1H	2.0E13	0.0	30.0E3	!
estimated!				

C6H5O2=C5H4O#+R5CHO 2.0E13 0.0 30.0E3 !  
estimated!  
!see DA COSTA01!

!MF

C6H5O2+R300H=C6H500H+O2 2.0E11 0.00 -1300  
C6H500H=C6H50#+R20H 1.5E16 0.00 43000

!REACTIONS OF PHENOXY RADICALS!

!\*\*\*CO elimination!

C6H50#=B2C0+C5H5# 2.5E11 0.0 43.8E3 !  
<BAULCH92>!

!\*\*\*Combinations!

!--C6H50#+R1H(+M)=C6H50H#(+M) 2.5E14 0.0 0.0 !  
<FRENKLACH>!

C6H50#+R1H(+M)=C6H50H#(+M) 1.0E14 0.0 0.0 !  
estimated!

LOW /1.0E94 -21.84 13.9E3/ !

<FRENKLACH>!

TROE /0.043 304 60000 5896/

O2/0.4/ B2C0/0.75/ C02/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/  
C6H50#+R1H=C5H6#+B2C0 1.1E53 -10.7 41.4E3 !  
<TAN96>!

C6H50#+B10=OC6H40H 2.6E10 0.47 0.8E3 !  
<LIN95>!

C6H50#+B10=OC6H40+R1H 8.5E13 0.0 0.0 !  
<FRANCK94>!

C6H50#+B10=C5H5#+C02 1.0E13 0.0 0.0 !  
<FRANCK94>!

!REACTIONS OF HYDROXYPHENOXY RADICALS!

!\*\*\*CO elimination!

OC6H40H=B2C0+C5H40H# 7.4E11 0.0 43.8E3 !  
estimated!

!as for phenoxy radicals!

!REACTIONS OF CYCLOPENTADIENYL RADICALS!

!\*\*\*Isomerization!

C5H5#=1C5H5 1.0E14 0.0 45.5E3 !  
<BRAUN89>!

!1C5H5 = ch///c/ch//ch/ch2(.), DH298 =31kcal/mol!

!MF car 1C5H6 n'intervient qu'ici

!1C5H5+R1H=1C5H6 1.0E14 0.0 0.0 !  
estimated!

1C5H5=C3H3+C2H2 2.0E13 0.0 50.0E3 !  
estimated!

!DH298 =43kcal/mol, Eadd=7 kcal/mol!

!\*\*\*Reactions with O2!

C5H5#+O2=R5CHO+C4H4O <ZHONG98>! !***Combinations!	1.2E19	-2.48	11.0E3	!
C5H6# = C5H5# + R1H ! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>	5.0E15		0.00	7.87E4
C5H5#+B10=C5H40#+R1H <ZHONG98>!	5.8E13	-0.02	0.02E3	!
C5H5#+B10=>2C2H2+R5CHO <ZHONG98>!	3.2E13	-0.17	0.44E3	!
C5H5#+R20H=>C4H6Z2+B2CO [PENGLON- RODA]	4e14	0.0	4500	!
C5H5#+R20H=C5H50H# calculated!	1.0E13	0.0	0.0	!
C5H5#+R300H=C5H50#+R20H calculated!	3.0E12	0.0	0.0	!
!calculation by KINGAS!				
C5H5#+C5H5#=>C10H10# estimated!	2.0E12	0.0	0.0	!
C10H10#=>C5H5#+C5H5# calculated!	3.2E15	0.0	57.5E3	!
!***disproportionnations!				
C5H5#+R300H=>C5H6#+O2 estimated!	2.5E9	1.0	3.5E3	!
!estimated as for allylic radicals (HEYBERGER02)/10!				
!REACTIONS OF CYCLOPENTADIONYL RADICALS!				
!***Decompositions by beta-scission!				
C5H50#=>2C2H2+R5CHO estimated!	2.0E13	0.0	30.0E3	!
C5H50#=C5H40#+R1H estimated!	2.0E13	0.0	30.0E3	!
!see DA COSTA01!				
!***Combinations!				
C5H50#+R1H=C5H50H# estimated!	1.0E14	0.0	0.0	!
!***no disproportionnations considered!				
!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!				
C5H40H#+O2=C5H40#+R300H estimated!	1.0E13	0.0	5.0E3	!
C5H40H#+R1H=C5H50H# estimated!	1.0E14	0.0	0.0	!
C5H40H#+B10=CO2+C2H2+R10C2H3V estimated!	3.2E13	-0.17	0.44E3	!
!C5H40H#+R300H=>R20H+CO2+R10C2H3V+C2H2 estimated!	3.0E12	0.0	0.0	!
C5H40H#+R300H=>R20H+R20H+C5H40#	3.0E12	0.0	0.0	! mf
C5H40H#+R300H=>C5H50H#+O2 estimated!	2.5E9	1.0	3.5E3	!
!Reactions derived from those of cyclopentadienyl radicals!				

C5H40H#+C6H50#=C5H40#+C6H50H# 1.0E12 0.0 0.0 !  
estimated!

!  
\*\*\*\*\*!  
\*\*\*\*\*!  
!\*  
!\* SECONDARY MECHANISM OF THE OXIDATION OF BENZENE!!\*  
!  
\*\*\*\*\*!  
\*\*\*\*\*!

!REACTIONS OF ORTHOBENZOQUINONE!

OC6H40=>C5H40#+B2C0 1.0E12 0.0 40.0E3 !  
<ALZUETA00>!

OC6H40+R1H=>2B2C0+C2H2+R10C2H3V 5.2E13 0.0 3.2E3 !

estimated!  
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!

!OC6H40+R1H=>H2+2B2C0+C2H2+R9C2H 1.6E6 2.5 9.8E3 !

estimated!

!OC6H40+R20H=>H20+2B2C0+C2H2+R9C2H 4.4E6 2.0 1.4E3 !

estimated!

!estimated as the metathesis of 4 tertiary vinylic H-atoms (HEYBERGER02)!

!REACTIONS OF PHENOL AND DERIVED RADICALS!

C6H50H#=C5H6#+B2C0 1.0E12 0.0 61.2E3 !  
<HORN98>!

C6H50H#+O2=R300H+C6H50# 1.0E13 0.0 38.9E3 !  
<ALZUETA00>!

C6H50H#+B10=OC6H40H+R1H 1.6E13 0.0 3.4E3 !

estimated!

!as the addition of O-atoms to toluene (DACOSTA01)!

C6H50H#+R1H=C6H50#+H2 1.2E14 0.0 12.4E3 !  
<ALZUETA00>!

C6H50H#+B10=C6H50#+R20H 1.3E13 0.0 2.9E3 !  
<ALZUETA00>!

C6H50H#+R20H=C6H50#+H20 1.4E8 1.4 -0.96E3 !  
<SHANDROSS96>!

C6H50H#+R300H=C6H50#+H202 1.0E12 0.0 10.0E3 !  
<ALZUETA00>!

C6H50H#+R4CH3=C6H50#+CH4 1.8E11 0.0 7.7E3 !  
<MULCAHY65>!

C6H50H#+C6H5#=C6H50#+C6H6# 4.9E12 0.0 4.4E3 !  
<ALZUETA00>!

!C6H50H#+C5H5#=C6H50#+C5H6# 4.9E11 0.0 9.4E3 !

estimated!

!C6H5OH##+C3H5Y=C6H50##+C3H6Y estimated!	4.9E11	0.0	9.4E3	!
!C6H5OH##+iC4H5=C6H50##+C4H6Z2 estimated!	4.9E11	0.0	9.4E3	!
C6H50H##+C5H5#=C6H50##+C5H6#	2.67e14	0.0	25.238e3	
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>				
C6H50H##+C3H5Y=C6H50##+C3H6Y	2.67e14	0.0	25.238e3	!mf
<Lovell Int. J. Chem. Kinet.21(1989)547>				
C6H50H##+iC4H5=C6H50##+C4H6Z2	2.67e14	0.0	25.238e3	
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>				

!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!

C6H50H##+R1H=C6H40H##+H2 <SHANDROSS96>!	1.7E14	0.0	16.0E3	!
C6H50H##+B10=C6H40H##+R20H estimated!	2.0E13	0.0	14.7E3	!
C6H50H##+R20H=C6H40H##+H2O <SHANDROSS96>!	1.4E13	0.0	4.6E3	!
C6H50H##+R300H=C6H40H##+H2O2 estimated!	4.0E11	0.0	28.9E3	!
C6H50H##+R4CH3=C6H40H##+CH4 estimated!	2.0E12	0.0	15.0E3	!

!as the H-abstractions from benzene!

C6H40H##+O2=OC6H40H+B10 estimated!	2.1E13	0.0	6.1E3	!
!as for phenyl radicals (FRANCK94)!				
C6H40H##+R1H=C6H50H# estimated!	1.0E14	0.0	0.0	!
C6H40H##+R4CH3=HOC6H4CH3	5.0E12	0.0	0.0	!mf

!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!

C5H6##+O2=>C5H5##+R300H <INGHAM94>!	1.4E12	0.0	31.6E3	!
!C5H6##+R1H=C5H7# estimated!	5.2E13	0.0	3.2E3	!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!				
C5H6##+B10=>C5H50##+R1H <ZHONG98>!	8.9E12	-0.15	590.0	!
C5H6##+R1H=C5H5##+H2 <ROY97>!	2.8E13	0.0	2.0E3	!
C5H6##+B10=C5H5##+R20H <ZHONG98>!	4.8E4	2.7	1.1E3	!
C5H6##+R20H=C5H5##+H2O <ZHONG98>!	3.1E6	2.0	0.0	!
C5H6##+R300H=C5H5##+H2O2 <ZHONG98>!	1.1E4	2.6	12.9E3	!
C5H6##+R4CH3=C5H5##+CH4 <ZHONG98>!	1.8E-1	4.0	0.0	!
C5H6##+C3H5Y=C5H5##+C3H6Y astoluene!	1.6E12	0.0	15.1E3	!

C5H6#+nC4H5=C5H5#+C4H6Z2 astoluene!	1.6E12	0.0	11.1E3	!
C5H6#+iC4H5=C5H5#+C4H6Z2 astoluene!	1.6E12	0.0	15.1E3	!
!C5H6#+C3H5Y=C5H5#+C3H6Y estimated!	6.0E12	0.0	0.0	!
!C5H6#+nC4H5=C5H5#+C4H6Z2 estimated!	6.0E12	0.0	0.0	!
!C5H6#+iC4H5=C5H5#+C4H6Z2 <EMDEE92>!	6.0E12	0.0	0.0	!
!C5H7#=>C2H2+C3H5Y estimated!	2.0E13	0.0	35.5E3	!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by HEYBERGER02!				
!C5H7#+O2=C5H6#+R300H estimated!	7.9E11	0.0	5.0E3	!
!oxidation of an alkylic radical!				
!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!				
C5H40#=>2C2H2+B2C0 <ALZUETA00>!	5.7E32	-6.76	68.5E3	!
!C5H40#=B2C0+C4H4 roda PENGLOAN!	1.00e12	0.0	53000	!
C5H40#+R1H=B2C0+nC4H5 estimated!	2.6E13	0.0	3.2E3	!
!estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!				
C5H40#+B10=C4H4+C02 <ALZUETA00>!	1.0E13	0.0	2.0E3	!
C5H40#+R1H=C5H30#+H2 idem C6H6#+R1H=C6H5#+H2	8.13E7	2.031	15.88E3	!MF
C5H40#+B10=C5H30#+R20H <ALZUETA00>!	1.4E13	0.0	14.7E3	!
C5H40#+R20H=C5H30#+H2O <ALZUETA00>!	1.1E8	1.42	1.4E3	!
C5H30#=>C2H2+B2C0+R9C2H estimated!	2.0E13	0.0	51.0E3	!
!estimated as the decomposition of lC6H5!				
C5H30#+O2=>C02+C2H2+R12CHC0Z <ALZUETA00>!	9.7E58	-13.47	38.2E3	!
C5H50H#+R1H=C5H50#+H2 <ALZUETA00>!	4.0E13	0.0	6.1E3	!
C5H50H#+B10=C5H50#+R20H <ALZUETA00>!	1.0E13	0.0	4.6E3	!
C5H50H#+R20H=C5H50#+H2O <ALZUETA00>!	1.0E13	0.0	1.7E3	!

!Estimated from the same reaction for CH30H!

C5H50H#+R1H=C5H40H#+H2 estimated!	1.4E13	0.0	2.0E3	!
C5H50H#+B10=C5H40H#+R20H estimated!	4.8E4	2.7	1.1E3	!
C5H50H#+R20H=C5H40H#+H2O estimated!	1.5E6	2.0	0.0E3	!

!estimated from the same reaction for cyclopentadiene!

!REACTIONS OF VINYLKETENE!

!additions decomposition

C4H40+R1H=>R10C2H3V+CH2COZ estimated!	1.3E13	0.0	3.0E3	!
C4H40+R1H=>C2H4Z+R12CHCOZ estimated!	1.3E13	0.0	3.0E3	!
C4H40+R1H=>sC3H5+B2CO estimated!	1.3E13	0.0	1.5E3	!
C4H40+R20H=>C2H3CHO+R5CHO estimated!	1.4E12	0.0	-1.0E3	!
C4H40+R20H=>CO2+C3H5Y estimated!	1.4E12	0.0	-1.0E3	!
C4H40+B10=>R13CH2CHO+R12CHCOZ estimated!	6.0E4	2.56	-1.1E3	!
C4H40+B10=>2CH2COZ estimated!	6.0E4	2.56	-1.1E3	!

!estimated as the addition of radicals to a double bond (HEYBERGER02)!

!metatheses/decomposition

C4H40+R1H=>C2H2+R12CHCOZ+H2 estimated!	8.2E5	2.5	12.3E3	!
C4H40+R1H=>C3H3+B2CO+H2 estimated!	4.1E5	2.5	9.8E3	!
C4H40+R20H=>C2H2+R12CHCOZ+H2O estimated!	2.2E6	2.0	2.8E3	!
C4H40+R20H=>C3H3+B2CO+H2O estimated!	1.1E6	2.0	1.5E3	!
C4H40+B10=>C2H2+R12CHCOZ+R20H estimated!	1.2E11	0.7	8.7E3	!
C4H40+B10=>C3H3+B2CO+R20H estimated!	6.0E10	0.7	8.7E3	!

!estimated as the metatheses of vinylic H-atoms (HEYBERGER02)!

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!\* \*!  
!\* MECHANISM FOR THE GAS PHASE OXIDATION OF TOLUENE  
\*!  
!\* \*!  
!\* efficiency coefficients for O2, CO, CO2, H2O, N2, AR, HE, C6H6#  
and toluene\*!  
!\* \*!



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!\* PRIMARY MECHANISM OF THE OXIDATION OF TOLUENE \*!  
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!\* \*!  
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!\*\*\*\*\*!  
!\*REACTIONS OF TOLUENE MOLECULES\*!  
!\*\*\*\*\*!

!\*\*UMIMOLECULAR INITIATIONS

toluene=benzyl+R1H 2.09E15 0.0 87.51E3 !  
<Oehlschlaeger07>! Zhenyu  
toluene=C6H5#+R4CH3 2.66E16 0.0 97.88E3 !  
<Oehlschlaeger07> Zhenyu

!\*\*BIMOLECULAR INITIATION

toluene+O2=benzyl+R300H 1.8E12 0.0 39.7E3 !<BAULCH94>!  
!toluene+O2=benzyl+R300H 2.18e7 2.50 46045 !  
mf<Oehlschlaeger06>!

!\*\*ADDITIONS

toluene+R1H=C6H6#+R4CH3 5.67E8 1.43 5.65E3 !Calcul CBS-  
QB3 Fournet Zhenyu

toluene+B10=OC6H4CH3+R1H 1.7E13 0.0 3.6E3 !<TAPPE89>!  
!toluene+R20H=HOC6H4CH3+R1H 2.3E12 0.0 -0.36E3 !<BAULCH92>!  
toluene+R20H=HOC6H4CH3+R1H 1.3E13 0.0 10.6E3 !<BAULCH94>as  
benzene!

toluene+R20H=C6H50H#+R4CH3 7.83E2 2.884 3.2193E3 !Seta V Nakajima  
V Miyoshi JPCA 2006 Zhenyu  
!toluene+R20H=C6H50H#+R4CH3 1E5 2.58 1134.0 !Olive as  
benzene+OH

!\*\*METATHESES

!\*\*METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

toluene+R1H=benzyl+H2 2.92E6 2.372 5.81E3 !Calcul CBS-QB3  
Fournet Zhenyu

toluene+B10=benzyl+R20H <HOFFMANN90>!	6.3E11	0.0	0.0	!
toluene+R20H=benzyl+H2O	5.2E09	1.0	0.87E3	!<BAULCH94>!
toluene+R300H=benzyl+H2O2	4.0E11	0.0	14.0E3	!<BAULCH94>!
toluene+R4CH3=benzyl+CH4 Fournet Zhenyu	3.91E0	3.76	6.98E3	!Calcul CBS-QB3

! ajout MF

toluene+R7CH30=benzyl+CH30H	2.12E+10	0.0	3000.0	!PITZ2001
toluene+R8CH300=benzyl+CH300H	1.02E+04	2.5	12339.3	!PITZ2001

  

!toluene+R5CHO=benzyl+HCHO	3.77E13	0.0	23.7874E3	!MEHL 09 Zhenyu
benzyl+HCHO = toluene+R5CHO	1.26e8	1.9	18.183E3	
benzyl+CH3CHO = toluene+R14CH3CO	1.26e8	1.9	18.183E3	

  

toluene+R10C2H3V=benzyl+C2H4Z	4.0e12	0.0	8.0e3	!<COLKET94>!
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toluene+C3H5Y=benzyl+C3H6Y	1.6E12	0.0	15.1E3	!<estimated(a)>!
toluene+C3H3=benzyl+pC3H4	1.6E12	0.0	15.1E3	!<estimated(a)>!
toluene+iC4H5=benzyl+C4H6Z2 <estimated(a)>!	1.6E12	0.0	15.1E3	!
toluene+nC4H5=benzyl+C4H6Z2 <estimated(a)>!	1.6E12	0.0	11.1E3	!
toluene+C5H5#=benzyl+C5H6#	1.6E11	0.0	15.1E3	!<estimated(a)>!

!(a) :Rate constant taken equal to that of the H-abstraction with methyl radicals proposed !  
!by COLKETT94 with A divided by 10 for cyclic radicals !  
! and with an activation energy 4 kcal/mol higher for resonance stabilised radicals!

  

!ajout MF

toluene+C6H5O2=benzyl+C6H500H PITZ2001			1.02E+04	2.5	12339.3	!
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toluene+C6H5#=benzyl+C6H6#	7.9E13	0.0	12.0E3	!<HECKMANN96>!
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toluene+C6H50#=benzyl+C6H50H# <estimated(a)>! peut etre trop rapide	1.6E11	0.0	15.1E3	!
toluene+C6H4CH3=benzyl+toluene <estimated(b)>!	7.9E13	0.0	12.0E3	!
toluene+OC6H4CH3=benzyl+HOC6H4CH3 <estimated(a)>!	1.6E11	0.0	15.1E3	!
toluene+C6H5CH200=benzyl+C6H5CH200H <estimated(c)>!	4.0E11	0.0	14.0E3	!
toluene+C6H5CH20=benzyl+C6H5CH20H <estimated(a)>!	1.6E11	0.0	11.1E3	!
toluene+HOC6H4CH2=benzyl+HOC6H4CH3 <estimated(a)>!	1.6E11	0.0	15.1E3	!

!(b) :Rate constant taken equal to that of the H-abstraction with phenyl radicals proposed !  
!by HECKMANN96!  
!(c) :Rate constant taken equal to that of the H-abstraction with H02 radicals proposed !  
!by BAULCH94!

!\*\*METATHESES WITH ABSTRACTION OF PHENYLIC H-ATOM!

toluene+R1H=C6H4CH3+H2 1.22E08 2.031 15.88E3 !as  
C6H6#+R1H=C6H5#+H2 CBS-QB3 Fournet Zhenyu  
toluene+B10=C6H4CH3+R20H 2.0E13 0.0 14.7E3 !<estimated(d)>!  
  
toluene+R20H=C6H4CH3+H2O 1.36E4 2.7 0.6196E3 !<Seta06>! in Sakai07 Zhenyu  
toluene+R300H=C6H4CH3+H2O2 9.2E12 0.0 28.81E3 !<Baulch94>! in Sakai07 Zhenyu  
toluene+R4CH3=C6H4CH3+CH4 2.07E0 3.861 13.3E3 !as  
C6H6#+R4CH3=C6H5#+CH4 CBS-QB3 Fournet Zhenyu

!\*\*\*\*\*!  
!\*REACTIONS OF BENZYL RADICALS\*!  
!\*\*\*\*\*!

!\*\*DECOMPOSITION BY BETA-SCISSION

benzyl=>C5H5#+C2H2 6.0E13 0.0 70.0E3 !<Colket94>!  
benzyl=>C3H3+C4H4 2.0E14 0.0 83.6E3 !<Colket94>!

!\*\*REACTIONS WITH OXYGEN

benzyl+O2=C6H5CH2O 4.6E11 0.0 -377.0 !<FENTER94>!  
benzyl+O2=C6H5CH2O+B10 6.3E12 0.0 40.0E3 !<BREZYNSKY84>!

!\*\*TERMINATION REACTIONS

benzyl+B10=C6H5#+HCHO 3.5E13 0.0 0.0 !<EMDEE92>!  
benzyl+B10=C6H5CHO+R1H 1.0E14 0.0 0.0 !  
<estimated(e)>!

!(e) : This rate constant is that proposed by <HIPPLER90-2> divided by 4  
!(LINSTEDT96?? has used 3.5E13)!

benzyl+R8CH300=>C6H5CH2O+R7CH3O 5.0E12 0.0 0.0  
benzyl+R17C2H500=>C6H5CH2O+R15C2H5O 5.0E12 0.0 0.0

benzyl+R20H=C6H5CH2OH 2.0E13 0.0 0.0 !<HIPLER91>!

!MFbenzyl+R300H=C6H5CH2O 5.0E12 0.0 0.0 !<HIPPLER92>!  
benzyl+R300H=C6H5CH2O 8.21E4 2.20 -5.13E3 !MF<da  
silva-bozzelli- proceedings comb inst 32(2009)287-294>!

2benzyl=bibenzyl 5.01E12 0.0 0.454E3 !  
<0ehlschlaeger05>! in Sakai07 Zhenyu

etC6H5 = benzyl + R4CH3 6.1e15 0.0 75120 !<BAULCH94>!

!\*\*\*\*\*!  
 !\*REACTIONS OF METHYL PHENYL RADICALS\*!  
 !\*\*\*\*\*!

!\*\*reactions with oxygen

!mfC6H4CH3+O2=OC6H4CH3+B10 2.6E13 0.0 6.1E3 !

<estimated(f)>!

!mfC6H4CH3+O2=OC6H4O+R4CH3 3.0E13 0.0 9.0E3 !

<estimated(f)>!

!(f) : Rate constant taken equal to that of the similar reaction in the case of phenyl!

!radicals!

!ajout mf

C6H4CH3+O2=>OOC6H4CH3 3.72E13 -0.22 -711

!2008DAS/BOZ3566-3575

OOC6H4CH3=>C6H4CH3+O2 6.36E19 -1.372 48.74E3

!2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4CH3+B10 1.27E15 -0.25

3.85E4

!2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4O+R4CH3 5.0E11 0.00

46400

!

!\*\*\*termination reactions!

C6H4CH3+R1H=toluene 1.0E14 0.0 0.0 !

<estimated(g)>!

!(g) : Rate constant taken equal to that of the recombination of H atoms with alkyl !

!radicals as proposed by Allara!

C6H4CH3+B10=OC6H4CH3 1.0E14 0.0 0.0 !

<estimated(f)>!

C6H4CH3+R2OH=HOC6H4CH3 1.0E13 0.0 0.0 !

<estimated(f)>!

C6H4CH3+R4CH3=C8H10# 1.2E06 1.96 -3.7E3 !

<estimation(fbise)>!

!(fbise) : Rate constant taken equal to that of the similar reaction in the case of phenyl!

!radicals: Rao, skinner, 1989 J.P.C. (93,1864)!

C6H4CH3+R3OOH=OC6H4CH3+R2OH 5.0E12 0.0 0.0 !

<estimated(f)>!

C6H4CH3 +R1H = benzyl + R1H 1.0E13 0.0 0.0 !<MILLER92>!

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYL PEROXY RADICALS\*!  
 !\*\*\*\*\*!

!\*\*isomerisation-decomposition reactions

C6H5CH200=C6H5CH0+R20H 3.4E9 1.0 37.5E3 !  
 <estimated(h)>!  
 !(h) : Rate constant of the isomerisation :!  
 !A = ekBT/h x rpd x exp ((Dnirotx3.5)/R), Ea = 23 (4 membered transition  
 ring)!  
 !+ 14.5 (secondary allylic H-atom)!

!\*\*Combination reactions  
 !MF C6H5CH200+R1H=C6H5CH200H 1.0E14 0.0 0.0E3 !  
 <estimated(g)>!

!\*\*dispropotionnation reactions!  
 C6H5CH200+R300H=C6H5CH200H+O2 2.0E11 0.0 -1.3E3 !  
 <estimated(i)>!  
 2C6H5CH200=C6H5CH20H+C6H5CH0+O2 1.4E10 0.0 -725.0 !  
 <estimated(i)>!  
 C6H5CH200+C6H5CH200=2C6H5CH20+O2 6.3E10 0.0 -725.0 !  
 <estimated(i)>!  
 !(i) : Rate constant taken equal to that the disproportionnation of  
 peroxyalkyl radicals !  
 !as proposed by Warth!

! ajout MF  
 C6H5CH200+R1H=C6H5CH20+R20H 3.80E14 -0.19  
 1.89E3 !<da silva J Chem Theory Comput 2009>  
 C6H5CH200+R1H=C6H5CH200H 4.35e60 -15.92 11.40E3  
 !<da silva J Chem Theory Comput 2009>  
 C6H5CH200+R1H=benzyl+R300H 1.96E4 2.47 1.43E3  
 !<da silva J Chem Theory Comput 2009>

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYL ALCOXY RADICALS\*!  
 !\*\*\*\*\*!

!\*\*Decomposition by beta-scission \*\*\*\*\*  
 C6H5CH20=R1H+C6H5CH0 2.0E13 0.0 27.5E3 !  
 <estimated(j)>! INHIBE  
 C6H5CH20=C6H5#+HCHO 2.0E13 0.0 27.5E3 !  
 <estimated(j)>! ACCELERE  
 !DH = 23.59 kcal/mol!  
 !(j) For these beta-scissions involving the breaking of a C-C or a C-H  
 bond, A-factor !  
 !is an average value for beta-scissions [Heyberger] and activation  
 energies have been!  
 ! estimated from thermochemistry and to obtain the best results!

!C6H5CH20=R1H+C6H5CH0 5.26E28 -5.081 22.25E3 !  
 mf<Da silva-bozzelli J phys chem 25(2009)6979>!  
 !C6H5CH20=C6H6#+R5CH0 2.37E32 -6.095 28.81E3 !  
 mf<Da silva-bozzelli J phys chem 25(2009)6979>!  
 !C6H5CH20=C6H5#+HCHO 7.21E33 -6.21 36.85E3 !  
 mf<Da silva-bozzelli J phys chem 25(2009)6979>!

!C6H5CH2O=R1H+C6H5CHO 1.00e14 0.00 2.91e4 !  
mf<Mehl Proc comb inst 33(2011)193>!  
!C6H5CH2O=C6H5#+HCHO 1.46e20 -2.00 3.51e4 !  
mf<Mehl Proc comb inst 33(2011)193>!

!\*\*\*reactions with oxygen  
C6H5CH2O+O2=R3OOH+C6H5CHO 6.0E10 0.0 1.6E3 !  
<estimated(k)>!  
!(k) : Rate constant taken equal to that of the similar reaction in the  
case of ethoxy!  
!radicals as proposed by BAULCH92!

!\*\*\*\*\*!  
!\*REACTIONS OF CRESOXY RADICALS\*!  
!\*\*\*\*\*!

!\*\*OC6H4CH3=HOC6H4CH2 2.9E9 1.0 3.2E3 !<estimated(h')>!  
!(h') : Rate constant of the isomerisation :!  
!A =  $ekbT/h \times rpd \times \exp((Dnirot \times 3.5)/R)$ , Ea = 5.9 + 5 (5 membered  
transition ring)!  
!+ 7.3 (primary alkyllic H-atom by CH3O)!

!OC6H4CH3=HOC6H4CH2 1.1E9 1.0 22.9E3 !  
! A x2/5 only for ortho isomere, Ea= 5.9(RSE)+17 (H allylique p by R00.  
close bde)

!\*\*CO elimination with rearrangement  
!OC6H4CH3=>R1H+C6H6#+B2CO 7.5E11 0.0 43.8E3 !  
<FRANCK94>!  
OC6H4CH3=>R1H+C6H6#+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
!OC6H4CH3=>R10C2H3V+C4H4+B2CO 3.0E11 0.0 43.8E3!<FRANCK94>!  
!OC6H4CH3=>C2H2+iC4H5+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
!OC6H4CH3=>C2H2+C4H4+R1H+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
OC6H4CH3=>C3H3+aC3H4+B2CO 1.5E11 0.0 43.8E3 !  
<FRANCK94>!

!\*\*termination reactions!  
OC6H4CH3+R1H=HOC6H4CH3 1.0E14 0.0 0.0E3 !  
<estimated(g)>!

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

!\*  
\*!

!\* SECONDARY MECHANISM OF THE OXIDATION OF TOLUENE

\*!

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

!*****!
!*REACTIONS OF BENZALDEHYDE AND DERIVED RADICALS*!
!*****!

! Amorcage
!C6H5CHO+O2=C6H5CO+R300H      2.0E13  0.0  38.9E3      !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R300H      7.0E11  0.0  39.5E3 !RODA RODA
C6H5CHO = C6H5CO + R1H      3.98E15 0.0 83.74E3 !NIST GRELA86!

! Addition
C6H5CHO+R1H=C6H6#+R5CHO      5.8E13  0.0  8.1E3      !
<estimated(m)>!
!(m) : Rate constant taken equal to that of the same reaction in the case
of toluene!

! Metatheses
C6H5CHO+R1H=C6H5CO+H2      4.0E13  0.0  3.2E3      !
<estimated(n)>!
!(n) : Rate constant estimated from the parameters proposed by WARNATZ84
for acetaldehyde!
!with an activation energy 1 kcal/mol lower due to the resonance
stabilisation of the!
! obtained radical!

C6H5CHO+B10=C6H5CO+R20H      6.0E12  0.0  1.8E3 !<BAULCH94>!
C6H5CHO+R20H=C6H5CO+H2O      7.8E12  0.0  0.0  !<BAULCH94>!
C6H5CHO+R300H=C6H5CO+H2O2  3.0E12  0.0  11.0E3 !<estimated(o)>!
C6H5CHO+R4CH3=C6H5CO+CH4    2.0E-6  5.6  2.5E3 !MF <BAULCH94>!

C6H5CHO+R11C2H5=C6H5CO+C2H6  1.3E12  0.0  7.5E3 !<estimated(o)>!
!(o) : Rate constant estimated from the parameters proposed by BAULCH94
(HO2, CH3) and by !
!HOLHEIN70 (C2H5) for acetaldehyde with an activation energy 1 kcal/mol
lower due to the !
!resonance stabilisation of the obtained radical!

C6H5CHO+C3H5Y=C6H5CO+C3H6Y  1.3E12  0.0  11.5E3      !
<estimated(p)>!
C6H5CHO+iC4H5=C6H5CO+C4H6Z2  1.3E12  0.0  11.5E3      !
<estimated(p)>!
C6H5CHO+nC4H5=C6H5CO+C4H6Z2  1.3E12  0.0  7.5E3      !
<estimated(p)>!
C6H5CHO+benzyl=toluene+C6H5CO  1.3E11  0.0  11.5E3      !
<estimated(p)>
C6H5CHO+C6H5O#=C6H5CO+C6H5OH#  1.3E11  0.0  11.5E3      !
<estimated(p)>
C6H5CHO+OC6H4CH3=C6H5CO+HOC6H4CH3  1.3E11  0.0  11.5E3      !
<estimated(p)>

```

```

C6H5CHO+C5H5#=#C6H5CO+C5H6#      1.3E11      0.0  11.5E3      !
<estimated(p)>
!(p) :Rate constant taken equal to that of the H-abstraction with ethyl
radicals !
! with A divided by 10 for cyclic radicals and with an activation
energy !
!4 kcal/mol higher for resonance stabilised radicals!

C6H5CHO+HOC6H4CH2=C6H5CO+HOC6H4CH3  1.3E11      0.0  11.5E3      !
<estimated(p)>
C6H5CHO+C6H5#=#C6H5CO+C6H6#      1.3E11      0.0  11.5E3      !<estimated(p)>

C6H5CO=C6H5#+B2CO                    4E14      0.0      29.5e3      !
<SOLLY71>!
!Author(s):  Solly, R.K.; Benson, S.W.
!Title:  Kinetics of the gas-phase unimolecular decomposition of the
benzoyl radical
!Journal:  J. Am. Chem. Soc.
!Volume:  93
!Page(s):  2127
!Year:  1971

!*****!
!*REACTIONS OF BENZYL HYDROPEROXYDE*!
!*****!

!MFC6H5CH2OOH=C6H5CH2O+R2OH          1.5E16      0.0  42.0E3      !
<estimated(r)>!
!(r) : Rate constant taken equal to that the decomposition of
hydroperoxide species !
! proposed by Bounaceur <SAHETCHIAN>!
!MFC6H5CH2OOH=C6H5CH2O+R2OH          2.03E47          -10.27
50.71E3  !<da silva J Chem Theory Comput 2009>
C6H5CH2OOH=C6H5CH2O+R2OH            3.29E13          0.42      39.89E3      !
MF<da silva Proc comb inst 32(2009)287-294>
C6H5CH2OOH=C6H5CHO+H2O               7.45E8           1.19
46.04E3  !MF<da silva Proc comb inst 32(2009)287-294>

!*****!
!*REACTIONS OF CRESOL AND DERIVED RADICALS*!
!*****!

! amorage
HOC6H4CH3+O2=OC6H4CH3+R3OOH        1.0E13      0.0  38.9E3      !
<estimated(s)>! ralenti
!A=1E13 pour phenol!
!(s) : Rate constant taken equal to that of the same reaction for
phenol !

!HOC6H4CH3+O2=HOC6H4CH2+R3OOH      2.1E13      0.0      38.0E3      !
<EMDEE92*2>!
HOC6H4CH3+O2=HOC6H4CH2+R3OOH      2.1E12      0.0      38.6E3      !
RODA <estimated(aaa)>!

```



! addition  
HOC6H4CH3+R1H=C6H5OH#+R4CH3 5.8E13 0.0 8.1E3  
!<estimated(t)>!  
!(t) : Rate constant taken equal to that of the same reaction for toluene  
!

!HOC6H4CH2+B10=C6H4OH#+HCHO 8E13 0.0 0.0

! metatheses

HOC6H4CH3+R1H=OC6H4CH3+H2 1.2E14 0.0 12.4E3 !  
<estimated(s)>!  
HOC6H4CH3+B10=OC6H4CH3+R2OH 1.3E13 0.0 2.9E3 !  
<estimated(s)>!  
HOC6H4CH3+R2OH=OC6H4CH3+H2O 1.4E8 1.4 -0.96E3 !  
<estimated(s)>!  
HOC6H4CH3+R300H=OC6H4CH3+H2O2 1.0E12 0.0 10.0E3 !  
<estimated(s)>!  
HOC6H4CH3+R4CH3=OC6H4CH3+CH4 1.8E11 0.0 7.7E3 !  
<estimated(s)>!  
HOC6H4CH3+C6H5#=OC6H4CH3+C6H6# 4.9E12 0.0 4.4E3 !  
<estimated(s)>!  
HOC6H4CH3+C5H5#=OC6H4CH3+C5H6# 4.9E11 0.0 9.4E3 !  
<estimated(s)>!  
HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y 4.9E11 0.0 9.4E3 !  
<estimated(s)>!  
HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2 4.9E11 0.0 9.4E3 !  
<estimated(s)>!  
HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH# 4.9E11 0.0 9.4E3 !  
<estimated(s)>!

HOC6H4CH3+R1H=HOC6H4CH2+H2 1.2E14 0.0 8.4E3 !  
<estimated(t)>!  
HOC6H4CH3+B10=HOC6H4CH2+R2OH 6.3E11 0.0  
0.0 !<estimated(t)>!  
HOC6H4CH3+R2OH=HOC6H4CH2+H2O 5.2E9 1.0 0.87E3 !  
<estimated(t)>!  
HOC6H4CH3+R300H=HOC6H4CH2+H2O2 4.0E11 0.0 14.0E3 !  
<estimated(t)>!  
HOC6H4CH3+R4CH3=HOC6H4CH2+CH4 1.6E12 0.0 11.1E3 !  
<estimated(t)>!  
HOC6H4CH3+C3H5Y=HOC6H4CH2+C3H6Y 1.6E12 0.0 15.1E3 !  
<estimated(t)>!  
HOC6H4CH3+C3H3=HOC6H4CH2+pC3H4 1.6E12 0.0 15.1E3 !  
<estimated(t)>!  
HOC6H4CH3+iC4H5=HOC6H4CH2+C4H6Z2 1.6E12 0.0 15.1E3 !  
<estimated(t)>!  
HOC6H4CH3+nC4H5=HOC6H4CH2+C4H6Z2 1.6E12 0.0 11.1E3 !  
<estimated(t)>!

$\text{HOC6H4CH3} + \text{C5H5\#} = \text{HOC6H4CH2} + \text{C5H6\#}$  1.6E11 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H5\#} = \text{HOC6H4CH2} + \text{C6H6\#}$  7.9E13 0.0 12.0E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H50\#} = \text{HOC6H4CH2} + \text{C6H50H\#}$  1.6E11 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H4CH3} = \text{HOC6H4CH2} + \text{toluene}$  7.9E13 0.0 12.0E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{OC6H4CH3} = \text{HOC6H4CH2} + \text{HOC6H4CH3}$  1.6E11 0.0  
 15.1E3 !<estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H5CH200} = \text{HOC6H4CH2} + \text{C6H5CH200H}$  4.0E11 0.0  
 14.0E3 !<estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H5CH20} = \text{HOC6H4CH2} + \text{C6H5CH20H}$  1.6E11 0.0  
 11.1E3 !<estimated(t)>!

$\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH200}$  4.6E11 0.0 -377.0 !  
 <estimated(u)>!

$\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH20} + \text{B10}$  6.3E12 0.0 40.0E3 !  
 <estimated(u)>!

$\text{HOC6H4CH2} + \text{R300H} = \text{HOC6H4CH20} + \text{R20H}$  5.0E12 0.0 0.0 !  
 <estimated(u)>!

!(u) : Rate constant taken equal to that of the same reaction for benzyl radicals !

$\text{HOC6H4CH2} + \text{R1H} = \text{HOC6H4CH3}$  1.0E14 0.0 0.0 !  
 <estimated(g)>!

$\text{HOC6H4CH2} + \text{R4CH3} = \text{C6H50H\#} + \text{C2H4Z}$  5.0E12 0.0 0.0 !  
 <estimated(g)>!

$\text{HOC6H4CH200} = \text{C6H40HCHO} + \text{R20H}$  3.4E9 1.0 37.5E3 !<estimated(v)>!  
 !(v) : Rate constant taken equal to that of the same reaction for benzyl peroxy radicals !

$\text{HOC6H4CH20} = \text{R1H} + \text{C6H40HCHO}$  2.0E13 0.0 27.5E3 !  
 <estimated(w)>!

$\text{HOC6H4CH20} = \text{C6H40H\#\#} + \text{HCHO}$  2.0E13 0.0 27.5E3 !  
 <estimated(w)>!

$\text{HOC6H4CH20} + \text{O2} = \text{R300H} + \text{C6H40HCHO}$  6.0E10 0.0 1.6E3 !  
 <estimated(w)>!

!(w) : Rate constant taken equal to that of the same reaction for benzyl alcoxy radicals !

$\text{C6H40HCHO} + \text{R1H} = \text{C6H40HCO} + \text{H2}$  4.0E13 0.0 3.2E3 !<estimated(x)>!

$\text{C6H40HCHO} + \text{B10} = \text{C6H40HCO} + \text{R20H}$  6.0E12 0.0 1.8E3 !  
 <estimated(x)>!

$\text{C6H40HCHO} + \text{R20H} = \text{C6H40HCO} + \text{H20}$  7.8E12 0.0 0.0 !  
 <estimated(x)>!

$\text{C6H40HCHO} + \text{R300H} = \text{C6H40HCO} + \text{H202}$  3.0E12 0.0 11.0E3 !  
 <estimated(x)>!

$\text{C6H40HCHO} + \text{R4CH3} = \text{C6H40HCO} + \text{CH4}$  2.0E-6 5.6 1.5E3 !  
 <estimated(x)>!

!(x) : Rate constant taken equal to that of the same reaction for benzaldehyde !

C6H40HC0=C6H40H#+B2C0 2.0E13 0.0 30.5E3 !  
 <estimated(y)>  
 !(y) : Rate constant taken equal to that of the same reaction for C6H5C0  
 radicals !

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

C6H5CH20H+O2=R300H+C6H5CHOH 1.4E12 0.0 34.0E3 !RODA  
 <estimated(aaa)>!  
 C6H5CH20H+O2=C6H5CH20+R300H 2.0E14 0.0 41.4E3 !  
 <EMDEE92>!

C6H5CH20H+R1H=C6H6#+R6CH20H 5.8E13 0.0 8.1E3 !  
 <estimated(t)>!

C6H5CH20H+R1H=C6H5CHOH+H2 8.0E13 0.0 6.4E3 !<estimated(t')>!

C6H5CH20H+B10=C6H5CHOH+R20H 4.2E11 0.0 -2.0E3 !  
 <estimated(t')>!

C6H5CH20H+R20H=C6H5CHOH+H2O 3.5E9 1.0 -1.13E3 !  
 <estimated(t')>!

C6H5CH20H+R300H=C6H5CHOH+H2O2 2.7E11 0.0 12.0E3 !  
 <estimated(t')>!

C6H5CH20H+R4CH3=C6H5CHOH+CH4 1.1E12 0.0 9.1E3 !  
 <estimated(t')>!

C6H5CH20H+C3H5Y=C6H5CHOH+C3H6Y 1.1E12 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+iC4H5=C6H5CHOH+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+nC4H5=C6H5CHOH+C4H6Z2 1.112 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+C6H5#=C6H5CHOH+C6H6# 5.2E13 0.0 10.0E3 !  
 <estimated(t')>!

C6H5CH20H+C6H4CH3=C6H5CHOH+toluene 5.2E13 0.0 10.0E3 !  
 <estimated(t')>!

C6H5CH20H+C6H50#=C6H5CHOH+C6H50H# 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+benzyl=C6H5CHOH+toluene 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+OC6H4CH3=C6H5CHOH+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+HOC6H4CH2=C6H5CHOH+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!

C6H5CH20H+C5H5#=C6H5CHOH+C5H6# 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!

!t': estimated as toluene with A x(2/3) to take into account the number  
 of abstractable !

!H atoms and Ea -2 kcal/mol due to the OH substitution!

C6H5CHOH=C6H5CHO+R1H 2.0E13 0. 36.373E3 !MF

DHr=36.79 correlation baptiste E=0.6\*DHr+14.3

!R15C2H50=CH3CHO+R1H 2.0E14 0. 23.3E3 !(243, -

243)<HEICKLEN88NIST>!

!\*\*\*\*\*!  
 !\*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

!\*\* Amorзages monomolйculaires

etC6H5 = R1H + C8H9# 4.3E14 0.0 83.6E3 !<kingas>!

!\*\* Amorзages bimolйculaires

etC6H5+O2=C8H9#+R300H 1.4E12 0.0 34.0E3 !  
 <estimated(aaa)>!  
 etC6H5+O2=C8H9#-1+R300H 1.2E13 0.0 49.0E3 !  
 <exgas>!

!\*\* Additions ipso

etC6H5+R1H=C6H6#+R11C2H5 5.8E13 0.0 8.1E3 !  
 <estimated(t)>!

!\*\* Metatheses

etC6H5+R1H=C8H9#+H2 8.0E13 0.0 6.4E3  
 !<estimated(t">!  
 etC6H5+B10=C8H9#+R20H 4.2E11 0.0 -2.0 !  
 <estimated(t">!  
 etC6H5+R20H=C8H9#+H20 3.5E9 1.0 -1.13E3 !  
 <estimated(t">!  
 etC6H5+R300H=C8H9#+H202 2.7E11 0.0 12.0E3  
 !<estimated(t">!  
 etC6H5+R4CH3=C8H9#+CH4 1.1E12 0.0 9.1E3 !  
 <estimated(t">!  
 etC6H5+C3H5Y=C8H9#+C3H6Y 1.1E12 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+iC4H5=C8H9#+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+nC4H5=C8H9#+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+C6H5O#=#C8H9#+C6H5OH# 1.1E11 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+benzyl=C8H9#+toluene 1.1E11 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t">!  
 etC6H5+C5H5#=#C8H9#+C5H6# 1.1E11 0.0 13.1E3 !  
 <estimated(t">!

!t": estimated as toluene with A x(2/3) to take into account the number of abstractable !

!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

etC6H5+R1H=C8H9#-1+H2 7.2E8 1.5 6.79E3 !MF  
 correlation Dean-Bozzelli 2000

```

etC6H5+B10=C8H9#-1+R20H      5.1E8      1.5      5.05E3      !MF
correlation Dean-Bozzelli 2000
etC6H5+R20H=C8H9#-1+H2O      3.6E6      2.0      4.82E2      !MF
correlation Dean-Bozzelli 2000
etC6H5+R300H=C8H9#-1+H2O2    4.2E4      2.69    1.85E4      !MF
correlation Dean-Bozzelli 2000
etC6H5+R4CH3=C8H9#-1+CH4    2.43E6      1.87    1.03E4      !MF correlation
Dean-Bozzelli 2000

!mfetC6H5+C6H5#=C6H6#+C8H9#      5.27E13    0.0      12.0E3      !ajout MF as
2/3 toluene <HECKMANN96>!
etC6H5+C6H5#=C6H6#+C8H9#      5.27E13    0.0      9.0E3      !test mf

etC6H5+C6H5#=C6H6#+C8H9#-1    5.85E10    0.0      3.83E3      !ajout MF as
C5H12/4 <Park, Int J. Chem. Kinet.33(2001)64-69>

! Ajout ipso MF
etC6H5+B10=C6H5O#+R11C2H5    1.7E13    0.0      3.6E3      !MF as toluene !
<TAPPE89>!
etC6H5+R20H=C6H5OH#+R11C2H5  1.3E13    0.0      10.6E3     !MF as toluene
<BAULCH94>as benzene
!etC6H5+R4CH3=toluene+R11C2H5 1.2E12    0.0      1.59E4     !MF as benzene
<Robaugh, J. Phys. Chem.90(1986)4159 - 4163>
etC6H5+R4CH3=toluene+R11C2H5 1.2E12    0.0      1.24E4     ! MF as benzene-
kcal <Robaugh, J. Phys. Chem.90(1986)4159 - 4163>

! ** Decompositions

C8H9#-1=C2H4Z+C6H5#          2.0E13    0.0      35.5E3     !MF correlation exgas
C8H9# =R1H+styrene           3.1e13    0.0      50670      !<MULLER88>
C8H9#-1=R1H+styrene           4.0E13    0.0      33.58E3    !MF <Sirjean,
J.Phys.Chem.A 2008>

! ** Reactions of derived radicals
C8H9#+O2=R300H+styrene      6.90E11      0.0
15.2E3      !<est (exgas-sylvain)>!

!C8H9#+R300H=R20H+R4CH3+C6H5CHO      3.27E12      0.0
0.0      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R300H=R20H+R1H+C6H5COCH3      7.80E10      0.0
0.0      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
!C8H9#+R300H=>R20H+C6H5#+CH3CHO      2.54E11      0.0
0.0      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

C8H9#+R300H=C8H9#OOH      3.60E12      0.0
0.0      !MF KINGAS
C8H9#OOH=R20H+C8H9#O      5.00E15
0.0      42500      !MF
C8H9#O=R4CH3+C6H5CHO      2.69E13      0.0
12117      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>
C8H9#O=C6H5#+CH3CHO      1.74E14
0.0      20458      !MF as but-3-en-1-oxy <Rauk, Can.J.Chem
81(2003)431-442>

```

C8H9#-1+O2=R300H+styrene 2.5E3	2.60E11		0.0	
C8H9#-1+R300H=R20H+HCHO+benzyl 0.0 !<kingas>!	5.00E12		0.0	
!*****! !*REACTIONS OF STYRENE AND DERIVED RADICALS*! !*****!				
styrene+O2=R300H+C6H5C2H2 <asbutadiene/2>!	2.0E13	0.0	57.9E3	!
!C4H6Z2+O2=iC4H5+R300H <LEUNG95>!	4.0E13	0.0	57.9E3	!
!styrene+B10=C6H5#+R13CH2CHO <asbutadiene/2>!	3.0E08	1.45	0.9E3	!
! ENLEVE PAR BENOIT ET PAG styrene+R20H=benzyl+HCHO butadiene/2!	1.4E12	0.0	-0.9E3	!<as
styrene+R20H=C6H5CHO+R4CH3 idem rñaction prñcñdente as C3H6Y <TSAnG91>	1.4E12	0.0	-0.9E3	!MF
!C4H6Z2+B10=C3H5Y+R1H+B2C0 <LEUNG95, BREZINSKY84>!	6.0E08	1.45	0.9E3	!
!C4H6Z2+R20H=C3H5Y+HCHO <LINSTEDT96>!	2.8E12	0.0	-0.9E3	!
!C4H6Z2+R20H=CH3CHO+R10C2H3V <fromLINSTEDT96>!	5.6E12	0.0	-0.9E3	!
styrene+R1H=C6H5C2H2+H2 butadiene/2>!	3.3E5	2.53	9.2E3	!MF<as
styrene+R20H=C6H5C2H2+H2O butadiene/2>!	1.5E6	2.0	0.4E3	!<as
styrene+R4CH3=C6H5C2H2+CH4 butadiene/2>	3.5E13	0.0	15.5E3	!<as
!C4H6Z2+R1H=iC4H5+H2 <WANG97>!	6.6E5	2.53	9.2E3	!
!C4H6Z2+R20H=iC4H5+H2O <WANG97>!	3.1E6	2.0	0.4E3	!
!C4H6Z2+R4CH3=iC4H5+CH4 <WU87-3kcal>!	7.0E13	0.0	15.5E3	!
C6H5C2H2+O2=C6H5C0+HCHO <asMebel C2H3+O2>! **	4.5E16	-1.39	1.0E3	!
!*Addition Zhenyu*!				
C6H5C2H2+R1H=C6H5#C2H+H2 0.0 !in Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120 (1996) 119-167.	1.0E13	0.0		

C6H5C2H2+R20H=C6H5#C2H+H2O 1.0E13 0.0 0.0 !in  
Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120  
(1996) 119-167.

! ajout d'un amorçage Roda  
C6H5#C2H => C6H5# + R9C2H 2.2e16 0.0 98.0e3 ! MF  
as toluene

!\*\*\*\*\*!  
!\*REACTIONS OF C5H5CCH AND DERIVED RADICALS\*!  
!\*\*\*\*\*!

!\*Addition Zhenyu\*!  
!C5H5CCH=C5H5#+R9C2H 4.2E15 0.0 125.0E3 !  
<KInGAS1500>! pC3H4=R9C2H+R4CH3  
!C5H5CCH+R1H=C5H5#+C2H2 2.0E10 0.0 0.0  
!Lindstedt96  
!C5H5CCH+R1H=C3H3+C4H4 6.0E10 0.0 0.0  
!Lindstedt96  
!C5H5CCH+R20H=C5H5#+CH2COZ 4.3E11 0.0 -0.8E3  
!<BOODAGHIANs87>! pC3H4+R20H=CH2COZ+R4CH3  
!C5H4CCH2=C5H5CCH 2.5E12 0.0 59.0E3 !  
<HIDAKA89>! aC3H4=pC3H4  
!C5H4CCH2+R1H=C5H5CCH+R1H 8.5E12 0.0 2.0E3 !  
<WAGnER72>! aC3H4+R1H(+M)=tC3H5(+M)  
!C5H4CCH2+R20H=C5H5#+CH2COZ 2.0E12 0.0 -0.2E3 !<LIU88>!  
aC3H4+R20H=CH2COZ+R4CH3

!\*\*\*\*\*!  
!\*REACTIONS OF BIBENZYL AND DERIVED RADICALS\*!  
!\*\*\*\*\*!

bibenzyl=C14H13#+R1H 1.0E16 0.0 83.66E3 !  
<Oehlschlaeger05>! in Sakai07 Zhenyu  
bibenzyl+O2=C14H13#+R300H 2.8E12 0.0 35.0E3 !<est  
aaaa!  
bibenzyl+R1H=C14H13#+H2 5.4E4 2.5 -1.9E3 !  
Table A-I-21 Zhenyu  
bibenzyl+B10=C14H13#+R20H 8.4E11 0.0 -2.0 !  
<estimated(t'')>!  
bibenzyl+R20H=C14H13#+H2O 7.0E9 1.0 -1.13E3 !  
<estimated(t'')>!  
bibenzyl+R300H=C14H13#+H2O2 5.4E11 0.0 12.0E3 !  
<estimated(t'')>!  
bibenzyl+R4CH3=C14H13#+CH4 2.2E12 0.0 9.1E3 !  
<estimated(t'')>!  
bibenzyl+C6H50#=C14H13#+C6H50H# 2.2E12 0.0 13.1e3 !  
<estimated(t'')>!  
bibenzyl+benzyl=C14H13#+toluene 2.2E12 0.0 9.1E3 !  
<Oehlschlaeger05>! in Sakai07 Zhenyu

bibenzyl+C3H5Y=C14H13#+C3H6Y 2.2E12 0.0 13.1E3 !  
<estimated(t'')>!  
!t'': estimated as toluene with A x(4/3) to take into account the number  
of abstractable !  
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

!Ajout ipso MF  
bibenzyl+R1H=C6H6#+C8H9#-1 5.67E8 1.43 5.65E3 !Calcul CBS-  
QB3 Fournet as toluene  
bibenzyl+R20H=C6H50H#+C8H9#-1 7.83E2 2.884 3.2193E3 !Seta V  
Nakajima V Miyoshi JPCA 2006  
C14H13#=stilbene+R1H 7.94E15 0.0 51.864E3 !  
<Oehlschlaeger05>! in Sakai07 Zhenyu  
C14H13#+O2= stilbene+R300H 1.6E12 0.00 15200 !as allylique  
C14H13#+R300H=>R20H+C6H5CH0+benzyl 8.21E4 2.20 -5.13E3 ! as benzyl

!\*\*\*\*\*!  
!\* REACTIONS OF STILBENE \*!  
!\*\*\*\*\*!

!Ajout Ipso MF  
stilbene+R1H=>C6H6#+C2H2+C6H5# 5.67E8 1.43 5.65E3 !Calcul CBS-  
QB3 Fournet as toluene  
stilbene+R20H=C6H50H#+C6H5C2H2 7.83E2 2.884 3.2193E3 !Seta V  
Nakajima V Miyoshi JPCA 2006

! ajout MF  
stilbene+R20H=C6H5CH0+benzyl 1.0E13 0.0 5.94E3 !  
<Baulch05> as C2H4

!\*\*\*\*\*!  
!\* Reactions of naphthalene \*!  
!\*\*\*\*\*!  
2C5H5#=naphthalene+H2 4.3E36 -6.3 22.835E3 ! A.M. Dean, J.  
Phys. Chem. 94 (1990) 1432-1439.  
C6H5#+iC4H3=naphthalene 3.18E23 -3.2 2.13E3 ! H.Y. Zhang, J.T.  
McKinnon, CST 107 (1995) 261-300.  
C6H5#+C4H4=naphthalene+R1H 3.3E33 -5.7 12.75E3 ! J. Appel, H.  
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.  
benzyl+C3H3=>naphthalene+R1H+R1H 6.0E11 0.0 0.0 ! M.B. Colket,  
D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.  
C6H5C2H2+C2H2=naphthalene+R1H 1.6E16 -1.33 3.3E3 ! J. Appel, H.  
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.

naphthalene+O2=R300H+naphthyl 8.0E13 0.0 63.4E3 !  
like benzene <ALZUETA00>A\*8/6!  
naphthalene+B10=>indenyl+B2C0+R1H 2.7E13 0.0 3.6E3 !like  
benzene <Nicovich82>A\*8/6!  
naphthalene+R1H=naphthyl+H2 8.0E8 1.8 16.8E3 !like  
benzene <MEBEL97>A\*8/6!  
naphthalene+B10=naphthyl+R20H 2.7E13 0.0 14.7E3 !like  
benzene <LINDSTEDT94>A\*8/6!



naphthalene+R20H=naphthyl+H2O	2.1E8	1.42	1.45E3	!like
benzene <BAULCH92>A*8/6!				
naphthalene+R300H=naphthyl+H2O2	7.3E12	0.0	28.9E3	!like
benzene <BAULCH94>A*8/6!				
naphthalene+R4CH3=naphthyl+CH4	2.7E12	0.0	15.0E3	!like
benzene <ZHANG89>A*8/6!				

naphthyl+R1H=naphthalene	1.0E14	0.0	0.0E3	!as n-
buthylbenzene				
naphthyl+O2=>indenyl+B2CO+B10	2.6E13	0.0	6.1E3	!as n-
buthylbenzene				
naphthyl+B10=>indenyl+B2CO	1.0E14	0.0	0.0	!as n-
buthylbenzene				
naphthyl+R300H=>indenyl+B2CO+R20H	5.0E12	0.0	0.0	!as n-
buthylbenzene				
naphthyl+R20H=>indenyl+B2CO+R1H	1.0E13	0.0	0.0	!as n-
buthylbenzene				

```

!*****!
!* Reactions of indene and derived radicals      *!
! Indene C6H4#/CH2/CH//CH/                      *!
! Indenyl C6H4#/CH/CH//CH/                      *!
! ph#C3H2 C6H5#/CH(./)C///CH                   *!
!*****!

```

indene+R20H=>C2H4Z+C6H5CO	1.37E12	0.0	-1.04E3	!Slavinskaya
indene+R20H=>R10C2H3V+B2CO+C6H6#	1.37E12	0.0	-1.04E3	!Est.
!indene+R20H=>o-methylbenzyl+B2CO	1.37E12	0.0	-1.04E3	

indene+O2=R300H+indenyl	1.4E12	0.0	31.03E3	! as n-
buthylbenzene mais E = DH de reaction				
indene+B10=indenyl+R20H	1.76E11	0.7	3.25E3	! A-I-21
secondary A*2				
indene+R1H=indenyl+H2	1.08E5	2.5	-1.9E3	! A-I-21
secondary A*2				
indene+R20H=indenyl+H2O	6.0E6	2.0	-1.52E3	! A-I-21
secondary A*2				
indene+R4CH3=indenyl+CH4	2.0E11	0.0	7.3E3	! A-I-21
secondary A*2				
indene+R300H=H2O2+indenyl	1.28E4	2.6	12.4E3	! A-I-21
secondary A*2				

!indene+R1H=ph#C3H4Y	5.8E13	0.0	8.1E3	!ipso-addition
!indene+R1H=ph#C3H4-1	5.8E13	0.0	8.1E3	!ipso-addition
indene+R1H=>C2H2+benzyl	1.16E14	0.0	8.1E3	!mf 2x ipso-addition

indenyl=>C5H5#+C4H2	5.0E13	0.0	75.0E3	!Slavinskaya09
5.0E13 0.0 37.5E3				
indenyl+R1H=indene	1.0E14	0.0	0.0	!as n-buthylbenzene
C6H5#+C3H3=indene	6.46E12	0.0	0.0	!Slavinskaya09
!indenyl+R300H=>C6H6#+B2CO+R9C2H+R20H	3.0E12	0.0	0.0	! Est.!
similar to C5H5#+H02				
indenyl+R300H=>C6H5#C2H+R5CHO+R20H	3.0E12	0.0	0.0	! Est.!
similar to C5H5#+H02				

```

indeny1+B10=>C6H6#+B2C0+R9C2H      5.8E13  -0.02  0.02E3 !Est.
C5H5#+B10=C5H40#+R1H
indeny1+B10=>C6H5#C2H+R5CHO         5.8E13  -0.02  0.02E3 !Est.
C5H5#+B10=C5H40#+R1H

indeny1+R20H=>styrene+B2C0      4.0E14  0.0    4.5E3  !Est.
C5H5#+OH=C4H6Z2+C0

!C9H70#=C9H60#+R1H                2.0E13  0.0    27.5E3  ! Est.like ph#CH20
!C9H70#=>C6H6#+B2C0+R9C2H        2.8E13  0.0    17.1E3  ! Est.CH3C0=CH3+C0
!C9H70#=C6H5#C2H+R5CHO            2.8E13  0.0    17.1E3  ! Est.CH3C0=CH3+C0

!END
END

```

### Механизм окисления смеси метилгексаноат/н-гептан/толуол

```

ELEMENTS
H O C N AR
END
SPECIES

```

```

! Biradicals :
B10
B2C0
B3C
B4CH
B5CH2
B6CH2

```

```

! Primary molecules :
! Reactants:
C7H16-1
C8H18-1
H2
H2O
O2

```

H2O2  
CH4  
HCHO  
CH3OH  
CO2  
CH3OOH  
C2H2  
C2H4Z  
C2H6  
CH2COZ  
CH3CHO  
C2H5OH  
C2H3OH  
C2H5OOH  
CH3COOOH  
C3H6Y  
C3H8  
C4H8Y  
C4H10  
C2H5CHO  
C3H7OH  
C2H6CO  
C3H8CO  
C4H6Z2  
C2H3CHOZ  
C7H16  
C8H18  
C5H10Z  
C7H14Z  
C6H12Z  
C7H14Y  
C8H16Y  
C8H16Z  
C5H10Y  
C4H100L  
C4H1002P  
C3H802P  
C5H12  
C5H100A  
C4H80A  
C5H120L  
C6H14

! Secondary molecules :

C6H120A  
C7H140A  
C9H18Z  
C10H20Z  
C13H26Z  
C12H24Z  
C11H22Z  
!C14H28Z  
C8H160A  
C9H180A

C12H240A  
C11H220A  
C10H200A  
C13H260A  
C3H60LY  
C3H602PY  
C4H60AY  
C4H80LY  
C6H10Y2  
C7H12Y2  
C10H18Y2  
C11H20Y2  
C8H14Y2  
C4H802PY  
C5H80AY  
C5H100LY  
C12H22Y2  
C9H16Y2  
C7H140LY  
C7H1402PY  
C8H140AY  
C8H160LY  
!C14H26Y2  
!C15H28Y2  
C8H1602PY  
C9H160AY  
C9H180LY  
!C16H30Y2  
C13H24Y2  
C5H1002PY  
C6H100AY  
C6H120LY  
C4H60KZ  
C5H80KZ  
C6H100KZ  
C7H120KZ

! Cyclic primary molecules :  
C2H40E#3

! Cyclic secondary molecules :  
C3H60E#3  
C4H80E#3  
C5H100E#3  
C7H140E#3  
C6H120E#3  
C8H160E#3  
C9H180E#3  
C10H200E#3  
C13H260E#3  
C12H240E#3  
C11H220E#3  
!C14H280E#3

! Benzenic primary molecules :

! Free radicals :

R1H ! .h  
R2OH ! .oh  
R3OOH ! .o/oh  
R4CH3 ! .ch3  
R5CHO ! .ch//o  
R6CH2OH ! .ch2/oh  
R7CH3O ! .o/ch3  
R8CH3OO ! .o/o/ch3  
R9C2H ! .c///ch  
R10C2H3V ! .ch//ch2  
R11C2H5 ! .ch2/ch3  
R12CHCOZ ! .ch//c//o  
R13CH2CHO ! .ch2/ch//o  
R14CH3CO ! .c(/o)/ch3  
R15C2H5O ! .o/ch2/ch3  
R16C2H4OOH ! .ch2/ch2/o/oh  
R17C2H5OO ! .o/o/ch2/ch3  
R18CH3COOO ! .o/o/c(/o)/ch3  
R19C3H7 ! .ch2/ch2/ch3  
R20C4H9 ! .ch2/ch2/ch2/ch3  
R21CH3OCO ! .c(/o)/o/ch3  
!R22CO2H ! .c(/o)/oh  
!R23C2H3O2B ! .ch2/c(/o)/oh  
!R24C2H4OH ! .ch2/ch2/oh  
!R25C2H4OH ! .ch(/oh)/ch3  
R23C2H4OH ! c.h2-ch2-oh  
R24C2H4OH ! ch3-c.h-oh  
R25C2H5CO ! ch3-ch2-c.o  
  
R26C7H15 ! .ch(/ch2/ch2/ch3)2  
R27C7H15 ! .ch2/ch2/ch2/ch2/ch2/ch2/ch3  
R28C7H15 ! .ch(/ch3)/ch2/ch2/ch2/ch2/ch3  
R29C7H15 ! .ch(/ch2/ch3)/ch2/ch2/ch2/ch3  
R30C8H17 ! .ch2/c(/ch3)2/ch2/ch(/ch3)2  
R31C8H17 ! .ch2/ch(/ch3)/ch2/c(/ch3)3  
R32C8H17 ! .c(/ch3)2/ch2/c(/ch3)3  
R33C8H17 ! .ch(/ch(/ch3)2)/c(/ch3)3  
R34C4H9 ! .ch(/ch3)/ch2/ch3  
R35C5H11 ! .ch2/ch2/ch2/ch2/ch3  
R36C4H9 ! .ch2/ch(/ch3)2  
R37C5H11 ! .ch2/c(/ch3)3  
R38C4H9 ! .c(/ch3)3  
R39C5H11 ! .ch(/ch2/ch3)2  
R40C5H11 ! .ch(/ch3)/ch2/ch2/ch3  
R41C6H13 ! .ch2/ch2/ch2/ch2/ch2/ch3  
R42C7H15 ! .c(/ch3)2/ch2/ch(/ch3)2  
R43C3H7 ! .ch(/ch3)2  
R44C7H15 ! .ch(/ch3)/ch2/c(/ch3)3

!Cyclic free radicals:

!Benzenic free radicals:

! lumped Free radicals :

RC3H5Y  
RC4H7Y  
RC3H50  
RC7H13Y  
RC8H15Y  
RC5H9Y  
RC5H90  
RC4H70  
RC3H503  
RC6H110  
RC7H130  
RC5H903  
RC4H703  
RC6H1103  
RC7H1303  
RC8H150  
RC9H170  
RC12H230  
RC11H210  
RC10H190  
RC13H250  
RC8H1503  
RC9H1703  
RC11H23  
RC12H2303  
RC10H21  
RC11H2103  
RC9H19  
RC10H1903  
RC12H25  
RC13H2503  
RC6H11Y

! lumped Cyclic free radicals :

N2

AR

!!!!!!!!!!!!Especies rajoutées pour le мйса toлуине

aC3H4	!ch2//ch//ch2	propadiene = allene
pC3H4	!ch///c/ch3	propyne
C4H2	!ch///c/c///ch	butadiyne = diacetylene
C4H4	!ch2//ch/c///ch	1-buten-3-yne ou vinyl
acetylene		
C4H6-12	!ch2//c//ch/ch3	1,2-butadiene ou
мйthyl allиne		
C4H6-1	!ch///c/ch2/ch3	1-butyne
C4H6-2	!ch3/c///c/ch3	2-butyne
iC4H8	!ch2//c(ch3)/ch3	2methyl-propene
C5H8	!ex ch2//ch/ch2/ch//ch2	pentadiene
iC5H8	!ex ch3/c(ch3)//c//ch2	
!iC5H10	!ex ch3/ch(ch3)/ch//ch2	
!C5H10	!ex ch2//ch/ch2/ch2/ch3	pentene

C5H8#	!c(#1)h2/ch2/ch//ch/ch2/1	cyclopentene
C5H6#	!c(#1)h//ch/ch//ch/ch2/1	cyclopentadiene
C6H6#	!c(#1)h&ch&ch&ch&ch&ch&1	benzene
toluene	!c(#1)h&ch&ch&ch&ch&ch&1(/ch3)	
MCP	!c(#1)h2/ch2/ch//ch/ch(/ch3)/1	methylcyclopentene
MCPD	!c(#1)h//ch/ch//ch/ch(/ch3)/1	methylcyclopentadiene
C5H40#	!o//c(#1)/ch//ch/ch//ch/1	
C3H2	!.ch//c//c(.)h	
C2H40#3	!c(#1)h2/o/ch2/1	
C2H3CHO	!ch(/o)/ch//ch2	2-propenal
cC3H4	!c(#1)h2/ch//ch/1	cyclopropene
cC3H6	!c(#1)h2/ch2/ch2/1	cyclopropane
tC4H4	!ch2//c//c//ch2	1,2,3 butatriene
C6H2	!ch//c/c//c/c//ch	hexatriyne
cC4H6	!c(#1)h2/ch//ch/ch2/1	cyclobutene
lC6H4	!ch//c/ch//ch/c//ch	
!lC6H6	!ch2//ch/c//c/ch//ch2	!MF car n'intervient plus (une rñaction)
lC6H8	!ch2//ch/ch//ch/ch//ch2	
C6H8#	!c(#1)h2/ch//ch/ch2/ch//ch/1	cyclohexadiene
C6H10#	!c(#1)h2/ch//ch/ch2/ch2/ch2/1	cyclohexene
C8H10#	!c(#1)h2/ch//ch/ch//ch/ch//ch/ch2/1	cyclooctatriene
!Espes excitees		
OHE		
CHE		
iC3H7	!.ch(/ch3)2	
C3H3	!ch//c/ch2(.)	
C3H5Y	!.ch2/ch//ch2	
tC3H5	!ch2//c./ch3	
sC3H5	!.ch//ch/ch3	
nC4H3	!.ch//ch/c//ch	
iC4H3	!ch2//c./c//ch	
nC4H5	!.ch//ch/ch//ch2	
iC4H5	!ch2//c./ch//ch2	
C4H5-1s	!ch//c/ch./ch3	
C4H5-1p	!.ch2/ch2/c//ch	
C4H5-2	!.ch2/c//c/ch3	
lC6H5	!ch//c/ch//ch/ch//ch(.)	
lC6H7	!ex .ch//ch/ch//ch/ch//ch2	
!lC6H9	!ex .ch//ch/ch//ch/ch2/ch3	!MF car n'intervient plus (une rñaction)
C6H4#	!.c(#1)&ch&ch&ch&c(.)&1	
C6H5#	!.c(#1)&ch&ch&ch&ch&1	
C6H7#	!.c(#1)h/ch//ch/ch2/ch//ch/1	
C6H9Z#	!.c(#1)h/ch//ch/ch2/ch2/ch2/1	
C4H7-1	!.ch2/ch2/ch//ch2	
C4H7-2	!ch3/c./ch/ch3	
C4H7Y	!ch3/c./h/ch//ch2	
C4H7T	!ch2//c./ch2/ch3	
iC4H7	!.ch//c(/ch3)2	
C4H7V	!.c(/ch3)//ch/ch3	
!C5H7Y	!ch2//ch/ch//ch/c(.)h2	
!iC5H7Y	!ch2//c(/c(.)h2)/ch//ch2	
C5H9Y	!ch2//ch/c(.)h/ch2/ch3	

```

iC5H9      !.ch2/ch(/ch3)/ch//ch2
!iC5H9Y    !ch3/c(./ch3)/ch//ch2
CH2CHCO    !.ch2/ch//c//o
cC3H3      !.c(#1)h/ch//ch/1
! MECHANISM OF BENZENE
! Molecules
C4H4O      !ch2//ch/ch//c//o          vinylketene
!lC5H6     !ch///c/ch//ch/ch3          !MF car
n'intervient plus (une rñaction)
C5H5OH#    !c(#1)h//ch/ch//ch/ch(/oh)/1    cyclopentadienol
C6H5OH#    !c(#1)h&ch&ch&ch&ch&c(/oh)&1    phñnol
OC6H4O     !o//c(#1)/ch//ch/ch//ch/c(/o)/1    orthobenzoquinone
C6H5#C2H   !ch///c/c(#1)&ch&ch&ch&ch&ch/1    phenylacetylene
etC6H5     !c(#1)h&ch&ch&ch&ch&c(/ch2/ch3)&1    ethylbenzene
styrene    !c(#1)h&ch&ch&ch&ch&c(/ch//ch2)&1
!C6H5C3H3 !c(#1)h&ch&ch&ch&ch&c(/ch//c//ch2)&1 !MF car n'intervient plus
(une rñaction)
C10H10#    !c(#1)h(c(#1)h/ch//ch/ch//ch/1)/ch//ch/ch//ch/1 !
bicyclopentadienyl
C6H5CHO    !c(#1)h&ch&ch&ch&ch&c(/ch//o)&1    benzaldehyde
biphenyl   !c(#1)h&ch&ch&ch&ch&c(/c(#2)h&ch&ch&ch&c&c2)&1
C6H5OOH

```

! Radicals

```

C5H5#      !c(#1)(.)h/ch//ch/ch//ch/1
lC5H5      !.c///c/ch//ch/ch3
C5H3O#     !.c(#1)//ch/ch//ch/c(/o)&1
C5H5O#     !c(#1)h//ch/ch//ch/ch(/o(.))&1
C5H4OH#    !.c(#1)//ch/ch//ch/ch(/oh)&1
C6H5O#     !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5O2     !.c(#1)&ch&ch&ch&ch&c(/o/o(.))&1
C6H4OH#    !.c(#1)&ch&ch&ch&ch&c(/oh)&1
OC6H4OH    !c(#1)h&ch&ch&ch&ch(/o(.))&c(/oh)&1

```

!MECHANISM OF TOLUENE

```

HOC6H4CH3 !oh/c(#1)&ch&ch&ch&ch&c(/ch3)&1 cresol
C6H4OHCHO !oh/c(#1)&ch&ch&ch&ch&c(/ch//o)&1
C6H5CH2OH !c(#1)h&ch&ch&ch&ch&c(/ch2/oh)&1
C6H5CH2OOH !c(#1)h&ch&ch&ch&ch&c(/ch2/o/oh)&1
bibenzyl   !ok
stilbene   !ok
benzyl     !c(#1)h&ch&ch&ch&ch&c(/c(. )h2)&1
C6H4CH3    !c(#1)h&ch&ch&ch&ch&c(/ch3)&1
C6H4OHCO   !oh/c(#1)&ch&ch&ch&ch&c(/c(. )//o)&1
HOC6H4CH2O !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o/o(.))&1
OC6H4CH3   !o(. )/c(#1)&ch&ch&ch&ch&c(/ch3)&1
HOC6H4CH2  !oh/c(#1)&ch&ch&ch&ch&c(/c(. )h2)&1
C6H5CO     !c(#1)h&ch&ch&ch&ch&c(/o(.))&1
C6H5CHOH   !c(#1)h&ch&ch&ch&ch&c(/c(. )h/oh)&1
C6H5CH2O   !c(#1)h&ch&ch&ch&ch&c(/ch2/o(.))&1
HOC6H4CH2O !oh/c(#1)&ch&ch&ch&ch&c(/ch2/o(.))&1
C6H5CH2OO  !c(#1)h&ch&ch&ch&ch&c(/ch2/o/o(.))&1
C8H9#      !c(#1)h&ch&ch&ch&ch&c(/c(. )h2/ch2)&1

```



C8H9#-1 !c(#1)h&ch&ch&ch&ch&c(/ch2/c(. )h2)&1  
 C6H5C2H2 !c(#1)h&ch&ch&ch&ch&c(/ch//c(. )h)&1  
 C14H13# !bibenzyl -H

!MECHANISM OF CYCLOPENTENE!

!C5H8-12 !ch2//c//ch/ch2/ch3  
 !C5H7# !.c(#1)h/ch2/ch//ch/ch2/1  
 !C5H7#Y !c(#1)h2/c(. )h/ch//ch/ch2/1  
 !C5H7#V !c(#1)h2/ch2/c(. )//ch/ch2/1  
 !C5H7-1s !ch(. )//ch/ch2/ch//ch2  
 !C5H7-2t !ch2//ch/ch2/c(. )//ch2  
 !C5H7-4t !ch3/c(. )//ch/ch//ch2  
 !C5H7-3t !ch3/ch//c(. )/ch//ch2  
 !C5H7-5p !ch2(. )/ch2/ch2/c///ch  
 !C5H7-12-5p !ch2(. )/ch2/ch//c//ch2  
 !C5H9# !.c(#1)h/ch2/ch2/ch2/ch2/1  
 !C5H9 !(.)ch2/ch2/ch2/ch//ch2  
 !RMCP1 !c(#1)h(. )/ch2/ch//ch/ch(/ch3)/1  
 !RMCP2 !c(#1)h2/ch2/ch//ch/ch(/ch2(. ))/1  
 !RMCPY1 !c(#1)h2/ch(. )/ch//ch/ch(/ch3)/1  
 !RMCPY2 !c(#1)h2/ch2/ch//ch/c(. )(/ch3)/1  
 !RMCPD !c(#1)h//ch/ch//ch/ch(/ch2(. ))/1  
 !RMCPDY !c(#1)h//ch/ch//ch/c(. )(/ch3)/1

!\*Espèces ajoutées\*!

!mfC5H5C2H2 !c(#1)h//ch/ch//ch/c(/ch//c(. )h)&1  
 !C5H4CCH2 !c(#1)h//ch/ch//ch/c(/c//ch2)/1  
 !C5H5CCH !c(#1)h//ch/ch//ch/ch(/c//ch)/1  
 !C6H5COCH3 !C6H5x/CO/CH3  
 C8H9#00H !C6H5#ch(/ooh)/ch3 !c(#1)h&ch&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1  
 C8H9#0 !C6H5#ch(/o(. ))/ch3 !  
 c(#1)h&ch&ch&ch&ch&c(/ch(/o(. ))/ch3)&1  
 00C6H4CH3 !o(. )/o/c(#1)&ch&ch&ch&ch&c(/ch3)&1  
 !C6H5OCH2C6H5 !c(#1)h&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1  
 !To10CH2C6H5 !ch3/c(#1)&ch&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1  
 !PhenolCH2bz !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1  
 !PhenolC2H4bz !h/o/c(#1)&ch&ch&ch&ch&c(/ch2/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1  
 CH3bzOHCH2bz !h/o/c(#1)&ch&ch&c(/ch3)&ch&c(/ch2/c(#2)&ch&ch&ch&ch&ch&2)&1  
 !Benzaldtol !  
 c(#1)h&ch&ch&ch&ch&c(/c(/o)/o/c(#2)&ch&ch&c(/ch3)&ch&ch&2)&1  
 !HOC6H4CHO !h/o/c(#1)&ch&ch&ch&c(/ch//o)&ch&1  
 !C6H5C4H7 !c(#1)h&ch&ch&ch&ch&c(/ch2/ch2/ch//ch2)&1  
 naphthalene  
 !benzofuran  
 C8H80# !c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch2/2  
 C8H70# !c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch(. )/ch2/2  
 C8H70#-1 !c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch(. )/2  
 naphthyl  
 indenyl  
 indene  
 !cumene  
 !CH3styre

C9H11#-1  
 C2H3C6H4CH2  
 !phenanthrene  
 !C6H5CH2CHO  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 \*\*\*\*\*

!!! MEthylEtHaNOate sPECiEs !!!

MEMj  
 ME2j ME2\*0 ME2j\*0  
 !!! MEthylPrOPaNOate sPECiEs !!!  
 MP2j MP3j MP2D3j MP2D2j MP2DMj MPMj  
 !!! MEthylButaNOate sPECiEs !!!  
 MB2j MB3j MB4j MBMj  
 MB3D2j MB2DMj MB3DMj MB2D3j

!!! MEthylPENTaNOate sPECiEs !!!

MPE5j MPE4j MPE3j MPE2j MPEMj MPE4D3j MPE4D2j  
 MPE3D2j MPE4D2D MPE

!  
 ME MP MP2D MB MP2D MB3D MB2D MB2D-z MB3D20 MPE4D MPE3D MPE2D  
 !

NC4H9CO  
 CH3CHCO  
 C2H5CHO  
 C2H3CO  
 CH2CCO  
 C3H7CO  
 sC3H5CO  
 aC3H5CO  
 C2H3CO2  
 !C4H7-3 C4H7-4

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!!! Methyl Hexanoate Species

!!!!!!!!!!!!!!!!!!!!  
 MHX MHX5d MHX4d MHX3d MHX2d  
 MHX6j MHX5j MHX4j MHX3j MHX2j MHXmj  
 MHX5d4j MHX4d3j MHX3d2j

HXAoj C5H8CO  
 !!!!!!!!!!!!!  
 HCCCCO

END

REACTIONS

!(k = A T\*\*b exp(-E/RT)) A units: mole-cm-sec-K, E units cal/mole

!  
 ! -----  
 ! PRIMARY REACTIONS  
 ! -----

! molecular elimination :  
 ! unimolecular initiations :

C7H16-1=>R19C3H7+R20C4H9 2.0E+0017 0.000 85750.3 ! UI 1 KB  
 C7H16-1=>R11C2H5+R35C5H11 1.6E+0017 0.000 85815.5 ! UI 2 KB

C7H16-1=>R4CH3+R41C6H13	3.2E+0017	0.000	87654.8	! UI 3 KB
C8H18-1=>R4CH3+R42C7H15	1.2E+0018	0.000	81845.9	! UI 4 KB
C8H18-1=>R36C4H9+R38C4H9	2.4E+0017	0.000	78804.1	! UI 5 KB
C8H18-1=>R43C3H7+R37C5H11	4.6E+0017	0.000	83562.0	! UI 6 KB
C8H18-1=>R4CH3+R44C7H15	8.0E+0017	0.000	87665.1	! UI 7 KB

! bimolecular initiations :

C7H16-1+O2=>R300H+R26C7H15	1.4E+0013	0.000	50652.5	! BI 8 CN
C7H16-1+O2=>R300H+R27C7H15	4.2E+0013	0.000	53033.1	! BI 9 CN
C7H16-1+O2=>R300H+R28C7H15	2.8E+0013	0.000	50588.2	! BI 10 CN
C7H16-1+O2=>R300H+R29C7H15	2.8E+0013	0.000	50652.5	! BI 11 CN
C8H18-1+O2=>R300H+R30C8H17	6.3E+0013	0.000	53033.0	! BI 12 CN
C8H18-1+O2=>R300H+R31C8H17	4.2E+0013	0.000	52333.1	! BI 13 CN
C8H18-1+O2=>R300H+R32C8H17	7.0E+0012	0.000	47243.3	! BI 14 CN
C8H18-1+O2=>R300H+R33C8H17	1.4E+0013	0.000	50652.7	! BI 15 CN

! additions :

! additions with oxygen:

! isomerisations :

R20C4H9=R34C4H9	3.3E+0009	1.000	37000.0	! IS 16 KB
R26C7H15=R28C7H15	6.7E+0009	1.000	37000.0	! IS 17 KB
R26C7H15=R27C7H15	1.7E+0009	1.000	19800.0	! IS 18 KB
R27C7H15=R29C7H15	9.9E+0007	1.000	37000.0	! IS 19 KB
R27C7H15=R28C7H15	1.7E+0007	1.000	17400.0	! IS 20 KB
R28C7H15=R29C7H15	5.7E+0008	1.000	17300.0	! IS 21 KB
R30C8H17=R33C8H17	3.3E+0009	1.000	37000.0	! IS 22 KB
R30C8H17=R32C8H17	2.9E+0008	1.000	15300.0	! IS 23 KB
R30C8H17=R31C8H17	3.0E+0008	1.000	14500.0	! IS 24 KB
R31C8H17=R33C8H17	3.3E+0009	1.000	37000.0	! IS 25 KB
R35C5H11=R39C5H11	3.3E+0009	1.000	37000.0	! IS 26 KB
R35C5H11=R40C5H11	5.7E+0008	1.000	17300.0	! IS 27 KB

! Decomposition of 00Q00H into branching agents:

! beta-scissions :

R19C3H7=>R4CH3+C2H4Z	2.0E+0013	0.000	31000.0	! DE 28 CN
R19C3H7=>R1H+C3H6Y	3.0E+0013	0.000	38000.0	! DE 29 CN
R20C4H9=>R11C2H5+C2H4Z	2.0E+0013	0.000	28700.0	! DE 30 CW
R20C4H9=>R1H+C4H8Y	3.0E+0013	0.000	38000.0	! DE 31 CN
R26C7H15=>R11C2H5+C5H10Z	4.0E+0013	0.000	28700.0	! DE 32 CW
R26C7H15=>R1H+C7H14Z	6.0E+0013	0.000	38000.0	! DE 33 CN
R27C7H15=>R35C5H11+C2H4Z	2.0E+0013	0.000	28700.0	! DE 34 CW
R27C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	! DE 35 CN
R28C7H15=>R20C4H9+C3H6Y	2.0E+0013	0.000	28700.0	! DE 36 CW
R28C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	! DE 37 CN
DUPLICATE				
R28C7H15=>R1H+C7H14Z	3.0E+0013	0.000	39000.0	! DE 38 CN
DUPLICATE				
R29C7H15=>R19C3H7+C4H8Y	2.0E+0013	0.000	28700.0	! DE 39 CW
R29C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	! DE 40 CN
DUPLICATE				
R29C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	! DE 41 CN

DUPLICATE

R29C7H15=>R4CH3+C6H12Z	2.0E+0013	0.000	31000.0	!	DE 42	CN
R30C8H17=>R36C4H9+C4H8Y	2.0E+0013	0.000	28700.0	!	DE 43	CW
R30C8H17=>R4CH3+C7H14Y	4.0E+0013	0.000	31000.0	!	DE 44	CN
R31C8H17=>R37C5H11+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 45	CW
R31C8H17=>R4CH3+C7H14Z	2.0E+0013	0.000	31000.0	!	DE 46	CN
R31C8H17=>R1H+C8H16Y	1.5E+0013	0.000	37500.0	!	DE 47	CN
R32C8H17=>R38C4H9+C4H8Y	2.0E+0013	0.000	26700.0	!	DE 48	
R32C8H17=>R1H+C8H16Y	6.0E+0013	0.000	39000.0	!	DE 49	CN
R32C8H17=>R1H+C8H16Z	3.0E+0013	0.000	38000.0	!	DE 50	CN
R33C8H17=>R4CH3+C7H14Z	4.0E+0013	0.000	31000.0	!	DE 51	CN
R33C8H17=>R4CH3+C7H14Y	6.0E+0013	0.000	31000.0	!	DE 52	CN
R33C8H17=>R1H+C8H16Z	3.0E+0013	0.000	37500.0	!	DE 53	CN
R34C4H9=>R4CH3+C3H6Y	2.0E+0013	0.000	31000.0	!	DE 54	CN
R34C4H9=>R1H+C4H8Y	3.0E+0013	0.000	38000.0	!	DE 55	CN

DUPLICATE

R34C4H9=>R1H+C4H8Y	3.0E+0013	0.000	39000.0	!	DE 56	CN
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DUPLICATE

R35C5H11=>R19C3H7+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 57	CW
R35C5H11=>R1H+C5H10Z	3.0E+0013	0.000	38000.0	!	DE 58	CN
R36C4H9=>R4CH3+C3H6Y	4.0E+0013	0.000	31000.0	!	DE 59	CN
R36C4H9=>R1H+C4H8Y	3.0E+0013	0.000	37500.0	!	DE 60	CN
R37C5H11=>R4CH3+C4H8Y	6.0E+0013	0.000	31000.0	!	DE 61	CN
R38C4H9=>R1H+C4H8Y	9.0E+0013	0.000	39000.0	!	DE 62	CN
R39C5H11=>R4CH3+C4H8Y	4.0E+0013	0.000	31000.0	!	DE 63	CN
R39C5H11=>R1H+C5H10Y	6.0E+0013	0.000	38000.0	!	DE 64	CN
R40C5H11=>R11C2H5+C3H6Y	2.0E+0013	0.000	28700.0	!	DE 65	CW
R40C5H11=>R1H+C5H10Z	3.0E+0013	0.000	39000.0	!	DE 66	CN
R40C5H11=>R1H+C5H10Y	3.0E+0013	0.000	38000.0	!	DE 67	CN
R41C6H13=>R20C4H9+C2H4Z	2.0E+0013	0.000	28700.0	!	DE 68	CW
R41C6H13=>R1H+C6H12Z	3.0E+0013	0.000	38000.0	!	DE 69	CN
R42C7H15=>R43C3H7+C4H8Y	2.0E+0013	0.000	27700.0	!	DE 70	
R42C7H15=>R1H+C7H14Y	3.0E+0013	0.000	38000.0	!	DE 71	CN

DUPLICATE

R42C7H15=>R1H+C7H14Y	6.0E+0013	0.000	39000.0	!	DE 72	CN
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DUPLICATE

R43C3H7=>R1H+C3H6Y	6.0E+0013	0.000	39000.0	!	DE 73	CN
R44C7H15=>R38C4H9+C3H6Y	2.0E+0013	0.000	26700.0	!	DE 74	
R44C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE 75	CN

DUPLICATE

R44C7H15=>R1H+C7H14Z	3.0E+0013	0.000	39000.0	!	DE 76	CN
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DUPLICATE

! decomposition of R(.)C0 free radicals

! decomposition to o-rings :

! oxidations :

R26C7H15+O2=>C7H14Z+R300H	3.9E+0012	0.000	5000.0	!	OX 77	CN
R27C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 78	CN
R28C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 79	CN

DUPLICATE

R28C7H15+O2=>C7H14Z+R300H	8.1E+0011	0.000	5000.0	!	OX 80	CN
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DUPLICATE

R29C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	!	OX 81	CN
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DUPLICATE  
R29C7H15+O2=>C7H14Z+R300H 1.9E+0012 0.000 5000.0 ! OX 82 CN  
DUPLICATE  
R31C8H17+O2=>C8H16Y+R300H 6.4E+0011 0.000 5000.0 ! OX 83 CN  
R32C8H17+O2=>C8H16Y+R300H 1.6E+0012 0.000 5000.0 ! OX 84 CN  
R32C8H17+O2=>C8H16Z+R300H 1.9E+0012 0.000 5000.0 ! OX 85 CN  
R33C8H17+O2=>C8H16Z+R300H 6.4E+0011 0.000 5000.0 ! OX 86 CN  
R38C4H9+O2=>C4H8Y+R300H 1.6E+0012 0.000 5000.0 ! OX 87 CW  
R43C3H7+O2=>C3H6Y+R300H 2.3E+0012 0.000 5000.0 ! OX 88 CW

! oxidations of R(.) (OH) radicals:

! metathesis :

B10+C7H16-1=>R20H+R26C7H15 2.6E+0013 0.000 5200.0 ! ME 89 CW  
B10+C7H16-1=>R20H+R27C7H15 1.0E+0014 0.000 7850.0 ! ME 90 CW  
B10+C7H16-1=>R20H+R28C7H15 5.2E+0013 0.000 5200.0 ! ME 91 CW  
B10+C7H16-1=>R20H+R29C7H15 5.2E+0013 0.000 5200.0 ! ME 92 CW  
B10+C8H18-1=>R20H+R30C8H17 1.5E+0014 0.000 7850.0 ! ME 93 CW  
B10+C8H18-1=>R20H+R31C8H17 1.0E+0014 0.000 7850.0 ! ME 94 CW  
B10+C8H18-1=>R20H+R32C8H17 1.0E+0013 0.000 3280.0 ! ME 95 CW  
B10+C8H18-1=>R20H+R33C8H17 2.6E+0013 0.000 5200.0 ! ME 96 CW  
C7H16-1+R1H=>H2+R26C7H15 9.0E+0006 2.000 5000.0 ! ME 97 CW  
C7H16-1+R1H=>H2+R27C7H15 5.7E+0007 2.000 7700.0 ! ME 98 CW  
C7H16-1+R1H=>H2+R28C7H15 1.8E+0007 2.000 5000.0 ! ME 99 CW  
C7H16-1+R1H=>H2+R29C7H15 1.8E+0007 2.000 5000.0 ! ME 100 CW  
C8H18-1+R1H=>H2+R30C8H17 8.6E+0007 2.000 7700.0 ! ME 101 CW  
C8H18-1+R1H=>H2+R31C8H17 5.7E+0007 2.000 7700.0 ! ME 102 CW  
C8H18-1+R1H=>H2+R32C8H17 4.2E+0006 2.000 2400.0 ! ME 103 CN  
C8H18-1+R1H=>H2+R33C8H17 9.0E+0006 2.000 5000.0 ! ME 104 CW  
C7H16-1+R20H=>H20+R26C7H15 2.6E+0006 2.000 -765.0 ! ME 105 CW  
C7H16-1+R20H=>H20+R27C7H15 5.4E+0006 2.000 450.0 ! ME 106 CW  
C7H16-1+R20H=>H20+R28C7H15 5.2E+0006 2.000 -765.0 ! ME 107 CW  
C7H16-1+R20H=>H20+R29C7H15 5.2E+0006 2.000 -765.0 ! ME 108 CW  
C8H18-1+R20H=>H20+R30C8H17 8.1E+0006 2.000 450.0 ! ME 109 CW  
C8H18-1+R20H=>H20+R31C8H17 5.4E+0006 2.000 450.0 ! ME 110 CW  
C8H18-1+R20H=>H20+R32C8H17 1.1E+0006 2.000 -1865.0 ! ME 111 CW  
C8H18-1+R20H=>H20+R33C8H17 2.6E+0006 2.000 -765.0 ! ME 112 CW  
C7H16-1+R300H=>H202+R26C7H15 4.0E+0011 0.000 15500.0 ! ME 113 CN  
C7H16-1+R300H=>H202+R27C7H15 1.2E+0012 0.000 17000.0 ! ME 114 CN  
C7H16-1+R300H=>H202+R28C7H15 8.0E+0011 0.000 15500.0 ! ME 115 CN  
C7H16-1+R300H=>H202+R29C7H15 8.0E+0011 0.000 15500.0 ! ME 116 CN  
C8H18-1+R300H=>H202+R30C8H17 1.8E+0012 0.000 17000.0 ! ME 117 CN  
C8H18-1+R300H=>H202+R31C8H17 1.2E+0012 0.000 17000.0 ! ME 118 CN  
C8H18-1+R300H=>H202+R32C8H17 2.0E+0011 0.000 14000.0 ! ME 119 CN  
C8H18-1+R300H=>H202+R33C8H17 4.0E+0011 0.000 15500.0 ! ME 120 CN  
C7H16-1+R4CH3=>CH4+R26C7H15 2.0E+0011 0.000 9600.0 ! ME 121 CN  
C7H16-1+R4CH3=>CH4+R27C7H15 6.0E-0001 4.000 8200.0 ! ME 122 CN  
C7H16-1+R4CH3=>CH4+R28C7H15 4.0E+0011 0.000 9600.0 ! ME 123 CN  
C7H16-1+R4CH3=>CH4+R29C7H15 4.0E+0011 0.000 9600.0 ! ME 124 CN  
C8H18-1+R4CH3=>CH4+R30C8H17 9.0E-0001 4.000 8200.0 ! ME 125 CN  
C8H18-1+R4CH3=>CH4+R31C8H17 6.0E-0001 4.000 8200.0 ! ME 126 CN  
C8H18-1+R4CH3=>CH4+R32C8H17 1.0E+0011 0.000 7900.0 ! ME 127 CW  
C8H18-1+R4CH3=>CH4+R33C8H17 2.0E+0011 0.000 9600.0 ! ME 128 CN  
C7H16-1+R5CHO=>HCHO+R26C7H15 1.0E+0007 1.900 17000.0 ! ME 129 CN

C7H16-1+R5CHO=>HCHO+R27C7H15	2.0E+0005	2.500	18500.0	!	ME 130	CN
C7H16-1+R5CHO=>HCHO+R28C7H15	2.2E+0007	1.900	17000.0	!	ME 131	CN
C7H16-1+R5CHO=>HCHO+R29C7H15	2.2E+0007	1.900	17000.0	!	ME 132	CN
C8H18-1+R5CHO=>HCHO+R30C8H17	3.1E+0005	2.500	18500.0	!	ME 133	CN
C8H18-1+R5CHO=>HCHO+R31C8H17	2.0E+0005	2.500	18500.0	!	ME 134	CN
C8H18-1+R5CHO=>HCHO+R32C8H17	3.4E+0004	2.500	13500.0	!	ME 135	CN
C8H18-1+R5CHO=>HCHO+R33C8H17	1.0E+0007	1.900	17000.0	!	ME 136	CN
C7H16-1+R6CH2OH=>CH3OH+R26C7H15	6.0E+0001	2.950	12000.0	!	ME 137	CN
C7H16-1+R6CH2OH=>CH3OH+R27C7H15	2.0E+0002	2.950	14000.0	!	ME 138	CN
C7H16-1+R6CH2OH=>CH3OH+R28C7H15	1.2E+0002	2.950	12000.0	!	ME 139	CN
C7H16-1+R6CH2OH=>CH3OH+R29C7H15	1.2E+0002	2.950	12000.0	!	ME 140	CN
C8H18-1+R6CH2OH=>CH3OH+R30C8H17	3.0E+0002	2.950	14000.0	!	ME 141	CN
C8H18-1+R6CH2OH=>CH3OH+R31C8H17	2.0E+0002	2.950	14000.0	!	ME 142	CN
C8H18-1+R6CH2OH=>CH3OH+R32C8H17	1.2E+0002	2.760	10800.0	!	ME 143	CN
C8H18-1+R6CH2OH=>CH3OH+R33C8H17	6.0E+0001	2.950	12000.0	!	ME 144	CN
C7H16-1+R7CH3O=>CH3OH+R26C7H15	1.5E+0011	0.000	4500.0	!	ME 145	CN
C7H16-1+R7CH3O=>CH3OH+R27C7H15	3.2E+0011	0.000	7300.0	!	ME 146	CN
C7H16-1+R7CH3O=>CH3OH+R28C7H15	2.9E+0011	0.000	4500.0	!	ME 147	CN
C7H16-1+R7CH3O=>CH3OH+R29C7H15	2.9E+0011	0.000	4500.0	!	ME 148	CN
C8H18-1+R7CH3O=>CH3OH+R30C8H17	4.9E+0011	0.000	7300.0	!	ME 149	CN
C8H18-1+R7CH3O=>CH3OH+R31C8H17	3.2E+0011	0.000	7300.0	!	ME 150	CN
C8H18-1+R7CH3O=>CH3OH+R32C8H17	2.3E+0010	0.000	2900.0	!	ME 151	CN
C8H18-1+R7CH3O=>CH3OH+R33C8H17	1.5E+0011	0.000	4500.0	!	ME 152	CN
C7H16-1+R8CH3OO=>CH3OOH+R26C7H15	3.0E+0012	0.000	17500.0	!	ME 153	CN
C7H16-1+R8CH3OO=>CH3OOH+R27C7H15	1.2E+0013	0.000	20000.0	!	ME 154	CN
C7H16-1+R8CH3OO=>CH3OOH+R28C7H15	6.0E+0012	0.000	17500.0	!	ME 155	CN
C7H16-1+R8CH3OO=>CH3OOH+R29C7H15	6.0E+0012	0.000	17500.0	!	ME 156	CN
C8H18-1+R8CH3OO=>CH3OOH+R30C8H17	1.8E+0013	0.000	20000.0	!	ME 157	CN
C8H18-1+R8CH3OO=>CH3OOH+R31C8H17	1.2E+0013	0.000	20000.0	!	ME 158	CN
C8H18-1+R8CH3OO=>CH3OOH+R32C8H17	1.5E+0012	0.000	15000.0	!	ME 159	CN
C8H18-1+R8CH3OO=>CH3OOH+R33C8H17	3.0E+0012	0.000	17500.0	!	ME 160	CN
C7H16-1+R11C2H5=>C2H6+R26C7H15	2.0E+0011	0.000	11000.0	!	ME 161	CN
C7H16-1+R11C2H5=>C2H6+R27C7H15	6.0E+0011	0.000	13500.0	!	ME 162	CR
C7H16-1+R11C2H5=>C2H6+R28C7H15	4.0E+0011	0.000	11000.0	!	ME 163	CN
C7H16-1+R11C2H5=>C2H6+R29C7H15	4.0E+0011	0.000	11000.0	!	ME 164	CN
C8H18-1+R11C2H5=>C2H6+R30C8H17	9.0E+0011	0.000	13500.0	!	ME 165	CR
C8H18-1+R11C2H5=>C2H6+R31C8H17	6.0E+0011	0.000	13500.0	!	ME 166	CR
C8H18-1+R11C2H5=>C2H6+R32C8H17	1.0E+0011	0.000	9200.0	!	ME 167	CN
C8H18-1+R11C2H5=>C2H6+R33C8H17	2.0E+0011	0.000	11000.0	!	ME 168	CN
C7H16-1+R38C4H9=>C4H10+R26C7H15	1.0E+0011	0.000	12700.0	!	ME 169	CR
C7H16-1+R38C4H9=>C4H10+R27C7H15	3.0E+0011	0.000	15000.0	!	ME 170	CR
C7H16-1+R38C4H9=>C4H10+R28C7H15	2.0E+0011	0.000	12700.0	!	ME 171	CR
C7H16-1+R38C4H9=>C4H10+R29C7H15	2.0E+0011	0.000	12700.0	!	ME 172	CR
C8H18-1+R38C4H9=>C4H10+R30C8H17	4.5E+0011	0.000	15000.0	!	ME 173	CR
C8H18-1+R38C4H9=>C4H10+R31C8H17	3.0E+0011	0.000	15000.0	!	ME 174	CR
C8H18-1+R38C4H9=>C4H10+R32C8H17	5.0E+0010	0.000	11100.0	!	ME 175	CR

C8H18-1+R38C4H9=>C4H10+R33C8H17 1.0E+0011 0.000 12700.0 ! ME 176 CR

! combinations :

R1H+R38C4H9=>C4H10 8.3E+0012 0.000 0.0 ! CO 177 KB  
R1H+R43C3H7=>C3H8 8.3E+0012 0.000 0.0 ! CO 178 KB  
R2OH+R38C4H9=>C4H100L 5.7E+0012 0.000 0.0 ! CO 179 KB  
R2OH+R43C3H7=>C3H70H 5.9E+0012 0.000 0.0 ! CO 180 KB  
R300H+R38C4H9=>C4H1002P 4.5E+0012 0.000 0.0 ! CO 181 KB  
R300H+R43C3H7=>C3H802P 4.8E+0012 0.000 0.0 ! CO 182 KB  
R4CH3+R38C4H9=>C5H12 1.5E+0013 0.000 0.0 ! CO 183 KB  
R4CH3+R43C3H7=>C4H10 1.5E+0013 0.000 0.0 ! CO 184 KB  
R5CH0+R38C4H9=>C5H100A 4.9E+0012 0.000 0.0 ! CO 185 KB  
R5CH0+R43C3H7=>C4H80A 5.2E+0012 0.000 0.0 ! CO 186 KB  
R6CH2OH+R38C4H9=>C5H120L 4.8E+0012 0.000 0.0 ! CO 187 KB  
R6CH2OH+R43C3H7=>C4H100L 5.1E+0012 0.000 0.0 ! CO 188 KB  
R11C2H5+R38C4H9=>C6H14 4.9E+0012 0.000 0.0 ! CO 189 KB  
R11C2H5+R43C3H7=>C5H12 5.2E+0012 0.000 0.0 ! CO 190 KB  
R38C4H9+R38C4H9=>C8H18 2.0E+0012 0.000 0.0 ! CO 191 KB  
R38C4H9+R43C3H7=>C7H16 4.3E+0012 0.000 0.0 ! CO 192 KB  
R43C3H7+R43C3H7=>C6H14 2.3E+0012 0.000 0.0 ! CO 193 KB

! dismutations :

! -----  
! SECONDARY MECHANISM  
! -----

! Peroxide decomposition

! Hydroperoxide decomposition

C4H1002P=>R2OH+R11C2H5+CH3CHO 1.5E+0016 0.000 43000.0 ! DHP 194  
C3H802P=>R2OH+R11C2H5+HCHO 1.5E+0016 0.000 43000.0 ! DHP 195  
C3H602PY=>R2OH+R1H+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 196  
C4H802PY=>R2OH+R4CH3+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 197  
C7H1402PY=>R2OH+R20C4H9+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 198  
C8H1602PY=>R2OH+R35C5H11+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 199  
C5H1002PY=>R2OH+R11C2H5+C2H3CHOZ 1.5E+0016 0.000 43000.0 ! DHP 200

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

! Aldohydroperoxide decomposition

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions

C3H8+R1H=>H2+R19C3H7 5.7E+0007 2.000 7700.0 ! MH 201  
DUPLICATE  
C3H8+R1H=>H2+R19C3H7 9.0E+0006 2.000 5000.0 ! MH 202

DUPLICATE					
C3H8+R20H=>H2O+R19C3H7	5.4E+0006	2.000	450.0	!	MH 203
DUPLICATE					
C3H8+R20H=>H2O+R19C3H7	2.6E+0006	2.000	-765.0	!	MH 204
DUPLICATE					
C3H8+R300H=>H2O2+R19C3H7	1.2E+0012	0.000	17000.0	!	MH 205
DUPLICATE					
C3H8+R300H=>H2O2+R19C3H7	4.0E+0011	0.000	15500.0	!	MH 206
DUPLICATE					
C3H8+R4CH3=>CH4+R19C3H7	6.0E-0001	4.000	8200.0	!	MH 207
DUPLICATE					
C3H8+R4CH3=>CH4+R19C3H7	2.0E+0011	0.000	9600.0	!	MH 208
DUPLICATE					
C3H8+R8CH300=>CH300H+R19C3H7	1.2E+0013	0.000	20000.0	!	MH 209
DUPLICATE					
C3H8+R8CH300=>CH300H+R19C3H7	3.0E+0012	0.000	17500.0	!	MH 210
DUPLICATE					
C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	!	MH 211
DUPLICATE					
C3H8+R11C2H5=>C2H6+R19C3H7	2.0E+0011	0.000	11000.0	!	MH 212
DUPLICATE					
C4H10+R1H=>H2+R20C4H9	5.7E+0007	2.000	7700.0	!	MH 213
DUPLICATE					
C4H10+R1H=>H2+R20C4H9	1.8E+0007	2.000	5000.0	!	MH 214
DUPLICATE					
C4H10+R20H=>H2O+R20C4H9	5.4E+0006	2.000	450.0	!	MH 215
DUPLICATE					
C4H10+R20H=>H2O+R20C4H9	5.2E+0006	2.000	-765.0	!	MH 216
DUPLICATE					
C4H10+R300H=>H2O2+R20C4H9	1.2E+0012	0.000	17000.0	!	MH 217
DUPLICATE					
C4H10+R300H=>H2O2+R20C4H9	8.0E+0011	0.000	15500.0	!	MH 218
DUPLICATE					
C4H10+R4CH3=>CH4+R20C4H9	6.0E-0001	4.000	8200.0	!	MH 219
DUPLICATE					
C4H10+R4CH3=>CH4+R20C4H9	4.0E+0011	0.000	9600.0	!	MH 220
DUPLICATE					
C4H10+R8CH300=>CH300H+R20C4H9	1.2E+0013	0.000	20000.0	!	MH 221
DUPLICATE					
C4H10+R8CH300=>CH300H+R20C4H9	6.0E+0012	0.000	17500.0	!	MH 222
DUPLICATE					
C4H10+R11C2H5=>C2H6+R20C4H9	6.0E+0011	0.000	13500.0	!	MH 223
DUPLICATE					
C4H10+R11C2H5=>C2H6+R20C4H9	4.0E+0011	0.000	11000.0	!	MH 224
DUPLICATE					
C5H12+R1H=>H2+R35C5H11	5.7E+0007	2.000	7700.0	!	MH 225
DUPLICATE					
C5H12+R1H=>H2+R35C5H11	2.7E+0007	2.000	5000.0	!	MH 226
DUPLICATE					
C5H12+R20H=>H2O+R35C5H11	5.4E+0006	2.000	450.0	!	MH 227
DUPLICATE					
C5H12+R20H=>H2O+R35C5H11	7.8E+0006	2.000	-765.0	!	MH 228
DUPLICATE					
C5H12+R300H=>H2O2+R35C5H11	1.2E+0012	0.000	17000.0	!	MH 229



DUPLICATE				
C5H12+R300H=>H2O2+R35C5H11	1.2E+0012	0.000	15500.0	! MH 230
DUPLICATE				
C5H12+R4CH3=>CH4+R35C5H11	6.0E-0001	4.000	8200.0	! MH 231
DUPLICATE				
C5H12+R4CH3=>CH4+R35C5H11	6.0E+0011	0.000	9600.0	! MH 232
DUPLICATE				
C5H12+R8CH300=>CH300H+R35C5H11	1.2E+0013	0.000	20000.0	! MH 233
DUPLICATE				
C5H12+R8CH300=>CH300H+R35C5H11	9.0E+0012	0.000	17500.0	! MH 234
DUPLICATE				
C5H12+R11C2H5=>C2H6+R35C5H11	6.0E+0011	0.000	13500.0	! MH 235
DUPLICATE				
C5H12+R11C2H5=>C2H6+R35C5H11	6.0E+0011	0.000	11000.0	! MH 236
DUPLICATE				
C6H14+R1H=>H2+R41C6H13	5.7E+0007	2.000	7700.0	! MH 237
DUPLICATE				
C6H14+R1H=>H2+R41C6H13	3.6E+0007	2.000	5000.0	! MH 238
DUPLICATE				
C6H14+R20H=>H2O+R41C6H13	5.4E+0006	2.000	450.0	! MH 239
DUPLICATE				
C6H14+R20H=>H2O+R41C6H13	1.0E+0007	2.000	-765.0	! MH 240
DUPLICATE				
C6H14+R300H=>H2O2+R41C6H13	1.2E+0012	0.000	17000.0	! MH 241
DUPLICATE				
C6H14+R300H=>H2O2+R41C6H13	1.6E+0012	0.000	15500.0	! MH 242
DUPLICATE				
C6H14+R4CH3=>CH4+R41C6H13	6.0E-0001	4.000	8200.0	! MH 243
DUPLICATE				
C6H14+R4CH3=>CH4+R41C6H13	8.0E+0011	0.000	9600.0	! MH 244
DUPLICATE				
C6H14+R8CH300=>CH300H+R41C6H13	1.2E+0013	0.000	20000.0	! MH 245
DUPLICATE				
C6H14+R8CH300=>CH300H+R41C6H13	1.2E+0013	0.000	17500.0	! MH 246
DUPLICATE				
C6H14+R11C2H5=>C2H6+R41C6H13	6.0E+0011	0.000	13500.0	! MH 247
DUPLICATE				
C6H14+R11C2H5=>C2H6+R41C6H13	8.0E+0011	0.000	11000.0	! MH 248
DUPLICATE				
! 0-ring decomposition				
C3H60E#3+R1H=>H2+R4CH3+CH2COZ	2.9E+0007	2.000	7700.0	! DE# 249
DUPLICATE				
C3H60E#3+R1H=>H2+R4CH3+CH2COZ	1.3E+0007	2.000	5000.0	! DE# 250
DUPLICATE				
C3H60E#3+R20H=>H2O+R4CH3+CH2COZ	2.7E+0006	2.000	450.0	! DE# 251
DUPLICATE				
C3H60E#3+R20H=>H2O+R4CH3+CH2COZ	3.9E+0006	2.000	-765.0	! DE# 252
DUPLICATE				
C3H60E#3+R300H=>H2O2+R4CH3+CH2COZ	6.0E+0011	0.000	17000.0	! DE# 253
DUPLICATE				
C3H60E#3+R300H=>H2O2+R4CH3+CH2COZ	6.0E+0011	0.000	15500.0	! DE# 254
DUPLICATE				
C3H60E#3+R4CH3=>CH4+R4CH3+CH2COZ	3.0E-0001	4.000	8200.0	! DE# 255

DUPLICATE					
C3H60E#3+R4CH3=>CH4+R4CH3+CH2COZ	3.0E+0011	0.000	9600.0	!	DE# 256
DUPLICATE					
C3H60E#3+R8CH300=>CH300H+R4CH3+CH2COZ	6.0E+0012	0.000	20000.0	!	DE# 257
DUPLICATE					
C3H60E#3+R8CH300=>CH300H+R4CH3+CH2COZ	4.5E+0012	0.000	17500.0	!	DE# 258
DUPLICATE					
C3H60E#3+R11C2H5=>C2H6+R4CH3+CH2COZ	3.0E+0011	0.000	13500.0	!	DE# 259
DUPLICATE					
C3H60E#3+R11C2H5=>C2H6+R4CH3+CH2COZ	3.0E+0011	0.000	11000.0	!	DE# 260
DUPLICATE					
C4H80E#3+R1H=>H2+R11C2H5+CH2COZ	2.9E+0007	2.000	7700.0	!	DE# 261
DUPLICATE					
C4H80E#3+R1H=>H2+R11C2H5+CH2COZ	2.3E+0007	2.000	5000.0	!	DE# 262
DUPLICATE					
C4H80E#3+R20H=>H2O+R11C2H5+CH2COZ	2.7E+0006	2.000	450.0	!	DE# 263
DUPLICATE					
C4H80E#3+R20H=>H2O+R11C2H5+CH2COZ	6.5E+0006	2.000	-765.0	!	DE# 264
DUPLICATE					
C4H80E#3+R300H=>H2O2+R11C2H5+CH2COZ	6.0E+0011	0.000	17000.0	!	DE# 265
DUPLICATE					
C4H80E#3+R300H=>H2O2+R11C2H5+CH2COZ	1.0E+0012	0.000	15500.0	!	DE# 266
DUPLICATE					
C4H80E#3+R4CH3=>CH4+R11C2H5+CH2COZ	3.0E-0001	4.000	8200.0	!	DE# 267
DUPLICATE					
C4H80E#3+R4CH3=>CH4+R11C2H5+CH2COZ	5.0E+0011	0.000	9600.0	!	DE# 268
DUPLICATE					
C4H80E#3+R8CH300=>CH300H+R11C2H5+CH2COZ	6.0E+0012	0.000	20000.0	!	DE# 269
DUPLICATE					
C4H80E#3+R8CH300=>CH300H+R11C2H5+CH2COZ	7.5E+0012	0.000	17500.0	!	DE# 270
DUPLICATE					
C4H80E#3+R11C2H5=>C2H6+R11C2H5+CH2COZ	3.0E+0011	0.000	13500.0	!	DE# 271
DUPLICATE					
C4H80E#3+R11C2H5=>C2H6+R11C2H5+CH2COZ	5.0E+0011	0.000	11000.0	!	DE# 272
DUPLICATE					
C5H100E#3+R1H=>H2+R19C3H7+CH2COZ	2.9E+0007	2.000	7700.0	!	DE# 273
DUPLICATE					
C5H100E#3+R1H=>H2+R19C3H7+CH2COZ	3.2E+0007	2.000	5000.0	!	DE# 274
DUPLICATE					
C5H100E#3+R20H=>H2O+R19C3H7+CH2COZ	2.7E+0006	2.000	450.0	!	DE# 275
DUPLICATE					
C5H100E#3+R20H=>H2O+R19C3H7+CH2COZ	9.1E+0006	2.000	-765.0	!	DE# 276
DUPLICATE					

C5H100E#3+R300H=>H2O2+R19C3H7+CH2COZ 277	6.0E+0011	0.000	17000.0	! DE#
DUPLICATE				
C5H100E#3+R300H=>H2O2+R19C3H7+CH2COZ 278	1.4E+0012	0.000	15500.0	! DE#
DUPLICATE				
C5H100E#3+R4CH3=>CH4+R19C3H7+CH2COZ 279	3.0E-0001	4.000	8200.0	! DE#
DUPLICATE				
C5H100E#3+R4CH3=>CH4+R19C3H7+CH2COZ 280	7.0E+0011	0.000	9600.0	! DE#
DUPLICATE				
C5H100E#3+R8CH300=>CH300H+R19C3H7+CH2COZ DE# 281	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C5H100E#3+R8CH300=>CH300H+R19C3H7+CH2COZ DE# 282	1.0E+0013	0.000	17500.0	!
DUPLICATE				
C5H100E#3+R11C2H5=>C2H6+R19C3H7+CH2COZ DE# 283	3.0E+0011	0.000	13500.0	!
DUPLICATE				
C5H100E#3+R11C2H5=>C2H6+R19C3H7+CH2COZ DE# 284	7.0E+0011	0.000	11000.0	!
DUPLICATE				
C7H140E#3+R1H=>H2+R20C4H9+C2H3CHOZ DUPLICATE	2.9E+0007	2.000	7700.0	! DE# 285
DUPLICATE				
C7H140E#3+R1H=>H2+R20C4H9+C2H3CHOZ DUPLICATE	5.0E+0007	2.000	5000.0	! DE# 286
DUPLICATE				
C7H140E#3+R20H=>H2O+R20C4H9+C2H3CHOZ 287	2.7E+0006	2.000	450.0	! DE#
DUPLICATE				
C7H140E#3+R20H=>H2O+R20C4H9+C2H3CHOZ 288	1.4E+0007	2.000	-765.0	! DE#
DUPLICATE				
C7H140E#3+R300H=>H2O2+R20C4H9+C2H3CHOZ DE# 289	6.0E+0011	0.000	17000.0	!
DUPLICATE				
C7H140E#3+R300H=>H2O2+R20C4H9+C2H3CHOZ DE# 290	2.2E+0012	0.000	15500.0	!
DUPLICATE				
C7H140E#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ 291	3.0E-0001	4.000	8200.0	! DE#
DUPLICATE				
C7H140E#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ 292	1.1E+0012	0.000	9600.0	! DE#
DUPLICATE				
C7H140E#3+R8CH300=>CH300H+R20C4H9+C2H3CHOZ 20000.0 ! DE# 293	6.0E+0012	0.000		
DUPLICATE				
C7H140E#3+R8CH300=>CH300H+R20C4H9+C2H3CHOZ 17500.0 ! DE# 294	1.7E+0013	0.000		
DUPLICATE				
C7H140E#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ DE# 295	3.0E+0011	0.000	13500.0	!

DUPLICATE  
 C7H140E#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ 1.1E+0012 0.000 11000.0 !  
 DE# 296  
 DUPLICATE  
 C6H120E#3+R1H=>H2+R19C3H7+C2H3CHOZ 2.9E+0007 2.000 7700.0 ! DE# 297  
 DUPLICATE  
 C6H120E#3+R1H=>H2+R19C3H7+C2H3CHOZ 4.1E+0007 2.000 5000.0 ! DE# 298  
 DUPLICATE  
 C6H120E#3+R20H=>H20+R19C3H7+C2H3CHOZ 2.7E+0006 2.000 450.0 ! DE#  
 299  
 DUPLICATE  
 C6H120E#3+R20H=>H20+R19C3H7+C2H3CHOZ 1.1E+0007 2.000 -765.0 ! DE#  
 300  
 DUPLICATE  
 C6H120E#3+R300H=>H202+R19C3H7+C2H3CHOZ 6.0E+0011 0.000 17000.0 !  
 DE# 301  
 DUPLICATE  
 C6H120E#3+R300H=>H202+R19C3H7+C2H3CHOZ 1.8E+0012 0.000 15500.0 !  
 DE# 302  
 DUPLICATE  
 C6H120E#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 3.0E-0001 4.000 8200.0 ! DE#  
 303  
 DUPLICATE  
 C6H120E#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 9.0E+0011 0.000 9600.0 ! DE#  
 304  
 DUPLICATE  
 C6H120E#3+R8CH300=>CH300H+R19C3H7+C2H3CHOZ 6.0E+0012 0.000  
 20000.0 ! DE# 305  
 DUPLICATE  
 C6H120E#3+R8CH300=>CH300H+R19C3H7+C2H3CHOZ 1.3E+0013 0.000  
 17500.0 ! DE# 306  
 DUPLICATE  
 C6H120E#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ 3.0E+0011 0.000 13500.0 !  
 DE# 307  
 DUPLICATE  
 C6H120E#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ 9.0E+0011 0.000 11000.0 !  
 DE# 308  
 DUPLICATE  
 C8H160E#3+R1H=>H2+R20C4H9+C4H60KZ 2.9E+0007 2.000 7700.0 ! DE# 309  
 DUPLICATE  
 C8H160E#3+R1H=>H2+R20C4H9+C4H60KZ 5.9E+0007 2.000 5000.0 ! DE# 310  
 DUPLICATE  
 C8H160E#3+R20H=>H20+R20C4H9+C4H60KZ 2.7E+0006 2.000 450.0 ! DE# 311  
 DUPLICATE  
 C8H160E#3+R20H=>H20+R20C4H9+C4H60KZ 1.7E+0007 2.000 -765.0 ! DE#  
 312  
 DUPLICATE  
 C8H160E#3+R300H=>H202+R20C4H9+C4H60KZ 6.0E+0011 0.000 17000.0 ! DE#  
 313  
 DUPLICATE  
 C8H160E#3+R300H=>H202+R20C4H9+C4H60KZ 2.6E+0012 0.000 15500.0 ! DE#  
 314  
 DUPLICATE

C8H160E#3+R4CH3=>CH4+R20C4H9+C4H60KZ	3.0E-0001	4.000	8200.0	! DE#
315				
DUPLICATE				
C8H160E#3+R4CH3=>CH4+R20C4H9+C4H60KZ	1.3E+0012	0.000	9600.0	! DE#
316				
DUPLICATE				
C8H160E#3+R8CH300=>CH300H+R20C4H9+C4H60KZ	6.0E+0012	0.000	20000.0	!
DE# 317				
DUPLICATE				
C8H160E#3+R8CH300=>CH300H+R20C4H9+C4H60KZ	2.0E+0013	0.000	17500.0	!
DE# 318				
DUPLICATE				
C8H160E#3+R11C2H5=>C2H6+R20C4H9+C4H60KZ	3.0E+0011	0.000	13500.0	!
DE# 319				
DUPLICATE				
C8H160E#3+R11C2H5=>C2H6+R20C4H9+C4H60KZ	1.3E+0012	0.000	11000.0	!
DE# 320				
DUPLICATE				
C9H180E#3+R1H=>H2+R35C5H11+C4H60KZ	2.9E+0007	2.000	7700.0	! DE# 321
DUPLICATE				
C9H180E#3+R1H=>H2+R35C5H11+C4H60KZ	6.8E+0007	2.000	5000.0	! DE# 322
DUPLICATE				
C9H180E#3+R20H=>H20+R35C5H11+C4H60KZ	2.7E+0006	2.000	450.0	! DE#
323				
DUPLICATE				
C9H180E#3+R20H=>H20+R35C5H11+C4H60KZ	2.0E+0007	2.000	-765.0	! DE#
324				
DUPLICATE				
C9H180E#3+R300H=>H202+R35C5H11+C4H60KZ	6.0E+0011	0.000	17000.0	!
DE# 325				
DUPLICATE				
C9H180E#3+R300H=>H202+R35C5H11+C4H60KZ	3.0E+0012	0.000	15500.0	!
DE# 326				
DUPLICATE				
C9H180E#3+R4CH3=>CH4+R35C5H11+C4H60KZ	3.0E-0001	4.000	8200.0	! DE#
327				
DUPLICATE				
C9H180E#3+R4CH3=>CH4+R35C5H11+C4H60KZ	1.5E+0012	0.000	9600.0	! DE#
328				
DUPLICATE				
C9H180E#3+R8CH300=>CH300H+R35C5H11+C4H60KZ	6.0E+0012	0.000		
20000.0 ! DE# 329				
DUPLICATE				
C9H180E#3+R8CH300=>CH300H+R35C5H11+C4H60KZ	2.3E+0013	0.000		
17500.0 ! DE# 330				
DUPLICATE				
C9H180E#3+R11C2H5=>C2H6+R35C5H11+C4H60KZ	3.0E+0011	0.000	13500.0	!
DE# 331				
DUPLICATE				
C9H180E#3+R11C2H5=>C2H6+R35C5H11+C4H60KZ	1.5E+0012	0.000	11000.0	!
DE# 332				
DUPLICATE				
C10H200E#3+R1H=>H2+R35C5H11+C5H80KZ	2.9E+0007	2.000	7700.0	! DE#
333				

DUPLICATE					
C10H200E#3+R1H=>H2+R35C5H11+C5H80KZ	7.7E+0007	2.000	5000.0	!	DE#
334					
DUPLICATE					
C10H200E#3+R20H=>H20+R35C5H11+C5H80KZ	2.7E+0006	2.000	450.0	!	DE#
335					
DUPLICATE					
C10H200E#3+R20H=>H20+R35C5H11+C5H80KZ	2.2E+0007	2.000	-765.0	!	DE#
336					
DUPLICATE					
C10H200E#3+R300H=>H202+R35C5H11+C5H80KZ	6.0E+0011	0.000	17000.0	!	
DE# 337					
DUPLICATE					
C10H200E#3+R300H=>H202+R35C5H11+C5H80KZ	3.4E+0012	0.000	15500.0	!	
DE# 338					
DUPLICATE					
C10H200E#3+R4CH3=>CH4+R35C5H11+C5H80KZ	3.0E-0001	4.000	8200.0	!	DE#
339					
DUPLICATE					
C10H200E#3+R4CH3=>CH4+R35C5H11+C5H80KZ	1.7E+0012	0.000	9600.0	!	DE#
340					
DUPLICATE					
C10H200E#3+R8CH300=>CH300H+R35C5H11+C5H80KZ	6.0E+0012	0.000	20000.0	!	
! DE# 341					
DUPLICATE					
C10H200E#3+R8CH300=>CH300H+R35C5H11+C5H80KZ	2.6E+0013	0.000	17500.0	!	
! DE# 342					
DUPLICATE					
C10H200E#3+R11C2H5=>C2H6+R35C5H11+C5H80KZ	3.0E+0011	0.000	13500.0	!	
DE# 343					
DUPLICATE					
C10H200E#3+R11C2H5=>C2H6+R35C5H11+C5H80KZ	1.7E+0012	0.000	11000.0	!	
DE# 344					
DUPLICATE					
C13H260E#3+R1H=>H2+R26C7H15+C6H100KZ	2.9E+0007	2.000	7700.0	!	DE#
345					
DUPLICATE					
C13H260E#3+R1H=>H2+R26C7H15+C6H100KZ	1.0E+0008	2.000	5000.0	!	DE#
346					
DUPLICATE					
C13H260E#3+R20H=>H20+R26C7H15+C6H100KZ	2.7E+0006	2.000	450.0	!	DE#
347					
DUPLICATE					
C13H260E#3+R20H=>H20+R26C7H15+C6H100KZ	3.0E+0007	2.000	-765.0	!	DE#
348					
DUPLICATE					
C13H260E#3+R300H=>H202+R26C7H15+C6H100KZ	6.0E+0011	0.000	17000.0	!	
DE# 349					
DUPLICATE					
C13H260E#3+R300H=>H202+R26C7H15+C6H100KZ	4.6E+0012	0.000	15500.0	!	
DE# 350					
DUPLICATE					
C13H260E#3+R4CH3=>CH4+R26C7H15+C6H100KZ	3.0E-0001	4.000	8200.0	!	
DE# 351					

DUPLICATE  
 C13H260E#3+R4CH3=>CH4+R26C7H15+C6H100KZ      2.3E+0012    0.000    9600.0    !  
 DE# 352  
 DUPLICATE  
 C13H260E#3+R8CH300=>CH300H+R26C7H15+C6H100KZ      6.0E+0012    0.000    20000.0  
 ! DE# 353  
 DUPLICATE  
 C13H260E#3+R8CH300=>CH300H+R26C7H15+C6H100KZ      3.5E+0013    0.000    17500.0  
 ! DE# 354  
 DUPLICATE  
 C13H260E#3+R11C2H5=>C2H6+R26C7H15+C6H100KZ      3.0E+0011    0.000  
 13500.0    ! DE# 355  
 DUPLICATE  
 C13H260E#3+R11C2H5=>C2H6+R26C7H15+C6H100KZ      2.3E+0012    0.000  
 11000.0    ! DE# 356  
 DUPLICATE  
 C12H240E#3+R1H=>H2+R41C6H13+C6H100KZ      2.9E+0007    2.000    7700.0    ! DE#  
 357  
 DUPLICATE  
 C12H240E#3+R1H=>H2+R41C6H13+C6H100KZ      9.5E+0007    2.000    5000.0    ! DE#  
 358  
 DUPLICATE  
 C12H240E#3+R20H=>H20+R41C6H13+C6H100KZ      2.7E+0006    2.000    450.0    ! DE#  
 359  
 DUPLICATE  
 C12H240E#3+R20H=>H20+R41C6H13+C6H100KZ      2.7E+0007    2.000    -765.0    ! DE#  
 360  
 DUPLICATE  
 C12H240E#3+R300H=>H202+R41C6H13+C6H100KZ      6.0E+0011    0.000    17000.0    !  
 DE# 361  
 DUPLICATE  
 C12H240E#3+R300H=>H202+R41C6H13+C6H100KZ      4.2E+0012    0.000    15500.0    !  
 DE# 362  
 DUPLICATE  
 C12H240E#3+R4CH3=>CH4+R41C6H13+C6H100KZ      3.0E-0001    4.000    8200.0    !  
 DE# 363  
 DUPLICATE  
 C12H240E#3+R4CH3=>CH4+R41C6H13+C6H100KZ      2.1E+0012    0.000    9600.0    !  
 DE# 364  
 DUPLICATE  
 C12H240E#3+R8CH300=>CH300H+R41C6H13+C6H100KZ      6.0E+0012    0.000    20000.0  
 ! DE# 365  
 DUPLICATE  
 C12H240E#3+R8CH300=>CH300H+R41C6H13+C6H100KZ      3.2E+0013    0.000    17500.0  
 ! DE# 366  
 DUPLICATE  
 C12H240E#3+R11C2H5=>C2H6+R41C6H13+C6H100KZ      3.0E+0011    0.000  
 13500.0    ! DE# 367  
 DUPLICATE  
 C12H240E#3+R11C2H5=>C2H6+R41C6H13+C6H100KZ      2.1E+0012    0.000  
 11000.0    ! DE# 368  
 DUPLICATE  
 C11H220E#3+R1H=>H2+R41C6H13+C5H80KZ      2.9E+0007    2.000    7700.0    ! DE#  
 369

DUPLICATE				
C11H220E#3+R1H=>H2+R41C6H13+C5H80KZ	8.6E+0007	2.000	5000.0	! DE#
370				
DUPLICATE				
C11H220E#3+R20H=>H20+R41C6H13+C5H80KZ	2.7E+0006	2.000	450.0	! DE#
371				
DUPLICATE				
C11H220E#3+R20H=>H20+R41C6H13+C5H80KZ	2.5E+0007	2.000	-765.0	! DE#
372				
DUPLICATE				
C11H220E#3+R300H=>H202+R41C6H13+C5H80KZ	6.0E+0011	0.000	17000.0	!
DE# 373				
DUPLICATE				
C11H220E#3+R300H=>H202+R41C6H13+C5H80KZ	3.8E+0012	0.000	15500.0	!
DE# 374				
DUPLICATE				
C11H220E#3+R4CH3=>CH4+R41C6H13+C5H80KZ	3.0E-0001	4.000	8200.0	! DE#
375				
DUPLICATE				
C11H220E#3+R4CH3=>CH4+R41C6H13+C5H80KZ	1.9E+0012	0.000	9600.0	! DE#
376				
DUPLICATE				
C11H220E#3+R8CH300=>CH300H+R41C6H13+C5H80KZ	6.0E+0012	0.000	20000.0	!
! DE# 377				
DUPLICATE				
C11H220E#3+R8CH300=>CH300H+R41C6H13+C5H80KZ	2.9E+0013	0.000	17500.0	!
! DE# 378				
DUPLICATE				
C11H220E#3+R11C2H5=>C2H6+R41C6H13+C5H80KZ	3.0E+0011	0.000	13500.0	!
DE# 379				
DUPLICATE				
C11H220E#3+R11C2H5=>C2H6+R41C6H13+C5H80KZ	1.9E+0012	0.000	11000.0	!
DE# 380				
DUPLICATE				
! C14H280E#3+R1H=>H2+R26C7H15+C7H120KZ	2.9E+0007	2.000	7700.0	! DE#
381				
DUPLICATE				
! C14H280E#3+R1H=>H2+R26C7H15+C7H120KZ	1.1E+0008	2.000	5000.0	! DE#
382				
DUPLICATE				
! C14H280E#3+R20H=>H20+R26C7H15+C7H120KZ	2.7E+0006	2.000	450.0	! DE#
383				
DUPLICATE				
! C14H280E#3+R20H=>H20+R26C7H15+C7H120KZ	3.3E+0007	2.000	-765.0	!
DE# 384				
DUPLICATE				
! C14H280E#3+R300H=>H202+R26C7H15+C7H120KZ	6.0E+0011	0.000	17000.0	!
DE# 385				
DUPLICATE				
! C14H280E#3+R300H=>H202+R26C7H15+C7H120KZ	5.0E+0012	0.000	15500.0	!
DE# 386				
DUPLICATE				
! C14H280E#3+R4CH3=>CH4+R26C7H15+C7H120KZ	3.0E-0001	4.000	8200.0	!
DE# 387				



DUPLICATE  
 !C14H280E#3+R4CH3=>CH4+R26C7H15+C7H120KZ      2.5E+0012   0.000   9600.0   !  
 DE# 388  
 DUPLICATE  
 !C14H280E#3+R8CH300=>CH300H+R26C7H15+C7H120KZ      6.0E+0012   0.000  
 20000.0   ! DE# 389  
 DUPLICATE  
 !C14H280E#3+R8CH300=>CH300H+R26C7H15+C7H120KZ      3.8E+0013   0.000  
 17500.0   ! DE# 390  
 DUPLICATE  
 !C14H280E#3+R11C2H5=>C2H6+R26C7H15+C7H120KZ      3.0E+0011   0.000   13500.0  
 ! DE# 391  
 DUPLICATE  
 !C14H280E#3+R11C2H5=>C2H6+R26C7H15+C7H120KZ      2.5E+0012   0.000   11000.0  
 ! DE# 392  
 DUPLICATE

! Metatheses of oxetanes, furanes and pyranes  
 ! decompositions of cyclo-ether radicals  
 ! Addition of oxygen on cyclo-ether radicals  
 !    O2 elimination  
 !    Isomerization  
 !    Cylo-ether keto-hydroperoxide ester formation  
 !    Decomposition of cylo-ether keto-hydroperoxide ester  
 ! Isomerization of peroxy-radicals  
 !Addition of oxygen on cyclo-peroxy radicals  
 ! Formation of cyclo-ether ketohydroperoxydes  
 ! Decomposition of cyclo-ether ketohydroperoxydes  
 ! Olefin reactions  
 ! addition of H and CH3 on olefins  
 C3H6Y+R1H=>R19C3H7      1.3E+0013   0.000   1560.0   ! ADZ 393  
 DUPLICATE  
 C3H6Y+R1H=>R19C3H7      1.3E+0013   0.000   3260.0   ! ADZ 394  
 DUPLICATE  
 C4H8Y+R1H=>R20C4H9      1.3E+0013   0.000   1560.0   ! ADZ 395  
 DUPLICATE  
 C4H8Y+R1H=>R20C4H9      1.3E+0013   0.000   3260.0   ! ADZ 396  
 DUPLICATE  
 C4H8Y+R4CH3=>C3H6Y+R11C2H5      9.6E+0010   0.000   8000.0   ! ADZ 397  
 C5H10Z+R1H=>R35C5H11      1.3E+0013   0.000   1560.0   ! ADZ 398  
 DUPLICATE  
 C5H10Z+R1H=>R35C5H11      1.3E+0013   0.000   3260.0   ! ADZ 399  
 DUPLICATE  
 C5H10Z+R4CH3=>C4H8Y+R11C2H5      1.7E+0011   0.000   7400.0   ! ADZ 400  
 C5H10Z+R4CH3=>C3H6Y+R19C3H7      9.6E+0010   0.000   8000.0   ! ADZ 401  
 C7H14Z+R1H=>R26C7H15      1.3E+0013   0.000   1560.0   ! ADZ 402

DUPLICATE  
 C7H14Z+R1H=>R26C7H15 1.3E+0013 0.000 3260.0 ! ADZ 403  
 DUPLICATE  
 C7H14Z+R4CH3=>C4H8Y+R20C4H9 1.7E+0011 0.000 7400.0 ! ADZ 404  
 C7H14Z+R4CH3=>C3H6Y+R35C5H11 9.6E+0010 0.000 8000.0 ! ADZ 405  
 C6H12Z+R1H=>R41C6H13 1.3E+0013 0.000 1560.0 ! ADZ 406  
 DUPLICATE  
 C6H12Z+R1H=>R41C6H13 1.3E+0013 0.000 3260.0 ! ADZ 407  
 DUPLICATE  
 C6H12Z+R4CH3=>C4H8Y+R19C3H7 1.7E+0011 0.000 7400.0 ! ADZ 408  
 C6H12Z+R4CH3=>C3H6Y+R20C4H9 9.6E+0010 0.000 8000.0 ! ADZ 409  
 C7H14Y+R1H=>R26C7H15 1.3E+0013 0.000 1560.0 ! ADZ 410  
 DUPLICATE  
 C7H14Y+R1H=>R26C7H15 1.3E+0013 0.000 3260.0 ! ADZ 411  
 DUPLICATE  
 C7H14Y+R4CH3=>C4H8Y+R20C4H9 1.7E+0011 0.000 7400.0 ! ADZ 412  
 C7H14Y+R4CH3=>C3H6Y+R35C5H11 9.6E+0010 0.000 8000.0 ! ADZ 413  
 C8H16Y+R1H=>R30C8H17 1.3E+0013 0.000 1560.0 ! ADZ 414  
 DUPLICATE  
 C8H16Y+R1H=>R30C8H17 1.3E+0013 0.000 3260.0 ! ADZ 415  
 DUPLICATE  
 C8H16Y+R4CH3=>C4H8Y+R35C5H11 1.7E+0011 0.000 7400.0 ! ADZ 416  
 C8H16Y+R4CH3=>C3H6Y+R41C6H13 9.6E+0010 0.000 8000.0 ! ADZ 417  
 C8H16Z+R1H=>R30C8H17 1.3E+0013 0.000 1560.0 ! ADZ 418  
 DUPLICATE  
 C8H16Z+R1H=>R30C8H17 1.3E+0013 0.000 3260.0 ! ADZ 419  
 DUPLICATE  
 C8H16Z+R4CH3=>C4H8Y+R35C5H11 1.7E+0011 0.000 7400.0 ! ADZ 420  
 C8H16Z+R4CH3=>C3H6Y+R41C6H13 9.6E+0010 0.000 8000.0 ! ADZ 421  
 C5H10Y+R1H=>R35C5H11 1.3E+0013 0.000 1560.0 ! ADZ 422  
 DUPLICATE  
 C5H10Y+R1H=>R35C5H11 1.3E+0013 0.000 3260.0 ! ADZ 423  
 DUPLICATE  
 C5H10Y+R4CH3=>C4H8Y+R11C2H5 1.7E+0011 0.000 7400.0 ! ADZ 424  
 C5H10Y+R4CH3=>C3H6Y+R19C3H7 9.6E+0010 0.000 8000.0 ! ADZ 425  
 C9H18Z+R4CH3=>C4H8Y+R41C6H13 1.7E+0011 0.000 7400.0 ! ADZ 426  
 C9H18Z+R4CH3=>C3H6Y+R26C7H15 9.6E+0010 0.000 8000.0 ! ADZ 427  
 C10H20Z+R4CH3=>C4H8Y+R26C7H15 1.7E+0011 0.000 7400.0 ! ADZ 428  
 C10H20Z+R4CH3=>C3H6Y+R30C8H17 9.6E+0010 0.000 8000.0 ! ADZ 429  
 C11H22Z+R4CH3=>C4H8Y+R30C8H17 1.7E+0011 0.000 7400.0 ! ADZ 430  
 C9H18Z+R1H=>4C2H4Z+R4CH3 9.6E+0010 0.000 8000.0 ! ADZ 431  
 C10H20Z+R1H=>4C2H4Z+R11C2H5 9.6E+0010 0.000 8000.0 ! ADZ 432  
 C13H26Z+R1H=>6C2H4Z+R4CH3 9.6E+0010 0.000 8000.0 ! ADZ 433  
 C12H24Z+R1H=>5C2H4Z+R11C2H5 9.6E+0010 0.000 8000.0 ! ADZ 434  
 C11H22Z+R1H=>5C2H4Z+R4CH3 9.6E+0010 0.000 8000.0 ! ADZ 435  
 !C14H28Z+R1H=>6C2H4Z+R11C2H5 9.6E+0010 0.000 8000.0 ! ADZ 436  
  
 ! addition of OH on olefins  
 C3H6Y+R20H=>R4CH3+CH3CHO 1.4E+0012 0.000 -1040.0 ! ADZ 437  
 C3H6Y+R20H=>R11C2H5+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 438  
 C4H8Y+R20H=>R4CH3+C2H5CHO 1.4E+0012 0.000 -1040.0 ! ADZ 439  
 C4H8Y+R20H=>R19C3H7+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 440  
 C5H10Z+R20H=>R4CH3+C4H8OA 1.4E+0012 0.000 -1040.0 ! ADZ 441  
 C5H10Z+R20H=>R20C4H9+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 442

C7H14Z+R20H=>R4CH3+C6H120A	1.4E+0012	0.000	-1040.0	!	ADZ 443
C7H14Z+R20H=>R41C6H13+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 444
C6H12Z+R20H=>R4CH3+C5H100A	1.4E+0012	0.000	-1040.0	!	ADZ 445
C6H12Z+R20H=>R35C5H11+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 446
C7H14Y+R20H=>R4CH3+C6H120A	1.4E+0012	0.000	-1040.0	!	ADZ 447
C7H14Y+R20H=>R41C6H13+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 448
C8H16Y+R20H=>R4CH3+C7H140A	1.4E+0012	0.000	-1040.0	!	ADZ 449
C8H16Y+R20H=>R26C7H15+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 450
C8H16Z+R20H=>R4CH3+C7H140A	1.4E+0012	0.000	-1040.0	!	ADZ 451
C8H16Z+R20H=>R26C7H15+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 452
C5H10Y+R20H=>R4CH3+C4H80A	1.4E+0012	0.000	-1040.0	!	ADZ 453
C5H10Y+R20H=>R20C4H9+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 454
C9H18Z+R20H=>R4CH3+C8H160A	1.4E+0012	0.000	-1040.0	!	ADZ 455
C9H18Z+R20H=>R30C8H17+HCHO	1.4E+0012	0.000	-1040.0	!	ADZ 456
C10H20Z+R20H=>R4CH3+C9H180A	1.4E+0012	0.000	-1040.0	!	ADZ 457
C13H26Z+R20H=>R4CH3+C12H240A	1.4E+0012	0.000	-1040.0	!	ADZ 458
C12H24Z+R20H=>R4CH3+C11H220A	1.4E+0012	0.000	-1040.0	!	ADZ 459
C11H22Z+R20H=>R4CH3+C10H200A	1.4E+0012	0.000	-1040.0	!	ADZ 460
!C14H28Z+R20H=>R4CH3+C13H260A	1.4E+0012	0.000	-1040.0	!	ADZ 461

C10H20Z+R20H=>HCHO+R4CH3+4C2H4Z	1.4E+0012	0.000	-1040.0	!	FOH 462
C13H26Z+R20H=>HCHO+R11C2H5+5C2H4Z	1.4E+0012	0.000	-1040.0	!	FOH 463
C12H24Z+R20H=>HCHO+R4CH3+5C2H4Z	1.4E+0012	0.000	-1040.0	!	FOH 464
C11H22Z+R20H=>HCHO+R11C2H5+4C2H4Z	1.4E+0012	0.000	-1040.0	!	FOH 465
!C14H28Z+R20H=>HCHO+R4CH3+6C2H4Z	1.4E+0012	0.000	-1040.0	!	FOH 466

! addition of O on olefins

C3H6Y+B10=>CH2COZ+R1H+R4CH3	1.2E+0005	2.560	-1130.0	!	A0Z 467
C4H8Y+B10=>CH2COZ+R1H+R11C2H5	1.2E+0005	2.560	-1130.0	!	A0Z 467
C5H10Z+B10=>CH2COZ+R1H+R19C3H7	1.2E+0005	2.560	-1130.0	!	A0Z 467
C7H14Z+B10=>CH2COZ+R1H+R35C5H11	1.2E+0005	2.560	-1130.0	!	A0Z 467
C6H12Z+B10=>CH2COZ+R1H+R20C4H9	1.2E+0005	2.560	-1130.0	!	A0Z 467
C7H14Y+B10=>CH2COZ+R1H+R35C5H11	1.2E+0005	2.560	-1130.0	!	A0Z 467
C8H16Y+B10=>CH2COZ+R1H+R41C6H13	1.2E+0005	2.560	-1130.0	!	A0Z 467
C8H16Z+B10=>CH2COZ+R1H+R41C6H13	1.2E+0005	2.560	-1130.0	!	A0Z 467
C5H10Y+B10=>CH2COZ+R1H+R19C3H7	1.2E+0005	2.560	-1130.0	!	A0Z 467
C9H18Z+B10=>CH2COZ+R1H+R26C7H15	1.2E+0005	2.560	-1130.0	!	A0Z 467
C10H20Z+B10=>CH2COZ+R1H+R30C8H17	1.2E+0005	2.560	-1130.0	!	A0Z 467
!C13H26Z+B10=>CH2COZ+R4CH3+R1H+5C2H4Z	7.8E+0013	0.000	5200.0	!	A0Z 467
!C12H24Z+B10=>CH2COZ+R11C2H5+R1H+4C2H4Z	7.8E+0013	0.000	5200.0	!	A0Z 467
!C11H22Z+B10=>CH2COZ+R4CH3+R1H+4C2H4Z	7.8E+0013	0.000	5200.0	!	A0Z 467
!C14H28Z+B10=>CH2COZ+R11C2H5+R1H+5C2H4Z	7.8E+0013	0.000	5200.0	!	A0Z 467

! retroene reactions

C5H10Z=>C3H6Y+C2H4Z	8.0E+0012	0.000	56500.0	!	RTZ 467
C7H14Z=>C3H6Y+C4H8Y	8.0E+0012	0.000	56500.0	!	RTZ 468
C6H12Z=>C3H6Y+C3H6Y	8.0E+0012	0.000	56500.0	!	RTZ 469
C7H14Y=>C3H6Y+C4H8Y	8.0E+0012	0.000	56500.0	!	RTZ 470
C8H16Y=>C3H6Y+C5H10Z	8.0E+0012	0.000	56500.0	!	RTZ 471
C8H16Z=>C3H6Y+C5H10Z	8.0E+0012	0.000	56500.0	!	RTZ 472

C5H10Y=>C3H6Y+C2H4Z	8.0E+0012	0.000	56500.0	! RTZ 473
C9H18Z=>C3H6Y+C6H12Z	8.0E+0012	0.000	56500.0	! RTZ 474
C10H20Z=>C3H6Y+C7H14Z	8.0E+0012	0.000	56500.0	! RTZ 475
C13H26Z=>C3H6Y+C10H20Z	8.0E+0012	0.000	56500.0	! RTZ 476
C12H24Z=>C3H6Y+C9H18Z	8.0E+0012	0.000	56500.0	! RTZ 477
C11H22Z=>C3H6Y+C8H16Z	8.0E+0012	0.000	56500.0	! RTZ 478
!C14H28Z=>C3H6Y+C11H22Z	8.0E+0012	0.000	56500.0	! RTZ 479

! addition of 00H on olefins

C3H6Y+R300H=>R20H+C3H60E#3	1.0E+0012	0.000	14200.0	! ADZ 480
C4H8Y+R300H=>R20H+C4H80E#3	1.0E+0012	0.000	14200.0	! ADZ 481
C5H10Z+R300H=>R20H+C5H100E#3	1.0E+0012	0.000	14200.0	! ADZ 482
C7H14Z+R300H=>R20H+C7H140E#3	1.0E+0012	0.000	14200.0	! ADZ 483
C6H12Z+R300H=>R20H+C6H120E#3	1.0E+0012	0.000	14200.0	! ADZ 484
C7H14Y+R300H=>R20H+C7H140E#3	1.0E+0012	0.000	14200.0	! ADZ 485
C8H16Y+R300H=>R20H+C8H160E#3	1.0E+0012	0.000	14200.0	! ADZ 486
C8H16Z+R300H=>R20H+C8H160E#3	1.0E+0012	0.000	14200.0	! ADZ 487
C5H10Y+R300H=>R20H+C5H100E#3	1.0E+0012	0.000	14200.0	! ADZ 488
C9H18Z+R300H=>R20H+C9H180E#3	1.0E+0012	0.000	14200.0	! ADZ 489
C10H20Z+R300H=>R20H+C10H200E#3	1.0E+0012	0.000	14200.0	! ADZ 490
C13H26Z+R300H=>R20H+C13H260E#3	1.0E+0012	0.000	14200.0	! ADZ 491
C12H24Z+R300H=>R20H+C12H240E#3	1.0E+0012	0.000	14200.0	! ADZ 492
C11H22Z+R300H=>R20H+C11H220E#3	1.0E+0012	0.000	14200.0	! ADZ 493
!C14H28Z+R300H=>R20H+C14H280E#3	1.0E+0012	0.000	14200.0	! ADZ 494

! olefin to dienes

C5H10Z+R1H=>H2+C4H6Z2+R4CH3	5.4E+0004	2.500	-1900.0	! MZ 495
DUPLICATE				
C5H10Z+R1H=>H2+C4H6Z2+R4CH3	2.9E+0007	2.000	7700.0	! MZ 496
DUPLICATE				
C5H10Z+R1H=>H2+C4H6Z2+R4CH3	9.0E+0006	2.000	5000.0	! MZ 497
DUPLICATE				
C5H10Z+R20H=>H20+C4H6Z2+R4CH3	3.0E+0006	2.000	-1520.0	! MZ 498
DUPLICATE				
C5H10Z+R20H=>H20+C4H6Z2+R4CH3	2.7E+0006	2.000	450.0	! MZ 499
DUPLICATE				
C5H10Z+R20H=>H20+C4H6Z2+R4CH3	2.6E+0006	2.000	-765.0	! MZ 500
DUPLICATE				
C5H10Z+R300H=>H202+C4H6Z2+R4CH3	6.4E+0003	2.600	12400.0	! MZ 501
DUPLICATE				
C5H10Z+R300H=>H202+C4H6Z2+R4CH3	6.0E+0011	0.000	17000.0	! MZ 502
DUPLICATE				
C5H10Z+R300H=>H202+C4H6Z2+R4CH3	4.0E+0011	0.000	15500.0	! MZ 503
DUPLICATE				
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	1.0E+0011	0.000	7300.0	! MZ 504
DUPLICATE				
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	3.0E-0001	4.000	8200.0	! MZ 505
DUPLICATE				
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3	2.0E+0011	0.000	9600.0	! MZ 506
DUPLICATE				
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3	1.0E+0012	0.000	14550.0	! MZ 507

DUPLICATE

C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3 508	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3 509	3.0E+0012	0.000	17500.0	! MZ
DUPLICATE				
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	1.5E+0000	3.500	4140.0	! MZ 510
DUPLICATE				
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	3.0E+0011	0.000	13500.0	! MZ 511
DUPLICATE				
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	2.0E+0011	0.000	11000.0	! MZ 512
DUPLICATE				
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	5.4E+0004	2.500	-1900.0	! MZ 513
DUPLICATE				
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	2.9E+0007	2.000	7700.0	! MZ 514
DUPLICATE				
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	2.7E+0007	2.000	5000.0	! MZ 515
DUPLICATE				
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7	3.0E+0006	2.000	-1520.0	! MZ 516
DUPLICATE				
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7	2.7E+0006	2.000	450.0	! MZ 517
DUPLICATE				
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7	7.8E+0006	2.000	-765.0	! MZ 518
DUPLICATE				
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7	6.4E+0003	2.600	12400.0	! MZ 519
DUPLICATE				
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7	6.0E+0011	0.000	17000.0	! MZ 520
DUPLICATE				
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7	1.2E+0012	0.000	15500.0	! MZ 521
DUPLICATE				
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	1.0E+0011	0.000	7300.0	! MZ 522
DUPLICATE				
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	3.0E-0001	4.000	8200.0	! MZ 523
DUPLICATE				
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	6.0E+0011	0.000	9600.0	! MZ 524
DUPLICATE				
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7 525	1.0E+0012	0.000	14550.0	! MZ
DUPLICATE				
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7 526	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7 527	9.0E+0012	0.000	17500.0	! MZ
DUPLICATE				
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	1.5E+0000	3.500	4140.0	! MZ 528
DUPLICATE				
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7 529	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7 530	6.0E+0011	0.000	11000.0	! MZ
DUPLICATE				
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5	5.4E+0004	2.500	-1900.0	! MZ 531

DUPLICATE					
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5	2.9E+0007	2.000	7700.0	!	MZ 532
DUPLICATE					
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5	1.8E+0007	2.000	5000.0	!	MZ 533
DUPLICATE					
C6H12Z+R20H=>H2O+C4H6Z2+R11C2H5	3.0E+0006	2.000	-1520.0	!	MZ 534
DUPLICATE					
C6H12Z+R20H=>H2O+C4H6Z2+R11C2H5	2.7E+0006	2.000	450.0	!	MZ 535
DUPLICATE					
C6H12Z+R20H=>H2O+C4H6Z2+R11C2H5	5.2E+0006	2.000	-765.0	!	MZ 536
DUPLICATE					
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5	6.4E+0003	2.600	12400.0	!	MZ 537
DUPLICATE					
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5	6.0E+0011	0.000	17000.0	!	MZ 538
DUPLICATE					
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5	8.0E+0011	0.000	15500.0	!	MZ 539
DUPLICATE					
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5	1.0E+0011	0.000	7300.0	!	MZ 540
DUPLICATE					
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5	3.0E-0001	4.000	8200.0	!	MZ 541
DUPLICATE					
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5	4.0E+0011	0.000	9600.0	!	MZ 542
DUPLICATE					
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5	1.0E+0012	0.000	14550.0	!	MZ 543
DUPLICATE					
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5	6.0E+0012	0.000	20000.0	!	MZ 544
DUPLICATE					
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5	6.0E+0012	0.000	17500.0	!	MZ 545
DUPLICATE					
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5	1.5E+0000	3.500	4140.0	!	MZ 546
DUPLICATE					
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5	3.0E+0011	0.000	13500.0	!	MZ 547
DUPLICATE					
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5	4.0E+0011	0.000	11000.0	!	MZ 548
DUPLICATE					
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	5.4E+0004	2.500	-1900.0	!	MZ 549
DUPLICATE					
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	2.9E+0007	2.000	7700.0	!	MZ 550
DUPLICATE					
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9	3.6E+0007	2.000	5000.0	!	MZ 551
DUPLICATE					
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9	3.0E+0006	2.000	-1520.0	!	MZ 552
DUPLICATE					
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9	2.7E+0006	2.000	450.0	!	MZ 553
DUPLICATE					
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9	1.0E+0007	2.000	-765.0	!	MZ 554
DUPLICATE					
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9	6.4E+0003	2.600	12400.0	!	MZ 555
DUPLICATE					

C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 556
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9 DUPLICATE	1.6E+0012	0.000	15500.0	! MZ 557
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 558
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 559
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 DUPLICATE	8.0E+0011	0.000	9600.0	! MZ 560
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 561 DUPLICATE	1.0E+0012	0.000	14550.0	! MZ
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 562 DUPLICATE	6.0E+0012	0.000	20000.0	! MZ
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 563 DUPLICATE	1.2E+0013	0.000	17500.0	! MZ
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 DUPLICATE	1.5E+0000	3.500	4140.0	! MZ 564
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 565 DUPLICATE	3.0E+0011	0.000	13500.0	! MZ
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 566 DUPLICATE	8.0E+0011	0.000	11000.0	! MZ
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 567
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 568
C9H18Z+R1H=>H2+C4H6Z2+R35C5H11 DUPLICATE	4.5E+0007	2.000	5000.0	! MZ 569
C9H18Z+R20H=>H2O+C4H6Z2+R35C5H11 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 570
C9H18Z+R20H=>H2O+C4H6Z2+R35C5H11 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 571
C9H18Z+R20H=>H2O+C4H6Z2+R35C5H11 DUPLICATE	1.3E+0007	2.000	-765.0	! MZ 572
C9H18Z+R300H=>H2O2+C4H6Z2+R35C5H11 DUPLICATE	6.4E+0003	2.600	12400.0	! MZ 573
C9H18Z+R300H=>H2O2+C4H6Z2+R35C5H11 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 574
C9H18Z+R300H=>H2O2+C4H6Z2+R35C5H11 DUPLICATE	2.0E+0012	0.000	15500.0	! MZ 575
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 576
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 577
C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11 DUPLICATE	1.0E+0012	0.000	9600.0	! MZ 578
C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 579 DUPLICATE	1.0E+0012	0.000	14550.0	! MZ

C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 580	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 581	1.5E+0013	0.000	17500.0	! MZ
DUPLICATE				
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 582	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 583	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 584	1.0E+0012	0.000	11000.0	! MZ
DUPLICATE				
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 585
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 586
C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 DUPLICATE	5.4E+0007	2.000	5000.0	! MZ 587
C10H20Z+R20H=>H2O+C4H6Z2+R41C6H13 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 588
C10H20Z+R20H=>H2O+C4H6Z2+R41C6H13 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 589
C10H20Z+R20H=>H2O+C4H6Z2+R41C6H13 DUPLICATE	1.5E+0007	2.000	-765.0	! MZ 590
C10H20Z+R300H=>H2O2+C4H6Z2+R41C6H13 591	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
C10H20Z+R300H=>H2O2+C4H6Z2+R41C6H13 592	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
C10H20Z+R300H=>H2O2+C4H6Z2+R41C6H13 593	2.4E+0012	0.000	15500.0	! MZ
DUPLICATE				
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 594
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 595
C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 DUPLICATE	1.2E+0012	0.000	9600.0	! MZ 596
C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 597	1.0E+0012	0.000	14550.0	!
DUPLICATE				
C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 598	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 599	1.8E+0013	0.000	17500.0	!
DUPLICATE				
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 600	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				



C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 601	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 602	1.2E+0012	0.000	11000.0	! MZ
DUPLICATE				
! C13H26Z+R1H=>H2+C4H6Z2+R4CH3+4C2H4Z 603	5.4E+0004	2.500	-1900.0	! MZ
! C13H26Z+R20H=>H2O+C4H6Z2+R4CH3+4C2H4Z 604	3.0E+0006	2.000	-1520.0	! MZ
! C13H26Z+R300H=>H2O2+C4H6Z2+R4CH3+4C2H4Z MZ 605	6.4E+0003	2.600	12400.0	!
! C13H26Z+R4CH3=>CH4+C4H6Z2+R4CH3+4C2H4Z 606	1.0E+0011	0.000	7300.0	! MZ
! C13H26Z+R8CH300=>CH300H+C4H6Z2+R4CH3+4C2H4Z ! MZ 607	1.0E+0011	0.000	7300.0	!
! C13H26Z+R11C2H5=>C2H6+C4H6Z2+R4CH3+4C2H4Z MZ 608	1.5E+0000	3.500	4140.0	!
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 609
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 610
C12H24Z+R1H=>H2+C4H6Z2+R30C8H17 DUPLICATE	7.2E+0007	2.000	5000.0	! MZ 611
C12H24Z+R20H=>H2O+C4H6Z2+R30C8H17 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 612
C12H24Z+R20H=>H2O+C4H6Z2+R30C8H17 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 613
C12H24Z+R20H=>H2O+C4H6Z2+R30C8H17 DUPLICATE	2.1E+0007	2.000	-765.0	! MZ 614
C12H24Z+R300H=>H2O2+C4H6Z2+R30C8H17 615	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
C12H24Z+R300H=>H2O2+C4H6Z2+R30C8H17 616	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
C12H24Z+R300H=>H2O2+C4H6Z2+R30C8H17 617	3.2E+0012	0.000	15500.0	! MZ
DUPLICATE				
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 618
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 619
C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17 DUPLICATE	1.6E+0012	0.000	9600.0	! MZ 620
C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17 MZ 621	1.0E+0012	0.000	14550.0	!
DUPLICATE				
C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17 MZ 622	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17 MZ 623	2.4E+0013	0.000	17500.0	!
DUPLICATE				

C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 624	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 625	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 626	1.6E+0012	0.000	11000.0	! MZ
DUPLICATE				
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15 627	5.4E+0004	2.500	-1900.0	! MZ
DUPLICATE				
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15 628	2.9E+0007	2.000	7700.0	! MZ
DUPLICATE				
C11H22Z+R1H=>H2+C4H6Z2+R26C7H15 629	6.3E+0007	2.000	5000.0	! MZ
DUPLICATE				
C11H22Z+R20H=>H20+C4H6Z2+R26C7H15 630	3.0E+0006	2.000	-1520.0	! MZ
DUPLICATE				
C11H22Z+R20H=>H20+C4H6Z2+R26C7H15 631	2.7E+0006	2.000	450.0	! MZ
DUPLICATE				
C11H22Z+R20H=>H20+C4H6Z2+R26C7H15 632	1.8E+0007	2.000	-765.0	! MZ
DUPLICATE				
C11H22Z+R300H=>H202+C4H6Z2+R26C7H15 633	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
C11H22Z+R300H=>H202+C4H6Z2+R26C7H15 634	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
C11H22Z+R300H=>H202+C4H6Z2+R26C7H15 635	2.8E+0012	0.000	15500.0	! MZ
DUPLICATE				
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15 636	1.0E+0011	0.000	7300.0	! MZ
DUPLICATE				
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15 637	3.0E-0001	4.000	8200.0	! MZ
DUPLICATE				
C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15 638	1.4E+0012	0.000	9600.0	! MZ
DUPLICATE				
C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15 MZ 639	1.0E+0012	0.000	14550.0	!
DUPLICATE				
C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15 MZ 640	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15 MZ 641	2.1E+0013	0.000	17500.0	!
DUPLICATE				
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15 642	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15 643	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15 644	1.4E+0012	0.000	11000.0	! MZ
DUPLICATE				

!C14H28Z+R1H=>H2+C4H6Z2+R11C2H5+4C2H4Z	5.4E+0004	2.500	-1900.0	! MZ 645
!C14H28Z+R20H=>H20+C4H6Z2+R11C2H5+4C2H4Z	3.0E+0006	2.000	-1520.0	! MZ 646
!C14H28Z+R300H=>H202+C4H6Z2+R11C2H5+4C2H4Z	6.4E+0003	2.600	12400.0	! MZ 647
!C14H28Z+R4CH3=>CH4+C4H6Z2+R11C2H5+4C2H4Z	1.0E+0011	0.000	7300.0	! MZ 648
!C14H28Z+R8CH300=>CH300H+C4H6Z2+R11C2H5+4C2H4Z	1.0E+0011	0.000	7300.0	! MZ 649
!C14H28Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5+4C2H4Z	1.5E+0000	3.500	4140.0	! MZ 650
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	8.8E+0010	0.700	3250.0	! MZ 651
DUPLICATE				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	5.1E+0013	0.000	7850.0	! MZ 652
DUPLICATE				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	2.6E+0013	0.000	5200.0	! MZ 653
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	8.8E+0010	0.700	3250.0	! MZ 654
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	5.1E+0013	0.000	7850.0	! MZ 655
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	7.8E+0013	0.000	5200.0	! MZ 656
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	8.8E+0010	0.700	3250.0	! MZ 657
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	5.1E+0013	0.000	7850.0	! MZ 658
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	5.2E+0013	0.000	5200.0	! MZ 659
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	8.8E+0010	0.700	3250.0	! MZ 660
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	5.1E+0013	0.000	7850.0	! MZ 661
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	1.0E+0014	0.000	5200.0	! MZ 662
DUPLICATE				
C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	8.8E+0010	0.700	3250.0	! MZ 663
DUPLICATE				
C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	5.1E+0013	0.000	7850.0	! MZ 664
DUPLICATE				
C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	1.3E+0014	0.000	5200.0	! MZ 665
DUPLICATE				
C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	8.8E+0010	0.700	3250.0	! MZ 666
DUPLICATE				
C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	5.1E+0013	0.000	7850.0	! MZ 667
DUPLICATE				
C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	1.6E+0014	0.000	5200.0	! MZ 668
DUPLICATE				
C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	8.8E+0010	0.700	3250.0	! MZ 669
DUPLICATE				
C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	5.1E+0013	0.000	7850.0	! MZ 670
DUPLICATE				
C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	2.1E+0014	0.000	5200.0	! MZ 671
DUPLICATE				

C11H22Z+B10=>R20H+C4H6Z2+R26C7H15 DUPLICATE	8.8E+0010	0.700	3250.0	! MZ 672
C11H22Z+B10=>R20H+C4H6Z2+R26C7H15 DUPLICATE	5.1E+0013	0.000	7850.0	! MZ 673
C11H22Z+B10=>R20H+C4H6Z2+R26C7H15 DUPLICATE	1.8E+0014	0.000	5200.0	! MZ 674

! Metathesis with YH

C3H6Y+R1H=>RC3H5Y+H2	1.7E+0005	2.500	2510.0	! MES 675
C3H6Y+R20H=>RC3H5Y+H2O	3.0E+0006	2.000	-298.0	! MES 676
C3H6Y+R300H=>RC3H5Y+H2O2	9.6E+0003	2.600	13900.0	! MES 677
C3H6Y+R4CH3=>RC3H5Y+CH4	2.2E+0000	3.500	5670.0	! MES 678
C3H6Y+R8CH300=>RC3H5Y+CH300H	2.0E+0012	0.000	17050.0	! MES 679
C3H6Y+R11C2H5=>RC3H5Y+C2H6	2.2E+0000	3.500	6640.0	! MES 680
C4H8Y+R1H=>RC4H7Y+H2 DUPLICATE	5.4E+0004	2.500	-1900.0	! MES 681
C4H8Y+R1H=>RC4H7Y+H2 DUPLICATE	2.9E+0007	2.000	7700.0	! MES 682
C4H8Y+R20H=>RC4H7Y+H2O DUPLICATE	3.0E+0006	2.000	-1520.0	! MES 683
C4H8Y+R20H=>RC4H7Y+H2O DUPLICATE	2.7E+0006	2.000	450.0	! MES 684
C4H8Y+R300H=>RC4H7Y+H2O2 DUPLICATE	6.4E+0003	2.600	12400.0	! MES 685
C4H8Y+R300H=>RC4H7Y+H2O2 DUPLICATE	6.0E+0011	0.000	17000.0	! MES 686
C4H8Y+R4CH3=>RC4H7Y+CH4 DUPLICATE	1.0E+0011	0.000	7300.0	! MES 687
C4H8Y+R4CH3=>RC4H7Y+CH4 DUPLICATE	3.0E-0001	4.000	8200.0	! MES 688
C4H8Y+R8CH300=>RC4H7Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 689
C4H8Y+R8CH300=>RC4H7Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 690
C4H8Y+R11C2H5=>RC4H7Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 691
C4H8Y+R11C2H5=>RC4H7Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 692
C7H14Y+R1H=>RC7H13Y+H2 DUPLICATE	5.4E+0004	2.500	-1900.0	! MES 693
C7H14Y+R1H=>RC7H13Y+H2 DUPLICATE	2.9E+0007	2.000	7700.0	! MES 694
C7H14Y+R1H=>RC7H13Y+H2 DUPLICATE	2.7E+0007	2.000	5000.0	! MES 695
C7H14Y+R20H=>RC7H13Y+H2O DUPLICATE	3.0E+0006	2.000	-1520.0	! MES 696
C7H14Y+R20H=>RC7H13Y+H2O DUPLICATE	2.7E+0006	2.000	450.0	! MES 697
C7H14Y+R20H=>RC7H13Y+H2O DUPLICATE	7.8E+0006	2.000	-765.0	! MES 698
C7H14Y+R300H=>RC7H13Y+H2O2 DUPLICATE	6.4E+0003	2.600	12400.0	! MES 699
C7H14Y+R300H=>RC7H13Y+H2O2 DUPLICATE	6.0E+0011	0.000	17000.0	! MES 700

C7H14Y+R300H=>RC7H13Y+H202 DUPLICATE	1.2E+0012	0.000	15500.0	! MES 701
C7H14Y+R4CH3=>RC7H13Y+CH4 DUPLICATE	1.0E+0011	0.000	7300.0	! MES 702
C7H14Y+R4CH3=>RC7H13Y+CH4 DUPLICATE	3.0E-0001	4.000	8200.0	! MES 703
C7H14Y+R4CH3=>RC7H13Y+CH4 DUPLICATE	6.0E+0011	0.000	9600.0	! MES 704
C7H14Y+R8CH300=>RC7H13Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 705
C7H14Y+R8CH300=>RC7H13Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 706
C7H14Y+R8CH300=>RC7H13Y+CH300H DUPLICATE	9.0E+0012	0.000	17500.0	! MES 707
C7H14Y+R11C2H5=>RC7H13Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 708
C7H14Y+R11C2H5=>RC7H13Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 709
C7H14Y+R11C2H5=>RC7H13Y+C2H6 DUPLICATE	6.0E+0011	0.000	11000.0	! MES 710
C8H16Y+R1H=>RC8H15Y+H2 DUPLICATE	5.4E+0004	2.500	-1900.0	! MES 711
C8H16Y+R1H=>RC8H15Y+H2 DUPLICATE	2.9E+0007	2.000	7700.0	! MES 712
C8H16Y+R1H=>RC8H15Y+H2 DUPLICATE	3.6E+0007	2.000	5000.0	! MES 713
C8H16Y+R20H=>RC8H15Y+H20 DUPLICATE	3.0E+0006	2.000	-1520.0	! MES 714
C8H16Y+R20H=>RC8H15Y+H20 DUPLICATE	2.7E+0006	2.000	450.0	! MES 715
C8H16Y+R20H=>RC8H15Y+H20 DUPLICATE	1.0E+0007	2.000	-765.0	! MES 716
C8H16Y+R300H=>RC8H15Y+H202 DUPLICATE	6.4E+0003	2.600	12400.0	! MES 717
C8H16Y+R300H=>RC8H15Y+H202 DUPLICATE	6.0E+0011	0.000	17000.0	! MES 718
C8H16Y+R300H=>RC8H15Y+H202 DUPLICATE	1.6E+0012	0.000	15500.0	! MES 719
C8H16Y+R4CH3=>RC8H15Y+CH4 DUPLICATE	1.0E+0011	0.000	7300.0	! MES 720
C8H16Y+R4CH3=>RC8H15Y+CH4 DUPLICATE	3.0E-0001	4.000	8200.0	! MES 721
C8H16Y+R4CH3=>RC8H15Y+CH4 DUPLICATE	8.0E+0011	0.000	9600.0	! MES 722
C8H16Y+R8CH300=>RC8H15Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 723
C8H16Y+R8CH300=>RC8H15Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 724
C8H16Y+R8CH300=>RC8H15Y+CH300H DUPLICATE	1.2E+0013	0.000	17500.0	! MES 725
C8H16Y+R11C2H5=>RC8H15Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 726
C8H16Y+R11C2H5=>RC8H15Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 727

C8H16Y+R11C2H5=>RC8H15Y+C2H6	8.0E+0011	0.000	11000.0	! MES 728
DUPLICATE				
C5H10Y+R1H=>RC5H9Y+H2	5.4E+0004	2.500	-1900.0	! MES 729
DUPLICATE				
C5H10Y+R1H=>RC5H9Y+H2	2.9E+0007	2.000	7700.0	! MES 730
DUPLICATE				
C5H10Y+R1H=>RC5H9Y+H2	9.0E+0006	2.000	5000.0	! MES 731
DUPLICATE				
C5H10Y+R20H=>RC5H9Y+H20	3.0E+0006	2.000	-1520.0	! MES 732
DUPLICATE				
C5H10Y+R20H=>RC5H9Y+H20	2.7E+0006	2.000	450.0	! MES 733
DUPLICATE				
C5H10Y+R20H=>RC5H9Y+H20	2.6E+0006	2.000	-765.0	! MES 734
DUPLICATE				
C5H10Y+R300H=>RC5H9Y+H202	6.4E+0003	2.600	12400.0	! MES 735
DUPLICATE				
C5H10Y+R300H=>RC5H9Y+H202	6.0E+0011	0.000	17000.0	! MES 736
DUPLICATE				
C5H10Y+R300H=>RC5H9Y+H202	4.0E+0011	0.000	15500.0	! MES 737
DUPLICATE				
C5H10Y+R4CH3=>RC5H9Y+CH4	1.0E+0011	0.000	7300.0	! MES 738
DUPLICATE				
C5H10Y+R4CH3=>RC5H9Y+CH4	3.0E-0001	4.000	8200.0	! MES 739
DUPLICATE				
C5H10Y+R4CH3=>RC5H9Y+CH4	2.0E+0011	0.000	9600.0	! MES 740
DUPLICATE				
C5H10Y+R8CH300=>RC5H9Y+CH300H	1.0E+0012	0.000	14550.0	! MES 741
DUPLICATE				
C5H10Y+R8CH300=>RC5H9Y+CH300H	6.0E+0012	0.000	20000.0	! MES 742
DUPLICATE				
C5H10Y+R8CH300=>RC5H9Y+CH300H	3.0E+0012	0.000	17500.0	! MES 743
DUPLICATE				
C5H10Y+R11C2H5=>RC5H9Y+C2H6	1.5E+0000	3.500	4140.0	! MES 744
DUPLICATE				
C5H10Y+R11C2H5=>RC5H9Y+C2H6	3.0E+0011	0.000	13500.0	! MES 745
DUPLICATE				
C5H10Y+R11C2H5=>RC5H9Y+C2H6	2.0E+0011	0.000	11000.0	! MES 746
DUPLICATE				
C3H6Y+B10=>RC3H5Y+R20H	1.7E+0011	0.700	5900.0	! MES 747
C4H8Y+B10=>RC4H7Y+R20H	8.8E+0010	0.700	3250.0	! MES 748
DUPLICATE				
C4H8Y+B10=>RC4H7Y+R20H	5.1E+0013	0.000	7850.0	! MES 749
DUPLICATE				
C7H14Y+B10=>RC7H13Y+R20H	8.8E+0010	0.700	3250.0	! MES 750
DUPLICATE				
C7H14Y+B10=>RC7H13Y+R20H	5.1E+0013	0.000	7850.0	! MES 751
DUPLICATE				
C7H14Y+B10=>RC7H13Y+R20H	7.8E+0013	0.000	5200.0	! MES 752
DUPLICATE				
C8H16Y+B10=>RC8H15Y+R20H	8.8E+0010	0.700	3250.0	! MES 753
DUPLICATE				
C8H16Y+B10=>RC8H15Y+R20H	5.1E+0013	0.000	7850.0	! MES 754
DUPLICATE				
C8H16Y+B10=>RC8H15Y+R20H	1.0E+0014	0.000	5200.0	! MES 755

DUPLICATE  
 C5H10Y+B10=>RC5H9Y+R20H 8.8E+0010 0.700 3250.0 ! MES 756  
 DUPLICATE  
 C5H10Y+B10=>RC5H9Y+R20H 5.1E+0013 0.000 7850.0 ! MES 757  
 DUPLICATE  
 C5H10Y+B10=>RC5H9Y+R20H 2.6E+0013 0.000 5200.0 ! MES 758  
 DUPLICATE

! Addition of .Y on YH

RC3H5Y+C5H10Y=>R10C2H3V+C6H12Z 6.0E+0009 0.000 11400.0 ! ADY 759  
 RC3H5Y+C8H16Y=>R10C2H3V+C9H18Z 6.0E+0009 0.000 11400.0 ! ADY 760  
 RC3H5Y+C7H14Y=>R10C2H3V+C8H16Z 6.0E+0009 0.000 11400.0 ! ADY 761  
 RC3H5Y+C4H8Y=>R10C2H3V+C5H10Z 6.0E+0009 0.000 11400.0 ! ADY 762  
 RC3H5Y+C3H6Y=>R10C2H3V+C4H8Y 6.0E+0009 0.000 11400.0 ! ADY 763  
 RC4H7Y+C5H10Y=>R10C2H3V+C7H14Z 6.0E+0009 0.000 11400.0 ! ADY 764  
 RC4H7Y+C8H16Y=>R10C2H3V+C10H20Z 6.0E+0009 0.000 11400.0 ! ADY 765  
 RC4H7Y+C7H14Y=>R10C2H3V+C9H18Z 6.0E+0009 0.000 11400.0 ! ADY 766  
 RC4H7Y+C4H8Y=>R10C2H3V+C6H12Z 6.0E+0009 0.000 11400.0 ! ADY 767  
 RC4H7Y+C3H6Y=>R10C2H3V+C5H10Z 6.0E+0009 0.000 11400.0 ! ADY 768  
 RC7H13Y+C5H10Y=>R10C2H3V+C10H20Z 6.0E+0009 0.000 11400.0 ! ADY 769  
 RC7H13Y+C8H16Y=>R10C2H3V+C13H26Z 6.0E+0009 0.000 11400.0 ! ADY 770  
 RC7H13Y+C7H14Y=>R10C2H3V+C12H24Z 6.0E+0009 0.000 11400.0 ! ADY 771  
 RC7H13Y+C4H8Y=>R10C2H3V+C9H18Z 6.0E+0009 0.000 11400.0 ! ADY 772  
 RC7H13Y+C3H6Y=>R10C2H3V+C8H16Z 6.0E+0009 0.000 11400.0 ! ADY 773  
 RC8H15Y+C5H10Y=>R10C2H3V+C11H22Z 6.0E+0009 0.000 11400.0 ! ADY 774  
 !RC8H15Y+C8H16Y=>R10C2H3V+C14H28Z 6.0E+0009 0.000 11400.0 ! ADY 775  
 RC8H15Y+C7H14Y=>R10C2H3V+C13H26Z 6.0E+0009 0.000 11400.0 ! ADY 776  
 RC8H15Y+C4H8Y=>R10C2H3V+C10H20Z 6.0E+0009 0.000 11400.0 ! ADY 777  
 RC8H15Y+C3H6Y=>R10C2H3V+C9H18Z 6.0E+0009 0.000 11400.0 ! ADY 778  
 RC5H9Y+C5H10Y=>R10C2H3V+C8H16Z 6.0E+0009 0.000 11400.0 ! ADY 779  
 RC5H9Y+C8H16Y=>R10C2H3V+C11H22Z 6.0E+0009 0.000 11400.0 ! ADY 780  
 RC5H9Y+C7H14Y=>R10C2H3V+C10H20Z 6.0E+0009 0.000 11400.0 ! ADY 781  
 RC5H9Y+C4H8Y=>R10C2H3V+C7H14Z 6.0E+0009 0.000 11400.0 ! ADY 782  
 RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z 6.0E+0009 0.000 11400.0 ! ADY 783

! Alkohol reactions

C3H7OH+R1H=>H2+R2OH+C3H6Y 2.9E+0007 2.000 7700.0 ! MOL 784  
 DUPLICATE  
 C3H7OH+R1H=>H2+R2OH+C3H6Y 1.8E+0007 2.000 5000.0 ! MOL 785  
 DUPLICATE  
 C3H7OH+R1H=>H2+R11C2H5+HCHO 2.4E+0006 2.000 6525.0 ! MOL 786  
 C3H7OH+R2OH=>H2O+R2OH+C3H6Y 2.7E+0006 2.000 450.0 ! MOL 787  
 DUPLICATE  
 C3H7OH+R2OH=>H2O+R2OH+C3H6Y 5.2E+0006 2.000 -765.0 ! MOL 788  
 DUPLICATE  
 C3H7OH+R2OH=>H2O+R11C2H5+HCHO 4.0E+0005 2.000 -475.0 ! MOL 789  
 C3H7OH+R300H=>H2O2+R2OH+C3H6Y 6.0E+0011 0.000 17000.0 ! MOL 790  
 DUPLICATE  
 C3H7OH+R300H=>H2O2+R2OH+C3H6Y 8.0E+0011 0.000 15500.0 ! MOL 791  
 DUPLICATE  
 C3H7OH+R300H=>H2O2+R11C2H5+HCHO 5.4E+0004 2.000 15025.0 ! MOL 792  
 C3H7OH+R4CH3=>CH4+R2OH+C3H6Y 3.0E-0001 4.000 8200.0 ! MOL 793  
 DUPLICATE  
 C3H7OH+R4CH3=>CH4+R2OH+C3H6Y 4.0E+0011 0.000 9600.0 ! MOL 794

DUPLICATE  
 C3H70H+R4CH3=>CH4+R11C2H5+HCHO 3.9E+0004 2.000 7525.0 ! MOL 795  
 C3H70H+R8CH300=>CH300H+R20H+C3H6Y 1.6E+0011 0.000 7300.0 ! MOL 796  
 DUPLICATE  
 C3H70H+R8CH300=>CH300H+R20H+C3H6Y 2.9E+0011 0.000 4500.0 ! MOL 797  
 DUPLICATE  
 C3H70H+R8CH300=>CH300H+R11C2H5+HCHO 0.0E+0000 0.000 0.0 ! MOL 798  
 C3H70H+R11C2H5=>C2H6+R20H+C3H6Y 3.0E+0011 0.000 13500.0 ! MOL 799  
 DUPLICATE  
 C3H70H+R11C2H5=>C2H6+R20H+C3H6Y 4.0E+0011 0.000 11000.0 ! MOL 800  
 DUPLICATE  
 C3H70H+R11C2H5=>C2H6+R11C2H5+HCHO 2.3E+0004 2.000 10525.0 ! MOL 801  
 C4H100L+R1H=>H2+R20H+C4H8Y 2.9E+0007 2.000 7700.0 ! MOL 802  
 DUPLICATE  
 C4H100L+R1H=>H2+R20H+C4H8Y 2.7E+0007 2.000 5000.0 ! MOL 803  
 DUPLICATE  
 C4H100L+R1H=>H2+R19C3H7+HCHO 2.4E+0006 2.000 6525.0 ! MOL 804  
 C4H100L+R20H=>H20+R20H+C4H8Y 2.7E+0006 2.000 450.0 ! MOL 805  
 DUPLICATE  
 C4H100L+R20H=>H20+R20H+C4H8Y 7.8E+0006 2.000 -765.0 ! MOL 806  
 DUPLICATE  
 C4H100L+R20H=>H20+R19C3H7+HCHO 4.0E+0005 2.000 -475.0 ! MOL 807  
 C4H100L+R300H=>H202+R20H+C4H8Y 6.0E+0011 0.000 17000.0 ! MOL 808  
 DUPLICATE  
 C4H100L+R300H=>H202+R20H+C4H8Y 1.2E+0012 0.000 15500.0 ! MOL 809  
 DUPLICATE  
 C4H100L+R300H=>H202+R19C3H7+HCHO 5.4E+0004 2.000 15025.0 ! MOL 810  
 C4H100L+R4CH3=>CH4+R20H+C4H8Y 3.0E-0001 4.000 8200.0 ! MOL 811  
 DUPLICATE  
 C4H100L+R4CH3=>CH4+R20H+C4H8Y 6.0E+0011 0.000 9600.0 ! MOL 812  
 DUPLICATE  
 C4H100L+R4CH3=>CH4+R19C3H7+HCHO 3.9E+0004 2.000 7525.0 ! MOL 813  
 C4H100L+R8CH300=>CH300H+R20H+C4H8Y 1.6E+0011 0.000 7300.0 ! MOL 814  
 DUPLICATE  
 C4H100L+R8CH300=>CH300H+R20H+C4H8Y 4.4E+0011 0.000 4500.0 ! MOL 815  
 DUPLICATE  
 C4H100L+R8CH300=>CH300H+R19C3H7+HCHO 0.0E+0000 0.000 0.0 ! MOL 816  
 C4H100L+R11C2H5=>C2H6+R20H+C4H8Y 3.0E+0011 0.000 13500.0 ! MOL 817  
 DUPLICATE  
 C4H100L+R11C2H5=>C2H6+R20H+C4H8Y 6.0E+0011 0.000 11000.0 ! MOL 818  
 DUPLICATE  
 C4H100L+R11C2H5=>C2H6+R19C3H7+HCHO 2.3E+0004 2.000 10525.0 ! MOL  
 819  
 C5H120L+R1H=>H2+R20H+C5H10Z 2.9E+0007 2.000 7700.0 ! MOL 820  
 DUPLICATE  
 C5H120L+R1H=>H2+R20H+C5H10Z 3.6E+0007 2.000 5000.0 ! MOL 821  
 DUPLICATE  
 C5H120L+R1H=>H2+R20C4H9+HCHO 2.4E+0006 2.000 6525.0 ! MOL 822  
 C5H120L+R20H=>H20+R20H+C5H10Z 2.7E+0006 2.000 450.0 ! MOL 823  
 DUPLICATE  
 C5H120L+R20H=>H20+R20H+C5H10Z 1.0E+0007 2.000 -765.0 ! MOL 824  
 DUPLICATE  
 C5H120L+R20H=>H20+R20C4H9+HCHO 4.0E+0005 2.000 -475.0 ! MOL 825  
 C5H120L+R300H=>H202+R20H+C5H10Z 6.0E+0011 0.000 17000.0 ! MOL 826



DUPLICATE  
 C5H120L+R300H=>H202+R20H+C5H10Z 1.6E+0012 0.000 15500.0 ! MOL 827  
 DUPLICATE  
 C5H120L+R300H=>H202+R20C4H9+HCHO 5.4E+0004 2.000 15025.0 ! MOL 828  
 C5H120L+R4CH3=>CH4+R20H+C5H10Z 3.0E-0001 4.000 8200.0 ! MOL 829  
 DUPLICATE  
 C5H120L+R4CH3=>CH4+R20H+C5H10Z 8.0E+0011 0.000 9600.0 ! MOL 830  
 DUPLICATE  
 C5H120L+R4CH3=>CH4+R20C4H9+HCHO 3.9E+0004 2.000 7525.0 ! MOL 831  
 C5H120L+R8CH300=>CH300H+R20H+C5H10Z 1.6E+0011 0.000 7300.0 ! MOL 832  
 DUPLICATE  
 C5H120L+R8CH300=>CH300H+R20H+C5H10Z 5.8E+0011 0.000 4500.0 ! MOL 833  
 DUPLICATE  
 C5H120L+R8CH300=>CH300H+R20C4H9+HCHO 0.0E+0000 0.000 0.0 ! MOL 834  
 C5H120L+R11C2H5=>C2H6+R20H+C5H10Z 3.0E+0011 0.000 13500.0 ! MOL 835  
 DUPLICATE  
 C5H120L+R11C2H5=>C2H6+R20H+C5H10Z 8.0E+0011 0.000 11000.0 ! MOL 836  
 DUPLICATE  
 C5H120L+R11C2H5=>C2H6+R20C4H9+HCHO 2.3E+0004 2.000 10525.0 ! MOL 837  
 C3H70H+B10=>R20H+R20H+C3H6Y 3.9E+0013 0.000 5200.0 ! MOL 838  
 DUPLICATE  
 C3H70H+B10=>R20H+R20H+C3H6Y 4.0E+0013 0.000 5200.0 ! MOL 839  
 DUPLICATE  
 C3H70H+B10=>R20H+R11C2H5+HCHO 1.3E+0006 2.000 5025.0 ! MOL 840  
 C4H100L+B10=>R20H+R20H+C4H8Y 3.9E+0013 0.000 5200.0 ! MOL 841  
 DUPLICATE  
 C4H100L+B10=>R20H+R20H+C4H8Y 6.0E+0013 0.000 5200.0 ! MOL 842  
 DUPLICATE  
 C4H100L+B10=>R20H+R19C3H7+HCHO 1.3E+0006 2.000 5025.0 ! MOL 843  
 C5H120L+B10=>R20H+R20H+C5H10Z 3.9E+0013 0.000 5200.0 ! MOL 844  
 DUPLICATE  
 C5H120L+B10=>R20H+R20H+C5H10Z 8.0E+0013 0.000 5200.0 ! MOL 845  
 DUPLICATE  
 C5H120L+B10=>R20H+R20C4H9+HCHO 1.3E+0006 2.000 5025.0 ! MOL 846

! Aldehydes metathesis

C2H5CHO+R1H=>H2+RC3H50 4.0E+0013 0.000 4200.0 ! ADZ 847  
 C2H5CHO+R20H=>H20+RC3H50 4.2E+0012 0.000 500.0 ! ADZ 848  
 C2H5CHO+R300H=>H202+RC3H50 1.0E+0012 0.000 10000.0 ! ADZ 849  
 C2H5CHO+R4CH3=>CH4+RC3H50 2.0E-0006 5.600 2500.0 ! ADZ 850  
 C2H5CHO+R11C2H5=>C2H6+RC3H50 1.3E+0012 0.000 8500.0 ! ADZ 851  
 C5H100A+R1H=>H2+RC5H90 4.0E+0013 0.000 4200.0 ! ADZ 852  
 C5H100A+R20H=>H20+RC5H90 4.2E+0012 0.000 500.0 ! ADZ 853  
 C5H100A+R300H=>H202+RC5H90 1.0E+0012 0.000 10000.0 ! ADZ 854  
 C5H100A+R4CH3=>CH4+RC5H90 2.0E-0006 5.600 2500.0 ! ADZ 855  
 C5H100A+R11C2H5=>C2H6+RC5H90 1.3E+0012 0.000 8500.0 ! ADZ 856  
 C4H80A+R1H=>H2+RC4H70 4.0E+0013 0.000 4200.0 ! ADZ 857  
 C4H80A+R20H=>H20+RC4H70 4.2E+0012 0.000 500.0 ! ADZ 858  
 C4H80A+R300H=>H202+RC4H70 1.0E+0012 0.000 10000.0 ! ADZ 859  
 C4H80A+R4CH3=>CH4+RC4H70 2.0E-0006 5.600 2500.0 ! ADZ 860  
 C4H80A+R11C2H5=>C2H6+RC4H70 1.3E+0012 0.000 8500.0 ! ADZ 861

C6H120A+R1H=>H2+RC6H110 4.0E+0013 0.000 4200.0 ! ADZ 862  
C6H120A+R20H=>H20+RC6H110 4.2E+0012 0.000 500.0 ! ADZ 863  
C6H120A+R300H=>H202+RC6H110 1.0E+0012 0.000 10000.0 ! ADZ 864  
C6H120A+R4CH3=>CH4+RC6H110 2.0E-0006 5.600 2500.0 ! ADZ 865  
C6H120A+R11C2H5=>C2H6+RC6H110 1.3E+0012 0.000 8500.0 ! ADZ 866  
C7H140A+R1H=>H2+RC7H130 4.0E+0013 0.000 4200.0 ! ADZ 867  
C7H140A+R20H=>H20+RC7H130 4.2E+0012 0.000 500.0 ! ADZ 868  
C7H140A+R300H=>H202+RC7H130 1.0E+0012 0.000 10000.0 ! ADZ 869  
C7H140A+R4CH3=>CH4+RC7H130 2.0E-0006 5.600 2500.0 ! ADZ 870  
C7H140A+R11C2H5=>C2H6+RC7H130 1.3E+0012 0.000 8500.0 ! ADZ 871  
C8H160A+R1H=>H2+RC8H150 4.0E+0013 0.000 4200.0 ! ADZ 872  
C8H160A+R20H=>H20+RC8H150 4.2E+0012 0.000 500.0 ! ADZ 873  
C8H160A+R300H=>H202+RC8H150 1.0E+0012 0.000 10000.0 ! ADZ 874  
C8H160A+R4CH3=>CH4+RC8H150 2.0E-0006 5.600 2500.0 ! ADZ 875  
C8H160A+R11C2H5=>C2H6+RC8H150 1.3E+0012 0.000 8500.0 ! ADZ 876  
C9H180A+R1H=>H2+RC9H170 4.0E+0013 0.000 4200.0 ! ADZ 877  
C9H180A+R20H=>H20+RC9H170 4.2E+0012 0.000 500.0 ! ADZ 878  
C9H180A+R300H=>H202+RC9H170 1.0E+0012 0.000 10000.0 ! ADZ 879  
C9H180A+R4CH3=>CH4+RC9H170 2.0E-0006 5.600 2500.0 ! ADZ 880  
C9H180A+R11C2H5=>C2H6+RC9H170 1.3E+0012 0.000 8500.0 ! ADZ 881  
C12H240A+R1H=>H2+RC12H230 4.0E+0013 0.000 4200.0 ! ADZ 882  
C12H240A+R20H=>H20+RC12H230 4.2E+0012 0.000 500.0 ! ADZ 883  
C12H240A+R300H=>H202+RC12H230 1.0E+0012 0.000 10000.0 ! ADZ 884  
C12H240A+R4CH3=>CH4+RC12H230 2.0E-0006 5.600 2500.0 ! ADZ 885  
C12H240A+R11C2H5=>C2H6+RC12H230 1.3E+0012 0.000 8500.0 ! ADZ 886  
C11H220A+R1H=>H2+RC11H210 4.0E+0013 0.000 4200.0 ! ADZ 887  
C11H220A+R20H=>H20+RC11H210 4.2E+0012 0.000 500.0 ! ADZ 888  
C11H220A+R300H=>H202+RC11H210 1.0E+0012 0.000 10000.0 ! ADZ 889  
C11H220A+R4CH3=>CH4+RC11H210 2.0E-0006 5.600 2500.0 ! ADZ 890  
C11H220A+R11C2H5=>C2H6+RC11H210 1.3E+0012 0.000 8500.0 ! ADZ 891  
C10H200A+R1H=>H2+RC10H190 4.0E+0013 0.000 4200.0 ! ADZ 892  
C10H200A+R20H=>H20+RC10H190 4.2E+0012 0.000 500.0 ! ADZ 893  
C10H200A+R300H=>H202+RC10H190 1.0E+0012 0.000 10000.0 ! ADZ 894  
C10H200A+R4CH3=>CH4+RC10H190 2.0E-0006 5.600 2500.0 ! ADZ 895  
C10H200A+R11C2H5=>C2H6+RC10H190 1.3E+0012 0.000 8500.0 ! ADZ 896  
C13H260A+R1H=>H2+RC13H250 4.0E+0013 0.000 4200.0 ! ADZ 897  
C13H260A+R20H=>H20+RC13H250 4.2E+0012 0.000 500.0 ! ADZ 898  
C13H260A+R300H=>H202+RC13H250 1.0E+0012 0.000 10000.0 ! ADZ 899  
C13H260A+R4CH3=>CH4+RC13H250 2.0E-0006 5.600 2500.0 ! ADZ 900  
C13H260A+R11C2H5=>C2H6+RC13H250 1.3E+0012 0.000 8500.0 ! ADZ 901  
  
C4H60AY+R1H=>H2+R10C2H3V+CH2COZ 4.0E+0013 0.000 4200.0 ! ADZ 902  
C4H60AY+R20H=>H20+R10C2H3V+CH2COZ 4.0E+0012 0.000 500.0 ! ADZ 903  
C4H60AY+R300H=>H202+R10C2H3V+CH2COZ 1.0E+0012 0.000 10000.0 ! ADZ  
904  
C4H60AY+R4CH3=>CH4+R10C2H3V+CH2COZ 2.0E-0006 0.000 2500.0 ! ADZ 905  
C4H60AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ 1.3E+0012 0.000 8500.0 ! ADZ  
906  
C5H80AY+R1H=>H2+RC3H5Y+CH2COZ 4.0E+0013 0.000 4200.0 ! ADZ 907  
C5H80AY+R20H=>H20+RC3H5Y+CH2COZ 4.0E+0012 0.000 500.0 ! ADZ 908  
C5H80AY+R300H=>H202+RC3H5Y+CH2COZ 1.0E+0012 0.000 10000.0 ! ADZ 909  
C5H80AY+R4CH3=>CH4+RC3H5Y+CH2COZ 2.0E-0006 0.000 2500.0 ! ADZ 910  
C5H80AY+R11C2H5=>C2H6+RC3H5Y+CH2COZ 1.3E+0012 0.000 8500.0 ! ADZ  
911

!C8H140AY+R1H=>H2+R10C2H3V+CH2COZ+2C2H4Z 4.0E+0013 0.000 4200.0 !  
 ADZ 912  
 !C8H140AY+R20H=>H20+R10C2H3V+CH2COZ+2C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 913  
 !C8H140AY+R300H=>H202+R10C2H3V+CH2COZ+2C2H4Z 1.0E+0012 0.000 10000.0  
 ! ADZ 914  
 !C8H140AY+R4CH3=>CH4+R10C2H3V+CH2COZ+2C2H4Z 2.0E-0006 0.000  
 2500.0 ! ADZ 915  
 !C8H140AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+2C2H4Z 1.3E+0012 0.000  
 8500.0 ! ADZ 916  
 !C9H160AY+R1H=>H2+RC3H5Y+CH2COZ+2C2H4Z 4.0E+0013 0.000 4200.0 ! ADZ  
 917  
 !C9H160AY+R20H=>H20+RC3H5Y+CH2COZ+2C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 918  
 !C9H160AY+R300H=>H202+RC3H5Y+CH2COZ+2C2H4Z 1.0E+0012 0.000  
 10000.0 ! ADZ 919  
 !C9H160AY+R4CH3=>CH4+RC3H5Y+CH2COZ+2C2H4Z 2.0E-0006 0.000 2500.0 !  
 ADZ 920  
 !C9H160AY+R11C2H5=>C2H6+RC3H5Y+CH2COZ+2C2H4Z 1.3E+0012 0.000 8500.0  
 ! ADZ 921  
 !C6H100AY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z 4.0E+0013 0.000 4200.0 !  
 ADZ 922  
 !C6H100AY+R20H=>H20+R10C2H3V+CH2COZ+C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 923  
 !C6H100AY+R300H=>H202+R10C2H3V+CH2COZ+C2H4Z 1.0E+0012 0.000 10000.0  
 ! ADZ 924  
 !C6H100AY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z 2.0E-0006 0.000 2500.0 !  
 ADZ 925  
 !C6H100AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z 1.3E+0012 0.000 8500.0  
 ! ADZ 926

! Keto radicals decomposition

RC3H50=>B2CO+R11C2H5 1.8E+0014 0.000 15600.0 ! COR 927  
 RC5H90=>B2CO+R20C4H9 1.8E+0014 0.000 15600.0 ! COR 928  
 RC4H70=>B2CO+R19C3H7 1.8E+0014 0.000 15600.0 ! COR 929  
 RC6H110=>B2CO+R35C5H11 1.8E+0014 0.000 15600.0 ! COR 930  
 RC7H130=>B2CO+R41C6H13 1.8E+0014 0.000 15600.0 ! COR 931  
 RC8H150=>B2CO+R26C7H15 1.8E+0014 0.000 15600.0 ! COR 932  
 RC9H170=>B2CO+R30C8H17 1.8E+0014 0.000 15600.0 ! COR 933  
 RC12H230=>B2CO+R4CH3+5C2H4Z 1.8E+0014 0.000 15600.0 ! COR 934  
 RC11H210=>B2CO+R11C2H5+4C2H4Z 1.8E+0014 0.000 15600.0 ! COR 935  
 RC10H190=>B2CO+R4CH3+4C2H4Z 1.8E+0014 0.000 15600.0 ! COR 936  
 RC13H250=>B2CO+R11C2H5+5C2H4Z 1.8E+0014 0.000 15600.0 ! COR 937

! keto radicals addition to O2

RC3H50+O2=>RC3H503 3.0E+0019 -2.500 0.0 ! COR 938  
 RC5H90+O2=>RC5H903 3.0E+0019 -2.500 0.0 ! COR 939  
 RC4H70+O2=>RC4H703 3.0E+0019 -2.500 0.0 ! COR 940  
 RC6H110+O2=>RC6H1103 3.0E+0019 -2.500 0.0 ! COR 941  
 RC7H130+O2=>RC7H1303 3.0E+0019 -2.500 0.0 ! COR 942  
 RC8H150+O2=>RC8H1503 3.0E+0019 -2.500 0.0 ! COR 943  
 RC9H170+O2=>RC9H1703 3.0E+0019 -2.500 0.0 ! COR 944  
 RC12H230+O2=>RC12H2303 3.0E+0019 -2.500 0.0 ! COR 945

RC11H210+O2=>RC11H2103	3.0E+0019	-2.500	0.0	!	COR	946
RC10H190+O2=>RC10H1903	3.0E+0019	-2.500	0.0	!	COR	947
RC13H250+O2=>RC13H2503	3.0E+0019	-2.500	0.0	!	COR	948

! Peracide radical decomposition

RC3H503=>C2H4Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	949
RC5H903=>C4H8Y+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	950
RC4H703=>C3H6Y+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	951
RC6H1103=>C5H10Y+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	952
RC7H1303=>C6H12Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	953
RC8H1503=>C7H14Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	954
RC9H1703=>C8H16Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	955
RC12H2303=>C11H22Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	956
RC11H2103=>C10H20Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	957
RC10H1903=>C9H18Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	958
RC13H2503=>C12H24Z+R20H+C02	4.5E+0011	0.000	25000.0	!	PER	959

! Ketones reactions

!C2H6CO+R1H=>H2+CH2COZ+R4CH3	5.7E+0007	2.000	7700.0	!	MK	960
!C2H6CO+R20H=>H20+CH2COZ+R4CH3	5.4E+0006	2.000	450.0	!	MK	961
!C2H6CO+R300H=>H202+CH2COZ+R4CH3	1.2E+0012	0.000	17000.0	!	MK	962
!C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3	6.0E-0001	4.000	8200.0	!	MK	963
!C2H6CO+R8CH300=>CH300H+CH2COZ+R4CH3	1.2E+0013	0.000	20000.0	!	MK	964
!C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3	6.0E+0011	0.000	13500.0	!	MK	965
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	5.7E+0007	2.000	7700.0	!	MK	966
DUPLICATE						
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	9.0E+0006	2.000	5000.0	!	MK	967
DUPLICATE						
C3H8CO+R20H=>H20+CH2COZ+R11C2H5	5.4E+0006	2.000	450.0	!	MK	968
DUPLICATE						
C3H8CO+R20H=>H20+CH2COZ+R11C2H5	2.6E+0006	2.000	-765.0	!	MK	969
DUPLICATE						
C3H8CO+R300H=>H202+CH2COZ+R11C2H5	1.2E+0012	0.000	17000.0	!	MK	970
DUPLICATE						
C3H8CO+R300H=>H202+CH2COZ+R11C2H5	4.0E+0011	0.000	15500.0	!	MK	971
DUPLICATE						
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	6.0E-0001	4.000	8200.0	!	MK	972
DUPLICATE						
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	2.0E+0011	0.000	9600.0	!	MK	973
DUPLICATE						
C3H8CO+R8CH300=>CH300H+CH2COZ+R11C2H5	1.2E+0013	0.000	20000.0	!	MK	974
DUPLICATE						
C3H8CO+R8CH300=>CH300H+CH2COZ+R11C2H5	3.0E+0012	0.000	17500.0	!	MK	975
DUPLICATE						
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	6.0E+0011	0.000	13500.0	!	MK	976
DUPLICATE						
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	2.0E+0011	0.000	11000.0	!	MK	977
DUPLICATE						

! Unsaturated ester reactions  
! Esters metathesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis  
! Addition on unsaturated esters

! Carboxylic acid reactions  
! Carboxylic acid metathesis

! Carboxylic acid decomposition

! Alcohol ene to dienes

C3H60LY+R1H=>H2+HCHO+R10C2H3V	5.4E+0004	2.500	-1900.0	! ROH 978
C3H60LY+R20H=>H2O+HCHO+R10C2H3V	3.0E+0006	2.000	-1520.0	! ROH 979
C3H60LY+R300H=>H2O2+HCHO+R10C2H3V	6.4E+0003	2.600	12400.0	! ROH 980
C3H60LY+R4CH3=>CH4+HCHO+R10C2H3V	1.0E+0011	0.000	7300.0	! ROH 981
C3H60LY+R8CH300=>CH300H+HCHO+R10C2H3V	1.0E+0012	0.000	14550.0	! ROH 982
C3H60LY+R11C2H5=>C2H6+HCHO+R10C2H3V	1.5E+0000	3.500	4140.0	! ROH 983
C4H80LY+R1H=>H2+HCHO+RC3H5Y	5.4E+0004	2.500	-1900.0	! ROH 984
C4H80LY+R20H=>H2O+HCHO+RC3H5Y	3.0E+0006	2.000	-1520.0	! ROH 985
C4H80LY+R300H=>H2O2+HCHO+RC3H5Y	6.4E+0003	2.600	12400.0	! ROH 986
C4H80LY+R4CH3=>CH4+HCHO+RC3H5Y	1.0E+0011	0.000	7300.0	! ROH 987
C4H80LY+R8CH300=>CH300H+HCHO+RC3H5Y	1.0E+0012	0.000	14550.0	! ROH 988
C4H80LY+R11C2H5=>C2H6+HCHO+RC3H5Y	1.5E+0000	3.500	4140.0	! ROH 989
C5H100LY+R1H=>H2+HCHO+RC4H7Y	5.4E+0004	2.500	-1900.0	! ROH 990
C5H100LY+R20H=>H2O+HCHO+RC4H7Y	3.0E+0006	2.000	-1520.0	! ROH 991
C5H100LY+R300H=>H2O2+HCHO+RC4H7Y	6.4E+0003	2.600	12400.0	! ROH 992
C5H100LY+R4CH3=>CH4+HCHO+RC4H7Y	1.0E+0011	0.000	7300.0	! ROH 993
C5H100LY+R8CH300=>CH300H+HCHO+RC4H7Y	1.0E+0012	0.000	14550.0	! ROH 994
C5H100LY+R11C2H5=>C2H6+HCHO+RC4H7Y	1.5E+0000	3.500	4140.0	! ROH 995
C7H140LY+R1H=>H2+HCHO+RC6H11Y	5.4E+0004	2.500	-1900.0	! ROH 996
C7H140LY+R20H=>H2O+HCHO+RC6H11Y	3.0E+0006	2.000	-1520.0	! ROH 997
C7H140LY+R300H=>H2O2+HCHO+RC6H11Y	6.4E+0003	2.600	12400.0	! ROH 998
C7H140LY+R4CH3=>CH4+HCHO+RC6H11Y	1.0E+0011	0.000	7300.0	! ROH 999
C7H140LY+R8CH300=>CH300H+HCHO+RC6H11Y	1.0E+0012	0.000	14550.0	! ROH 1000
C7H140LY+R11C2H5=>C2H6+HCHO+RC6H11Y	1.5E+0000	3.500	4140.0	! ROH 1001
C8H160LY+R1H=>H2+HCHO+RC7H13Y	5.4E+0004	2.500	-1900.0	! ROH 1002
C8H160LY+R20H=>H2O+HCHO+RC7H13Y	3.0E+0006	2.000	-1520.0	! ROH 1003
C8H160LY+R300H=>H2O2+HCHO+RC7H13Y	6.4E+0003	2.600	12400.0	! ROH 1004
C8H160LY+R4CH3=>CH4+HCHO+RC7H13Y	1.0E+0011	0.000	7300.0	! ROH 1005
C8H160LY+R8CH300=>CH300H+HCHO+RC7H13Y	1.0E+0012	0.000	14550.0	! ROH 1006

C8H160LY+R11C2H5=>C2H6+HCHO+RC7H13Y 1.5E+0000 3.500 4140.0 ! ROH  
 1007  
 C9H180LY+R1H=>H2+HCHO+RC8H15Y 5.4E+0004 2.500 -1900.0 ! ROH 1008  
 C9H180LY+R20H=>H2O+HCHO+RC8H15Y 3.0E+0006 2.000 -1520.0 ! ROH 1009  
 C9H180LY+R300H=>H2O2+HCHO+RC8H15Y 6.4E+0003 2.600 12400.0 ! ROH  
 1010  
 C9H180LY+R4CH3=>CH4+HCHO+RC8H15Y 1.0E+0011 0.000 7300.0 ! ROH 1011  
 C9H180LY+R8CH300=>CH300H+HCHO+RC8H15Y 1.0E+0012 0.000 14550.0 ! ROH  
 1012  
 C9H180LY+R11C2H5=>C2H6+HCHO+RC8H15Y 1.5E+0000 3.500 4140.0 ! ROH  
 1013  
 C6H120LY+R1H=>H2+HCHO+RC5H9Y 5.4E+0004 2.500 -1900.0 ! ROH 1014  
 C6H120LY+R20H=>H2O+HCHO+RC5H9Y 3.0E+0006 2.000 -1520.0 ! ROH 1015  
 C6H120LY+R300H=>H2O2+HCHO+RC5H9Y 6.4E+0003 2.600 12400.0 ! ROH 1016  
 C6H120LY+R4CH3=>CH4+HCHO+RC5H9Y 1.0E+0011 0.000 7300.0 ! ROH 1017  
 C6H120LY+R8CH300=>CH300H+HCHO+RC5H9Y 1.0E+0012 0.000 14550.0 ! ROH  
 1018  
 C6H120LY+R11C2H5=>C2H6+HCHO+RC5H9Y 1.5E+0000 3.500 4140.0 ! ROH  
 1019

! Additions on dienes

C4H6Z2+R20H=>RC3H5Y+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1020!!!!!!!ds  
 мйса toluene

!

!C4H6Z2+R20H=>RC3H5Y+HCHO 3.0E+0012 0.000 -1040.0 !

!

C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V 1.0E+0005 2.500 -1900.0 ! AD 1021  
 C6H10Y2+R20H=>H2O+C4H6Z2+R10C2H3V 6.0E+0006 2.000 -1520.0 ! AD 1022  
 C6H10Y2+R300H=>H2O2+C4H6Z2+R10C2H3V 1.2E+0004 2.600 12400.0 ! AD  
 1023  
 C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD 1024  
 C6H10Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD  
 1025  
 C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V 3.0E+0000 3.500 4140.0 ! AD  
 1026  
 C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y 1.0E+0005 2.500 -1900.0 ! AD 1027  
 C7H12Y2+R20H=>H2O+C4H6Z2+RC3H5Y 6.0E+0006 2.000 -1520.0 ! AD 1028  
 C7H12Y2+R300H=>H2O2+C4H6Z2+RC3H5Y 1.2E+0004 2.600 12400.0 ! AD 1029  
 C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD 1030  
 C7H12Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD  
 1031  
 C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y 3.0E+0000 3.500 4140.0 ! AD  
 1032  
 !C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+2C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1033  
 !C10H18Y2+R20H=>H2O+C4H6Z2+R10C2H3V+2C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1034  
 !C10H18Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1035  
 !C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1036  
 !C10H18Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1037

!C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1038  
 !C11H20Y2+R1H=>H2+C4H6Z2+RC3H5Y+2C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1039  
 !C11H20Y2+R20H=>H2O+C4H6Z2+RC3H5Y+2C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1040  
 !C11H20Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+2C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1041  
 !C11H20Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+2C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1042  
 !C11H20Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1043  
 !C11H20Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+2C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1044  
 !C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1045  
 !C8H14Y2+R20H=>H2O+C4H6Z2+R10C2H3V+C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1046  
 !C8H14Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1047  
 !C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1048  
 !C8H14Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1049  
 !C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1050  
 !C12H22Y2+R1H=>H2+C4H6Z2+R10C2H3V+3C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1051  
 !C12H22Y2+R20H=>H2O+C4H6Z2+R10C2H3V+3C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1052  
 !C12H22Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+3C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1053  
 !C12H22Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1054  
 !C12H22Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1055  
 !C12H22Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+3C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1056  
 !C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1057  
 !C9H16Y2+R20H=>H2O+C4H6Z2+RC3H5Y+C2H4Z 6.0E+0006 2.000 -1520.0 ! AD  
 1058  
 !C9H16Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+C2H4Z 1.2E+0004 2.600 12400.0 !  
 AD 1059  
 !C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0 ! AD  
 1060  
 !C9H16Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0  
 ! AD 1061  
 !C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z 3.0E+0000 3.500 4140.0 !  
 AD 1062  
 !C14H26Y2+R1H=>H2+C4H6Z2+R10C2H3V+4C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1063  
 !C14H26Y2+R20H=>H2O+C4H6Z2+R10C2H3V+4C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1064

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!C14H26Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+4C2H4Z      1.2E+0004  2.600  12400.0
! AD 1065
!C14H26Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+4C2H4Z      2.0E+0011  0.000
7300.0 ! AD 1066
!C14H26Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+4C2H4Z      2.0E+0011  0.000
7300.0 ! AD 1067
!C14H26Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+4C2H4Z      3.0E+0000  3.500
4140.0 ! AD 1068
!C15H28Y2+R1H=>H2+C4H6Z2+RC3H5Y+4C2H4Z      1.0E+0005  2.500  -1900.0 ! AD
1069
!C15H28Y2+R20H=>H2O+C4H6Z2+RC3H5Y+4C2H4Z      6.0E+0006  2.000  -1520.0 !
AD 1070
!C15H28Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+4C2H4Z      1.2E+0004  2.600
12400.0 ! AD 1071
!C15H28Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+4C2H4Z      2.0E+0011  0.000  7300.0 !
AD 1072
!C15H28Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+4C2H4Z      2.0E+0011  0.000
7300.0 ! AD 1073
!C15H28Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+4C2H4Z      3.0E+0000  3.500  4140.0
! AD 1074
!C16H30Y2+R1H=>H2+C4H6Z2+R10C2H3V+5C2H4Z      1.0E+0005  2.500  -1900.0 !
AD 1075
!C16H30Y2+R20H=>H2O+C4H6Z2+R10C2H3V+5C2H4Z      6.0E+0006  2.000
-1520.0 ! AD 1076
!C16H30Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+5C2H4Z      1.2E+0004  2.600  12400.0
! AD 1077
!C16H30Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+5C2H4Z      2.0E+0011  0.000
7300.0 ! AD 1078
!C16H30Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+5C2H4Z      2.0E+0011  0.000
7300.0 ! AD 1079
!C16H30Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+5C2H4Z      3.0E+0000  3.500
4140.0 ! AD 1080
!C13H24Y2+R1H=>H2+C4H6Z2+RC3H5Y+3C2H4Z      1.0E+0005  2.500  -1900.0 ! AD
1081
!C13H24Y2+R20H=>H2O+C4H6Z2+RC3H5Y+3C2H4Z      6.0E+0006  2.000  -1520.0 !
AD 1082
!C13H24Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+3C2H4Z      1.2E+0004  2.600
12400.0 ! AD 1083
!C13H24Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+3C2H4Z      2.0E+0011  0.000  7300.0 !
AD 1084
!C13H24Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+3C2H4Z      2.0E+0011  0.000
7300.0 ! AD 1085
!C13H24Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+3C2H4Z      3.0E+0000  3.500  4140.0
! AD 1086

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! Diels Alder

! .Y termination

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RC3H5Y+R1H=>C3H6Y      1.0E+0014  0.000  0.0 ! TER
1087 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliy x10
RC3H5Y+R20H=>C3H60LY      1.0E+0013  0.000  0.0 ! TER 1088
RC3H5Y+R300H=>C3H602PY      5.0E+0012  0.000  0.0 ! TER 1089
RC3H5Y+R4CH3=>C4H8Y      1.0E+0013  0.000  0.0 ! TER 1090
RC3H5Y+R5CHO=>C4H60AY      1.0E+0013  0.000  0.0 ! TER 1091

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RC3H5Y+R6CH20H=>C4H80LY 1.0E+0013 0.000 0.0 ! TER 1092  
RC3H5Y+R8CH300=>HCH0+R7CH30+R10C2H3V 1.0E+0013 0.000 0.0 ! TER 1093  
RC3H5Y+R11C2H5=>C5H10Y 1.0E+0013 0.000 0.0 ! TER 1094  
RC4H7Y+R1H=>C4H8Y 1.0E+0014 0.000 0.0 ! TER  
1095!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliy x10  
RC4H7Y+R20H=>C4H80LY 1.0E+0013 0.000 0.0 ! TER 1096  
RC4H7Y+R300H=>C4H802PY 5.0E+0012 0.000 0.0 ! TER 1097  
RC4H7Y+R4CH3=>C5H10Y 1.0E+0013 0.000 0.0 ! TER 1098  
RC4H7Y+R5CHO=>C5H80AY 1.0E+0013 0.000 0.0 ! TER 1099  
RC4H7Y+R6CH20H=>C5H100LY 1.0E+0013 0.000 0.0 ! TER 1100  
RC4H7Y+R8CH300=>HCH0+R7CH30+RC3H5Y 1.0E+0013 0.000 0.0 ! TER 1101  
RC4H7Y+R11C2H5=>C6H12Z 1.0E+0013 0.000 0.0 ! TER 1102  
RC7H13Y+R1H=>C7H14Y 1.0E+0014 0.000 0.0 ! TER  
1103!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliy x10  
RC7H13Y+R20H=>C7H140LY 1.0E+0013 0.000 0.0 ! TER 1104  
RC7H13Y+R300H=>C7H1402PY 5.0E+0012 0.000 0.0 ! TER 1105  
RC7H13Y+R4CH3=>C8H16Y 1.0E+0013 0.000 0.0 ! TER 1106  
RC7H13Y+R5CHO=>C8H140AY 1.0E+0013 0.000 0.0 ! TER 1107  
RC7H13Y+R6CH20H=>C8H160LY 1.0E+0013 0.000 0.0 ! TER 1108  
RC7H13Y+R8CH300=>HCH0+R7CH30+RC6H11Y 1.0E+0013 0.000 0.0 ! TER 1109  
RC7H13Y+R11C2H5=>C9H18Z 1.0E+0013 0.000 0.0 ! TER 1110  
RC8H15Y+R1H=>C8H16Y 1.0E+0014 0.000 0.0 ! TER  
1111!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliy x10  
RC8H15Y+R20H=>C8H160LY 1.0E+0013 0.000 0.0 ! TER 1112  
RC8H15Y+R300H=>C8H1602PY 5.0E+0012 0.000 0.0 ! TER 1113  
RC8H15Y+R4CH3=>C9H18Z 1.0E+0013 0.000 0.0 ! TER 1114  
RC8H15Y+R5CHO=>C9H160AY 1.0E+0013 0.000 0.0 ! TER 1115  
RC8H15Y+R6CH20H=>C9H180LY 1.0E+0013 0.000 0.0 ! TER 1116  
RC8H15Y+R8CH300=>HCH0+R7CH30+RC7H13Y 1.0E+0013 0.000 0.0 ! TER 1117  
RC8H15Y+R11C2H5=>C10H20Z 1.0E+0013 0.000 0.0 ! TER 1118  
RC5H9Y+R1H=>C5H10Y 1.0E+0014 0.000 0.0 ! TER  
1119!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!multipliy x10  
RC5H9Y+R20H=>C5H100LY 1.0E+0013 0.000 0.0 ! TER 1120  
RC5H9Y+R300H=>C5H1002PY 5.0E+0012 0.000 0.0 ! TER 1121  
RC5H9Y+R4CH3=>C6H12Z 1.0E+0013 0.000 0.0 ! TER 1122  
RC5H9Y+R5CHO=>C6H100AY 1.0E+0013 0.000 0.0 ! TER 1123  
RC5H9Y+R6CH20H=>C6H120LY 1.0E+0013 0.000 0.0 ! TER 1124  
RC5H9Y+R8CH300=>HCH0+R7CH30+RC4H7Y 1.0E+0013 0.000 0.0 ! TER 1125  
RC5H9Y+R11C2H5=>C7H14Y 1.0E+0013 0.000 0.0 ! TER 1126  
RC3H5Y+RC3H5Y=>C6H10Y2 1.0E+0013 0.000 0.0 ! TER 1127  
RC3H5Y+RC4H7Y=>C7H12Y2 1.0E+0013 0.000 0.0 ! TER 1128  
RC3H5Y+RC7H13Y=>C10H18Y2 1.0E+0013 0.000 0.0 ! TER 1129  
RC3H5Y+RC8H15Y=>C11H20Y2 1.0E+0013 0.000 0.0 ! TER 1130  
RC3H5Y+RC5H9Y=>C8H14Y2 1.0E+0013 0.000 0.0 ! TER 1131  
RC4H7Y+RC4H7Y=>C8H14Y2 1.0E+0013 0.000 0.0 ! TER 1132  
RC4H7Y+RC7H13Y=>C11H20Y2 1.0E+0013 0.000 0.0 ! TER 1133  
RC4H7Y+RC8H15Y=>C12H22Y2 1.0E+0013 0.000 0.0 ! TER 1134  
RC4H7Y+RC5H9Y=>C9H16Y2 1.0E+0013 0.000 0.0 ! TER 1135  
!RC7H13Y+RC7H13Y=>C14H26Y2 1.0E+0013 0.000 0.0 ! TER 1136  
!RC7H13Y+RC8H15Y=>C15H28Y2 1.0E+0013 0.000 0.0 ! TER 1137  
RC7H13Y+RC5H9Y=>C12H22Y2 1.0E+0013 0.000 0.0 ! TER 1138  
!RC8H15Y+RC8H15Y=>C16H30Y2 1.0E+0013 0.000 0.0 ! TER 1139  
RC8H15Y+RC5H9Y=>C13H24Y2 1.0E+0013 0.000 0.0 ! TER 1140  
!RC8H15Y+RC6H11Y=>C14H26Y2 1.0E+0013 0.000 0.0 ! TER 1141

RC5H9Y+RC5H9Y=>C10H18Y2 1.0E+0013 0.000 0.0 ! TER 1142  
 RC5H9Y+RC6H11Y=>C11H20Y2 1.0E+0013 0.000 0.0 ! TER 1143

!  
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!especes excitees!

R1H+B10+M=OHE+M <HALL05>!	6.0E14	0.0	6.94E3	!
B4CH+O2=B2CO+OHE <HALL05>!	4.0E13	0.0	0.0	!
OHE+AR=R20H+AR <HALL05>!	5.2E10	0.5	0.0	!
OHE+H2O=R20H+H2O <HALL05>!	8.6E12	0.5	0.0	!
OHE+H2=R20H+H2 <HALL05>!	1.5E12	0.5	0.0	!
OHE+R1H=R20H+R1H <HALL05>!	1.5E12	0.5	0.0	!
OHE+O2=R20H+O2 <HALL05>!	1.5E12	0.5	0.0	!
OHE+B10=R20H+B10 <HALL05>!	1.5E12	0.5	0.0	!
OHE+R20H=R20H+R20H <HALL05>!	1.5E12	0.5	0.0	!
OHE=>R20H <HALL05>!	1.4E6	0.0	0.0	!
OHE+C02=R20H+C02 <HALL05>!	2.75E12	0.5	-968.	!
OHE+B2CO=R20H+B2CO <HALL05>!	3.23E12	0.5	-787.	!
OHE+CH4=R20H+CH4 <HALL05>!	3.36E12	0.5	-635.	!
R9C2H+B10=B2CO+CHE <HALL05>!	6.2E12	0.0	0.0	!
R9C2H+O2=C02+CHE <HALL05>!	2.17E10	0.0	0.0	!
CHE+AR=B4CH+AR <HALL05>!	4.0E10	0.5	0.0	!
CHE+O2=B4CH+O2 <HALL05>!	2.48E6	2.14	0.0	!
CHE+H2O=B4CH+H2O <HALL05>!	5.3E13	0.0	0.0	!
CHE+H2=B4CH+H2 <HALL05>!	1.47E14	0.0	1360.	!
CHE+C02=B4CH+C02 <HALL05>!	2.41E-1	4.3	-1694.	!
CHE+B2CO=B4CH+B2CO <HALL05>!	2.44E12	0.5	0.0	!
CHE+CH4=B4CH+CH4 <HALL05>!	1.73E13	0.0	167.	!
CHE=>B4CH <HALL05>!	1.86E6	0.0	0.0	!

!\*\*\*\*\*!  
! REACTIONS DE LA MATRICE O(0)C(y)H(z) !  
!\*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE H2\*\*\*\*\*!

R1H+R1H+M=H2+M 1.87E18 -1.00 0.00  
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ H2/0.0/ C2H6/3.0/  
AR/0.35/  
! N2/0.4/ HE/0.35/

!\*\*\*\*\* REACTIONS DE B4CH \*\*\*\*\*!

B4CH+R1H=B3C+H2 7.8E13 0. 0. !(2, -  
2)<PEETERS97>!

!\*\*\*\*\* REACTIONS DE B6CH2 \*\*\*\*\*!

B6CH2+M=B5CH2+M 1.51E13 0.0 0.0  
O2/.4/ B2C0/.75/ C02/1.5/ H20/6.5/ CH4/.48/ C2H4Z/1.6/  
AR/.24/  
B6CH2+R1H=B4CH+H2 3.0E13 0. 0. !(4, -  
4)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE B5CH2 \*\*\*\*\*!

B5CH2+R1H=B4CH+H2 6.0E12 0. -1.8E3 !(5, -  
5)<BAULCH94>!  
B5CH2+B3C=R9C2H+R1H 5.0E13 0. 0. !(6, -  
6)<RAnZI94>!  
B5CH2+B5CH2=>C2H2+R1H+R1H 1.2E14 0. 0.8E3 !  
(7)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE R4CH3 \*\*\*\*\*!

R4CH3+M=B5CH2+R1H+M 2.91E16 0.0 90.7E3  
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
R4CH3+R1H=B6CH2+H2 6.0E13 0. 15.0E3 !  
(9, -9)<BAULCH94>!  
R4CH3+B4CH=R10C2H3V+R1H 3.0E13 0. 0. !(10, -  
10)<DAGAUT91>  
R4CH3+B6CH2=C2H4Z+R1H 1.8E13 0. 0. !(11, -  
11)<TSAnG86>!  
R4CH3+B5CH2=C2H4Z+R1H 4.2E13 0. 0. !(12, -  
12)<BAULCH94>!  
R4CH3+B3C=C2H2+R1H 5.0E13 0. 0. !(13, -  
13)<RAnZI94>!  
R4CH3+R4CH3(+M)=>C2H6(+M) 3.61E13 0. 0. !  
(14)<BAULCH94>!  
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
LOW / 3.63E41 -7.0 2.76E3 /  
TROE / 0.62 73 1180 /  
C2H6(+M)=>R4CH3+R4CH3(+M) 1.8E21 -1.24 90.9E3 !(-  
14)<BAULCH94>!  
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/

LOW / 1.89E49 -8.24 93.7E3/  
 TROE / 0.62 73 1180 /  
 R4CH3+R4CH3=R11C2H5+R1H 3.0E13 0. 13.5E3 !(15, -  
 15)<BAULCH94>!  
 R4CH3+R4CH3=C2H4Z+H2 2.1E14 0. 19.3E3 !(16, -  
 16)<FRAnK86nIST>!

!\*\*\*\*\* REACTIONS DE CH4 \*\*\*\*\*!

R1H+R4CH3(+M)=>CH4(+M) 1.67E14 0. 0. !  
 (17)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/

LOW / 1.408E24 -1.8 0.0 /  
 TROE / 0.37 3315 61 /  
 CH4(+M)=>R4CH3+R1H(+M) 2.4E16 0. 105.0E3 !(-  
 17)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/

LOW / 1.29E18 0.00 90.9E3 /  
 TROE / 0 1350 1 7830 /  
 CH4(+CH4)=>R4CH3+R1H(+CH4) 2.4E16 0. 105.0E3 !(-  
 17')<BAULCH94>!

LOW / 8.43E17 0.00 90.9E3 /  
 TROE / 0.69 90 2210 /

CH4+R1H=R4CH3+H2 1.3E04 3. 8.0E3 !(18, -  
 18)<BAULCH94>!  
 CH4+B4CH=C2H4Z+R1H 3.0E13 0. -0.4E3 !(19, -  
 19)<DAGAUT91BAULCH94>!  
 CH4+B6CH2=R4CH3+R4CH3 4.2E13 0. 0. !(20, -  
 20)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE R9C2H \*\*\*\*\*!

R9C2H+B6CH2=C2H2+B4CH 1.8E13 0. 0. !(21, -  
 21)<TSAnG86>!  
 R9C2H+B5CH2=C2H2+B4CH 1.8E13 0. 0. !(22, -  
 22)<TSAnG86>!  
 R9C2H+CH4=C2H2+R4CH3 1.2E12 0. 0. !(23, -  
 23)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE C2H2 \*\*\*\*\*!

C2H2+M=R9C2H+R1H+M 1.14E17 0. 107.0E3 !(24, -  
 24)<BAULCH94>!  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 C2H2+R1H=R9C2H+H2 6.6E13 0. 27.7E3 !(25, -  
 25)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE R10C2H3V \*\*\*\*\*!

R10C2H3V(+M)=C2H2+R1H(+M) 2.0E14 0. 39.8E3 !(26, -  
 26)<BAULCH94>!  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 LOW / 1.19E42 -7.50 45.55E3 /  
 TROE / 0.35 1.0 1.E8/

R10C2H3V+R1H=C2H2+H2 27)<BAULCH94>!	1.2E13	0.	0.	!(27, -
R10C2H3V+B6CH2=C2H2+R4CH3 28)<TSAnG86>!	1.8E13	0.	0.	!(28, -
R10C2H3V+B5CH2=C2H2+R4CH3 29)<TSAnG86>!	1.8E13	0.	0.	!(29, -
R10C2H3V+R4CH3=CH4+C2H2 30)<TSAnG86>!	3.9E11	0.	0.	!(30, -
R10C2H3V+R9C2H=2C2H2 31)<TSAnG86>!	9.6E11	0.	0.	!(31, -
R10C2H3V+R10C2H3V=C2H4Z+C2H2 32)<TSAnG86>!	9.6E11	0.	0.	!(32, -

!\*\*\*\*\* REACTIONS DE C2H4Z \*\*\*\*\*!

C2H4Z+M=C2H2+H2+M 33)<BAULCH94>!	9.97E16	0.	71.6E3	!(33, -
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/				
C2H4Z+M=R10C2H3V+R1H+M 34)<BAULCH94>!	7.40E17	0.	96.7E3	!(34, -
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/				
!C2H4Z+R1H=R10C2H3V+H2 35)<BAULCH94>!	5.4E14	0.	14.8E3	!(35, -
C2H4Z+R1H=R10C2H3V+H2 35)SLAGLE96!	5.0E7	1.93	13.0E3	!(35, -
!C2H4Z+R4CH3=CH4+R10C2H3V 36)<BAULCH94>!	4.1E12	0.	11.1E3	!(36, -
C2H4Z+R4CH3=CH4+R10C2H3V 36)BACK89!	6.3E11	0.	16.0E3	!(36, -

!\*\*\*\*\* REACTIONS DE R11C2H5 \*\*\*\*\*!

!C2H4Z+R1H(+M)=>R11C2H5(+M)	3.97E09	1.28	1.3E3	
! 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/ ! LOW / 1.35E19 0.00 0.76E3 / ! TROE / 0.76 40 1025/				
R11C2H5(+M)=C2H4Z+R1H(+M)	8.2E13	0.	40.0E3	
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/ ! LOW / 3.40E17 0.00 33.4E3 / ! TROE / 0.75 97 1379/				
R11C2H5+R1H=C2H4Z+H2 38)<TSAnG86>!	1.8E12	0.	0.	!(38, -
R11C2H5+R1H=C2H6 39)<TSAnG86>!	3.6E13	0.	0.	!(39, -
R11C2H5+B6CH2=C2H4Z+R4CH3 40)<TSAnG86>!	9.0E12	0.	0.	!(40, -
R11C2H5+B5CH2=C2H4Z+R4CH3 41)<TSAnG86>!	1.8E13	0.	0.	!(41, -
R11C2H5+R4CH3=C2H4Z+CH4 42)<BAULCH94>!	1.1E12	0.	0.	!(42, -
R11C2H5+R9C2H=C2H2+C2H4Z 43)<TSAnG86>!	1.8E12	0.	0.	!(43, -

R11C2H5+R10C2H3V=2C2H4Z 44)<TSAnG86>!	4.8E11	0.	0.	!(44, -
R11C2H5+R10C2H3V=C2H2+C2H6 45)<TSAnG86>!	4.8E11	0.	0.	!(45, -
R11C2H5+R11C2H5=C2H4Z+C2H6 46)<BAULCH94>!	1.4E12	0.	0.	!(46, -

!\*\*\*\*\* REACTIONS DE C2H6 \*\*\*\*\*!

C2H6+M=C2H4Z+H2+M 47)<SCHULTZ85nIST>!	2.3E17	0.	67.4E3	!(47, -
C2H6+R1H=R11C2H5+H2 48)<BAULCH94>!	1.4E9	1.5	7.4E3	!(48, -
C2H6+B6CH2=R4CH3+R11C2H5 49)<TSAnG86>!	1.1E14	0.	0.	!(49, -
C2H6+R4CH3=R11C2H5+CH4 50)<BAULCH94>!	1.5E-7	6.0	5.8E3	!(50, -
C2H6+R9C2H=C2H2+R11C2H5 51)<TSAnG86>!	3.6E12	0.	0.	!(51, -
C2H6+R10C2H3V=R11C2H5+C2H4Z 52)<TSAnG86>!	6.0E2	3.3	10.5E3	!(52, -

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!\*\*\*\*\* REACTIONS DE LA MATRICE O(x)C(y)H(z) x>0 \*\*\*\*\*!

! REACTIONS DE LA MATRICE O(x)C(y)H(z) x>0 !  
!\*\*\*\*\*

!\*\*\*\*\* REACTIONS DE B10 \*\*\*\*\*!

B10+H2=R20H+R1H 53)<BAULCH94>!	5.1E4	2.67	6.2E3	!(53, -
B10+B4CH=B2C0+R1H 54)<BAULCH94>!	3.9E13	0.	0.	!(54, -
B10+B4CH=B3C+R20H 55)<MUR86nIS>!	1.5E13	0.	4.7E3	!(55, -
B10+B6CH2=>B2C0+2R1H <TSAnG86>!	1.5E13	0.	0.	!(56)
B10+B6CH2=B2C0+H2 <TSAnG86>!	1.5E13	0.	0.	!(57, -57)
B10+B5CH2=>B2C0+2R1H <BAULCH94>!	7.2E13	0.	0.	!(58)
B10+B5CH2=B2C0+H2 59)<BAULCH94>!	4.8E13	0.	0.	!(59, -
B10+R4CH3=HCH0+R1H 60)<BAULCH94>!	8.4E13	0.	0.	!(60, -
B10+R4CH3=R7CH30 61)<DEAn87nIS>!	8.0E15	-2.12	0.6E3	!(61, -

B10+CH4=R4CH3+R2OH 62)<BAULCH94>!	7.2E8	1.56	8.4E3	!(62, -
B10+R9C2H=B4CH+B2C0 63)<DAGAUT91>!	1.0E13	0.	0.	!(63, -
B10+C2H2=B5CH2+B2C0 64)<BAULCH LEEDS>!	2.17E06	2.1	1.6E3	!(64, -
B10+C2H2=R12CHCOZ+R1H 65)<BAULCH LEEDS>!	5.06E06	2.1	1.6E3	!(65, -
R20H+R9C2H=C2H2+B10 89)<TSANG86>! modif MF	1.8E13	0.	0.	!(89, -
B10+R10C2H3V=R4CH3+B2C0 66)<DAGAUT91>!	3.0E13	0.	0.	!(66, -
B10+R10C2H3V=CH2COZ+R1H 67)<TSAnG86>!	9.6E13	0.	0.	!(67, -
B10+C2H4Z=R4CH3+R5CHO 68)<BAULCH94>!	8.1E6	1.88	0.2E3	!(68, -
B10+C2H4Z=HCHO+B5CH2 69)<BAULCH94>!	4.00E5	1.88	0.2E3	!(69, -
B10+C2H4Z=CH2COZ+H2 70)<BAULCH94>!	6.6E5	1.88	0.2E3	!(70, -
B10+C2H4Z=R13CH2CHO+R1H 71)<BAULCH94>!	4.7E6	1.88	0.2E3	!(71, -
B10+C2H4Z=R20H+R10C2H3V 72)<MAHMUD87nIST>!	1.5E7	1.91	3.7E3	!(72, -
B10+R11C2H5=HCHO+R4CH3 73)<BAULCH94>!	1.1E13	0.	0.	!(73, -
B10+R11C2H5=CH3CHO+R1H 74)<BAULCH94>!	5.5e13	0.	0.	!(74, -
B10+R11C2H5=C2H4Z+R20H 75)<DAGAUT91>!	3.0E13	0.	0.	!(75, -
B10+C2H6=R11C2H5+R20H 76)<BAULCH94>!	1.0E9	1.5	5.8E3	!(76, -

!\*\*\*\*\* REACTIONS DE R20H \*\*\*\*\*!

R1H+B10+M=R20H+M	1.18E19	-1.0	0.0	
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
R1H+R20H+M=H20+M	5.53E+22	-2.0	0.0	
02/0.4/ B2C0/0.75/ C02/1.5/ H20/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/				
! N2/0.4/ HE/0.35/				
R20H+H2=R1H+H2O 79)<BAULCH94>!	1.0E8	1.6	3.3E3	!(79, -
R20H+B3C=B2C0+R1H 80)<RAnZI94>!	5.0E13	0.	0.	!(80, -
R20H+B4CH=R5CHO+R1H 81)<DAGAUT91>!	3.0E13	0.	0.	!(81, -
R20H+B6CH2=HCHO+R1H 82)<TSAnG86>!	3.0E13	0.	0.	!(82, -
R20H+B5CH2=HCHO+R1H 83)<TSAnG86>!	1.8E13	0.	0.	!(83, -
R20H+R4CH3=B6CH2+H2O 84)<BAULCH94>!	7.2E13	0.	2.7E3	!(84, -
R20H+R4CH3(+M)=CH3OH(+M) 85)<BAULCH94>!	6.0E13	0.	0.	!(85, -

	LOW	/1.4E44	-8.2	0./		
	TROE	/0.82	200.	1438./		
R20H+R4CH3=HCHO+H2 86)<DAGAUT91>!			3.2E12	-0.53	10.8E3	!(86, -
R20H+R4CH3=R7CH30+R1H 87)<DAGAUT91>!			5.7E12	-0.23	13.9E3	!(87, -
R20H+CH4=R4CH3+H2O 88)<BAULCH94>!			1.6E7	1.83	2.7E3	!(88, -
!R20H+R9C2H=C2H2+B10 89)<TSAnG86>!			1.8E13	0.	0.	!(89, -
R20H+R9C2H=B5CH2+B2C0 90)<TSAnG86>!			1.8E13	0.	0.	!(90, -
R20H+R9C2H=R12CHCOZ+R1H 91)<DAGAUT91>!			2.0E13	0.	0.	!(91, -
R20H+C2H2=R9C2H+H2O 92)<KONNOV00>!			3.385E+07	2.0	14000.0	!(92, -
R20H+C2H2=CH2COZ+R1H 93)<KONNOV00>!			1.100E+13	0.0	7170.0	!(93, -
R20H+C2H2=R4CH3+B2C0 94)<DAGAUT91>!			4.8E-4	4.	-2.0E3	!(94, -
R20H+R10C2H3V=C2H2+H2O 95)<TSAnG86>!			3.0E13	0.	0.	!(95, -
R20H+R10C2H3V=CH3CHO 96)<TSAnG86>!			3.0E13	0.	0.	!(96, -
R20H+C2H4Z=R10C2H3V+H2O 97)<BAULCH94>!			2.0E13	0.	5.9E3	!(97, -
R20H+C2H4Z=R4CH3+HCHO 98)<GLARBORG86>!			2.0E12	0.	0.9E3	!(98, -
R20H+R11C2H5=C2H4Z+H2O 99)<TSAnG86>!			2.4E13	0.	0.	!(99, -
R20H+R11C2H5=>R4CH3+R1H+HCHO <TSAnG86>!			2.4E13	0.	0.	!(100)
R20H+C2H6=R11C2H5+H2O 101)<BAULCH94>!			7.2E6	2.	0.9E3	!(101, -
R20H+R20H=H2O+B10 102)<BAULCH94>!			1.5E9	1.14	0.1E3	!(102, -
!***** REACTIONS DE H2O *****!						
H20+B4CH=R6CH20H 103)<BAULCH94>!			5.7E12	0.	-0.8E3	!(103, -
H20+B6CH2=CH30H 104)<TSAnG86>!			1.8E13	0.	0.	!(104, -
!REACTIONS DE B2C0!						
B2C0+R4CH3(+M)=R14CH3CO(+M) 105)<BAULCH94>!			5.0E11	0.	6.9E3	!(105, -
	LOW	/1.1E14	0.	3.8E3/		
	TROE	/0.5	1.0	1.0E8/		
B2C0+B10+M=C02+M 106)<TSAnG86>!			1.54E15	0.0	3.0E3	!(106, -
! O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/						
! N2/0.4/ HE/0.35/						
B2C0+R20H=C02+R1H 107)<BAULCH94>!			6.3E6	1.5	-0.5E3	!(107, -



!REACTIOnS DE R5CH0!

R5CH0+M=R1H+B2C0+M 108)<wAnG97>!	1.9E17	-1.	17.0E3	!(108, -
H2/2.0/ B2C0/1.5/ C02/2.0/ H20/6.0/				
R5CH0+R1H=H2+B2C0 109)<BAULCH94>!	9.0E13	0.	0.	!(109, -
R5CH0+R1H=B10+B5CH2 110)<TSUB0I81nIST>!	4.0E13	0.	102.5E3	!(110, -
R5CH0+B6CH2=R4CH3+B2C0 111)<TSAnG86>!	1.8E13	0.	0.	!(111, -
R5CH0+B5CH2=R4CH3+B2C0 112)<TSAnG86>!	1.8E13	0.	0.	!(112, -
R5CH0+R4CH3=CH4+B2C0 113)<TSAnG86>!	1.2E14	0.	0.	!(113, -
R5CH0+R4CH3=CH3CH0 114)<TSAnG86>!	1.8E13	0.	0.	!(114, -
R4CH3+HCH0=R5CH0+CH4 115)<BAULCH94>!	7.7E-8	6.1	1.97E3	!(115, -
R5CH0+R9C2H=C2H2+B2C0 116)<TSAnG86>!	6.0E13	0.	0.	!(116, -
R5CH0+R10C2H3V=C2H4Z+B2C0 117)<TSAnG86>!	9.0E13	0.	0.	!(117, -
R10C2H3V+HCH0=R5CH0+C2H4Z 118)<TSAnG86>!	5.4E3	2.81	5.9E3	!(118, -
R5CH0+R11C2H5=C2H6+B2C0 119)<TSAnG86>!	1.2E14	0.	0.	!(119, -
R11C2H5+HCH0=R5CH0+C2H6 120)<TSAnG86>!	5.57E3	2.81	5.86E3	!(120, -
R5CH0+B10=R1H+C02 121)<BAULCH94>!	3.0E13	0.	0.	!(121, -
R5CH0+B10=R20H+B2C0 122)<BAULCH94>!	3.0E13	0.	0.	!(122, -
R5CH0+R20H=H20+B2C0 123)<BAULCH94>!	1.1E14	0.	0.	!(123, -
R5CH0+R5CH0=HCH0+B2C0 124)<BAULCH94>!	3.0E13	0.	0.	!(124, -

!\*\*\*\*\* REACTIONS DE HCH0 \*\*\*\*\*!

HCH0+M=R5CH0+R1H+M 125)<BAULCH94>!	1.40E36	-5.54	96.8E3	!(125, -
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/				
HCH0+M=H2+B2C0+M 126)<BAULCH94>!	3.26E36	-5.54	96.8E3	!(126, -
O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/				
HCH0+R1H=R5CH0+H2 127)<BAULCH94>!	1.3E8	1.62	2.1E3	!(127, -
HCH0+B4CH=R13CH2CH0 128)<BAULCH94average>!	9.6E13	0.	-0.5E3	!(128, -
HCH0+B6CH2=R4CH3+R5CH0 129)<TSAnG86>!	1.2E12	0.	0.	!(129, -

HCHO+B10=R5CHO+R20H	4.1E11	0.57	2.7E3	!(130, -
130)<BAULCH94>!				
HCHO+R20H=R5CHO+H2O	7.82E07	1.63	-1.06E3	!MF

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!\*\*\*\*\* REACTIONS DE R7CH3O \*\*\*\*\*!

R7CH3O+M=HCHO+R1H+M	1.55E14	0.00	13.5E3	
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
!	N2/0.4/ HE/0.35/			
R7CH3O+R1H=HCHO+H2	1.8E13	0.	0.	!(133, -
133)<BAULCH94>!				
R7CH3O+B6CH2=R4CH3+HCHO	1.8E13	0.	0.	!(134, -
134)<TSAnG86>!				
R7CH3O+B5CH2=R4CH3+HCHO	1.8E13	0.	0.	!(135, -
135)<TSAnG86>!				
R7CH3O+R4CH3=HCHO+CH4	2.4E13	0.	0.	!(136, -
136)<TSAnG86>!				
R7CH3O+CH4=R4CH3+CH3OH	1.6E11	0.	8.8E3	!(137, -
137)<TSAnG86>!				
R7CH3O+R9C2H=HCHO+C2H2	2.4E13	0.	0.	!(138, -
138)<TSAnG86>!				
R7CH3O+R10C2H3V=HCHO+C2H4Z	2.4E13	0.	0.	!(139, -
139)<TSAnG86>!				
R7CH3O+C2H4Z=HCHO+R11C2H5	1.2E11	0.	6.7E3	!(140, -
140)<TSAnG86>!				
R7CH3O+R11C2H5=HCHO+C2H6	2.4E13	0.	0.	!(141, -
141)<TSAnG86>!				
R7CH3O+C2H6=R11C2H5+CH3OH	2.4E11	0.	7.0E3	!(142, -
142)<TSAnG86>!				
R7CH3O+B10=HCHO+R20H	1.8E12	0.	0.	!(143, -
143)<BAULCH94>!				
R7CH3O+R20H=HCHO+H2O	1.8E13	0.	0.	!(144, -
144)<TSAnG86>!				
R7CH3O+B2CO=R4CH3+CO2	1.6E13	0.	11.7E3	!(145, -
145)<TSAnG86>!				
R7CH3O+R5CHO=CH3OH+B2CO	9.1E13	0.	0.	!(146, -
146)<TSAnG86>!				
R7CH3O+HCHO=CH3OH+R5CHO	1.0E11	0.	3.0E3	!(147, -
147)<TSAnG86>!				
R7CH3O+R7CH3O=CH3OH+HCHO	6.0E13	0.	0.	!(148, -
148)<TSAnG86>!				

!\*\*\*\*\* REACTIONS DE R6CH2OH \*\*\*\*\*!

R6CH2OH+M=HCHO+R1H+M	1.26E16	0.00	30.0E3	!(149, -
149)<BAULCHLEEDS>!				
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
!	N2/0.4/ HE/0.35/			
R6CH2OH+R1H=R4CH3+R20H	9.6E13	0.	0.	!(150, -
150)<TSAnG87>!				
R6CH2OH+R1H=HCHO+H2	6.0E12	0.	0.	!(151, -
151)<TSAnG87>!				
R6CH2OH+H2=CH3OH+R1H	6.7E5	2.	13.4E3	!(152, -
152)<TSAnG87>!				

R6CH2OH+B6CH2=CH3CHO+R1H	1.8E13	0.	0.	!(153, -
153)<TSAnG87>!				
R6CH2OH+B5CH2=C2H4Z+R2OH	2.4E13	0.	0.	!(154, -
154)<TSAnG87>!				
R6CH2OH+B5CH2=R4CH3+HCHO	1.2E12	0.	0.	!(155, -
155)<TSAnG87>!				
R6CH2OH+R4CH3=C2H5OH	1.2E13	0.	0.	!(156, -
156)<TSAnG87>!				
R6CH2OH+R4CH3=CH4+HCHO	2.4E12	0.	0.	!(157, -
157)<TSAnG87>!				
R6CH2OH+CH4=CH3OH+R4CH3	21.7	3.1	16.2E3	!(158, -
158)<TSAnG87>!				
R6CH2OH+R9C2H=C2H2+HCHO	4.8E13	0.	0.	!(159, -
159)<TSAnG87>!				
!la constante de vitesse du processus 159 est globalisee!				
!R6CH2OH+R9C2H=C3H3+R2OH	1.2E13	0.	0.	!(159a, -
159a)<TSAnG87>!				
!R6CH2OH+R9C2H=C2H2+HCHO	3.6E13	0.	0.	!(159b, -
159b)<TSAnG87>!				
R6CH2OH+C2H2=R10C2H3V+HCHO	7.2E11	0.	9.0E3	!(160, -
160)<TSAnG87>!				
R6CH2OH+R10C2H3V=C2H4Z+HCHO	4.2E13	0.	0.	!(161, -
161)<TSAnG87>!				
!La constante de vitesse du processus 161 est globalisee!				
R6CH2OH+R11C2H5=C2H4Z+CH3OH	2.4E12	0.	0.	!(162, -
162)<TSAnG87>!				
R6CH2OH+R11C2H5=C2H6+HCHO	2.4E12	0.	0.	!(163, -
163)<TSAnG87>!				
R6CH2OH+C2H6=CH3OH+R11C2H5	199.	3.	14.0E3	!(164, -
164)<TSAnG87>!				
R6CH2OH+B10=HCHO+R2OH	4.2E13	0.	0.	!(165, -
165)<TSAnG87>!				
R6CH2OH+R2OH=H2O+HCHO	2.4E13	0.	0.	!(166, -
166)<TSAnG87>!				
!attention (167) metatheses dans les reactions de CH3OH!				
!R6CH2OH+H2O=CH3OH+R2OH	1.6E14	0.	26.3E3	!(167, -
167)<TSUB0I81nIST>!				
R6CH2OH+R5CHO=CH3OH+B2CO	1.2E14	0.	0.	!(168, -
168)<TSAnG87>!				
R6CH2OH+R5CHO=HCHO+HCHO	1.8E14	0.	0.	!(169, -
169)<TSAnG87>!				
R6CH2OH+HCHO=CH3OH+R5CHO	5.5E3	2.8	5.9E3	!(170, -
170)<TSAnG87>!				
R6CH2OH+R7CH3O=CH3OH+HCHO	2.4E13	0.	0.	!(171, -
171)<TSAnG87>!				
R6CH2OH+R6CH2OH=CH3OH+HCHO	1.4E13	0.	0.	!(172, -
172)<TSAnG87>!				
!la constante de vitesse du processus 172 est globalisee!				
!R6CH2OH+R6CH2OH=CH3OH+HCHO	4.8E12	0.	0.	!(172a, -
172a)<TSAnG87>!				
!R6CH2OH+R6CH2OH=HOCH2CH2OH	9.6E12	0.	0.	!(172b, -
172b)<TSAnG87>!				

!\*\*\*\*\* REACTIONS DE CH3OH \*\*\*\*\*!

CH3OH+R1H=R4CH3+H2O 173)<HIDAKA89nIST>!	2.0E14	0.	5.3E3	!(173, -
CH3OH+R1H=R7CH3O+H2 174)<TSAnG87>!	4.2E6	2.1	4.9E3	!(174, -
CH3OH+B6CH2=R6CH2OH+R4CH3 175)<TSAnG87>!	1.5E12	0.	0.	!(175, -
CH3OH+B5CH2=R4CH3+R6CH2OH 176)<TSAnG87>!	31.9	3.2	7.2E3	!(176, -
CH3OH+B5CH2=R4CH3+R7CH3O 177)<TSAnG87>!	14.4	3.1	6.9E3	!(177, -
CH3OH+R9C2H=C2H2+R6CH2OH 178)<TSAnG87>!	6.0E12	0.	0.	!(178, -
CH3OH+R9C2H=C2H2+R7CH3O 179)<TSAnG87>!	1.2E12	0.	0.	!(179, -
CH3OH+R10C2H3V=C2H4Z+R6CH2OH 180)<TSAnG87>!	31.9	3.2	7.2E3	!(180, -
CH3OH+R10C2H3V=C2H4Z+R7CH3O 181)<TSAnG87>!	14.4	3.1	6.9E3	!(181, -
CH3OH+B10=R6CH2OH+R2OH 182)<GROTHEER81nIST>!	3.4E13	0.	5.5E3	!(182, -
CH3OH+B10=R7CH3O+R2OH 183)<WARnATZ84>!	1.0E13	0.	4.7E3	!(183, -
!modification des metatheses avec OH!				
!CH3OH+R2OH=R7CH3O+H2O 184)<WARnATZ84>!	1.0E13	0.	1.7E3	!(184, -
CH3OH+R2OH=R6CH2OH+H2O 184a)<Atkinson86>85%!	3.1E06	2.	-3.4E2	!(184a, -
CH3OH+R2OH=R7CH3O+H2O 184b)<Atkinson86>15%!	5.4E05	2.	-3.4E2	!(184b, -
CH3OH+R7CH3O=CH3OH+R6CH2OH 185)<TSAnG87>!	3.0E11	0.	4.1E3	!(185, -

!\*\*\*\*\* REACTIONS DE R12CHCOD \*\*\*\*\*!

R12CHCOZ+M=B4CH+B2CO+M 186)<DAGAUT91>!	6.0E15	0.	58.8E3	!(186, -
R12CHCOZ+R1H=B5CH2+B2CO 187a)<BAULCH94>!	1.5E14	0.	0.	!(187a, -
R12CHCOZ+R1H=B6CH2+B2CO 187b)<PEETERS97>!	1.3E14	0.	0.	!(187b, -
R12CHCOZ+B5CH2=R9C2H+HCHO 188)<DAGAUT91>!	1.0E13	0.	2.0E3	!(188, -
R12CHCOZ+B5CH2=R10C2H3V+B2CO 189)<DAGAUT91>!	3.0E13	0.	0.	!(189, -
R12CHCOZ+B10=>B2CO+B2CO+R1H (190)<BAULCH94>!	9.6E13	0.	0.	!
R12CHCOZ+R2OH=>R5CHO+B2CO+R1H (191)<DAGAUT91>!	1.0E13	0.	0.	!

!\*\*\*\*\* REACTIONS DE CH2COD \*\*\*\*\*!

CH2COZ+M=B6CH2+B2CO+M 192)<FRAnK86nIST>!	6.57E15	0.0	57.6E3	!(192, -
! 02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ N2/0.4/ HE/0.35/				

CH2COZ+M=R12CHCOZ+R1H+M 193)<FRAnK86nIST>! 02/0.4/ B2CO/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/ ! N2/0.4/ HE/0.35/	2.7E17	0.	87.0E3	!(193, -
CH2COZ+R1H=R4CH3+B2CO 194)<BAULCH94>!	1.8E13	0.	3.4E3	!(194, -
CH2COZ+R1H=R12CHCOZ+H2 195)<DAGAUT91>!	5.0E13	0.	8.0E3	!(195, -
CH2COZ+B5CH2=C2H4Z+B2CO 196)<CAn0SA-MAS84nIST>!	1.3E14	0.	0.	!(196, -
CH2COZ+B10=B5CH2+C02 197)<DAGAUT91>!	1.8E12	0.	1.3E3	!(197, -
CH2COZ+B10=R12CHCOZ+R20H 198)<DAGAUT91>!	1.0E13	0.	8.0E3	!(198, -
CH2COZ+R20H=R12CHCOZ+H20 199)<DAGAUT91>!	7.5E12	0.	2.0E3	!(199, -
!CH2COZ+R20H=R5CHO+HCHO 200)<VAnD00REn77nIST>!	2.8E13	0.	0.	!(200, -
CH2COZ+R20H=R4CH3+C02 200a)<BAULCH LEEDS>!	2.52E12	0.	0.	!(200a, -
CH2COZ+R20H=R6CH20H+B2CO 200b)<BAULCH LEEDS>!	4.68E12	0.	0.	!(200b, -

!\*\*\*\*\* REACTIONS DE R14CH3CO \*\*\*\*\*!

R14CH3CO+R1H=R4CH3+R5CHO 201)<TSAnG86>!	9.6E13	0.	0.	!(201, -
R14CH3CO+B6CH2=R4CH3+CH2COZ 202)<TSAnG86>!	1.8E13	0.	0.	!(202, -
R14CH3CO+B5CH2=R4CH3+CH2COZ 203)<TSAnG86>!	1.8E13	0.	0.	!(203, -
R14CH3CO+B10=R4CH3+C02 204)<TSAnG86>!	9.6E12	0.	0.	!(204, -
R14CH3CO+R20H=CH2COZ+H20 205)<TSAnG86>!	1.2E13	0.	0.	!(205, -
R14CH3CO+R20H=>R4CH3+B2CO+R20H (206)<TSAnG86>!	3.0E13	0.	0.	!
R14CH3CO+R5CHO=CH3CHO+B2CO 207)<TSAnG86>!	9.0E12	0.	0.	!(207, -
R14CH3CO+HCHO=CH3CHO+R5CHO 208)<TSAnG86>!	1.8E11	0.	12.9E3	!(208, -
R14CH3CO+R7CH30=CH30H+CH2COZ 209)<TSAnG86>!	6.0E12	0.	0.	!(209, -
R14CH3CO+R7CH30=HCHO+CH3CHO 210)<TSAnG86>!	6.0E12	0.	0.	!(210, -
R14CH3CO+CH30H=CH3CHO+R6CH20H 211)<TSAnG87>!	4.85E3	3.	12.3E3	!(211, -
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 212)<TSAnG86>!	1.2E13	0.	0.	!(212, -

!\*\*\*\*\* REACTIONS DE R13CH2CHO \*\*\*\*\*!

!R13CH2CHO=R14CH3CO (213, -213)<COLKET75nIST>!	1.0E13	0.	47.0E3	!
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!R13CH2CHO=R1H+CH2COZ	1.6E13	0.	35.0E3	!
(214, -214)<COLKET75nIST>!				
R13CH2CHO=R4CH3+B2CO	2.93E12	0.29	40.3E3	!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.				
R13CH2CHO=R1H+CH2COZ	1.43E15	-0.15	45.6E3	!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.				

!\*\*\*\*\* REACTIONS DE CH3CHO \*\*\*\*\*!

!CH3CHO+R1H=H2+R14CH3CO	4.0E13	0.	4.2E3	!
(215, -215)<WARnATZ84>!				
!CH3CHO+R4CH3=R14CH3CO+CH4	2.0E-6	5.6	2.5E3	!
(216, -216)<BAULCH94>!				
!CH3CHO+R10C2H3V=C2H4Z+R14CH3CO	8.1E10	0.	3.7E3	!
(217, -217)<SCHERZER87>!				
!CH3CHO+R11C2H5=C2H6+R14CH3CO	1.3E12	0.	8.5E3	!
(218, -218)<HOHLEIn70>!				
!CH3CHO+B10=R14CH3CO+R2OH	1.4E13	0.	2.3E3	!
(219, -219)<CAVAnAGH90>!				
!CH3CHO+R2OH=R14CH3CO+H2O	4.2E12	0.	0.5E3	!
(220, -220)<CAVAnAGH90>!				
!CH3CHO+R7CH3O=R14CH3CO+CH3OH	2.4E11	0.	1.8E3	!
(221, -221)<CAVAnAGH90>!				
!CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO	2.5E7	0.	0.	!
(222, -222)<SCHUCHMann70nIST>!				

!\*\*\*\*\* REACTIONS DE C2H4O# \*\*\*\*\*!

C2H4O#3=CH4+B2CO	1.2E13	0.	57.2E3	!(223, -
223)<LIFSHITZ83nIST>!				
C2H4O#3=CH3CHO	7.3E13	0.	57.2E3	!(224, -
224)<LIFSHITZ83nIST>!				
C2H4O#3=R4CH3+R5CHO	3.6E13	0.	57.2E3	!(225, -
225)<LIFSHITZ83nIST>!				
C2H4O#3+R1H=H2+R13CH2CHO	2.0E13	0.	8.3E3	!(226, -
226)<LIFSHITZ83nIST*>!				
C2H4O#3+R1H=H2O+R10C2H3V	5.0E9	0.	5.0E3	!(227, -
227)<LIFSHITZ83nIST>!				
C2H4O#3+R1H=C2H4Z+R2OH	9.5E10	0.	5.0E3	!(228, -
228)<LIFSHITZ83nIST>!				
C2H4O#3+R4CH3=CH4+R13CH2CHO	1.1E12	0.	11.8E3	!(229, -
229)<BALDWIn84nIST*>!				
C2H4O#3+R4CH3=R11C2H5+HCHO	1.4E11	0.	7.6E3	!(230, -
230)<RAnZI94>!				
C2H4O#3+R4CH3=C2H4Z+R7CH3O	1.5E10	0.	7.6E3	!(231, -
231)<RAnZI94>!				
C2H4O#3+R9C2H=C2H2+R13CH2CHO	1.2E12	0.	9.8E3	!(232, -
232)<RAnZI94>!				
C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO	2.0E12	0.	9.3E3	!(233, -
233)<RAnZI94>!				
C2H4O#3+R11C2H5=C2H6+R13CH2CHO	6.8E11	0.	11.4E3	!(234, -
234)<RAnZI94>!				
C2H4O#3+B10=R2OH+R13CH2CHO	1.9E12	0.	5.2E3	!(235, -
235)<BOGAn78nIST>!				

C2H40#3+R20H=H2O+R13CH2CHO	1.8E13	0.	3.6E3	!(236, -
236)<BALDWIn84nIST*>!				
C2H40#3+R5CHO=HCHO+R13CH2CHO	3.7E12	0.	15.8E3	!(237, -
237)<RAnZI94>!				
C2H40#3+R7CH3O=CH3OH+R13CH2CHO	1.3E12	0.	5.8E3	!(238, -
238)<RAnZI94>!				
C2H40#3+R6CH2OH=CH3OH+R13CH2CHO	8.4E11	0.	13.4E3	!(239, -
239)<RAnZI94>!				
C2H40#3+R14CH3CO=CH3CHO+R13CH2CHO	4.0E12	0.	17.5E3	!(240, -
240)<RAnZI94>!				
C2H40#3+R13CH2CHO=CH3CHO+R13CH2CHO	6.8E11	0.	15.4E3	!(241, -
241)<RAnZI94>!				

!\* assuming that C2H3O decompose rapidly to R13CH2CHO!

!\*\*\*\*\* REACTIONS DE R15C2H5O \*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C2H5OH \*\*\*\*\*!

!Voir Plus bas meca 10a Luc Sy Tran

!\*\*\*\*\* REACTIONS DE O2 \*\*\*\*\*!

B10+B10+M=O2+M	5.40E13	0.	-1.79E3	!(244, -
244)<BAULCH94>!				
O2/0.4/ B2CO/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
!    N2/0.4/ HE/0.35/				
O2+R1H=R20H+B10	9.8E13	0.	14.8E3	!(245, -
245)<BAULCH94>!				
!O2+R1H+M=R300H+M	2.10E18	-0.8	0.00	!(246, -
246)<baseLeeds>!				
!    O2/0.4/ B2CO/0.75/ C02/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/				
!    N2/0.4/ HE/0.35/				
!O2+R1H+H2O=R300H+H2O	6.90E15	0.0	-2.10E3	!(246, -
246bis)<base Leeds>!				
O2+R1H(+M)=R300H(+M)	4.52E13	0.	0.	!(246, -
246)<COBOS85>!				
LOW /1.8E18	-0.8	0.00/		!k0
BAULCH94!				
TROE /0.5	1.0	1.0E8/		
O2/0.4/ B2CO/0.75/ C02/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/				
!    N2/0.4/ HE/0.35/				
!O2+R1H(+H2O)=R300H(+H2O)	1.63E14	0.	761.	!(246b, -
246b)<COBOS85>!				
O2+R1H(+H2O)=R300H(+H2O)	4.52E13	0.	0.	!(246b, -
246b)<BAULCH94>!				
LOW /6.9E15	0.0	-2080/		
TROE /0.45	1.0	1.0E8/		
O2+B3C=B2CO+B10	1.2E14	0.	0.	!(247, -
247)<RAnZI94>!				
O2+B4CH=R5CHO+B10	3.3E13	0.	0.	!(248, -
248)<DAGAUT91>!				
O2+B4CH=B2CO+R20H	3.2E13	0.	0.	!(249, -
249)<PEETERS97>!				

02+B6CH2=>B2CO+R20H+R1H (250)<BAULCH94>!	3.1E12	0.	0.	!
02+B5CH2=R5CHO+R20H 251)<DAGAUT91>!	4.3E10	0.	-0.5E3	!(251, -
02+B5CH2=C02+H2 252)<DAGAUT91>!	6.9E11	0.	0.5E3	!(252, -
02+B5CH2=>C02+R1H+R1H (253)<DAGAUT91>!	1.6E12	0.	1.0E3	!
02+B5CH2=B2CO+H2O 254)<DAGAUT91>!	1.9E10	0.	-1.0E3	!(254, -
02+B5CH2=>B2CO+R20H+R1H (255)<DAGAUT91>!	8.6E10	0.	-0.5E3	!
02+B5CH2=HCHO+B10 256)<DAGAUT91>!	1.0E14	0.	4.5E3	!(256, -
02+R4CH3(+M)=R8CH300(+M) 257)<BAULCH94>!	7.8E8	1.2	0.	!(257, -
	LOW /5.6E25	-3.3	0./	
	TROE /0.36	1.0	1.0E8/	
02+R4CH3=R7CH30+B10 258)<BAULCH94>!	1.3E14	0.	31.3E3	!(258, -
!02+R4CH3=R7CH30+B10 258)<HWAnG&RABInOVITCH99>!	1.6E13	0.	31.4E3	!(258, -
02+R4CH3=HCHO+R20H 259)<DAGAUT91>!	3.0E30	-4.69	36.6E3	!(259, -
02+CH4=R4CH3+R300H 260)<BAULCH94>!	4.0E13	0.	56.7E3	!(260, -
02+R9C2H=B2CO+R5CHO 261)<TIESEMA97/TSAnG86>!	3.8E13	-0.16	0.	!(261, -
02+R9C2H=R12CHCOZ+B10 262)<TIESEMA97/TSAnG86>!	9.0E12	-0.16	0.	!(262, -
02+C2H2=R9C2H+R300H 263)<TSAnG86>!	1.2E13	0.	74.5E3	!(263, -
!02+C2H2=R12CHCOZ+R20H 264)<DAGAUT91>!	2.0E8	1.5	30.1E3	!(264, -
02+C2H2=R5CHO+R5CHO 264)<BEnS0n95>!	7.0E7	1.8	30.6E3	!(264, -
!02+R10C2H3V=C2H2+R300H 265)<TSAnG86>!	1.2E11	0.	0.	!(265, -
!02+R10C2H3V=C2H2+R300H 265)<WAnG97>! !at 760 Torr	1.6E14	-0.83	2.5E3	!(265, -
!02+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	8.6E21	-2.97	3.3E3	!(266a, -
!02+R10C2H3V=B10+R13CH2CHO 266b)<WAnG97>! !at 20-90 Torr	1.2E13	-0.12	1.7E3	!(266b, -
!02+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	1.6E21	-2.78	2.5E3	!(266a, -
!02+R10C2H3V=B10+R13CH2CHO 266b)<WAnG97>!	2.5E12	0.057	0.9E3	!(266b, -



02+R10C2H3V=C2H2+R300H 265)<MEBEL nIST>!	1.34E6	1.61	-0.4E3	!(265, -
02+R10C2H3V=HCHO+R5CHO 266a)<MEBEL nIST>!	4.5E16	-1.39	1.0E3	!(266a, -
02+R10C2H3V=B10+R13CH2CHO 266b)<MEBEL nIST>!	3.3E11	-0.29	10.	!(266b, -
02+C2H4Z=R10C2H3V+R300H 267)<TSAnG86>!	4.2E13	0.	57.4E3	!(267, -
02+R11C2H5=R17C2H500 268)<WAGnER90>!	2.2E10	0.77	-0.6E3	!(268, -
02+R11C2H5=C2H4Z+R300H 269)<TSAnG86>!	8.4E11	0.	3.9E3	!(269, -
02+R11C2H5=R15C2H50+B10 270)<BOZZELLI90nIST>!	1.2E13	-0.2	27.9E3	!(270, -
02+R11C2H5=CH3CHO+R20H 271)<TSAnG86>!	6.0E10	0.	6.9E3	!(271, -
02+C2H6=R11C2H5+R300H 272)<BAULCH94>!	6.0E13	0.	51.7E3	!(272, -
02+R20H=R300H+B10 273)<TSAnG86>!	2.2E13	0.	52.5E3	!(273, -
02+B2CO=C02+B10 274)<TSAnG86>!	2.5E12	0.	47.7E3	!(274, -
!02+R5CHO=B2CO+R300H 275)<TSAnG86>!	5.1E13	0.	1.7E3	!(275, -
02+R5CHO=B2CO+R300H 275)<TIM0nEn88>!	7.6E12	0.	0.41E3	!(275, -
02+HCHO=R5CHO+R300H 276)<TSAnG86>!	2.0E13	0.	38.8E3	!(276, -
02+R7CH30=HCHO+R300H 277)<BAULCH94>!	2.2E10	0.	1.7E3	!(277, -
02+R6CH20H=HCHO+R300H 278)<TSAnG87>!	1.2E12	0.	0.	!(278, -
02+CH30H=R6CH20H+R300H 279)<TSAnG87>!	2.0E13	0.	44.9E3	!(279, -
02+R12CHCOZ=>B2CO+B2CO+R20H <DAGAUT91>!	1.5E12	0.	2.5E3	!(280)
!02+CH2COZ=HCHO+C02 281)<DAGAUT91>!bizarre	1.0E8	0.	0.	!(281, -
02+R14CH3CO=R18CH3C000 282)<COX90>!	2.4E12	0.	0.	!(282, -
02+R13CH2CHO=>HCHO+R20H+B2CO <COX90>!	5.9E9	0.	-1.4E3	!(283)
02+R13CH2CHO=CH2COZ+R300H 284)<COX90>!	1.0E10	0.	-1.4E3	!(284, -
02+CH3CHO=R14CH3CO+R300H 285)<COX90>!	5.0E13	0.	36.4E3	!(285, -
! ajout demande par Laetitia le 25 Avril 95				
02+CH3CHO=R13CH2CHO+R300H 285)<Ranzi94>!	1.0E13	0.5	46.0E3	!(285', -
02+C2H40#3=R300H+R13CH2CHO 286)<RAnZI94>!	5.0E13	0.	48.0E3	!(286, -
!02+R15C2H50=CH3CHO+R300H 287)<BAULCH94>!	6.0E10	0.	1.7E3	!(287, -

!\*\*\*\*\* REACTIONS DE R300H \*\*\*\*\*!

R300H+R1H=H2+O2 288)<BAULCH94>!	4.3E13	0.	1.4E3	!(288, -
R300H+R1H=2R2OH 289)<BAULCH94>!	1.7E14	0.	0.9E3	!(289, -
R300H+R1H=H2O+B10 290)<BAULCH94>!	3.0E13	0.	1.7E3	!(290, -
R300H+B6CH2=HCHO+R2OH 291)<TSAnG86>!	3.0E13	0.	0.	!(291, -
R300H+B5CH2=HCHO+R2OH 292)<TSAnG86>!	1.8E13	0.	0.	!(292, -
R300H+R4CH3=R7CH30+R2OH 293)<BAULCH94>!	1.8E13	0.	0.	!(293, -
!R300H+R4CH3=R7CH30+R2OH 293)<DAGAUT>	4.0E13	0.	5.0E3	!(293, -
R300H+CH4=R4CH3+H2O2 294)<BAULCH94>!	9.0E12	0.	24.6E3	!(294, -
R300H+R9C2H=R12CHCOZ+R2OH 295)<TSAnG86>!	1.8E13	0.	0.	!(295, -
R300H+C2H2=CH2COZ+R2OH 296)<TSAnG86>!	6.0E9	0.	8.0E3	!(296, -
!incertitude au moins un facteur 10				
R300H+R10C2H3V=>R2OH+R4CH3+B2CO <TSAnG86>!	3.0E13	0.	0.	!(297)
R300H+C2H4Z=CH3CHO+R2OH 298)<TSAnG86>!	6.0E9	0.	7.9E3	!(298, -
R300H+C2H4Z=C2H4O#3+R2OH 299)<BAULCH94>!	2.2E12	0.	17.2E3	!(299, -
R300H+R11C2H5=>R4CH3+HCHO+R2OH <TSAnG86>!	2.4E13	0.	0.	!(300)
R300H+R11C2H5=C2H4Z+H2O2 301)<TSAnG86>!	3.0E11	0.	0.	!(301, -
R300H+C2H6=R11C2H5+H2O2 302)<BAULCH94>!	1.3E13	0.	20.4E3	!(302, -
R300H+R2OH=H2O+O2 303)<BAULCH94>!	2.9E13	0.	-0.5E3	!(303, -
R300H+B2CO=C02+R2OH Phys. Chem. A 111(2007)4031 - 4042	1.57E05	2.18	17.9E3	!MF Wang, J.
R300H+R5CHO=>R2OH+R1H+C02 <TSAnG86>!	3.0E13	0.	0.	!(305)
R300H+HCHO=R5CHO+H2O2 306)<BAULCH94>!	3.0E12	0.	13.0E3	!(306, -
R300H+R7CH30=HCHO+H2O2 307)<TSAnG86>!	3.0E11	0.	0.	!(307, -
R300H+R6CH2OH=HCHO+H2O2 308)<TSAnG87>!	1.2E13	0.	0.	!(308, -
R300H+CH3OH=R6CH2OH+H2O2 309)<TSAnG87>!	9.6E10	0.	12.6E3	!(309, -
R300H+R14CH3CO=>R4CH3+C02+R2OH (310)<TSAnG86>!	3.0E13	0.	0.	!
R300H+CH3CHO=R14CH3CO+H2O2 311)<CAVANAGH90>!	1.0E12	0.	10.0E3	!(311, -

R300H+C2H4O#3=H2O2+R13CH2CHO 1.6E12 0. 15.0E3 !(312, -  
 312)<RAnZI94>  
 R300H+R300H=H2O2+O2 1.3E11 0. -1.63E3 !(313, -  
 313)<BAULCH 94>!  
 DUPLICATE  
 R300H+R300H=H2O2+O2 4.2E14 0. 11.98E3 !(313, -  
 313)<BAULCH 94>!  
 DUPLICATE

!\*\*\*\*\* REACTIONS DE H2O2 !\*\*\*\*\*!

!R20H+R20H(+ M)=>H2O2 (+ M) 7.23E13 -0.37 0.00  
 ! 02/0.4/ B2C0/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 !! N2/0.4/ HE/0.35/  
 ! LOW /5.53E19 -0.76 0.00 /  
 ! TROE /0.5 1 1.E8/  
 !H2O2(+M)=>R20H+R20H(+M) 3.00E14 0.00 48.5E3  
 ! 02/0.4/ B2C0/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 !! N2/0.4/ HE/0.35/  
 ! LOW /3.0E17 0.0 45.5E3/  
 ! TROE /0.5 1 1.E8/

! MF Troe, Comb.Flam. 158(2011)594-601

H2O2(+M)=R20H+R20H(+M) 1.99E12 0.9 4.8749E4 !<BAULCH94>!  
 AR/0.68/ 02/0.79/ N2/1.00/ C02/1.06/ H2O/5.1/ H2O2/5.2/  
 LOW /3.65e24 -2.3 4.8749E4/  
 TROE /0.43 1 1.E8/

H2O2+R1H=H2+R300H 1.7E12 0. 3.7E3 !(315, -  
 315)<BAULCH94>!  
 H2O2+R1H=H2O+R20H 1.0E13 0. 3.6E3 !(316, -  
 316)<BAULCH94>!  
 H2O2+B6CH2=R7CH30+R20H 3.0E13 0. 0. !(317, -  
 317)<TSAnG86>!  
 H2O2+R10C2H3V=C2H4Z+R300H 1.2E10 0. -0.6E3 !(318, -  
 318)<TSAnG86>!  
 H2O2+B10=R20H+R300H 6.6E11 0. 4.0E3 !(319, -  
 319)<BAULCH94>!  
 H2O2+R20H=H2O+R300H 7.8E12 0. 1.3E3 !(320, -  
 320)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE CO2 !\*\*\*\*\*!

CO2+B5CH2=HCHO+B2C0 2.3E10 0. 0. !(321, -  
 321)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE R8CH300 !\*\*\*\*\*!

R8CH300=HCHO+R20H 1.5E13 0. 47.0E3 !(322, -  
 322)<RAnZI94>!  
 R8CH300+R1H=R7CH30+R20H 9.6E13 0. 0. !(323, -  
 323)<TSAnG86>!  
 R8CH300+H2=CH300H+R1H 3.0E13 0. 26.0E3 !(324, -  
 324)<TSAnG86>!  
 R8CH300+B6CH2=HCHO+R7CH30 1.8E13 0. 0. !(325, -  
 325)<TSAnG86>!

R8CH300+B5CH2=HCHO+R7CH30 326)<TSAnG86>!	1.8E13	0.	0. ! (326, -
R8CH300+R4CH3=R7CH30+R7CH30 327)<CAVAnAGH90>!	5.0E12	0.	-1.4E3 ! (327, -
R8CH300+CH4=CH300H+R4CH3 328)<TSAnG86>!	1.8E11	0.	18.5E3 ! (328, -
R8CH300+R9C2H=R7CH30+R12CHCOZ 329)<TSAnG86>!	2.4E13	0.	0. ! (329, -
!R8CH300+C2H2=CH300H+R9C2H 330)<RAnZI94>! MF car i<<0	5.6E11	0.	24.5E3 ! (330, -
R8CH300+R10C2H3V=R7CH30+R13CH2CHO 331)<TSAnG86*>!	2.4E13	0.	0. ! (331, -
!* assuming that C2H30 decompose rapidly to R13CH2CHO!			
R8CH300+C2H4Z=R7CH30+C2H40#3 332)<nIKISHA81/MOSHKInA80nIST>!	1.1E15	0.	20.0E3 ! (332, -
R8CH300+C2H4Z=CH300H+R10C2H3V 333)<RAnZI94>!	3.9E12	0.	24.5E3 ! (333, -
R8CH300+R11C2H5=R7CH30+R15C2H50 334)<TSAnG86>!	2.4E13	0.	0. ! (334, -
R8CH300+C2H6=CH300H+R11C2H5 335)<TSAnG86>!	2.9E11	0.	14.9E3 ! (335, -
R8CH300+B10=R7CH30+O2 336)<TSAnG86>!	3.6E13	0.	0. ! (336, -
R8CH300+R20H=CH30H+O2 337)<TSAnG86>!	6.0E13	0.	0. ! (337, -
R8CH300+R20H=R7CH30+R300H 338)<RAnZI94>!	3.0E12	0.	0. ! (338, -
R8CH300+B2CO=R7CH30+CO2 339)<RAnZI94>!	1.0E14	0.	24.0E3 ! (339, -
R8CH300+R5CHO=>R7CH30+R1H+CO2 <TSAnG86>!	3.0E13	0.	0. ! (340)
R8CH300+HCHO=CH300H+R5CHO 341)<CAVAnAGH90>!	1.0E12	0.	12.1E3 ! (341, -
R8CH300+R7CH30=HCHO+CH300H 342)<TSAnG86>!	3.0E11	0.	0. ! (342, -
R8CH300+R6CH20H=>R7CH30+R20H+HCHO (343)<TSAnG87>!	1.2E13	0.	0. !
R8CH300+CH30H=CH300H+R6CH20H 344)<TSAnG87>!	1.8E12	0.	13.7E3 ! (344, -
R8CH300+CH30H=CH300H+R7CH30 345)<RAnZI94>!	2.8E11	0.	18.8E3 ! (345, -
R8CH300+CH2COZ=CH300H+R12CHCOZ 346)<RAnZI94>!	1.7E12	0.	27.0E3 ! (346, -
R8CH300+R14CH3CO=R4CH3+CO2+R7CH30 347)<TSAnG86>!	2.4E13	0.	0. ! (347, -
R8CH300+CH3CHO=CH300H+R14CH3CO 348)<CAVAnAGH90>!	1.0E12	0.	12.1E3 ! (348, -
R8CH300+CH3CHO=CH300H+R13CH2CHO 349)<RAnZI94>!	1.7E12	0.	19.2E3 ! (349, -
R8CH300+C2H40#3=CH300H+R13CH2CHO 350)<RAnZI94>!	2.2E12	0.	16.0E3 ! (350, -
R8CH300+R300H=CH300H+O2 351)<BAULCH94>!	2.5E11	0.	-1.6E3 ! (351, -

R8CH300+R300H=>O2+HCHO+H2O (352)<RAnZI94>!	5.0E10	0.	0. !
R8CH300+H2O2=CH300H+R300H 353)<TSAnG86>!	2.4E12	0.	9.9E3 !(353, -
R8CH300+R8CH300=CH30H+HCHO+O2 354)<BAULCH94>!	2.5E10	0.	-0.8E3 !(354, -
R8CH300+R8CH300=R7CH30+R7CH30+O2 355)<BAULCH94>!	2.5E10	0.	-0.8E3 !(355, -

!\*\*\*\*\* REACTIOns DE CH300H \*\*\*\*\*!

CH300H=R7CH30+R20H 356)<BAULCH94>!	6.0E14	0.	42.3E3 !(356, -
CH300H+B10=R8CH300+R20H 357)<BAULCH94average>!	2.0E13	0.	4.8E3 !(357, -
CH300H+R20H=H2O+R8CH300 358)<BAULCH94average>!	1.8E12	0.	-0.37E3 !(358, -
CH300H+R7CH30=>CH30H+R20H+HCHO (359)<RAnZI94>!	1.5E11	0.	6.5E3 !

!\*\*\*\*\* REACTIOns DE R17C2H500 \*\*\*\*\*!

R17C2H500=R16C2H400H 360)<HUGHES93>!	4.2E12	0.	36.9E3 !(360, -
R17C2H500+H2=C2H500H+R1H 361)<RAnZI94>!	7.9E12	0.	21.0E3 !(361, -
R17C2H500+R4CH3=R15C2H50+R7CH30 362)<RAnZI94>!	2.0E12	0.	-1.2E3 !(362, -
R17C2H500+CH4=C2H500H+R4CH3 363)<RAnZI94>!	3.9E12	0.	24.0E3 !(363, -
R17C2H500+C2H2=C2H500H+R9C2H 364)<RAnZI94>!	5.6E11	0.	24.4E3 !(364, -
R17C2H500+C2H4Z=C2H500H+R10C2H3V 365)<RAnZI94>!	3.9E12	0.	24.4E3 !(365, -
R17C2H500+C2H4Z=R15C2H50+C2H40#3 366)<MOSHKInA80nIST>!	2.3E16	0.	21.9E3 !(366, -
R17C2H500+C2H6=C2H500H+R11C2H5 367)<RAnZI94>!	5.1E12	0.	19.5E3 !(367, -
R17C2H500+H2O=C2H500H+R20H 368)<RAnZI94>!	5.6E12	0.	30.6E3 !(368, -
R17C2H500+B2C0=C02+R15C2H50 369)<RAnZI94>!	1.0E14	0.	24.0E3 !(369, -
R17C2H500+HCHO=C2H500H+R5CHO 370)<RAnZI94>!	4.5E12	0.	14.4E3 !(370, -
R17C2H500+CH30H=C2H500H+R7CH30 371)<RAnZI94>!	2.8E11	0.	18.4E3 !(371, -
R17C2H500+CH30H=C2H500H+R6CH20H 372)<RAnZI94>!	2.8E12	0.	19.5E3 !(372, -
R17C2H500+CH2C0Z=C2H500H+R12CHC0Z 373)<RAnZI94>!	1.7E12	0.	24.4E3 !(373, -
R17C2H500+CH3CHO=C2H500H+R14CH3C0 374)<RAnZI94>!	3.9E12	0.	14.4E3 !(374, -
R17C2H500+CH3CHO=C2H500H+R13CH2CHO 375)<RAnZI94>!	1.7E12	0.	19.5E3 !(375, -
R17C2H500+C2H40#3=C2H500H+R13CH2CHO 376)<RAnZI94>!	2.2E12	0.	16.3E3 !(376, -

R17C2H500+R300H=O2+C2H500H 3.9E11 0. -1.3E3 !(377, -  
 377)<BAULCH89>!  
 !Rate constant measured between 240 and 380K!  
 R17C2H500+H2O2=C2H500H+R300H 4.5E11 0. 10.8E3 !(378, -  
 378)<RAnZI94>!  
 R17C2H500+R8CH300=>R15C2H50+R7CH30+O2 2.0E11 0. 0. !  
 (379)<RAnZI94>!  
 R17C2H500+CH300H=C2H500H+R8CH300 1.1E12 0. 16.3E3 !(380, -  
 380)<RAnZI94>!  
 R17C2H500+R17C2H500=2R15C2H50+O2 4.1E10 0. 0.2E3 !(381, -  
 381)<LIGHTFOOT92>!  
 R17C2H500+R17C2H500=C2H50H+CH3CHO+O2 1.8E10 0. 0.2E3 !(382, -  
 382)<LIGHTFOOT92>!

!\*\*\*\*\* REACTIONS DE R16C2H400H \*\*\*\*\*!

R16C2H400H=C2H40#3+R20H 1.5E11 0. 20.0E3 !(383, -  
 383)<RAnZI94>!  
 R16C2H400H=R6CH20H+HCHO 2.5E13 0. 27.5E3 !(384, -  
 384)<RAnZI94>!  
 R16C2H400H=C2H4Z+R300H 2.0E13 0. 23.5E3 !(385, -  
 385)<RAnZI94>!

!\*\*\*\*\* REACTIONS DE C2H500H \*\*\*\*\*!

C2H500H=R15C2H50+R20H 4.0E15 0. 42.9E3 !(386, -  
 386)<BAULCH94>!  
 C2H500H+R1H=>CH3CHO+R20H+H2 3.2E13 0. 7.7E3 !  
 (387)<RAnZI94>!  
 C2H500H+R4CH3=>CH3CHO+R20H+CH4 5.7E11 0. 8.7E3 !  
 (388)<RAnZI94>!  
 C2H500H+R9C2H=>CH3CHO+R20H+C2H2 6.0E11 0. 9.2E3 !  
 (389)<RAnZI94>!  
 C2H500H+R10C2H3V=>CH3CHO+R20H+C2H4Z 1.0E12 0. 8.7E3 !  
 (390)<RAnZI94>!  
 C2H500H+R11C2H5=>CH3CHO+R20H+C2H6 3.4E11 0. 11.4E3 !  
 (391)<RAnZI94>!  
 C2H500H+R20H=>CH3CHO+R20H+H2O 5.9E12 0. 0.9E3 !  
 (392)<RAnZI94>!  
 C2H500H+R5CHO=>CH3CHO+R20H+HCHO 1.8E12 0. 16.7E3 !  
 (393)<RAnZI94>!  
 C2H500H+R7CH30=>CH3CHO+R20H+CH30H 6.3E11 0. 5.5E3 !  
 (394)<RAnZI94>!  
 C2H500H+R6CH20H=>CH3CHO+R20H+CH30H 4.2E11 0. 13.6E3 !  
 (395)<RAnZI94>!  
 C2H500H+R14CH3C0=>2CH3CHO+R20H 2.0E12 0. 18.5E3 !  
 (396)<RAnZI94>!  
 C2H500H+R13CH2CHO=>2CH3CHO+R20H 3.4E11 0. 15.7E3 !  
 (397)<RAnZI94>!  
 C2H500H+R300H=>CH3CHO+R20H+H2O2 8.0E11 0. 16.2E3 !  
 (398)<RAnZI94>!  
 C2H500H+R8CH300=>CH3CHO+R20H+CH300H 1.1E12 0. 16.7E3 !  
 (399)<RAnZI94>!  
 C2H500H+R17C2H500=>CH3CHO+R20H+C2H500H 1.1E12 0. 16.7E3 !  
 (400)<RAnZI94>!

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!***** REACTIONS DE R18CH3C000 ***** !
R18CH3C000+C2H4O#3=CH3C000H+R13CH2CHO      1.0E12      0.      9.3E3 !
(401, -402)<RAnZI94>!
R18CH3C000+R300H=CH3C000H+O2                5.5E10      0.      -2.6E3 !
(402, -402)<COX90>!
R18CH3C000+C2H500H=CH3C000H+R17C2H500      5.0E11      0.      9.2E3 !
(403, -403)<RAnZI94>!
R18CH3C000+C2H500H=>CH3CHO+R20H+CH3C000H  5.0E11      0.      9.2E3 !
(404)<RAnZI94>!
R18CH3C000+R18CH3C000=>2R4CH3+O2+2C02     1.7E12      0.      -1.0E3 !
(405)<CAVAnAGH90>!

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!***** REACTIONS DE CH3C000H ***** !
CH3C000H=>R4CH3+C02+R20H                    1.0E16      0.      40.0E3 !
(406)<CAVAnAGH90>!

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!\* Primary mechanism of the  
oxidation of Ethanol \*!

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!\* REACTIONS OF ETHANOL \*!

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

!Unimolecular initiation

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C2H50H(+M)=R11C2H5+R20H(+M)      2.95E+22   -2.16   96.6E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
      LOW   /3.80E+88   -19.70   114.5E+3/
      TROE  /2.094   16539   1.114   161.36/

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C2H50H(+M)=C2H4Z+H20(+M)         4.90E+9    1.36   65.8E+3
!Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!
      LOW   /2.404+8   -17.9   84.8E+3/
      TROE  /2.126   13568   0.969   160.4/

```

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C2H50H(+M)=R4CH3+R6CH20H(+M)     6.61E+23  -2.16   88.04E+3
!Tsang, J Chem Kinet 36,436-63,2004!
      LOW   /1.99E+85  -18.9   104.8E+3/
      TROE  /2.058   16911   1.071   135.3/

```

C2H50H(+M)=R23C2H40H+R1H(+M) 2.01E+17 -0.149 101.8E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!  
 LOW /4.902E+94 -21.65 123.1E+3/  
 !Reaction (c5),T=500-1800K  
 !LOW /2.716E+83 -21.47 38.44E+3/  
 !Reaction (c5),T=1800-3000K

C2H50H(+M)=R24C2H40H+R1H(+M) 7.54E+16 -0.275 94.05E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!  
 LOW /7.708E+96 -22.47 116.9E+3/  
 !T=500-1800K  
 !LOW /5.58E+82 -21.20 37824.5/  
 !T=1800-3000K

DUPLICATE

C2H50H(+M)=R15C2H50+R1H(+M) 2.70E+15 0.305 101.3E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011b!  
 LOW /2.794E+88 -19.76 121.0E+3/  
 !T=500-1800K;  
 !LOW /4.246E+91 -23.49 49435.8/  
 !T=1800-3000K,

DUPLICATE

!Bimolecular initiation

C2H50H+O2=R23C2H40H+R300H 2.100E+13 0.0 52400.0  
 C2H50H+O2=R24C2H40H+R300H 1.400E+13 0.0 46300.0  
 C2H50H+O2=R15C2H50+R300H 7.000E+12 0.0 55730.0

!Metatheses with abstraction of H-atom

!C2H50H+R20H=R23C2H40H+H2O 6.203E+03 2.68 -576.3  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!  
 C2H50H+R20H=R23C2H40H+H2O 3.60E+06 2.0 950.0  
 !Nancy, correlation Bozzelli 1999!

!C2H50H+R20H=R24C2H40H+H2O 1.307E+05 2.43 -1456.6  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!  
 C2H50H+R20H=R24C2H40H+H2O 2.40E+06 2.00 -2100.0  
 !Nancy, correlation Bozzelli 1999!

C2H50H+R20H=R15C2H50+H2O 2.812E+02 2.97 -580.3  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!

C2H50H+B10=R23C2H40H+R20H 9.69E+02 3.23 4658.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007

C2H50H+B10=R24C2H40H+R20H 1.45E+05 2.47 876.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H50H+B10=R15C2H50+R20H 1.46E-03 4.73 1727.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!



C2H50H+R1H=R23C2H40H+H2 !T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).	1.88E+03	3.20	7150.0	
C2H50H+R1H=R24C2H40H+H2 !T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).	1.79E+05	2.53	3420.0	
C2H50H+R1H=R15C2H50+H2 !T=300-1000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).	5.33E-23	10.58	-4459.0	
!C2H50H+R1H=R15C2H50+H2 !T=1000-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).	5.36E+4	2.53	8753.6	
!C2H50H+R4CH3=R23C2H40H+CH4 !T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).	6.99E-83	30.14	-15663.0	
C2H50H+R4CH3=R23C2H40H+CH4 !T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).	3.30E+02	3.30	12291.0	
!C2H50H+R4CH3=R24C2H40H+CH4 !T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).	1.02E-47	18.51	-9409.4	
C2H50H+R4CH3=R24C2H40H+CH4 !T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)	1.99E+01	3.37	7635.0	
!C2H50H+R4CH3=R15C2H50+CH4 !T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).	1.01E-51	19.68	-10323.5	
C2H50H+R4CH3=R15C2H50+CH4 !T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)	2.035E+0	3.57	7722.0	
C2H50H+R300H=R23C2H40H+H2O2 !correlation (Dean and Bozzelli 2000)	4.2E+04	2.69	19080	
C2H50H+R300H=R24C2H40H+H2O2 !correlation (Dean and Bozzelli 2000)	2.80E+04	2.69	15420	
C2H50H+R300H=R15C2H50+H2O2 Grana et al.2010	5.400E+04	2.0	15025.0	!
C2H50H+R11C2H5=R23C2H40H+C2H6 Konnov 2005!	1.500E+12	0.0	11700.0	!
C2H50H+R11C2H5=R24C2H40H+C2H6 Konnov 2005!	4.000E+13	0.0	10000.0	!
C2H50H+R11C2H5=R15C2H50+C2H6 Grana et al.2010!	2.300E+04	2.0	10525.0	!
C2H50H+R6CH2OH=R24C2H40H+CH3OH Konnov 2005!	4.000E+11	0.0	9700.0	!
C2H50H+R7CH3O=R24C2H40H+CH3OH Konnov 2005!	2.000E+11	0.0	7000.0	!
C2H50H+R15C2H5O=C2H50H+R24C2H40H Konnov 2005!	2.000E+11	0.0	7000.0	!

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!*****!
!*          REACTIOnS OF R23C2H4OH      *!
!*****!

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R23C2H4OH=C2H4Z+R20H          3.52E-34      11.84      -18737.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!          1.35E+43      -10.29      28035.5
!at 1 atm, T=300-1000K
!          7.93E+2       1.51       15180.3
!at 1 Torr, T=300-3000K
!          1.51E+33      -6.54      26960.4
!at 100 atm, T=300-1000K
!          4.90E-24      9.44      -12183.6
!at 100 atm, T=1000-3000K

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R23C2H4OH=R1H+C2H30H          3.33E+28      -5.26      35586.9
!at 1 atm, T=300-3000K.ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!          2.67E+15      -1.92      29386.8
!at 1 Torr, T=300-3000K.
!          2.67E+27      -4.44      37208.5
!at 100 atm, T=300-3000K

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```

R23C2H4OH=R24C2H40H          1.000E+11      0.0       39500.0
! A=Konnov 2005; Ea=Lin et al 2009, chemphyschem, 10(6),972-81

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R23C2H40H+O2=C2H30H+R300H          1.600E+12      0.0       5000.0

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!*****!
!*          REACTIOnS OF R24C2H40H      *!
!*****!

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R24C2H40H=CH3CHO+R1H          8.34E+27      -5.19      35576.9
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.
!!          8.96E+13      -1.61      28844.3
!at 1 Torr, T=300-3000K
!!          5.47E+27      -4.67      37685.4
!at 100 atm, T=300-3000K

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R24C2H40H=R1H+C2H30H          2.00E+28      -5.08      39380.5
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!          4.44E+21      -3.23      36570.6
!at 1 Torr, T=300-3000K
!!          1.22E+30      -5.17      41916.2
!at 100 atm, T=300-3000K

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R24C2H40H=R4CH3+HCHO          1.14E+22      -3.59      34662.9
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81
!!          5.92E+11      -1.04      28739.0
!at 1 Torr, T=300-3000K
!!          4.36E+23      -3.55      38679.0
!at 100 atm, T=300-3000K

```

R24C2H40H+O2=CH3CHO+R300H	5.26E+17	-1.637	838.0
!at 0.1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.			
!!R24C2H40H+O2=CH3CHO+R300H	5.28E+17	-1.637	839.0
!at 1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.			
R24C2H40H+O2=C2H3OH+R300H	5.33E+2	2.490	-402
!at 0.1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.			
!!R24C2H40H+O2=C2H3OH+R300H	7.62E+2	2.446	-296
!at 1 atm, T=300-2000K,Ref: DaSilva et al 2009, JphyschemA, 113,31.			
R24C2H40H+R1H=CH3CHO+H2	1.361E+09	1.29	2823.8
! T=100-2000K! ref: Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H=R6CH2OH+R4CH3	8.67E+16	-0.891	2903.3
!R\action (b2), Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H=C2H3OH+H2	4.896E+08	1.70	588.2
!R\action (b11), T=100-2000K! Ref: Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H(+M)=C2H5OH(+M)	3.607E+13	0.06	437.2
!R\action (b1), T=500-2000K!Ref: Lin et al 2011b, JphyschemA,115,3509-22,			
	LOW /2.767E+56	-15.72	
10.7E+03/			
	Duplicate		
R24C2H40H+R20H=CH3CHO+H2O	1.500E+13	0.0	0.0
!Konnov 2005			
R24C2H40H+B10=CH3CHO+R20H	9.040E+13	0.0	0.0
!Konnov 2005			
!*****!			
!* REACTIONs OF R15C2H50 *!			
!*****!			
R15C2H50=R4CH3+HCHO	4.4E-29	10.69	-16245.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.			
!!	1.03E+23	-3.82	19303.7
!at 1 atm, T=300-1000K,			
!!	2.71E+24	-4.50	21018.7
!at 1 Torr, T=300-1000K,			
!!	1.87E-28	10.39	-12910.9
!at 1 Torr, T=1000-3000K,			
!!	5.31E+21	-2.97	19560.1
!at 100 atm, T=300-1000K,			
!!	9.56E-17	7.66	-7408.3
!at 100 atm, T=1000-3000K,			
R15C2H50=R1H+CH3CHO	4.25E-32	11.49	-16541.5
!at 1 atm,T=1000-3000K ref: Lin et al 2009, chemphyschem, 10(6),972-81			
!!	1.33E+38	-8.61	25513.8
!at 1 atm,T=300-1000K			

!!	7.25E+31	-7.58	21370.4
!at 1 Torr, T=300-1000K			
!!	2.14E-34	11.63	-15651.2
!at 1 Torr, T=1000-3000K			
!!	2.61E+19	-2.15	21996.4
!at 100 atm, T=300-1000K			
!!	1.64E-27	10.5	-15315.4
!at 100 atm, T=1000-3000K			

R15C2H5O+O2=CH3CHO+R3OOH !(287, -287)<BAULCH94>!	6.0E+10	0.0	1.7E+3
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R15C2H5O+R2OH=CH3CHO+H2O !Marinov 1998	1.0E+13	0.0	0.0
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R15C2H5O+R1H=CH3CHO+H2 !T=100-2000K! Lin et al 2011b, JphyschemA, 115, 3509-22	7.47E+09	1.15	673.7
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R15C2H5O+R1H(+M)=C2H5OH(+M) !T=100-2000K! Lin et al 2011b, JphyschemA, 115, 3509-22	3.08E+11	0.894	12.9
	LOW / 3.772E+51	-15.55	
11.1E+3/			

DUPLICATE

R15C2H5O+B10=CH3CHO+R2OH !Konnov 2005	1.210E+14	0.0	0.0
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*****!
!*                               Secondary mechanism of the
oxidation of Ethanol                *!
!
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*****!
!
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!*****!
!*           REACTIONS OF C2H3OH           *!
!*****!

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!C2H3OH+B10=R13CH2CHO+R2OH !<PAG, Ullisier paras. des mıtathises d'atome H allylique secondaire>!	4.4E+10	0.7	3250.0
C2H3OH+B10=R13CH2CHO+R2OH !Acıtaldıhyde! (219, -219)<CAVAnAGH90>	1.4E+13	0.0	2.3E3

!C2H3OH+R1H=R13CH2CHO+H2 2.700E+04 2.5  
 -1900.0 !<PAG,Ulisier paras. des мѣtathises d'atome H allylique  
 secondaire>!  
 !C2H3OH+R1H=R13CH2CHO+H2 1477.2 3.077  
 7230 !T=300-3000!RAO 2011! J Phys Chem 2011,115  
 ! REV /1.41 3.721 24600/  
 C2H3OH+R1H=R13CH2CHO+H2 1.31E+5 2.58 1220.0  
 !Acѣtaldѣhyde! T=200-2500K!Klippenstein et al.2010. J Phys Chem  
 A,114,755-764.

!C2H3OH+R2OH=R13CH2CHO+H2O 1.500E+06 2.0  
 -1520.0 !<PAG,Ulisier paras. des мѣtathises d'atome H allylique  
 secondaire>!  
 C2H3OH+R2OH=R13CH2CHO+H2O 2.300E+10 0.73 -1100.0  
 !Acѣtaldѣhyde! Konnov 2005

!C2H3OH+R3OOH=R13CH2CHO+H2O2 3.200E+03 2.6  
 12400.0 !<PAG,Ulisier paras. des мѣtathises d'atome H allylique  
 secondaire>!  
 !C2H3OH+R3OOH=R13CH2CHO+H2O2 1.626E+12 0.0  
 16295.1 !Syn\_CH2H3OH! ajoutѣ le 20/10/2011 !Altarawneh et al 2011!  
 T=700-1300K!  
 C2H3OH+R3OOH=R13CH2CHO+H2O2 1.0E12 0.0 10.0E3  
 !Acѣtaldѣhyde!(311, -311)<CAVAnAGH90>!

!C2H3OH+R4CH3=R13CH2CHO+CH4 5.000E+10 0.0  
 7300.0 !<PAG,Ulisier paras. des мѣtathises d'atome H allylique  
 secondaire>!  
 C2H3OH+R4CH3=R13CH2CHO+CH4 2.0E-6 5.6 2.5E+3  
 !Acѣtaldѣhyde! (216, -216)<BAULCH94>!Nancy! T=300-125

!C2H3OH+R11C2H5=R13CH2CHO+C2H6 0.740 3.5 4140.0  
 !<PAG,Ulisier paras. des мѣtathises d'atome H allylique secondaire>!  
 C2H3OH+R11C2H5=R13CH2CHO+C2H6 1.3E12 0.0 8.5E3  
 !Acѣtaldѣhyde! (218, -218)<HOHLEIn70>

C2H3OH=CH3CHO 4.5E+06 1.8 5.1E+4  
 !Prof. Fournet  
 !!C2H3OH=CH3CHO 8.590E+11 0.318 55900.00  
 ! DaSilva 2006!  
 !! REV/ 1.050E+09 1.202  
 66300.00 /

!C2H3OH+R3OOH=CH3CHO+R3OOH 1.49E+05 1.67 6810.0  
 !P=1atm, T=300-2000K!Da silva 2009, Chem Phys Letters 483, 25-29  
 C2H3OH+R1H=CH3CHO+R1H 1.00E+13 0.00 1506.0  
 !T=300-2000K!form observation in Huynh et al 2009, j phys chem A  
 113,3177-3185:

!"The rate of this reaction is close to that of the H addition to C2H4:  
 C2H4 + H=C2H5, ref: Warnatz 1984

C2H3OH+R2OH=R4CH3+C02+H2 1.40E+12 0.00 -1040.0  
 !Nancy, tableau A-I-5

!C2H3OH+R2OH=HCHO+R6CH2OH !Nancy, tableau A-I-5	1.40E+12	0.00	-1040.0
!C2H4+OH<=>C2H3OH+H !Senosiain et al 2006	1.070E+04	2.600	4133.00
C2H4Z+R2OH=C2H3OH+R1H !Hippler et al 2000	4.000E+12	0.000	4880.00
!*****! !* REACTIONs OF CH3CHO *! !*****!			
CH3CHO+R2OH=R14CH3CO+H2O -1100.0 ! Konnov 2005!	2.300E+10	0.73	
CH3CHO+R1H=H2+R14CH3CO 1220.0 !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-764.	1.31E+5	2.58	
CH3CHO+R4CH3=R14CH3CO+CH4 2.5E+3 !(216, -216)<BAULCH94>! T=300-1250K	2.0E-6	5.6	
CH3CHO+B10=R14CH3CO+R2OH 2.3E3 !(219, -219)<CAVAnAGH90>!	1.4E+13	0.	
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO 3.7E3 !(217, -217)<SCHERZER87>T=480-520K!NIST	8.1E10	0.	
CH3CHO+R11C2H5=C2H6+R14CH3CO 8.5E3 !(218, -218)<HOHLEIn70>!	1.3E12	0.	
CH3CHO+R7CH3O=R14CH3CO+CH3OH 0.0 !Konnov 2005!	5.000E+12	0.0	
CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 11200.0 !Konnov 2005!	3.000E+12	0.0	
!CH3CHO+R2OH=R13CH2CHO+H2O 2000.0 !T=1000-1700K, P=1.2-2.8 atm. ref: Yasunaga et al 2008, J Chem Kin 2008,40,73-102	1.600E+13	0.0	
CH3CHO+R2OH=R13CH2CHO+H2O -619.98 !Mech Sandiego=ref:Juan Li's PhD thesis!	3.370e+11	0.0	
!CH3CHO+R1H=R13CH2CHO+H2 10.0E+3 !NIST! 2008YAS/KUB73-102! T=1000-1700K, P=1.2-2.8 atm	4.40E+14	0.0	
CH3CHO+R1H=R13CH2CHO+H2 5206.5 !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-764.	2.72E+03	3.1	
!CH3CHO+R4CH3=R13CH2CHO+CH4 11000.0 !2008YAS/KUB73-102!T=1000-1700K, P=1.2-2.8 atm	6.00E+12	0.0	
CH3CHO+R4CH3=R13CH2CHO+CH4 5727.0 !Marinov 1998	2.45E+1	3.15	
CH3CHO+B10=R13CH2CHO+R2OH 3556.0 !Marinov 1998	3.720E+13	-0.2	
!***** REACTIONS DE C2H5 *****!			
R11C2H5+R10C2H3V=>C4H8Y (61, -61)<TSAnG86>!	1.5E13	0.	0. !

!R11C2H5+R11C2H5=>C4H10 1.1E13 0. 0. !  
 (65, -65)<BAULCH94>!

!\*\*\*\*\* REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE \*\*\*\*\*!

C2H3CHO+R20H=CH2CHCO+H2O 1.0E13 0.0 0.0 !  
 <MARInOV>!  
 C2H3CHO+B10=CH2CHCO+R20H 7.2E12 0.0 2.0E3 !  
 <MARInOV>!  
 C2H3CHO+B10=CH2COZ+R5CHO+R1H 5.0E7 1.76 0.08E3 !  
 <MARInOV>!  
 C2H3CHO+R1H=CH2CHCO+H2 4.0E13 0.0 4.2E3 !  
 <MARInOV>!  
 C2H3CHO+R1H=C2H4Z+R5CHO 2.0E13 0.0 3.5E3 !  
 <MARInOV>!  
 C2H3CHO+O2=CH2CHCO+R300H 3.0E13 0.0 38.5E3 !  
 <MARInOV99>+ MF correlation Baptiste  
 CH2CHCO=R10C2H3V+B2CO 1.0E14 0.0 34.0E3 !  
 <MARInOV>!  
 CH2CHCO+B10=R10C2H3V+CO2 1.0E14 0.0 0.0 !  
 <MARInOV>!  
 C3H5Y+R300H=>C2H3CHO+R1H+R20H 7.0E18 -2.0 0.0 !  
 <TSAng91>!  
 C3H5Y+O2=C2H3CHO+R20H 1.8E13 -0.41 22.9E3 !  
 <BOZELLI93>!  
 C3H5Y+B10=C2H3CHO+R1H 1.8E14 0.0 0.0 !  
 <SLAGLE92>!

!\*\*\*\*\*  
 ! REACTIONS DES ESPECES NON OXYGENNS EN C3 !  
 !\*\*\*\*\*

!\*\*\*\*\* REACTIONS DE C3H2 \*\*\*\*\* (CHCCH(..))\*\*\*\*\*!

B4CH+C2H2=C3H2+R1H 2.1E14 0.0 -0.5E3 !  
 <MILLER92/BAULCH94>!  
 C3H2+B10=R9C2H+R1H+B2CO 3.0E13 0.0 0.0 !  
 <PEETERS97>!  
 C3H2+R20H=C2H2+R5CHO 5.0E13 0.0 0.0 !  
 <MILLER92>!  
 C3H2+O2=R12CHCOZ+B2CO+R1H 5.0E13 0.0 0.0 !  
 <MILLER92>!

!\*\*\*\*\* REACTIONS DE C3H3 \*\*\*\*\* (CHCCH2(..)) Propargyl\*\*\*\*\*stabilise par  
 resonance !

B6CH2+C2H2=C3H3+R1H 1.8E14 0.0 0.0 !  
 <MILLER87/BAULCH94>!  
 C3H3+R1H=C3H2+H2 2.0E13 0.0 0.0 !  
 <MILLER92/BRAUn89>!  
 C3H3+B10=R9C2H+HCHO 1.4E14 0.0 0.0 !  
 <MILLER92/SLAGUE91>!

C3H3+R20H=C3H2+H2O <MILLER92>!	2.0E13	0.0	0.0	!
C3H3+R20H=R10C2H3V+R5CHO <WAnG97>!	4.0E13	0.0	0.0	!
C2H2+R12CHCOZ=C3H3+B2CO <MILLER92>!	1.0E11	0.0	3.0E3	!
C3H3+O2=CH2COZ+R5CHO <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3	!
C3H2+R1H=C3H3 <est>!	1.0E14	0.0	0.0	!
C3H3+R300H=>R20H+R9C2H+HCHO <Heyberger>!	1.0E15	-0.8	0.0	!
C3H3+C3H3=C6H6# <STEIn90>shocktube!	1.0E12	0.0	0.0	!
C3H3+C3H3=C6H5#+R1H <STEIn90>flame!	1.0E12	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE pC3H4 \*\*\*\*\* (CH3CCH) Propyne \*\*\*\*\*!

!pC3H4=>aC3H4 !<HIDAKA89>!	2.1E12	0.0	60.0E3	
pC3H4+M=C3H3+R1H+M !<HIDAKA89>!	4.7E18	0.0	80.0E3	
C2H2+B5CH2=pC3H4 !<TSAnG86>!	3.5E12	0.0	0.0	
pC3H4=R9C2H+R4CH3 <KInGAS1500>!	4.2E15	0.0	125.0E3	!
pC3H4+O2=C3H3+R300H <est Ingham>!	2.1E12	0.0	40.8E3	!
pC3H4+R1H=C2H2+R4CH3 <hidaka89> !	1.3E5	2.5	1.00E3	!
pC3H4+R1H(+M)=tC3H5(+M) <WAGnER72>!	8.5E12	0.0	1.7E3	!
LOW /5.6E25	-7.27	6.58E3/		
!<Marinov97>!				
pC3H4+R1H(+M)=sC3H5(+M) <WAGnER72>!	5.8E12	0.0	3.1E3	!
LOW /3.8E25	-7.27	7.98E3/		
!<estimated>!				
pC3H4+R4CH3=C3H3+CH4 <asTSAnG91>!	2.2E0	3.5	5.7E3	!
pC3H4+R1H=C3H3+H2 <asTSAnG91>	1.7E5	2.5	2.5E3	!
pC3H4+R9C2H=C3H3+C2H2 !<asTSAnG91>!	3.6E12	0.0	0.0	
pC3H4+R10C2H3V=C3H3+C2H4Z <asTSAnG91>!	2.2E0	3.5	4.7E3	!
pC3H4+R11C2H5=C3H3+C2H6 <asTSAnG91>!	2.2E0	3.5	6.6E3	!



pC3H4+B10=R12CHCOZ+R4CH3 <WARNATZ84>!	1.5E13	0.0	2.1E3	!
pC3H4+B10=R20H+C3H3 <<ADUSEI, G.Y, 1996>!	3.4E4	2.16	4.8E3	!
pC3H4+R20H=CH2COZ+R4CH3 <BOODAGHIANs87>!	4.3E11	0.0	-0.8E3	!
pC3H4+R20H=R1H+C2H3CHO <asB00DAGHIANs87>!	4.3E11	0.0	-0.8E3	!
pC3H4+R20H=C3H3+H2O <asTSAnG91>!	3.1E6	2.0	-0.3E3	!
pC3H4+R300H=C2H4Z+B2CO+R20H as296<TSAnG86>!	6.0E9	0.0	8.0E3	!
pC3H4+R300H=C3H3+H2O2 <asTSAnG91>!	9.6E3	2.6	13.9E3	!
pC3H4+R7CH30=CH30H+C3H3 <Heyberger>!	2.0E12	0.0	4.0E3	!

!\*\*\*\*\* REACTIONS DE aC3H4 \*\*\*\*\* (CH2CCH2) Allene \*\*\*\*\*!

aC3H4=pC3H4 <HIDAKA89>!	2.5E12	0.0	59.0E3	!
aC3H4+M=C3H3+R1H+M <HIDAKA89>!	2.0E18	0.0	80.0E3	!
aC3H4+O2=C3H3+R300H <Estimation Ingham>!	2.8E13	0.0	39.0E3	!
aC3H4+R1H(+M)=C3H5Y(+M) 2.7E3 !<WAGnER72>!		4.0E12	0.0	
LOW /5.6E33	-5.0	4.44E3/		
!<Marinov97> !				
aC3H4+R1H(+M)=tC3H5(+M) <WAGnER72>!	8.5E12	0.0	2.0E3	!
LOW /1.1E34	-5.0	4.44E3/		
!<Marinov97>!				
C2H4Z+B4CH=aC3H4+R1H <BAULCH94base>!	1.3E14	0.0	-0.3E3	!
R10C2H3V+B5CH2=aC3H4+R1H <MILLER92>!	3.0E13	0.0	0.0	!
iC4H3+B5CH2=aC3H4+R9C2H <MILLER92>!	2.0E13	0.0	0.0	!
aC3H4+B10=R1H+B2CO+R10C2H3V <Aleksandrev nist>!	6.6E12	0.0	3.0E3	!
aC3H4+R20H=CH2COZ+R4CH3 <LIU88>!	2.0E12	0.0	-0.2E3	!
aC3H4+R20H=HCHO+R10C2H3V <LIU88>!	2.0E12	0.0	-0.2E3	!
aC3H4+R1H=C3H3+H2 <est.butatiene>!	1.3E6	2.53	9.2E3	!
aC3H4+B10=C3H3+R20H <fromAleksandrev nist>!	6.2E12	0.0	1.9E3	!
!d'après leur vitesse de réaction total et d'addition !				
aC3H4+R20H=C3H3+H2O <est.butadiene>!	6.2E6	2.0	0.4E3	!

aC3H4+R4CH3=C3H3+CH4 <WU87>!	2.0E12	0.0	7.7E3	!
aC3H4+R9C2H=C3H3+C2H2 <WU87>!	1.0E13	0.0	0.0	!
aC3H4+C3H5Y=C3H3+C3H6Y <DAGAUT92>	2.0E12	0.0	7.7E3	!
aC3H4+R7CH30=CH30H+C3H3 9.6E3		4.0E12	0.0	
!<correlations a partir de Heyberger>!				
aC3H4+R11C2H5=C2H6+C3H3 !<asbutadiene>!	5.0E14	0.0	19.8E3	
aC3H4+R10C2H3V=C2H4Z+C3H3 <asbutadiene>!	5.0E14	0.0	19.8E3	!
!aC3H4+R4CH3=C4H7T <Scherzer>!	5.7E10	0.0	6.8E3	!
!aC3H4+R4CH3=C4H7T !<Tsang91x2>!	3.4E11	0.0	7.4E3	
!aC3H4+R4CH3=iC4H7 !<Tsang73>!	1.6E11	0.0	5.0E3	
!aC3H4+R4CH3=C4H7T 7.4E3		0.8E11	0.0	
!<Tsang91x2/4>!				
aC3H4+R4CH3=iC4H7 !<Tsang73/3>!	0.4E11	0.0	5.0E3	

!fort effet de fall off, environ un facteur 4 pour 6.7 kPa et 1100 K (Tsang91)!

!aC3H4+C3H3=C6H6#+R1H <HIDAKA89>!	1.4E12	0.0	10.0E3	!
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!\*\*\*\*\* REACTIONS DE cC3H4 \*\*\*\*\* cyclopropene \*\*\*\*\*!

cC3H4=aC3H4 <Karni>	1.5E14	0.0	50.5E3	!
cC3H4=pC3H4 <Karni>	7.1E13	0.0	47.8E3	!
cC3H4+R1H=cC3H3+H2 <Heyberger>!	5.4E4	2.5	-1.9E3	!
cC3H4+R20H=cC3H3+H2O <Heyberger>!	3.0E6	2.0	-1.5E3	!
cC3H4+R20H=C2H4Z+R5CHO <Heyberger>!	2.8E12	0.0	-1.0E3	!
cC3H3+R300H=R20H+C2H2+R5CHO <Heyberger>!	1.0E15	-0.8	0.0	!
cC3H3+R4CH3=cC4H6 <estimation>!	1.0E13	0.0	0.0	!
cC3H3+R1H=cC3H4 <estimation>!	1.0E14	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE C3H5Y \*\*\*\*\* (CH2CHCH2(.)) Allyl \*\*\*\*\*stabilise par resonance !

!C3H5Y+R1H=C3H6Y <TSAnG91>!	2.0E13	0.0	0.0	!
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C3H5Y+R1H=aC3H4+H2	1.8E13	0.0	0.0	!
TSANG 91!*				
C3H5Y+R1H=C3H6Y	1.0E14	0.0	0.0	!
<allara>!!				

!rñaction importante pour la formation de propine!

C3H5Y+R4CH3=aC3H4+CH4	3.0E12	-0.32	-0.1E3	!
<TSAnG91>!				
C3H5Y+R4CH3=C4H8Y	1.0E14	-0.32	-0.1E3	!
<TSAnG91>!				
C3H5Y+R20H=aC3H4+H2O	6.03E12	0.0	0.0	!
Tsang 91!				
!peu d'effet de fall off!				
C3H5Y+R10C2H3V=aC3H4+C2H4Z	2.4E12	0.0	0.0	!
<TSAnG91>!				
!C3H5Y+R11C2H5=aC3H4+C2H6	9.6E11	0.0	-0.1E3	!
<TSAnG91>!				
C3H5Y+R11C2H5=aC3H4+C2H6	2.0E13	0.0	-0.1E3	!
<TSAnG91>MODIF!!!!				
C3H5Y+B10=R10C2H3V+HCHO	1.8E14	0.0	0.0	!
<SLAGLE90,LEUnG95>!				
!processus non elementaire impliquant la formation-decomposition de l'hydroperoxyde				
!C3H5Y+C3H3=C6H6#+2R1H	5.6E20	-2.535	1.7E3	!
<MARInOV97>!				
C3H5Y+C3H5Y=aC3H4+C3H6Y	8.4E10	0.0	-0.3E3	!
<TSAnG91>!				

!\*\*\*\*\* REACTIONS DE sC3H5 \*\*\*\*\* (CH3CHCH(.)) 2-methyl vinyl \*\*\*\*\*!

sC3H5=C3H5Y	5.0E13	0.0	37.0E3	!
<WEISSMAN89>!				
R4CH3+C2H2=sC3H5	6.0E11	0.0	7.7E3	!
<BAULCH94>!				

!\*\*\*\*\* REACTIONS DE tC3H5 \*\*\*\*\* (CH3C(. )CH2) 1-methyl vinyl \*\*\*\*\*!

tC3H5+R1H=aC3H4+H2	3.3E12	0.0	0.0	!
<DAGAUT90>!				
tC3H5+R4CH3=aC3H4+CH4	1.0E11	0.0	0.0	!
<DAGAUT90>!				
tC3H5+R10C2H3V=aC3H4+C2H4Z	1.0E12	0.0	0.0	!
<LEUnG95>!				
tC3H5+R11C2H5=aC3H4+C2H6	1.0E12	0.0	0.0	!
<LEUnG95>!				
tC3H5+B10=CH2COZ+R4CH3	1.8E14	0.0	0.0	!
<LEUnG95>!				
tC3H5+O2=R4CH3+B2CO+HCHO	4.3E12	0.0	0.0	!
<DAGAUT90>!				
tC3H5=C3H5Y	2.0E13	0.0	47.0E3	!
<Weissman89>!				

!\*\*\*\*\* REACTIONS DE C3H6Y \*\*\*\*\* (CH3CHCH2) propene \*\*\*\*\*!

C2H4Z+B6CH2=C3H6Y <BAULCH94>!	9.6E13	0.0	0.0	!
C2H4Z+B5CH2=C3H6Y <BAULCH94>!	3.2E12	0.0	5.1E3	!
!duplicate R10C2H3V+R4CH3=C3H6Y <TSAnG86>!	2.5E13	0.0	0.0	!
C2H4Z+R4CH3=C3H6Y+R1H <TSAnG86>!	6.6E11	0.0	15.9E3	!
R11C2H5+B6CH2=C3H6Y+R1H <TSAnG86>!	9.0E12	0.0	0.0	!
C2H6+B4CH=C3H6Y+R1H <BAULCH94>!	1.1E14	0.0	-0.3E3	!
C3H6Y+R1H=sC3H5+H2 <TSAnG92>!	7.83E5	2.5	12.28E3	!
C3H6Y+R1H=tC3H5+H2 <TSAnG92>!	3.9E5	2.5	5.82E3	!
C3H6Y+R1H=C3H5Y+H2 <TSAnG91>!	1.7E5	2.5	2.5E3	!
C3H6Y+R4CH3=C3H5Y+CH4 <TSAnG91>!	2.2E0	3.5	5.7E3	!
C3H6Y+R4CH3=sC3H5+CH4 <TSAnG91>!	8.4E-1	3.5	11.7E3	!
C3H6Y+R4CH3=tC3H5+CH4 <TSAnG91>!	1.3E0	3.5	12.9E3	!
C3H6Y+R11C2H5=C3H5Y+C2H6 <TSAnG91>!	2.2E0	3.5	6.6E3	!
!C3H6Y+B10=>CH2COZ+R1H+R4CH3 <TSAnG91>! MF!!ds мйса PRF	1.2E+5	2.56	-1130.0	!
C3H6Y+B10=C3H5Y+R20H <TSAnG91>!	1.7E11	0.7	5.9E3	!
!C3H6Y+R20H=HCHO+R11C2H5 <TSAnG91>! MF!!ds мйса PRF	1.45E12	0.0	-0.9E3	!
!C3H6Y+R20H=R4CH3+CH3CHO <TSAnG91>! MF!!ds мйса PRF	1.45E12	0.0	-0.9E3	!
C3H6Y+R20H=C3H5Y+H2O <TSAnG91>!	3.1E6	2.0	-0.3E3	!
C3H6Y+R20H=sC3H5+H2O <TSAnG91>!	1.1E6	2.0	1.45E3	!
C3H6Y+R20H=tC3H5+H2O <TSAnG91>!	2.1E6	2.0	2.8E3	!
C3H6Y+O2=C3H5Y+R300H <WALKER93>!	1.9E12	0.0	39.0E3	!
C3H6Y+R300H=C3H5Y+H2O2 <TSAnG91>!	9.6E3	2.6	13.9E3	!
C3H6Y+R9C2H=pC3H4+R10C2H3V 91 mehdi!	1.2E13	0.0	0.0	!TSANG

!\*\*\*\*\* REACTIONS DE cC3H6 \*\*\*\*\* cyclopropane \*\*\*\*\*!

cC3H6=C3H6Y	4.6E14	0.0	62.6E3	!
<Hidaka87>!				
cC3H6+R1H=C3H5Y+H2	1.6E14	0.0	11.7E3	!
<Marshall86>!				
cC3H6+R20H=C3H5Y+H20	7.0E7	1.5	1.0E3	!
<Dobe82>!				
cC3H6+R4CH3=C3H5Y+CH4	2.0E11	0.0	9.6E3	!
<Exgas>!				

!\*\*\*\*\* REACTIONS DE R19C3H7 et iC3H7 \*\*\*\*\* CH3CH2CH2(.) et CH3CH(.)CH3  
\*\*\*\*\* !

!R19C3H7 = R4CH3+C2H4Z	6.400E+12	0.00	31000.0!!
ds мйса PRF			
!R19C3H7 = R1H+C3H6Y	3.000E+13	0.00	38000.00!!
ds мйса PRF			
iC3H7 = R1H+C3H6Y	6.000E+13	0.00	39000.00
R19C3H7 = iC3H7	1.960E+10	1.00	38600.00
!R19C3H7+O2 =R300H+C3H6Y	1.600E+12	0.00	5000.00
R19C3H7+O2 =R300H+C3H6Y	3.7e16	-1.63	3420 !
2003DES/KLI4415-4427			
iC3H7+O2 = R300H+C3H6Y	1.400E+12	0.00	5000.00

!\*\*\*\*\* Propane (C3H8) chemistry \*\*\*\*\*!

R11C2H5+R4CH3=C3H8	3.4E13	0.	0.	!(59, -
59)<BAULCH94>!				
C3H8+O2=>R300H+iC3H7	1.4E+0013	0.000	50323.7	! BI 2 CN
C3H8+O2=>R300H+R19C3H7	4.2E+0013	0.000	53033.0	! BI 3 CN
B10+C3H8=>R20H+iC3H7	2.6E+0013	0.000	5200.0	! ME 15 CW
B10+C3H8=>R20H+R19C3H7	1.0E+0014	0.000	7850.0	! ME 16 CW
C3H8+R1H=>H2+iC3H7	9.0E+0006	2.000	5000.0	! ME 17 CW
!C3H8+R1H=>H2+R19C3H7	5.7E+0007	2.000	7700.0	! ME 18 CW!!ds
мйса PRF				
C3H8+R20H=>H2O+iC3H7	2.6E+0006	2.000	-765.0	! ME 19 CW
!C3H8+R20H=>H2O+R19C3H7	5.4E+0006	2.000	450.0	! ME 20 CW!!ds
мйса PRF				
C3H8+R300H=>H2O2+iC3H7	4.0E+0011	0.000	15500.0	! ME 21 CN
!C3H8+R300H=>H2O2+R19C3H7	1.2E+0012	0.000	17000.0	! ME 22 CN!!ds
мйса PRF				
C3H8+R4CH3=>CH4+iC3H7	2.0E+0011	0.000	9600.0	! ME 23 CN
!C3H8+R4CH3=>CH4+R19C3H7	6.0E-0001	4.000	8200.0	! ME 24 CN!!ds
мйса PRF				
C3H8+R5CHO=>HCHO+iC3H7	1.0E+0007	1.900	17000.0	! ME 25 CN
C3H8+R5CHO=>HCHO+R19C3H7	2.0E+0005	2.500	18500.0	! ME 26 CN
C3H8+R11C2H5=>C2H6+iC3H7	2.0E+0011	0.000	11000.0	! ME 33 CN
!C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	! ME 34 CR!!ds
мйса PRF				
C3H8+iC3H7=>C3H8+R19C3H7	8.4E-0003	4.200	8700.0	! ME 35 CN
R1H+iC3H7=>C3H8	8.3E+0012	0.000	0.0	! CO 36 K

!\*\*\*\*\*Reactions of Acetone\*\*\*\*\*!

!R14CH3CO+R4CH3=>C2H6CO	4.0E15	-0.8	0. !
(231, -231)<TSAnG86>!			

R14CH3CO+R4CH3=>C2H6CO	2.7E15	-0.8	0. !
(231, -231)<TSAnG86>! A/1.5 to improve the agreement simu/exp at low pressure.			
iC3H7+B10=>C2H6CO+R1H	1.0	0.0	0.0 !
Tsang88 (Nist)			
C2H6CO+O2=>R300H+CH2COZ+R4CH3	4.2E12	0.0	49.28E3 !
Kingas!			
C2H6CO+B10=>CH2COZ+R4CH3+R2OH	1.02E14	0.0	7.85E3 !
Buda!			
C2H6CO+R1H=>CH2COZ+R4CH3+H2	5.70E07	2.0	7.70E3
C2H6CO+R2OH=>CH2COZ+R4CH3+H2O	5.34E06	2.0	0.45E3
C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4	6.00E-1	4.0	8.20E3
C2H6CO+R300H=>CH2COZ+R4CH3+H2O2	1.20E12	0.0	17.0E3

!\*\*\*\*\*Reactions of Propanal\*\*\*\*\*!

!R5CHO+R11C2H5=>C2H5CHO	1.8E13	0.	0.
!(141, -141)<TSAnG86>!			
!C2H5CHO=R5CHO+R11C2H5	1.07E+14	0.0	62600
!Decottignies et al.COMBT.FLAME 2002, 130, 225-240			
R5CHO+R11C2H5=C2H5CHO	3.4E+13	0.0	0.0
!= "CH3+C2H5=C3H8".			
!C2H5CHO=R5CHO+R11C2H5	2.45E+15	0.0	72864.5
!Lifshitz et al.J. Phys. Chem., 94 (1990)			
R13CH2CHO+R4CH3=C2H5CHO	3.4E+13	0.0	0.0
!= "CH3+C2H5=C3H8".			
!C2H5CHO=R4CH3+R13CH2CHO	7.00E+15	0	81703
!Baulch et al 1992, J. Phys.Chem.Ref.Data 21 411-429.			
B10+C3H6Y=>C2H5CHO	1.000E+12	0	5000.0
!Mech Franssoldati			
!C2H5CHO+R1H=H2+B2CO+R11C2H5	4.0E13	0.0	4.2E3
!<Heyberger>! ADZ 714			
!C2H5CHO+R2OH=H2O+B2CO+R11C2H5	4.0E12	0.0	0.5E3
!<Heyberger>! ADZ 715			
!C2H5CHO=R4CH3+R13CH2CHO	2.00E+16	0	83800.
!Mech Franssoldati			
C2H5CHO+R1H=H2+R25C2H5CO	1.17E+11	0.0	6000
!Decottignies et al.2002.			
C2H5CHO+B10=R2OH+R25C2H5CO	5.000e+12	0.0	
1.790e+03 !Curran et al. Fuel (2011) 90(1) 331-338.			
C2H5CHO+R2OH=H2O+R25C2H5CO	2.690e+10	0.760	
-3.400e+02 !Curran et al. Fuel (2011) 90(1) 331-338.			
R25C2H5CO=B2CO+R11C2H5	2.95E+12	0.0	11100.0
!Decottignies et al.2002.			

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!\*\*\*\*\*

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

! REACTIONS DES ESPECES NON OXYGENES EN C4 !  
 !\*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C4H2 \*\*\*\*\* (CH//CC//CH) diacetylene \*\*\*\*\* !

R9C2H+R9C2H=C4H2 <TSAng86>!	1.8E13	0.0	0.0	!
2C2H2=C4H2+H2 <LEUnG95>!	1.5E13	0.0	42.7E3	!
C2H2+R9C2H=C4H2+R1H BAULCH94!	9.0E13	0.0	0.0	!
!C4H2+R1H=C2H2+R9C2H <MEREDITH86>!	6.0E14	0.0	15.4E3	!
C4H2+R20H=>R5CHO+C3H2 <LEEDS-website>!	6.7E12	0.0	-0.4E3	!
C4H2+O2=R12CHCOZ+R12CHCOZ <HIDAKA02>!!!	9.6E12	0.0	31.1E3	!
C4H2+R9C2H=>C6H2+R1H <MEREDITH86>!	4.0E13	0.0	0.0	!
C6H2+R1H=>C4H2+R9C2H <MEREDITH86>!	9.3E14	0.0	15.1E3	!

!\*\*\*\*\* REACTIONS DE nC4H3 \*\*\*\*\* (ΓCH//CHC//CH) \*\*\*\*\*!

nC4H3(+M)=C4H2+R1H(+M) <MILLER92>!	1.0E14	0.0	36.0E3	!
LOW /1.0E14 0.0 30E3/ TROE / 1.0 1.0 1.0E8/				
C3H3+B4CH=nC4H3+R1H <MILLER92>!	7.0E13	0.0	0.0	!
!C3H3+B4CH=nC4H3+R1H <MILLER92>!	5.0E13	0.0	0.0	!
R9C2H+R10C2H3V=nC4H3+R1H <TSAng86>!	1.8E13	0.0	0.0	!
nC4H3+R1H=iC4H3+R1H <WAnG97>20Torr!	2.4E11	0.79	2.41E3	!
nC4H3+R1H=C4H2+H2 <0.5*la cst de la react(c2h3+h)>!	0.6E13	0.0	0.0	!
2C2H2=nC4H3+R1H <LEUnG95>!	1.0E12	0.0	64.1E3	!
nC4H3+R20H=C4H2+H2O <0.5* la cst de la react(c2h3+oh)>!	1.5E13	0.0	0.0	!
!***				
!nC4H3+C2H2=C6H4#+R1H <WESTMORELANd89, p=2.6kPa>!	1.64E9	0.73	12.2E3	!
nC4H3+C2H2=C6H4#+R1H <WESTMORELANd89, p=101kPa>!	3.0E-11	6.48	6.6E3	!
!***				
!nC4H3+C2H2=1C6H4+R1H <WESTMORELANd89, p=2.6kPa>!	29.6	3.33	9.6E3	!
nC4H3+C2H2=1C6H4+R1H <WESTMORELANd89, p=101kPa>!	2.77E-7	5.59	6.0E3	!
!***				

!nC4H3+C2H2=1C6H5	1.73E11	-0.41	4.0E3	!
<WESTMORELANd89, p=2.6kPa>!				
nC4H3+C2H2=1C6H5	6.17E15	-1.51	4.8E3	!
<WESTMORELANd89, p=101kPa>!				
!***				
!nC4H3+C2H2=C6H5#	3.33E24	-3.89	9.2E3	!
<WESTMORELANd89, p=2.6kPa>!				
nC4H3+C2H2=C6H5#	7.0E14	-0.86	6.4E3	!
<WESTMORELANd89, p=101kPa>!				
!***				

!\*\*\*\*\* REACTIONS DE iC4H3 \*\*\*\*\* (CH2//CΓC///CH) \*\*\*\*\*

iC4H3=nC4H3	1.5E13	0.0	67.8E3	!
<LEUnG95>!				
iC4H3(+M)=C4H2+R1H(+M)	1.0E14	0.0	55.0E3	!
<MILLER92>!				
LOW /2.0E15 0.0 48E3/				
TROE /1.0 1.0 1.0E8/				
C3H2+B5CH2=iC4H3+R1H	1.2E14	0.0	0.8E3	!
as(7)<BAULCH94>!				
iC4H3+R1H=2C2H2	2.40E19	-1.6	2800	!
<WAnG97>20Torr! !				
C3H3+B4CH=iC4H3+R1H	7.0E13	0.0	0.0	!
<MILLER92>!				
iC4H3+R1H=C4H2+H2	1.2E13	0.0	0.0	!
<equiv a la cst de la react(c2h3+h)>!				
iC4H3+B10=CH2COZ+R9C2H	2.0E13	0.0	0.0	!
<MILLER92>!				
iC4H3+R20H=C4H2+H2O	3.0E13	0.0	0.0	!<
equiv a la cst de la react(c2h3+oh)>!				
iC4H3+O2=CH2COZ+R12CHCOZ	1.0E12	0.0	0.0	!
<MILLER92>!				
*				
iC4H3+R10C2H3V=2C3H3	4.0E12	0.0	0.0	!
MILLER 92 !				
iC4H3+R10C2H3V=>1C6H5+R1H	6.0E12	0.0	0.0	!
MILLER 92!				

!\*\*\*\*\* REACTIONS DE C4H4 \*\*\*\*\* (CH2//CHC///CH) vinylacetylene \*\*\*\*\*!

C3H3+B5CH2=C4H4+R1H	4.0E13	0.0	0.0	!
<MILLER92>!				
R10C2H3V+C2H2=>C4H4+R1H	2.0E13	0.0	25.1E3	!
(40, -40)<DOUTE95>!				
C4H4+R1H=>R10C2H3V+C2H2	2.0E13	0.0	12.4E3	!
<DOUTE95>				
C2H4Z+R9C2H=C4H4+R1H	1.2E13	0.0	0.0	!
(50, -50)<TSAnG86>!				
C4H4+R1H=nC4H3+H2	2.0E7	2.0	15.E3	!
<Miller 92>!				
C4H4+R1H=iC4H3+H2	3.0E7	2.0	5.E3	!
<Miller 92>!				



R9C2H+C4H4=>C2H2+iC4H3 <MEREDITH86>!	4.0E13	0.0	0.0 !
C2H2+iC4H3=>R9C2H+C4H4 <MEREDITH86>!	3.0E13	0.0	27.9E3 !
R10C2H3V+C4H4=>C2H4Z+nC4H3 <MEREDITH86>!	5.0E11	0.0	16.3E3 !
nC4H3+C2H4Z=>R10C2H3V+C4H4 <MEREDITH86>!	3.5E11	0.0	13.4E3 !
R10C2H3V+C4H4=>C2H4Z+iC4H3 <MEREDITH86>!	5.0E11	0.0	16.3E3 !
iC4H3+C2H4Z=>R10C2H3V+C4H4 <MEREDITH86>!	1.3E11	0.0	24.1E3 !
C4H4+C2H2=C6H5#+R1H BENSON !MF	1.0E09	0.0	30.02E3 !
C4H4+R10C2H3V=C6H6#+R1H <LInSTEDT96>!	1.9E12	0.0	2.5E3 !
C4H4+B10=aC3H4+B2C0 <LEUnG95>!	3.0E13	0.0	1.8E3 !
C4H4+B10=pC3H4+B2C0 <MILLER>!	2.7E13	0.0	1.8E3 !
C4H4+R20H=nC4H3+H20 <MILLER92>!	7.5E6	2.0	5.0E3 !
C4H4+R20H=iC4H3+H20 <MILLER92>!	1.0E7	2.0	2.0E3 !
aC3H4+aC3H4=C2H4Z+C4H4 <HIDAKA89>!	1.0E15	0.0	48.0E3 !

!\*\*\*\*\* REACTIONS DE tC4H4 \*\*\*\*\* (CH2//C//C//CH2) \*\*\*\*\*!

tC4H4+R20H=iC4H3+H20 <Marinov>!	2.0E7	2.0	2.0E3 !
tC4H4+R1H=iC4H3+H2 <Marinov>!	3.0E7	2.0	6.0E3 !

!\*\*\*\*\* REACTIONS DE nC4H5 \*\*\*\*\* (ΓCH//CHCH//CH2) \*\*\*\*\*

nC4H5(+M)=R1H+C4H4(+M) <MILLER92>!	1.0E14	0.0	37.0E3 !
LOW /1.00e+14 0.0 30000/			
nC4H5+R1H=C4H4+H2 <WAnG97>!	1.5E13	0.0	0.0 !
nC4H5+R1H=iC4H5+R1H <MILLER92>!	1.0E14	0.0	0.0 !
nC4H5+R4CH3=C5H8 <estimated> !	1.0E13	0.0	0.0 !
nC4H5=C2H2+R10C2H3V <HIDAKA96>!	1.0E14	0.0	43.9E3 !
!***			
!MF car lC6H6 n'intervient qu'ici			
!nC4H5+C2H2=lC6H6+R1H <WESTMORELANd89, p=2.6kPa>!	1.17E-15	7.84	2.0E3 !

!nC4H5+C2H2=1C6H6+R1H <WESTMORELANd89, p=101kPa>! !***	3.47E-15	7.73	2.5E3 !
!nC4H5+C2H2=C6H6#+R1H <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=C6H6#+R1H <WESTMORELANd89, p=101kPa>! !***	1.90E7	1.47	4.2E3 !
!nC4H5+C2H2=1C6H7 <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=1C6H7 <WESTMORELANd89, p=101kPa>! !***	2.38E8	1.18	3.7E3 !
!nC4H5+C2H2=C6H7# <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=C6H7# <WESTMORELANd89, p=101kPa>! !***	8.74E12	-1.27	3.6E3 !
!nC4H5+C2H2=C6H7# <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=C6H7# <WESTMORELANd89, p=101kPa>! !***	7.24E14	-1.38	4.0E3 !
!nC4H5+C2H2=C6H7# <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=C6H7# <WESTMORELANd89, p=101kPa>! !***	1.96E19	-3.35	5.2E3 !
!nC4H5+C2H2=C6H7# <WESTMORELANd89, p=2.6kPa>! nC4H5+C2H2=C6H7# <WESTMORELANd89, p=101kPa>! !***	7.12E21	-3.64	6.3E3 !
!R10C2H3V+nC4H5=1C6H7+R1H <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=1C6H7+R1H <WESTMORELANd89, p=101kPa>! !***	8.28E-28	11.89	5.0E3 !
!R10C2H3V+nC4H5=1C6H7+R1H <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=1C6H7+R1H <WESTMORELANd89, p=101kPa>! !***	3.55E-43	16.16	-0.2E3 !
!R10C2H3V+nC4H5=1C6H8 <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=1C6H8 <WESTMORELANd89, p=101kPa>! !***	2.90E15	-0.78	1.0E3 !
!R10C2H3V+nC4H5=1C6H8 <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=1C6H8 <WESTMORELANd89, p=101kPa>! !***	1.50E13	-0.075	0.1E3 !
!R10C2H3V+nC4H5=C6H8# <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=C6H8# <WESTMORELANd89, p=101kPa>! !***	5.50E15	-1.67	1.5E3 !
!R10C2H3V+nC4H5=C6H8# <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=C6H8# <WESTMORELANd89, p=101kPa>! !***	8.53E13	-1.11	0.8E3 !
!R10C2H3V+nC4H5=C6H6#+H2 <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=C6H6#+H2 <WESTMORELANd89, p=101kPa>! !***	2.80E-7	5.63	-1.9E3 !
!R10C2H3V+nC4H5=C6H6#+H2 <WESTMORELANd89, p=2.6kPa>! R10C2H3V+nC4H5=C6H6#+H2 <WESTMORELANd89, p=101kPa>! !***	1.84E-13	7.07	-3.6E3 !
nC4H5+R20H=C4H4+H2O <WAnG97>!	2.5E12	0.0	0.0 !
!nC4H5+O2=R5CHO+C2H3CHO as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>	1.7e29	-5.31	6.5E3 !MF
nC4H5+O2=R5CHO+C2H3CHO	5.67E28	-5.31	6.5E3 !MF
nC4H5+O2=C2H4Z+B2CO+R5CHO	1.13e29	-5.31	6.5E3 !MF
nC4H5+O2=C4H4+R300H MF as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>	5.19E15	-1.26	3.31e3 !
!***** REACTIONS DE iC4H5 ***** (CH2//CHC <sup>+</sup> //CH2) *****stabilise par resonnance			
iC4H5=nC4H5 <LEUnG95>!	1.5E13	0.0	67.8E3 !

iC4H5(+M)=R1H+C4H4(+M) <MILLER92>!	1.0E14	0.0	50.0E3 !
LOW /2.0E15 0.0 42000/			
iC4H5+R1H=C4H4+H2 <WAnG97>!	3.0E13	0.0	0.0 !
iC4H5+R4CH3=iC5H8 <estimated> !	1.0E13	0.0	0.0 !
2R10C2H3V=iC4H5+R1H <WAnG97>20Torr!	1.5E30	-4.95	13.0E3 !
!***2R10C2H3V=iC4H5+R1H <WAnG97>760Torr!	1.2E22	-2.44	13.7E3 !
iC4H5+R20H=C4H4+H20 <WAnG97>!	5.50E12	0.0	0.0 !
iC4H5+O2=HCHO+CH2CHCO estimй par{O2+C2H3=HCHO+CHO}!	4.5E16	-1.39	1.0E3 !
iC4H5+O2=C4H4+R300H estimй par {O2+C2H3=C2H2+O0H}!	1.34E6	1.61	-400 !

!\*\*\*\*\* REACTIONS DE C4H5-1s \*\*\*\*\* (CH3/CH<sup>+</sup>/C///CH) \*\*\*\*\*stabililise par resonance

!C4H5-1s=R1H+C4H4 <HIDAKA96>!	3.0E13	0.0	45.0E3 !
C4H5-1s=R1H+C4H4 add inverse!	6.0E13	0.0	50.4E3 !
! Les rйactions suivantes sont deduites de celles de C3H3			
C4H5-1s+R1H=C4H4+H2 <MILLER92/BRAUn89>!	2.0E13	0.0	0.0 !
C4H5-1s+B10=R9C2H+CH3CHO <MILLER92/SLAGUE91>!	1.4E14	0.0	0.0 !
C4H5-1s+R20H=C4H4+H20 <MILLER92>!	2.0E13	0.0	0.0 !
C4H5-1s+R20H=R5CHO+sC3H5 <WAnG97>!	4.0E13	0.0	0.0 !
C4H5-1s+O2=R5CHO+B2CO+C2H4Z <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3 !
C4H5-1s+C4H5-1s=C8H10# <STEIn90>shocktube!	1.0E12	0.0	0.0 !

!\*\*\*\*\* REACTIONS DE C4H5-1p \*\*\*\*\* (CH2<sup>+</sup>/CH2/C///CH) \*\*\*\*\*

!C4H5-1p=R1H+C4H4 <HIDAKA96>!	3.0E13	0.0	45.0E3 !
!C4H5-1p=R1H+C4H4 <HIDAKA96>!	4.0E13	0.0	38.8E3 !
C4H5-1p=R9C2H+C2H4Z <HIDAKA96>!	2.0E14	0.0	57.0E3 !
C4H5-1p+O2=C4H4+R300H PAG00!	1.6E12	0.0	5.0E3 !
C4H5-1p=C4H5-1s PAG00!	5.0E12	0.0	37.4E3 !

!\*\*\*\*\* REACTIONS DE C4H5-2 \*\*\*\*\* (CH3/C///C/CH2Γ) \*\*\*\*\*stabililise par  
resonnance

!C4H5-2=R1H+tC4H4 <fromHIDAKA96+5! C4H5-2=R1H+tC4H4 toto!	3.0E13 6.0E13	0.0 0.0	50.0E3 ! 54.3E3 !
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!C4H5-2=iC4H5 <fromHIDAKA96>! C4H5-2=iC4H5 PAG00! C4H5-2+C4H5-2=C8H10# <STEIn90>shocktube!	3.0E13 5.0E12 1.0E12	0.0 0.0 0.0	50.0E3 ! 50.5E3 ! 0.0 !
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! Les rñactions suivantes sont deduities de celles de C3H3

C4H5-2+B10=C3H3+HCHO <MILLER92/SLAGUE91>! C4H5-2+R20H=R10C2H3V+B2CO+R4CH3 <WAnG97>! C4H5-2+O2=CH2COZ+B2CO+R4CH3 <MILLER92/SLAGUE88>!	1.4E14 4.0E13 3.0E10	0.0 0.0 0.0	0.0 ! 0.0 ! 2.9E3 !
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!\*\*\*\*\* REACTIONS DE C4H6Z2 \*\*\*\*\* 1,3 Butadiene (CH2CHCHCH2) \*\*\*\*\*!

!R10C2H3V+R10C2H3V=C4H6Z2 <TSAnG86 P=2.6KPa T=1500>! !R10C2H3V+R10C2H3V=C4H6Z2 <HIDAKA96shocktube>! ! !C4H6Z2=C4H4+H2 <HIDAKA96> !C4H6Z2=iC4H5+R1H <HIDAKA96>! ! !C2H4Z+R10C2H3V=C4H6Z2+R1H <TSAnG86>! ! !C4H6Z2+R1H=nC4H5+H2 <WAnG97>! !C4H6Z2+R1H=iC4H5+H2 <WAnG97>! ! !C4H6Z2+R1H=C4H7-1 ESTIMATED *2! !C4H6Z2+R1H=C4H7Y ESTIMATED *2! !C4H6Z2+R1H=C4H7-1 ESTIMATED !C4H6Z2+R1H=C4H7Y ESTIMATED ! ! !C4H6Z2+R4CH3=nC4H5+CH4 <WU87>!	6.8E12 9.8E14 2.5E15 1.4E15 5.0E11 1.3E6 6.6E5 2.6E13 2.6E13 1.3E13 1.3E13 7.0E13	0.0 -0.5 0.0 0.0 0.0 2.53 2.53 0 0 0 0 0.0	0.0 ! 0.0 ! 94.7E3 ! 98.0E3 ! 7.3E3 ! 12.2E3 ! 9.2E3 ! 3.2E3 ! 1.56E3 ! 3.2E3 ! 1.56E3 ! 18.5E3 !
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!C4H6Z2+R4CH3=iC4H5+CH4 <WU87-3kcal>!	7.0E13	0.0	15.5E3	!
!C4H6Z2+R4CH3=C5H9Y 88 nist!	6.3E10	0.0	7.49E3	! PERRIN
!C4H6Z2+R4CH3=iC5H9 Estimated*2!	1.8E11	0.0	8.0E3	!
!C4H6Z2+R4CH3=C5H9Y PERRIN 88 nist!	6.31E10	0.0	7.49E3	!
!C4H6Z2+R4CH3=iC5H9 Estimated!	9.64E10	0.0	8.0E3	!
!				
!C4H6Z2+R10C2H3V=nC4H5+C2H4Z <HIDAKA96>!	5.0E14	0.0	22.8E3	!
!C4H6Z2+R10C2H3V=iC4H5+C2H4Z <HIDAKA96-3kcal>!	5.0E14	0.0	19.8E3	!
!				
!C4H6Z2+B10=C3H5Y+R1H+B2CO <LEUnG95, BREZInSKY84>!	6.0E08	1.45	0.9E3	!
!				
!R10C2H3V+C4H6Z2=C6H8#+R1H <frenklach >!	7.4E014	-0.66	8.42E3	!
!R10C2H3V+C4H6Z2=C6H8#+R1H <WESTMORELANd89, p=2.6kPa>!	2.28E12	-0.24	9.9E3	!
!R10C2H3V+C4H6Z2=C6H8#+R1H <WESTMORELANd89, p=101kPa>!	4.15E-11	6.39	2.4E3	!
!***				
!R10C2H3V+C4H6Z2=lC6H8+R1H <WESTMORELANd89, p=2.6kPa>!	1.0E10	1.05	14.0E3	!
!R10C2H3V+C4H6Z2=lC6H8+R1H <WESTMORELANd89, p=101kPa>!	2.48E-15	8.20	6.3E3	!
!***				
!C4H6Z2+C2H2=C6H8# <WESTMORELANd89>!	2.3E12	0.0	35.0E3	!
!***				
!MF car lC6H9 n'intervient qu'ici				
!R10C2H3V+C4H6Z2=lC6H9 <WESTMORELANd89, p=2.6kPa>!	5.48E28	-5.31	9.3E3	!
!R10C2H3V+C4H6Z2=lC6H9 <WESTMORELANd89, p=101kPa>!	1.48E12	-0.17	3.2E3	!
!***				
!R10C2H3V+C4H6Z2=C6H9Z# <WESTMORELANd89, p=2.6kPa>!	1.64E29	-6.12	9.6E3	!
!R10C2H3V+C4H6Z2=C6H9Z# <WESTMORELANd89, p=101kPa>!	7.06E13	-1.35	4.0E3	!
!***				
!C4H6Z2+C2H4Z=C6H10# <WESTMORELANd89>!	2.3E10	0.0	27.0E3	!
!				
!C4H6Z2+R20H=nC4H5+H2O <WAnG97>!	6.2E6	2.0	3.4E3	!
!C4H6Z2+R20H=iC4H5+H2O <WAnG97>!	3.1E6	2.0	0.4E3	!
!C4H6Z2+R20H=C3H5Y+HCHO <LInSTEDT96>!	2.8E12	0.0	-0.9E3	!

!C4H6Z2+R20H=CH3CHO+R10C2H3V <fromLIStEDT96>!	5.6E12	0.0	-0.9E3	!
!C4H6Z2+O2=iC4H5+R300H <LEUnG95>!	4.0E13	0.0	57.9E3	!
!C4H6Z2+C3H3=nC4H5+aC3H4 <HIDAKA96>!	1.0E13	0.0	22.5E3	!
!C4H6Z2+C3H3=iC4H5+aC3H4 <HIDAKA96-3kcal>!	1.0E13	0.0	19.5E3	!

!\*\*\*\*\* REACTIONS DE C4H6-12 \*\*\*\*\* (1,2) Butadiene (CH2CCHCH3) \*\*\*\*\*

!C4H6-12=C4H6Z2 <HIDAKA96>!	3.0E13	0.0	65.0E3	!
!C4H6-12=iC4H5+R1H <LEUnG95>!	4.2E15	0.0	92.6E3	!
!C4H6-12+R1H=R10C2H3V+C2H4Z <LEUnG95>!	4.0E11	0.0	0.0	!
!C4H6-12=C3H3+R4CH3 <kingas1500K>!	7.3E14	0.0	75.4E3	!
!C4H6-12+R1H=C4H7-2 <heyberger> !	1.3E13	0.0	1.6E3	!
!C4H6-12+R1H=C4H7Y <heyberger>!	1.2E11	0.69	3.0E3	!
!C4H6-12+R1H=C4H7T <heyberger> !	1.3E13	0.0	3.2E3	!
!C4H6-12+R1H=iC4H5+H2 <asTSAnG91>!	1.7E5	2.5	2.5E3	!
!C4H6-12+R4CH3=iC4H5+CH4 <asTSAnG91>!	2.2E0	3.5	5.7E3	!
!C4H6-12+R11C2H5=iC4H5+C2H6 <asTSAnG91>!	2.2E0	3.5	6.6E3	!
!C4H6-12+B10=iC4H5+R20H <asTSAnG91>!	1.7E11	0.7	5.9E3	!
!C4H6-12+R20H=iC4H5+H2O <asTSAnG91>!	3.1E6	2.0	-0.3E3	!
!C4H6-12+R300H=iC4H5+H2O2 <asTSAnG91>!	9.6E3	2.6	13.9E3	!

!\*\*\*\*\* REACTIONS DE (c-C4H6) \*\*\*\*\* methyl-cyclopropene \*\*\*\*\*

!B6CH2+pC3H4=cC4H6 <LEUnG95>!	1.8E14	0.0	0.0	!
!cC4H6=C4H6Z2 <LEUnG95>!	3.0E13	0.0	42.3E3	!
!cC4H6=C4H6-12 <LEUnG95>!	3.0E13	0.0	43.8E3	!

!\*\*\*\*\* REACTIONS DE (C4H6-1) \*\*\*\*\* 1 Butyne \*\*\*\*\*

!C4H6-1=C4H6-12 <HIDAKA96>!	2.5E13	0.0	65.0E3	!
!C4H6-1=C4H5-1s+R1H Kinga&dH Melius!	7.7E14	0.0	87.9E3	!

!C4H6-1=C4H5-1p+R1H Kingas!	9.1E14	0.0	99.6E3 !
!C4H6-1=>C3H3+R4CH3 <HIDAKA96>!	3.0E15	0.0	75.8E3 !
!C4H6-1+R1H=R4CH3+aC3H4 <HIDAKA96>!	1.3E5	2.5	1.0E3 !
!C4H6-1+R1H=R11C2H5+C2H2 <HIDAKA96>!	6.5E4	2.5	1.0E3 !
!C4H6-1+R1H=R4CH3+aC3H4 <asWAGnER72>!	3.2E12	0.0	1.7E3 !
!C4H6-1+R1H=R11C2H5+C2H2 <asWAGnER72>!	3.2E12	0.0	1.7E3 !
! Les rñactions suivantes sont deduities de celles de 1-C4H8 generes par EXGAS			
!C4H6-1+R1H=H2+C4H5-1s <EXGAS>!	5.4E4	2.5	-1.9E3 !
!C4H6-1+R4CH3=CH4+C4H5-1s <EXGAS>!	1.5E12	0.0	7.1E3 !
!C4H6-1+B10=R20H+C4H5-1s <EXGAS>!	8.8E10	0.7	3.2E3 !
!C4H6-1+R20H=H2O+C4H5-1s <EXGAS>!	3.0E6	2.0	-1.5E3 !
!C4H6-1+O2=>R300H+C4H5-1s <InGHAM95sec>!	1.4E12	0.0	36.0E3 !
!C4H6-1+O2=>R300H+C4H5-1s <InGHAM95sec>!	1.4E12	0.0	41.4E3 !
!C4H6-1+O2=>R300H+C4H5-1s <DAGAUT90sec>!	4.2E12	0.0	49.5E3 !
!C4H6-1+R300H=>H2O2+C4H5-1s <EXGAS>!	6.4E3	2.6	12.4E3 !
! Les rñactions suivantes sont deduities de celles generes par EXGAS pour H primaires			
!C4H6-1+R1H=H2+C4H5-1p <EXGAS>!	2.9E7	2.0	7.7E3 !
!C4H6-1+R4CH3=CH4+C4H5-1p <EXGAS>!MF	3.7	4.0	8.2E3 !
!C4H6-1+B10=R20H+C4H5-1p <EXGAS>!	5.1E13	0.0	7.8E3 !
!C4H6-1+R20H=>H2O+C4H5-1p <EXGAS>!	2.7E6	2.0	-0.4E3 !
!C4H6-1+O2=>R300H+C4H5-1p <EXGAS>!	1.2E13	0.0	49.0E3 !
!C4H6-1+R300H=>H2O2+C4H5-1p <EXGAS>!	6.0E11	0.0	17.0E3 !
! Les rñactions d'addition suivantes sont deduities de celles de pC3H4			
!C4H6-1+B10=R12CHCOZ+R11C2H5 <asWARnATZ84>!	1.5E13	0.0	2.1E3 !
!C4H6-1+R20H=CH2COZ+R11C2H5 <asB00DAGHIANs87>!	4.3E11	0.0	-0.8E3 !
!***** REACTIONS DE (C4H6-2)***** 2 Butyne *****			
!C4H6-2=C4H6Z2 <HIDAKA96>!	3.0E13	0.0	65.0E3 !

!C4H6-2=C4H6-12 <HIDAKA96>!	3.0E13	0.0	67.0E3 !
!C4H6-2=C4H5-2+R1H <HIDAKA96>!	2.0E14	0.0	87.3E3 !
!C4H6-2+R1H=R4CH3+pC3H4 <HIDAKA96>!	2.6E5	2.5	1.0E3 !
!C4H6-2+R1H=R4CH3+pC3H4 <asWAGnER72>	6.5E12	0.0	1.7E3 !

! Les rñactions suivantes sont deduites de celles de pC3H4

!C4H6-2+R1H=C4H5-2+H2 <asTSAnG91*2>!	3.4E5	2.5	2.5E3 !
!C4H6-2+R4CH3=C4H5-2+CH4 <asTSAnG91*2>!	4.4E0	3.5	5.7E3 !
!C4H6-2+B10=B2C0+R10C2H3V+R4CH3 <asWARnATZ84>!	1.5E13	0.0	2.1E3 !
!C4H6-2+B10=R20H+C4H5-2 <asTSAnG91*2>!	1.2E11	0.7	7.6E3 !
!C4H6-2+R20H=B2C0+C2H4Z+R4CH3 <asB00DAGHIANs87>!	4.3E11	0.0	-0.8E3 !
!C4H6-2+R20H=C4H5-2+H2O <asTSAnG91*2>!	6.2E6	2.0	-0.3E3 !
!C4H6-2+O2=C4H5-2+R300H <InGHAM95*2>+4!	4.2E12	0.0	44.0E3 !
!C4H6-2+R300H=C4H5-2+H2O2 <asTSAnG91*2>!	1.9E4	2.6	13.9E3 !

!\*\*\*\*\* Reactions de C4H7-1 (CH2=CH-CH2-CH2.)!

!C4H7-1=C4H7Y ESTIMATED !	3.34E09	1.0	39.1E3 !
!C4H7-1=C4H7V Estimated!	3.3E9	1.0	20.7E3 !
!C4H7-1=C2H4Z+R10C2H3V Estimated!	2.0E13	0.0	35.5E3 !
!C4H7-1+R4CH3=C5H10 Estimated !	2.0E13	0.0	0.0 !
!C4H7-1+R1H=C4H8Y Estimated!	1.0E14	0.0	0.0 !

!\*\*\*\*\* Reactions de C4H7Y (CH3-CH.-CH=CH2)!\*\*\*\*\*stabilise par resonance

!C4H7Y+R1H=C4H8Y asTSANG 91!!	2.0E13	0.0	0.0 !
!C4H7Y+R1H=H2+C4H6Z2 asTSANG 91!!	0.9E13	0.0	0.0 !
!C4H7Y+R1H=H2+C4H6-12 asTSANG 91!	0.9E13	0.0	0.0 !
!C4H7Y+R300H=R20H+C2H3CHO+R4CH3 <Heyberger>!	1.0E15	-0.8	0.0 !
!C4H7Y+R4CH3=iC5H10 Estimated !	0.5E13	0.0	0.0 !



!\*\*\*\*\*Reactions de C4H7V (CH3-CH2-CH=CH.)\*\*\*\*\*!  
 !C4H7V=C4H7Y 1.9E10 1.0 36.3E3 !  
 Heyberger!  
 !C4H7V=R11C2H5+C2H2 2.0E13 0.0 33.0E3 !  
 Heyberger!

!\*\*\*\*\*Reactions de C4H7-2 (CH3-C.=CH-CH3)\*\*\*\*\*!  
 !C4H7-2=C4H7Y 2.9E10 1.0 37.8E3 !  
 ESTIMATED !  
 !C4H7-2=R4CH3+pC3H4 2.0E13 0.0 31.5E3 !  
 ESTIMATED !

!\*\*\*\*\*Reactions de C4H7T (CH2=C.-CH2-CH3)\*\*\*\*\*!  
 !C4H7T=C4H7-1 3.34E09 1.0 40.6E3 !  
 ESTIMATED !  
 !C4H7T=C4H7Y 2.0E13 0.0 47.0E3 !  
 <Heyberger>!  
 !C4H7T=R4CH3+aC3H4 2.0E13 0.0 32.5E3 !  
 ESTIMATED !

!\*\*\*\*\*Reactions du 1-butene!  
 !C4H8Y+O2=C4H7Y+R300H 3.6E12 0.0 38.2E3 !  
 <Heyberger>!  
 !C4H8Y+R1H=C4H7Y+H2 5.4E4 2.5 -1.9E3 !  
 <Heyberger>!  
 !C4H8Y+R20H=>HCHO+R4CH3+C2H4Z 1.4E12 0.0 -1.0E3 !  
 <Heyberger>!  
 !C4H8Y+R20H=R4CH3+C2H5CHO 1.4E12 0.0 -1.0E3 !  
 <Heyberger>!!ds мйса PRF  
 !C4H8Y+R20H=C4H7Y+H2O 3.0E6 2.0 -1.52E3 !  
 <Heyberger>!  
 !C4H8Y+R4CH3=C4H7Y+CH4 1.0E11 0.0 7.3E3 !  
 <Heyberger>!  
 !C2H5CHO+R1H=H2+B2C0+R11C2H5 4.0E13 0.0 4.2E3 !  
 <Heyberger>!  
 !C2H5CHO+R20H=H2O+B2C0+R11C2H5 4.0E12 0.0 0.5E3 !  
 <Heyberger>!

!\*\*\*\*\*reactions de iC4H8\*\*\*\*\*!  
 !iC4H8+R20H=iC3H7+HCHO 1.4E12 0.0 -1040.0 !  
 (idem RF)  
 !iC4H8+R1H=>iC4H7+H2 3.5E5 2.5 2510 !  
 (idem RF)  
 !iC4H8+R20H=>iC4H7+H2O 6.0D+06 2.000 -298.0 !  
 MES 878<C.M.>!(idem RF)  
 !iC4H7+R1H=iC4H8 1.0E14 0.0 0.0 !  
 <estimation>!  
 !iC4H7+R300H=>R20H+HCHO+tC3H5 1.0E15 -0.8 0.0 !  
 <Heyberger>!

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!
*****
**!
!
*****
*****!
!*          MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE
*!
!*
*!
!* efficiency coefficients for O2, CO, CO2, H2O, AR, C6H6#
*!
!
*****
*****!
!*          PRIMARY MECHANISM OF THE OXIDATION OF BENZENE
*!
!
*****
*****!

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!REACTIONS OF BENZENE MOLECULES!

!\*\*\*Umimolecular inititiation!

C6H5#+R1H(+M)=C6H6#(+M)                    1.0E14            0.0            0.0            !  
<WANG97>!

LOW /6.6E75 -16.3 7.0E3/  
TROE /1.0 0.1 585 6113/

O2/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ AR/0.35/ C6H6#/3.0/

!\*\*\*Bimolecular inititiation!

C6H6#+O2=C6H5#+R300H                    6.0E13            0.0            63.4E3        !  
<ALZUETA00>!

!\*\*\*additions!

C6H6#+R1H=C6H7#                    3.2E13            0.0            3.2E3        !  
<MEBEL97>!

C6H6#+B10=C6H50#+R1H                    2.8E13            0.0            4.91E3        !  
<EMDEE92>!

C6H6#+R20H=C6H50H#+R1H                    1.3E13            0.0            10.6E3        !  
<BAULCH94>!

C6H6#+R9C2H=C6H5#C2H+R1H                    5.0E13            0.0            0.0            !  
<WANG97>!

C6H6#+R10C2H3V=styrene+R1H                    7.9E11            0.0            6.4E3        !  
<WANG97>!

!\*\*\*Metatheses!

!\*modif Zhenyu\*!

!C6H6#+R1H=C6H5#+H2                    6.0E8            1.8            16.8E3        !  
<MEBEL97>!

C6H6#+R1H=C6H5#+H2                    1.22E8            2.031            15.88E3        !  
calcul CBS-QB3 Fournet

C6H6#+B10=C6H5#+R20H                    2.0E13            0.0            14.7E3        !  
<LINDSTEDT94>!

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!*modif Zhenyu*!
!C6H6#+R20H=C6H5#+H20          1.6E8          1.42          1.45E3      !
<BAULCH92>!
C6H6#+R20H=C6H5#+H20          1.36E4          2.7           0.6196E3    !as
toluene+R20H=C6H4CH3+H20

!*modif Zhenyu*!
!C6H6#+R300H=C6H5#+H202       5.5E12          0.0           28.9E3      !
<BAULCH94>!
C6H6#+R300H=C6H5#+H202       9.2E12          0.0           28.81E3     !as
toluene+R300H=C6H4CH3+H202

!*modif Zhenyu*!
!C6H6#+R4CH3=C6H5#+CH4        2.0E12          0.0           15.0E3      !
<ZHANG89>!
C6H6#+R4CH3=C6H5#+CH4        2.07E0          3.861         13.3E3      !
calcul CBS-QB3 Fournet

C6H6#+R11C2H5=C6H5#+C2H6      6.3E11          0.0           15.0E3      !
<ZHANG89>!
C6H5#+C3H6Y=C6H6#+C3H5Y      7.94E13         0.0           11.94E3     !MF
<Heckmann,Hippler,Troe(1996)>
C6H6#+nC4H5=C6H5#+C4H6Z2     6.3E11          0.0           15.0E3      !
estimated!
C6H6#+iC4H5=C6H5#+C4H6Z2     6.3E11          0.0           20.0E3      !
estimated!

!REACTIONS OF C6H7# RADICALS!
!***Isomerization!
C6H7#=lC6H7                    2.5E14          0.7           41.8E3      !
<WEISSMAN89!

!***Decomposition by beta-scission!
!C6H7#=>C2H2+nC4H5            2.0E13          0.0           50.0E3      !
estimated!
!Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by
HEYBERGER02!
!***Oxidation!
C6H7#+O2=C6H6#+R300H          7.9E11          0.0           9.9E3       !
estimated!
!Oxidation of an allylic radical as proposed by HEYBERGER02!
!combimations!
C6H7#+R1H=C6H8#                1.0E14          0.0           0.0         !
estimated!
!***Disproportionnations!
C6H7#+R1H=C6H6#+H2            3.3E12          0.0           0.0         !
<RISTORI01>!
C6H7#+R20H=C6H6#+H20          1.0E13          0.0           0.0         !
estimated!
C6H7#+R4CH3=C6H6#+CH4         3.0E12          -0.32         -0.1E3      !
estimated!
C6H7#+C6H7#=C6H6#+C6H8#      8.4E10          0.0           -0.3E3      !
estimated!

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!analogy with the disproportionations of C<sub>3</sub>H<sub>5</sub>Y proposed by TSANG91!

!REACTIONS OF C<sub>6</sub>H<sub>5</sub># RADICALS!

!\*\*\*Isomerization!

C<sub>6</sub>H<sub>5</sub>#=lC<sub>6</sub>H<sub>5</sub> 5.0E13 0.0 72.5E3 !  
<BRAUN89>!

!lC<sub>6</sub>H<sub>5</sub> = ch///c/ch//ch/ch//ch(.)!

lC<sub>6</sub>H<sub>5</sub>=>2C<sub>2</sub>H<sub>2</sub>+R<sub>9</sub>C<sub>2</sub>H 2.0E13 0.0 51.0E3 !  
estimated!

!DH<sub>298</sub> =44kcal/mol, E<sub>add</sub>=7 kcal/mol!

lC<sub>6</sub>H<sub>5</sub>=lC<sub>6</sub>H<sub>4</sub>+R<sub>1</sub>H 2.0E12 0.0  
41.0E3 !estimated!

!lC<sub>6</sub>H<sub>4</sub> = ch///c/ch//ch/c///ch , DH<sub>298</sub> =38kcal/mol, E<sub>add</sub>=3 kcal/mol!

!from BRAUN89 at 1500 K!

!\*\*\*Reactions with O<sub>2</sub>!

C<sub>6</sub>H<sub>5</sub>#+O<sub>2</sub>=C<sub>6</sub>H<sub>5</sub>O<sub>2</sub> 2.2E19 -2.5 0.0 !  
estimated!

C<sub>6</sub>H<sub>5</sub>#+O<sub>2</sub>=C<sub>6</sub>H<sub>5</sub>O# +B<sub>10</sub> 2.6E13 0.0 6.1E3 !  
<FRANK94>!

C<sub>6</sub>H<sub>5</sub>#+O<sub>2</sub>=O C<sub>6</sub>H<sub>4</sub>O +R<sub>1</sub>H 3.0E13 0.0 9.0E3 !  
<FRANK94>!

!as the addition of oxygen to alkyl radicals proposed by GLAUDE99!

!\*\*\*Additions!

C<sub>6</sub>H<sub>5</sub>#+C<sub>2</sub>H<sub>2</sub>=C<sub>6</sub>H<sub>5</sub>#C<sub>2</sub>H+R<sub>1</sub>H 4.0E13 0.0 10.1E3 !  
<MARINOV97>!

C<sub>6</sub>H<sub>5</sub>#+C<sub>6</sub>H<sub>6</sub>#=biphenyl+R<sub>1</sub>H 5.6E12 -0.074 7.5E3 !  
<WANG97>!

!\*\*\*Combinations!

C<sub>6</sub>H<sub>5</sub>#+B<sub>10</sub>=C<sub>5</sub>H<sub>5</sub>#+B<sub>2</sub>C<sub>0</sub> 1.0E14 0.0 0.0 !  
<FRANK94>!

C<sub>6</sub>H<sub>5</sub>#+R<sub>20</sub>H=C<sub>6</sub>H<sub>5</sub>O# 1.0E13 0.0 0.0  
!calculated!

!toluene=C<sub>6</sub>H<sub>5</sub>#+R<sub>4</sub>CH<sub>3</sub> 1.0E16 0.0 97.0E3  
!<COLKET94>!

!calculation by KINGAS!

C<sub>6</sub>H<sub>5</sub>#+R<sub>5</sub>CHO=C<sub>6</sub>H<sub>5</sub>CHO 5.0E12 0.0 0.0 !  
estimated!

C<sub>6</sub>H<sub>5</sub>#+R<sub>10</sub>C<sub>2</sub>H<sub>3</sub>V=styrene 5.0E12 0.0 0.0 !  
estimated!

C<sub>6</sub>H<sub>5</sub>#+R<sub>11</sub>C<sub>2</sub>H<sub>5</sub>=etC<sub>6</sub>H<sub>5</sub> 5.0E12 0.0 0.0 !  
estimated!

C<sub>6</sub>H<sub>5</sub>#+R<sub>300</sub>H=C<sub>6</sub>H<sub>5</sub>O# +R<sub>20</sub>H 5.0E12 0.0 0.0 !  
estimated!

!C<sub>6</sub>H<sub>5</sub>C<sub>3</sub>H<sub>3</sub> n'intervient qu'ici

!C<sub>6</sub>H<sub>5</sub>#+C<sub>3</sub>H<sub>3</sub>=C<sub>6</sub>H<sub>5</sub>C<sub>3</sub>H<sub>3</sub> 3.0E12 0.0 0.0 !  
<D'ANNA98>!

C<sub>6</sub>H<sub>5</sub>#+C<sub>6</sub>H<sub>5</sub>#=biphenyl 3.8E31 -5.75 7.9E3 !  
<WANG97>!

!\*\*\*disproportionations!

C<sub>6</sub>H<sub>5</sub>#+R<sub>20</sub>H=C<sub>6</sub>H<sub>5</sub>O# +R<sub>1</sub>H 5.0E13 0.0 0.0 !  
<ALZUETA00>!

C6H5#+C6H7#=C6H6#+C6H6# 1.0E12 0.0 0.0 !  
<SHANDROSS96>!

!REACTIONS OF PHENYLPEROXY RADICALS!

!\*\*\*Decomposition by beta-scission!

!mfC6H5O2=OC6H4O+R1H 2.0E13 0.0 30.0E3 !  
estimated!

C6H5O2=C5H4O#+R5CHO 2.0E13 0.0 30.0E3 !  
estimated!

!see DA COSTA01!

!MF

C6H5O2+R300H=C6H500H+O2 2.0E11 0.00 -1300  
C6H500H=C6H50#+R20H 1.5E16 0.00 43000

!REACTIONS OF PHENOXY RADICALS!

!\*\*\*CO elimination!

C6H5O#=B2CO+C5H5# 2.5E11 0.0 43.8E3 !  
<BAULCH92>!

!\*\*\*Combinations!

! --C6H5O#+R1H(+M)=C6H5OH#(+M) 2.5E14 0.0 0.0 !  
<FRENKLACH>!

C6H5O#+R1H(+M)=C6H5OH#(+M) 1.0E14 0.0 0.0 !  
estimated!

LOW /1.0E94 -21.84 13.9E3/ !

<FRENKLACH>!

TROE /0.043 304 60000 5896/

O2/0.4/ B2CO/0.75/ C02/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/  
C6H5O#+R1H=C5H6#+B2CO 1.1E53 -10.7 41.4E3 !

<TAN96>!

C6H5O#+B10=OC6H4OH 2.6E10 0.47 0.8E3 !  
<LIN95>!

C6H5O#+B10=OC6H4O+R1H 8.5E13 0.0 0.0 !  
<FRANCK94>!

C6H5O#+B10=C5H5#+C02 1.0E13 0.0 0.0 !  
<FRANCK94>!

!REACTIONS OF HYDROXYPHENOXY RADICALS!

!\*\*\*CO elimination!

OC6H4OH=B2CO+C5H4OH# 7.4E11 0.0 43.8E3 !  
estimated!

!as for phenoxy radicals!

!REACTIONS OF CYCLOPENTADIENYL RADICALS!

!\*\*\*Isomerization!

C5H5#=1C5H5 1.0E14 0.0 45.5E3 !  
<BRAUN89>!

!1C5H5 = ch///c/ch//ch/ch2(.), DH298 =31kcal/mol!

!MF car 1C5H6 n'intervient qu'ici

!1C5H5+R1H=1C5H6 1.0E14 0.0 0.0 !  
estimated!

1C5H5=C3H3+C2H2 estimated! !DH298 =43kcal/mol, Eadd=7 kcal/mol!	2.0E13	0.0	50.0E3	!
!***Reactions with O2!				
C5H5#+O2=R5CHO+C4H4O <ZHONG98>!	1.2E19	-2.48	11.0E3	!
!***Combinations!				
C5H6# = C5H5# + R1H ! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>	5.0E15		0.00	7.87E4
C5H5#+B10=C5H40#+R1H <ZHONG98>!	5.8E13	-0.02	0.02E3	!
C5H5#+B10=>2C2H2+R5CHO <ZHONG98>!	3.2E13	-0.17	0.44E3	!
C5H5#+R20H=>C4H6Z2+B2CO [PENGLAN- RODA]	4e14	0.0	4500	!
C5H5#+R20H=C5H50H# calculated!	1.0E13	0.0	0.0	!
C5H5#+R300H=C5H50#+R20H calculated!	3.0E12	0.0	0.0	!
!calculation by KINGAS!				
C5H5#+C5H5#=>C10H10# estimated!	2.0E12	0.0	0.0	!
C10H10#=>C5H5#+C5H5# calculated!	3.2E15	0.0	57.5E3	!
!***disproportionnations!				
C5H5#+R300H=>C5H6#+O2 estimated!	2.5E9	1.0	3.5E3	!
!estimated as for allylic radicals (HEYBERGER02)/10!				
!REACTIONS OF CYCLOPENTADIONYL RADICALS!				
!***Decompositions by beta-scission!				
C5H50#=>2C2H2+R5CHO estimated!	2.0E13	0.0	30.0E3	!
C5H50#=C5H40#+R1H estimated!	2.0E13	0.0	30.0E3	!
!see DA COSTA01!				
!***Combinations!				
C5H50#+R1H=C5H50H# estimated!	1.0E14	0.0	0.0	!
!***no disproportionnations considered!				
!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!				
C5H40H#+O2=C5H40#+R300H estimated!	1.0E13	0.0	5.0E3	!
C5H40H#+R1H=C5H50H# estimated!	1.0E14	0.0	0.0	!
C5H40H#+B10=C02+C2H2+R10C2H3V estimated!	3.2E13	-0.17	0.44E3	!

!C5H40H##+R300H=>R20H+C02+R10C2H3V+C2H2 3.0E12 0.0 0.0 !  
 estimated!  
 C5H40H##+R300H=>R20H+R20H+C5H40# 3.0E12 0.0 0.0 ! mf  
 C5H40H##+R300H=>C5H50H##+O2 2.5E9 1.0 3.5E3 !  
 estimated!  
 !Reactions derived from those of cyclopentadienyl radicals!  
 C5H40H##+C6H50#=C5H40##+C6H50H# 1.0E12 0.0 0.0 !  
 estimated!

!  
 \*\*\*\*\*  
 \*\*\*\*\*!  
 !\*  
 !\* SECONDARY MECHANISM OF THE OXIDATION OF BENZENE!!\*  
 !  
 \*\*\*\*\*  
 \*\*\*\*\*!

!REACTIONS OF ORTHOBENZOQUINONE!  
 OC6H40=>C5H40##+B2C0 1.0E12 0.0 40.0E3 !  
 <ALZUETA00>!  
 OC6H40+R1H=>2B2C0+C2H2+R10C2H3V 5.2E13 0.0 3.2E3 !  
 estimated!  
 !estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!  
 !OC6H40+R1H=>H2+2B2C0+C2H2+R9C2H 1.6E6 2.5 9.8E3 !  
 estimated!  
 !OC6H40+R20H=>H2O+2B2C0+C2H2+R9C2H 4.4E6 2.0 1.4E3 !  
 estimated!  
 !estimated as the metathesis of 4 tertiary vinylic H-atoms (HEYBERGER02)!

!REACTIONS OF PHENOL AND DERIVED RADICALS!  
 C6H50H##=C5H6##+B2C0 1.0E12 0.0 61.2E3 !  
 <HORN98>!

C6H50H##+O2=R300H+C6H50# 1.0E13 0.0 38.9E3 !  
 <ALZUETA00>!

C6H50H##+B10=OC6H40H+R1H 1.6E13 0.0 3.4E3 !  
 estimated!

!as the addition of O-atoms to toluene (DACOSTA01)!  
 C6H50H##+R1H=C6H50##+H2 1.2E14 0.0 12.4E3 !  
 <ALZUETA00>!  
 C6H50H##+B10=C6H50##+R20H 1.3E13 0.0 2.9E3 !  
 <ALZUETA00>!  
 C6H50H##+R20H=C6H50##+H2O 1.4E8 1.4 -0.96E3 !  
 <SHANDROSS96>!  
 C6H50H##+R300H=C6H50##+H2O2 1.0E12 0.0 10.0E3 !  
 <ALZUETA00>!

C6H50H##+R4CH3=C6H50##+CH4 <MULCAHY65>!	1.8E11	0.0	7.7E3	!
C6H50H##+C6H5#=C6H50##+C6H6# <ALZUETA00>!	4.9E12	0.0	4.4E3	!
!C6H50H##+C5H5#=C6H50##+C5H6# estimated!	4.9E11	0.0	9.4E3	!
!C6H50H##+C3H5Y=C6H50##+C3H6Y estimated!	4.9E11	0.0	9.4E3	!
!C6H50H##+iC4H5=C6H50##+C4H6Z2 estimated!	4.9E11	0.0	9.4E3	!
C6H50H##+C5H5#=C6H50##+C5H6#	2.67e14	0.0	25.238e3	
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>				
C6H50H##+C3H5Y=C6H50##+C3H6Y <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	!mf
C6H50H##+iC4H5=C6H50##+C4H6Z2 !mf <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	

!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!

C6H50H##+R1H=C6H40H##+H2 <SHANDROSS96>!	1.7E14	0.0	16.0E3	!
C6H50H##+B10=C6H40H##+R20H estimated!	2.0E13	0.0	14.7E3	!
C6H50H##+R20H=C6H40H##+H20 <SHANDROSS96>!	1.4E13	0.0	4.6E3	!
C6H50H##+R300H=C6H40H##+H202 estimated!	4.0E11	0.0	28.9E3	!
C6H50H##+R4CH3=C6H40H##+CH4 estimated!	2.0E12	0.0	15.0E3	!
!as the H-abstractions from benzene!				
C6H40H##+O2=OC6H40H+B10 estimated!	2.1E13	0.0	6.1E3	!
!as for phenyl radicals (FRANCK94)!				
C6H40H##+R1H=C6H50H## estimated!	1.0E14	0.0	0.0	!
C6H40H##+R4CH3=HOC6H4CH3	5.0E12	0.0	0.0	!mf

!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!

C5H6##+O2=>C5H5##+R300H <INGHAM94>!	1.4E12	0.0	31.6E3	!
!C5H6##+R1H=C5H7# estimated!	5.2E13	0.0	3.2E3	!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!				
C5H6##+B10=>C5H50##+R1H <ZHONG98>!	8.9E12	-0.15	590.0	!
C5H6##+R1H=C5H5##+H2 <ROY97>!	2.8E13	0.0	2.0E3	!
C5H6##+B10=C5H5##+R20H <ZHONG98>!	4.8E4	2.7	1.1E3	!
C5H6##+R20H=C5H5##+H20 <ZHONG98>!	3.1E6	2.0	0.0	!



C5H6#+R300H=C5H5#+H2O2 <ZHONG98>!	1.1E4	2.6	12.9E3	!
C5H6#+R4CH3=C5H5#+CH4 <ZHONG98>!	1.8E-1	4.0	0.0	!
C5H6#+C3H5Y=C5H5#+C3H6Y astoluene!	1.6E12	0.0	15.1E3	!
C5H6#+nC4H5=C5H5#+C4H6Z2 astoluene!	1.6E12	0.0	11.1E3	!
C5H6#+iC4H5=C5H5#+C4H6Z2 astoluene!	1.6E12	0.0	15.1E3	!
!C5H6#+C3H5Y=C5H5#+C3H6Y estimated!	6.0E12	0.0	0.0	!
!C5H6#+nC4H5=C5H5#+C4H6Z2 estimated!	6.0E12	0.0	0.0	!
!C5H6#+iC4H5=C5H5#+C4H6Z2 <EMDEE92>!	6.0E12	0.0	0.0	!
!C5H7#=>C2H2+C3H5Y estimated!	2.0E13	0.0	35.5E3	!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by HEYBERGER02!				
!C5H7#+O2=C5H6#+R300H estimated!	7.9E11	0.0	5.0E3	!
!oxidation of an alkylic radical!				
!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!				
C5H40#=>2C2H2+B2CO <ALZUETA00>!	5.7E32	-6.76	68.5E3	!
!C5H40#=B2CO+C4H4 roda PENGLOAN!	1.00e12	0.0	53000	!
C5H40#+R1H=B2CO+nC4H5 estimated!	2.6E13	0.0	3.2E3	!
!estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!				
C5H40#+B10=C4H4+C02 <ALZUETA00>!	1.0E13	0.0	2.0E3	!
C5H40#+R1H=C5H30#+H2 idem C6H6#+R1H=C6H5#+H2	8.13E7	2.031	15.88E3	!MF
C5H40#+B10=C5H30#+R20H <ALZUETA00>!	1.4E13	0.0	14.7E3	!
C5H40#+R20H=C5H30#+H2O <ALZUETA00>!	1.1E8	1.42	1.4E3	!
C5H30#=>C2H2+B2CO+R9C2H estimated!	2.0E13	0.0	51.0E3	!
!estimated as the decomposition of lC6H5!				
C5H30#+O2=>C02+C2H2+R12CHCOZ <ALZUETA00>!	9.7E58	-13.47	38.2E3	!
C5H50H#+R1H=C5H50#+H2 <ALZUETA00>!	4.0E13	0.0	6.1E3	!
C5H50H#+B10=C5H50#+R20H <ALZUETA00>!	1.0E13	0.0	4.6E3	!

C5H5OH#+R2OH=C5H5O#+H2O 1.0E13 0.0 1.7E3 !  
<ALZUETA00>!

!Estimated from the same reaction for CH3OH!

C5H5OH#+R1H=C5H4OH#+H2 1.4E13 0.0 2.0E3 !  
estimated!

C5H5OH#+B10=C5H4OH#+R2OH 4.8E4 2.7 1.1E3 !  
estimated!

C5H5OH#+R2OH=C5H4OH#+H2O 1.5E6 2.0 0.0E3 !  
estimated!

!estimated from the same reaction for cyclopentadiene!

!REACTIONS OF VINYLKETENE!

!additions decomposition

C4H4O+R1H=>R10C2H3V+CH2COZ 1.3E13 0.0 3.0E3 !  
estimated!

C4H4O+R1H=>C2H4Z+R12CHCOZ 1.3E13 0.0 3.0E3 !  
estimated!

C4H4O+R1H=>sC3H5+B2CO 1.3E13 0.0 1.5E3 !  
estimated!

C4H4O+R2OH=>C2H3CHO+R5CHO 1.4E12 0.0 -1.0E3 !  
estimated!

C4H4O+R2OH=>CO2+C3H5Y 1.4E12 0.0 -1.0E3 !  
estimated!

C4H4O+B10=>R13CH2CHO+R12CHCOZ 6.0E4 2.56 -1.1E3 !  
estimated!

C4H4O+B10=>2CH2COZ 6.0E4 2.56 -1.1E3 !  
estimated!

!estimated as the addition of radicals to a double bond (HEYBERGER02)!

!metatheses/decomposition

C4H4O+R1H=>C2H2+R12CHCOZ+H2 8.2E5 2.5 12.3E3 !  
estimated!

C4H4O+R1H=>C3H3+B2CO+H2 4.1E5 2.5 9.8E3 !  
estimated!

C4H4O+R2OH=>C2H2+R12CHCOZ+H2O 2.2E6 2.0 2.8E3 !  
estimated!

C4H4O+R2OH=>C3H3+B2CO+H2O 1.1E6 2.0 1.5E3 !  
estimated!

C4H4O+B10=>C2H2+R12CHCOZ+R2OH 1.2E11 0.7 8.7E3 !  
estimated!

C4H4O+B10=>C3H3+B2CO+R2OH 6.0E10 0.7 8.7E3 !  
estimated!

!estimated as the metatheses of vinylic H-atoms (HEYBERGER02)!

!

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!\* \*

\*!

!\* \*

MECHANISM FOR THE GAS PHASE OXIDATION OF TOLUENE

\*!

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!*                                     *!
!* efficiency coefficients for O2, CO, CO2, H2O, N2, AR, HE, C6H6#
and toluene*!
!*                                     *!
!
*****!
*****!

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!*                                     *!
!* PRIMARY MECHANISM OF THE OXIDATION OF TOLUENE
*!
!*                                     *!
!
*****!
*****!

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!*****!
!*REACTIONS OF TOLUENE MOLECULES*!
!*****!

```

!\*\*UMIMOLECULAR INITIATIONS

```

toluene=benzyl+R1H          2.09E15  0.0  87.51E3  !
<Oehlschlaeger07>! Zhenyu
toluene=C6H5#+R4CH3        2.66E16  0.0  97.88E3  !
<Oehlschlaeger07> Zhenyu

```

!\*\*BIMOLECULAR INITIATION

```

toluene+O2=benzyl+R300H    1.8E12  0.0  39.7E3  !<BAULCH94>!
!toluene+O2=benzyl+R300H  2.18e7  2.50  46045  !
mf<Oehlschlaeger06>!

```

!\*\*ADDITIONS

```

toluene+R1H=C6H6#+R4CH3    5.67E8  1.43  5.65E3  !Calcul CBS-
QB3 Fournet Zhenyu

toluene+B10=OC6H4CH3+R1H   1.7E13  0.0  3.6E3  !<TAPPE89>!
!toluene+R20H=HOC6H4CH3+R1H 2.3E12  0.0  -0.36E3 !<BAULCH92>!
toluene+R20H=HOC6H4CH3+R1H 1.3E13  0.0  10.6E3 !<BAULCH94>as
benzene!

toluene+R20H=C6H50H#+R4CH3 7.83E2  2.884  3.2193E3 !Seta V Nakajima
V Miyoshi JPCA 2006 Zhenyu
!toluene+R20H=C6H50H#+R4CH3 1E5  2.58  1134.0 !Olive as
benzene+OH

```

```

!**METATHESES
!**METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

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```

toluene+R1H=benzyl+H2      2.92E6   2.372   5.81E3   !Calcul CBS-QB3
Fournet Zhenyu
toluene+B10=benzyl+R20H    6.3E11   0.0      0.0      !
<HOFFMANN90>!

toluene+R20H=benzyl+H2O    5.2E09   1.0      0.87E3   !<BAULCH94>!

toluene+R300H=benzyl+H2O2  4.0E11   0.0      14.0E3   !<BAULCH94>!
toluene+R4CH3=benzyl+CH4   3.91E0   3.76     6.98E3   !Calcul CBS-QB3
Fournet Zhenyu

! ajout MF
toluene+R7CH30=benzyl+CH30H 2.12E+10 0.0 3000.0      !PITZ2001
toluene+R8CH300=benzyl+CH300H 1.02E+04 2.5 12339.3 !PITZ2001

!toluene+R5CHO=benzyl+HCHO   3.77E13   0.0 23.7874E3   !MEHL 09 Zhenyu
benzyl+HCHO = toluene+R5CHO      1.26e8   1.9 18.183E3
benzyl+CH3CHO = toluene+R14CH3CO 1.26e8   1.9 18.183E3

toluene+R10C2H3V=benzyl+C2H4Z 4.0e12   0.0      8.0e3      !<COLKET94>!

toluene+C3H5Y=benzyl+C3H6Y   1.6E12   0.0      15.1E3   !<estimated(a)>!
toluene+C3H3=benzyl+pC3H4   1.6E12   0.0      15.1E3   !<estimated(a)>!
toluene+iC4H5=benzyl+C4H6Z2  1.6E12   0.0      15.1E3   !
<estimated(a)>!
toluene+nC4H5=benzyl+C4H6Z2  1.6E12   0.0      11.1E3   !
<estimated(a)>!
toluene+C5H5#=benzyl+C5H6#   1.6E11   0.0      15.1E3   !<estimated(a)>!
!(a) :Rate constant taken equal to that of the H-abstraction with methyl
radicals proposed !
!by COLKETT94 with A divided by 10 for cyclic radicals !
! and with an activation energy 4 kcal/mol higher for resonance
stabilised radicals!

!ajout MF
toluene+C6H5O2=benzyl+C6H500H 1.02E+04 2.5 12339.3      !
PITZ2001

toluene+C6H5#=benzyl+C6H6#   7.9E13   0.0      12.0E3   !<HECKMANN96>!

toluene+C6H50#=benzyl+C6H50H# 1.6E11   0.0      15.1E3   !
<estimated(a)>! peut etre trop rapide
toluene+C6H4CH3=benzyl+toluene 7.9E13   0.0      12.0E3   !
<estimated(b)>!
toluene+OC6H4CH3=benzyl+HOC6H4CH3 1.6E11   0.0      15.1E3   !
<estimated(a)>!
toluene+C6H5CH200=benzyl+C6H5CH200H 4.0E11   0.0      14.0E3   !
<estimated(c)>!

```

toluene+C6H5CH2O=benzyl+C6H5CH2OH 1.6E11 0.0 11.1E3 !  
 <estimated(a)>!  
 toluene+HOC6H4CH2=benzyl+HOC6H4CH3 1.6E11 0.0 15.1E3 !  
 <estimated(a)>!  
 !(b) :Rate constant taken equal to that of the H-abstraction with phenyl  
 radicals proposed !  
 !by HECKMANN96!  
 !(c) :Rate constant taken equal to that of the H-abstraction with HO2  
 radicals proposed !  
 !by BAULCH94!

!\*\*METATHESSES WITH ABSTRACTION OF PHENYLIC H-ATOM!

toluene+R1H=C6H4CH3+H2 1.22E08 2.031 15.88E3 !as  
 C6H6#+R1H=C6H5#+H2 CBS-QB3 Fournet Zhenyu  
 toluene+B10=C6H4CH3+R2OH 2.0E13 0.0 14.7E3 !<estimated(d)>!  
 toluene+R2OH=C6H4CH3+H2O 1.36E4 2.7 0.6196E3 !<Seta06>! in  
 Sakai07 Zhenyu  
 toluene+R300H=C6H4CH3+H2O2 9.2E12 0.0 28.81E3 !<Baulch94>! in  
 Sakai07 Zhenyu  
 toluene+R4CH3=C6H4CH3+CH4 2.07E0 3.861 13.3E3 !as  
 C6H6#+R4CH3=C6H5#+CH4 CBS-QB3 Fournet Zhenyu

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYL RADICALS\*!  
 !\*\*\*\*\*!

!\*\*DECOMPOSITION BY BETA-SCISSION

benzyl=>C5H5#+C2H2 6.0E13 0.0 70.0E3 !<Colket94>!  
 benzyl=>C3H3+C4H4 2.0E14 0.0 83.6E3 !<Colket94>!

!\*\*REACTIONS WITH OXYGEN

benzyl+O2=C6H5CH2OO 4.6E11 0.0 -377.0 !<FENTER94>!  
 benzyl+O2=C6H5CH2O+B10 6.3E12 0.0 40.0E3 !<BREZYNSKY84>!

!\*\*TERMINATION REACTIONS

benzyl+B10=C6H5#+HCHO 3.5E13 0.0 0.0 !<EMDEE92>!  
 benzyl+B10=C6H5CHO+R1H 1.0E14 0.0 0.0 !  
 <estimated(e)>!

!(e) : This rate constant is that proposed by <HIPPLER90-2> divided by 4  
 !(LINSTEDT96?? has used 3.5E13)!

benzyl+R8CH3OO=>C6H5CH2O+R7CH3O 5.0E12 0.0 0.0  
 benzyl+R17C2H5OO=>C6H5CH2O+R15C2H5O 5.0E12 0.0 0.0

benzyl+R2OH=C6H5CH2OH 2.0E13 0.0 0.0 !<HIPLER91>!

!MFbenzyl+R300H=C6H5CH2OOH 5.0E12 0.0 0.0 !<HIPPLER92>!  
 benzyl+R300H=C6H5CH2OOH 8.21E4 2.20 -5.13E3 !MF<da  
 silva-bozzelli- proceedings comb inst 32(2009)287-294>!

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2benzyl=bibenzyl          5.01E12  0.0 0.454E3  !
<Oehlschlaeger05>! in Sakai07 Zhenyu

etC6H5 = benzyl + R4CH3      6.1e15  0.0  75120  !<BAULCH94>!

!*****!
!*REACTIONS OF METHYL PHENYL RADICALS*!
!*****!

!**reactions with oxygen
!mfC6H4CH3+O2=OC6H4CH3+B10      2.6E13  0.0  6.1E3  !
<estimated(f)>!
!mfC6H4CH3+O2=OC6H4O+R4CH3      3.0E13  0.0  9.0E3  !
<estimated(f)>!
!(f) : Rate constant taken equal to that of the similar reaction in the
case of phenyl!
!radicals!

!ajout mf
C6H4CH3+O2=>OOC6H4CH3          3.72E13      -0.22      -711
      !2008DAS/BOZ3566-3575
OOC6H4CH3=>C6H4CH3+O2          6.36E19      -1.372      48.74E3
      !2008DAS/BOZ3566-3575
OOC6H4CH3=>OC6H4CH3+B10        1.27E15      -0.25
      3.85E4      !2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4O+R4CH3        5.0E11      0.00
      46400      !

!***termination reactions!
C6H4CH3+R1H=toluene            1.0E14  0.0  0.0  !
<estimated(g)>!
!(g) : Rate constant taken equal to that of the recombination of H atoms
with alkyl !
!radicals as proposed by Allara!

C6H4CH3+B10=OC6H4CH3          1.0E14  0.0  0.0  !
<estimated(f)>!
C6H4CH3+R2OH=HOC6H4CH3        1.0E13  0.0  0.0  !
<estimated(f)>!
C6H4CH3+R4CH3=C8H10#           1.2E06  1.96  -3.7E3  !
<estimation(fbis)>!
!(fbis) : Rate constant taken equal to that of the similar reaction in
the case of phenyl!
!radicals: Rao, skinner, 1989 J.P.C. (93,1864)!

C6H4CH3+R3OOH=OC6H4CH3+R2OH    5.0E12  0.0  0.0  !
<estimated(f)>!
C6H4CH3 +R1H = benzyl + R1H     1.0E13  0.0  0.0  !<MILLER92>!

!*****!

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!\*REACTIONS OF BENZYL PEROXY RADICALS\*!  
!\*\*\*\*\*!

!\*\*isomerisation-decomposition reactions

C6H5CH2OO=C6H5CHO+R2OH 3.4E9 1.0 37.5E3 !

<estimated(h)>!

!(h) : Rate constant of the isomerisation :!

!A =  $ekbT/h \times rpd \times \exp((Dnirot \times 3.5)/R)$ , Ea = 23 (4 membered transition ring)!

!+ 14.5 (secondary allylic H-atom)!

!\*\*Combination reactions

!MF C6H5CH2OO+R1H=C6H5CH2OOH 1.0E14 0.0 0.0E3 !

<estimated(g)>!

!\*\*dispropotionnation reactions!

C6H5CH2OO+R3OOH=C6H5CH2OOH+O2 2.0E11 0.0 -1.3E3 !

<estimated(i)>!

2C6H5CH2OO=C6H5CH2OH+C6H5CHO+O2 1.4E10 0.0 -725.0 !

<estimated(i)>!

C6H5CH2OO+C6H5CH2OO=2C6H5CH2O+O2 6.3E10 0.0 -725.0 !

<estimated(i)>!

!(i) : Rate constant taken equal to that the disproportionnation of peroxyalkyl radicals !

!as proposed by Warth!

! ajout MF

C6H5CH2OO+R1H=C6H5CH2O+R2OH 3.80E14 -0.19

1.89E3 !<da silva J Chem Theory Comput 2009>

C6H5CH2OO+R1H=C6H5CH2OOH 4.35e60 -15.92 11.40E3

!<da silva J Chem Theory Comput 2009>

C6H5CH2OO+R1H=benzyl+R3OOH 1.96E4 2.47 1.43E3

!<da silva J Chem Theory Comput 2009>

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

!\*REACTIONS OF BENZYL ALCOXY RADICALS\*!

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

!\*\*Decomposition by beta-scission \*\*\*\*\*

C6H5CH2O=R1H+C6H5CHO 2.0E13 0.0 27.5E3 !

<estimated(j)>! INHIBE

C6H5CH2O=C6H5#+HCHO 2.0E13 0.0 27.5E3 !

<estimated(j)>! ACCELERE

!DH = 23.59 kcal/mol!

!(j) For these beta-scissions involving the breaking of a C-C or a C-H bond, A-factor !

!is an average value for beta-scissions [Heyberger] and activation energies have been!

! estimated from thermochemistry and to obtain the best results!

!C6H5CH2O=R1H+C6H5CHO 5.26E28 -5.081 22.25E3 !  
mf<Da silva-bozzelli J phys chem 25(2009)6979>!  
!C6H5CH2O=C6H6#+R5CHO 2.37E32 -6.095 28.81E3 !  
mf<Da silva-bozzelli J phys chem 25(2009)6979>!  
!C6H5CH2O=C6H5#+HCHO 7.21E33 -6.21 36.85E3 !  
mf<Da silva-bozzelli J phys chem 25(2009)6979>!

!C6H5CH2O=R1H+C6H5CHO 1.00e14 0.00 2.91e4 !  
mf<Mehl Proc comb inst 33(2011)193>!  
!C6H5CH2O=C6H5#+HCHO 1.46e20 -2.00 3.51e4 !  
mf<Mehl Proc comb inst 33(2011)193>!

!\*\*\*reactions with oxygen  
C6H5CH2O+O2=R300H+C6H5CHO 6.0E10 0.0 1.6E3 !  
<estimated(k)>!  
!(k) : Rate constant taken equal to that of the similar reaction in the  
case of ethoxy!  
!radicals as proposed by BAULCH92!

!\*\*\*\*\*!  
!\*REACTIONS OF CRESOXY RADICALS\*!  
!\*\*\*\*\*!

!\*\*OC6H4CH3=HOC6H4CH2 2.9E9 1.0 3.2E3 !<estimated(h')>!  
!(h') : Rate constant of the isomerisation :!  
!A =  $k_bT/h \times rpd \times \exp((Dnirotx3.5)/R)$ , Ea = 5.9 + 5 (5 membered  
transition ring)!  
!+ 7.3 (primary alkyllic H-atom by CH3O)!

!OC6H4CH3=HOC6H4CH2 1.1E9 1.0 22.9E3 !  
! A x2/5 only for ortho isomere, Ea= 5.9(RSE)+17 (H allylique p by R00.  
close bde)

!\*\*CO elimination with rearrangement  
!OC6H4CH3=>R1H+C6H6#+B2CO 7.5E11 0.0 43.8E3 !  
<FRANCK94>!  
OC6H4CH3=>R1H+C6H6#+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
!OC6H4CH3=>R10C2H3V+C4H4+B2CO 3.0E11 0.0 43.8E3!<FRANCK94>!  
!OC6H4CH3=>C2H2+iC4H5+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
!OC6H4CH3=>C2H2+C4H4+R1H+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
OC6H4CH3=>C3H3+aC3H4+B2CO 1.5E11 0.0 43.8E3 !  
<FRANCK94>!

!\*\*termination reactions!  
OC6H4CH3+R1H=HOC6H4CH3 1.0E14 0.0 0.0E3 !  
<estimated(g)>!



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!*****!
!*REACTIONS OF BENZALDEHYDE AND DERIVED RADICALS*!
!*****!

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! Amorcage
!C6H5CHO+O2=C6H5CO+R300H      2.0E13  0.0  38.9E3      !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R300H      7.0E11  0.0  39.5E3 !RODA RODA
C6H5CHO = C6H5CO + R1H      3.98E15 0.0 83.74E3 !NIST GRELA86!

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! Addition
C6H5CHO+R1H=C6H6#+R5CHO      5.8E13  0.0  8.1E3      !
<estimated(m)>!
!(m) : Rate constant taken equal to that of the same reaction in the case
of toluene!

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```

! Metatheses
C6H5CHO+R1H=C6H5CO+H2      4.0E13  0.0  3.2E3      !
<estimated(n)>!
!(n) : Rate constant estimated from the parameters proposed by WARNATZ84
for acetaldehyde!
!with an activation energy 1 kcal/mol lower due to the resonance
stabilisation of the!
! obtained radical!

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C6H5CHO+B10=C6H5CO+R20H      6.0E12  0.0  1.8E3 !<BAULCH94>!
C6H5CHO+R20H=C6H5CO+H2O      7.8E12  0.0  0.0 !<BAULCH94>!
C6H5CHO+R300H=C6H5CO+H2O2  3.0E12  0.0  11.0E3 !<estimated(o)>!
C6H5CHO+R4CH3=C6H5CO+CH4  2.0E-6  5.6  2.5E3 !MF <BAULCH94>!

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C6H5CHO+R11C2H5=C6H5CO+C2H6  1.3E12  0.0  7.5E3 !<estimated(o)>!
!(o) : Rate constant estimated from the parameters proposed by BAULCH94
(HO2, CH3) and by !
!HOLHEIN70 (C2H5) for acetaldehyde with an activation energy 1 kcal/mol
lower due to the !
!resonance stabilisation of the obtained radical!

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```

C6H5CHO+C3H5Y=C6H5CO+C3H6Y  1.3E12  0.0  11.5E3      !
<estimated(p)>!
C6H5CHO+iC4H5=C6H5CO+C4H6Z2  1.3E12  0.0  11.5E3      !
<estimated(p)>!

```

$C_6H_5CHO+nC_4H_5=C_6H_5CO+C_4H_6Z_2$       1.3E12      0.0      7.5E3      !  
 <estimated(p)>!  
 $C_6H_5CHO+benzyl=toluene+C_6H_5CO$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+C_6H_5O\# =C_6H_5CO+C_6H_5OH\#$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+OC_6H_4CH_3=C_6H_5CO+HOC_6H_4CH_3$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+C_5H_5\# =C_6H_5CO+C_5H_6\#$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>

!(p) :Rate constant taken equal to that of the H-abstraction with ethyl radicals !  
 ! with A divided by 10 for cyclic radicals and with an activation energy !  
 !4 kcal/mol higher for resonance stabilised radicals!

$C_6H_5CHO+HOC_6H_4CH_2=C_6H_5CO+HOC_6H_4CH_3$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+C_6H_5\# =C_6H_5CO+C_6H_6\#$       1.3E11      0.0      11.5E3      !<estimated(p)>

$C_6H_5CO=C_6H_5\#+B_2CO$       4E14      0.0      29.5e3      !  
 <SOLLY71>!

!Author(s): Solly, R.K.; Benson, S.W.  
 !Title: Kinetics of the gas-phase unimolecular decomposition of the benzoyl radical  
 !Journal: J. Am. Chem. Soc.  
 !Volume: 93  
 !Page(s): 2127  
 !Year: 1971

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYL HYDROPEROXYDE\*!  
 !\*\*\*\*\*!

$!MFC_6H_5CH_2OOH=C_6H_5CH_2O+R_2OH$       1.5E16      0.0      42.0E3      !  
 <estimated(r)>!  
 !(r) : Rate constant taken equal to that the decomposition of hydroperoxide species !  
 ! proposed by Bounaceur <SAHETCHIAN>!  
 $!MFC_6H_5CH_2OOH=C_6H_5CH_2O+R_2OH$       2.03E47      -10.27  
           50.71E3      !<da silva J Chem Theory Comput 2009>  
 $C_6H_5CH_2OOH=C_6H_5CH_2O+R_2OH$       3.29E13      0.42      39.89E3      !  
 MF<da silva Proc comb inst 32(2009)287-294>  
 $C_6H_5CH_2OOH=C_6H_5CHO+H_2O$       7.45E8      1.19  
           46.04E3      !MF<da silva Proc comb inst 32(2009)287-294>

!\*\*\*\*\*!  
 !\*REACTIONS OF CRESOL AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

! amorcage  
 $HOC_6H_4CH_3+O_2=OC_6H_4CH_3+R_3OOH$       1.0E13      0.0      38.9E3      !  
 <estimated(s)>! ralenti

!A=1E13 pour phenol!  
 !(s) : Rate constant taken equal to that of the same reaction for phenol !

!HOC6H4CH3+O2=HOC6H4CH2+R300H 2.1E13 0.0 38.0E3 !  
 <EMDEE92\*2>!  
 HOC6H4CH3+O2=HOC6H4CH2+R300H 2.1E12 0.0 38.6E3 !  
 RODA <estimated(aaa)>!

! addition  
 HOC6H4CH3+R1H=C6H5OH#+R4CH3 5.8E13 0.0 8.1E3  
 !<estimated(t)>!  
 !(t) : Rate constant taken equal to that of the same reaction for toluene  
 !

!HOC6H4CH2+B10=C6H4OH#+HCHO 8E13 0.0 0.0

! metatheses  
 HOC6H4CH3+R1H=OC6H4CH3+H2 1.2E14 0.0 12.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+B10=OC6H4CH3+R20H 1.3E13 0.0 2.9E3 !  
 <estimated(s)>!  
 HOC6H4CH3+R20H=OC6H4CH3+H2O 1.4E8 1.4 -0.96E3 !  
 <estimated(s)>!  
 HOC6H4CH3+R300H=OC6H4CH3+H2O2 1.0E12 0.0 10.0E3 !  
 <estimated(s)>!  
 HOC6H4CH3+R4CH3=OC6H4CH3+CH4 1.8E11 0.0 7.7E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C6H5#=OC6H4CH3+C6H6# 4.9E12 0.0 4.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C5H5#=OC6H4CH3+C5H6# 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH# 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!

HOC6H4CH3+R1H=HOC6H4CH2+H2 1.2E14 0.0 8.4E3 !  
 <estimated(t)>!  
 HOC6H4CH3+B10=HOC6H4CH2+R20H 6.3E11 0.0  
 0.0 !<estimated(t)>!  
 HOC6H4CH3+R20H=HOC6H4CH2+H2O 5.2E9 1.0 0.87E3 !  
 <estimated(t)>!  
 HOC6H4CH3+R300H=HOC6H4CH2+H2O2 4.0E11 0.0 14.0E3 !  
 <estimated(t)>!  
 HOC6H4CH3+R4CH3=HOC6H4CH2+CH4 1.6E12 0.0 11.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C3H5Y} = \text{HOC6H4CH2} + \text{C3H6Y}$  1.6E12 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C3H3} = \text{HOC6H4CH2} + \text{pC3H4}$  1.6E12 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{iC4H5} = \text{HOC6H4CH2} + \text{C4H6Z2}$  1.6E12 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{nC4H5} = \text{HOC6H4CH2} + \text{C4H6Z2}$  1.6E12 0.0 11.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C5H5\#} = \text{HOC6H4CH2} + \text{C5H6\#}$  1.6E11 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H5\#} = \text{HOC6H4CH2} + \text{C6H6\#}$  7.9E13 0.0 12.0E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H50\#} = \text{HOC6H4CH2} + \text{C6H50H\#}$  1.6E11 0.0 15.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H4CH3} = \text{HOC6H4CH2} + \text{toluene}$  7.9E13 0.0 12.0E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{OC6H4CH3} = \text{HOC6H4CH2} + \text{HOC6H4CH3}$  1.6E11 0.0  
 15.1E3 !<estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H5CH200} = \text{HOC6H4CH2} + \text{C6H5CH200H}$  4.0E11 0.0  
 14.0E3 !<estimated(t)>!

$\text{HOC6H4CH3} + \text{C6H5CH20} = \text{HOC6H4CH2} + \text{C6H5CH20H}$  1.6E11 0.0  
 11.1E3 !<estimated(t)>!

$\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH200}$  4.6E11 0.0 -377.0 !  
 <estimated(u)>!

$\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH20} + \text{B10}$  6.3E12 0.0 40.0E3 !  
 <estimated(u)>!

$\text{HOC6H4CH2} + \text{R300H} = \text{HOC6H4CH20} + \text{R20H}$  5.0E12 0.0 0.0 !  
 <estimated(u)>!

!(u) : Rate constant taken equal to that of the same reaction for benzyl radicals !

$\text{HOC6H4CH2} + \text{R1H} = \text{HOC6H4CH3}$  1.0E14 0.0 0.0 !  
 <estimated(g)>!

$\text{HOC6H4CH2} + \text{R4CH3} = \text{C6H50H\#} + \text{C2H4Z}$  5.0E12 0.0 0.0 !  
 <estimated(g)>!

$\text{HOC6H4CH200} = \text{C6H40HCHO} + \text{R20H}$  3.4E9 1.0 37.5E3 !<estimated(v)>!  
 !(v) : Rate constant taken equal to that of the same reaction for benzyl peroxy radicals !

$\text{HOC6H4CH20} = \text{R1H} + \text{C6H40HCHO}$  2.0E13 0.0 27.5E3 !  
 <estimated(w)>!

$\text{HOC6H4CH20} = \text{C6H40H\#} + \text{HCHO}$  2.0E13 0.0 27.5E3 !  
 <estimated(w)>!

$\text{HOC6H4CH20} + \text{O2} = \text{R300H} + \text{C6H40HCHO}$  6.0E10 0.0 1.6E3 !  
 <estimated(w)>!

!(w) : Rate constant taken equal to that of the same reaction for benzyl alcoxy radicals !

$\text{C6H40HCHO} + \text{R1H} = \text{C6H40HCO} + \text{H2}$  4.0E13 0.0 3.2E3 !<estimated(x)>!  
 $\text{C6H40HCHO} + \text{B10} = \text{C6H40HCO} + \text{R20H}$  6.0E12 0.0 1.8E3 !  
 <estimated(x)>!

$C_6H_4OHC_6H_4O + R_2OH = C_6H_4OHC_6H_4O + H_2O$       7.8E12      0.0      0.0      !  
 <estimated(x)>!  
 $C_6H_4OHC_6H_4O + R_3OOH = C_6H_4OHC_6H_4O + H_2O_2$       3.0E12      0.0      11.0E3      !  
 <estimated(x)>!  
 $C_6H_4OHC_6H_4O + R_4CH_3 = C_6H_4OHC_6H_4O + CH_4$       2.0E-6      5.6      1.5E3      !  
 <estimated(x)>!  
 !(x) : Rate constant taken equal to that of the same reaction for  
 benzaldehyde !

$C_6H_4OHC_6H_4O = C_6H_4OH\# + B_2CO$       2.0E13      0.0      30.5E3      !  
 <estimated(y)>  
 !(y) : Rate constant taken equal to that of the same reaction for  $C_6H_5CO$   
 radicals !

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

$C_6H_5CH_2OH + O_2 = R_3OOH + C_6H_5CHOH$       1.4E12      0.0      34.0E3      !RODA  
 <estimated(aaa)>!  
 $C_6H_5CH_2OH + O_2 = C_6H_5CH_2O + R_3OOH$       2.0E14      0.0      41.4E3      !  
 <EMDEE92>!

$C_6H_5CH_2OH + R_1H = C_6H_6\# + R_6CH_2OH$       5.8E13      0.0      8.1E3      !  
 <estimated(t)>!

$C_6H_5CH_2OH + R_1H = C_6H_5CHOH + H_2$       8.0E13      0.0      6.4E3      !<estimated(t')>!  
 $C_6H_5CH_2OH + B_{10} = C_6H_5CHOH + R_{20H}$       4.2E11      0.0      -2.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + R_{20H} = C_6H_5CHOH + H_2O$       3.5E9      1.0      -1.13E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + R_{300H} = C_6H_5CHOH + H_2O_2$       2.7E11      0.0      12.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + R_4CH_3 = C_6H_5CHOH + CH_4$       1.1E12      0.0      9.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_3H_5Y = C_6H_5CHOH + C_3H_6Y$       1.1E12      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + iC_4H_5 = C_6H_5CHOH + C_4H_6Z_2$       1.1E12      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + nC_4H_5 = C_6H_5CHOH + C_4H_6Z_2$       1.1E12      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_6H_5\# = C_6H_5CHOH + C_6H_6\#$       5.2E13      0.0      10.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_6H_4CH_3 = C_6H_5CHOH + toluene$       5.2E13      0.0      10.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_6H_5O\# = C_6H_5CHOH + C_6H_5O\#$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + benzyl = C_6H_5CHOH + toluene$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + OC_6H_4CH_3 = C_6H_5CHOH + HOC_6H_4CH_3$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + HOC_6H_4CH_2 = C_6H_5CHOH + HOC_6H_4CH_3$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!

C6H5CH2OH+C5H5#=C6H5CHOH+C5H6# 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!  
 !t': estimated as toluene with A x(2/3) to take into account the number  
 of abstractable !  
 !H atoms and Ea -2 kcal/mol due to the OH substitution!

C6H5CHOH=C6H5CHO+R1H 2.0E13 0. 36.373E3 !MF  
 DHR=36.79 correlation baptiste E=0.6\*DHR+14.3  
 !R15C2H5O=CH3CHO+R1H 2.0E14 0. 23.3E3 !(243,-  
 243)<HEICKLEN88NIST>!

!\*\*\*\*\*!  
 !\*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

!\*\* Amorзages monomolйculaires

etC6H5 = R1H + C8H9# 4.3E14 0.0 83.6E3 !<kingas>!

!\*\* Amorзages bimolйculaires

etC6H5+O2=C8H9#+R300H 1.4E12 0.0 34.0E3 !  
 <estimated(aaa)>!  
 etC6H5+O2=C8H9#-1+R300H 1.2E13 0.0 49.0E3 !  
 <exgas>!

!\*\* Additions ipso

etC6H5+R1H=C6H6#+R11C2H5 5.8E13 0.0 8.1E3 !  
 <estimated(t)>!

!\*\* Metatheses

etC6H5+R1H=C8H9#+H2 8.0E13 0.0 6.4E3  
 !<estimated(t'')>!  
 etC6H5+B10=C8H9#+R20H 4.2E11 0.0 -2.0 !  
 <estimated(t'')>!  
 etC6H5+R20H=C8H9#+H20 3.5E9 1.0 -1.13E3 !  
 <estimated(t'')>!  
 etC6H5+R300H=C8H9#+H202 2.7E11 0.0 12.0E3  
 !<estimated(t'')>!  
 etC6H5+R4CH3=C8H9#+CH4 1.1E12 0.0 9.1E3 !  
 <estimated(t'')>!  
 etC6H5+C3H5Y=C8H9#+C3H6Y 1.1E12 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+iC4H5=C8H9#+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+nC4H5=C8H9#+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+C6H5O#=#C8H9#+C6H5OH# 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+benzyl=C8H9#+toluene 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!

etC6H5+C5H5#=C8H9#+C5H6# 1.1E11 0.0 13.1E3 !  
<estimated(t")>!

!t": estimated as toluene with A x(2/3) to take into account the number of abstractable !

!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

etC6H5+R1H=C8H9#-1+H2 7.2E8 1.5 6.79E3 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+B10=C8H9#-1+R20H 5.1E8 1.5 5.05E3 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+R20H=C8H9#-1+H2O 3.6E6 2.0 4.82E2 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+R300H=C8H9#-1+H2O2 4.2E4 2.69 1.85E4 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+R4CH3=C8H9#-1+CH4 2.43E6 1.87 1.03E4 !MF correlation  
Dean-Bozzelli 2000

!mfetC6H5+C6H5#=C6H6#+C8H9# 5.27E13 0.0 12.0E3 !ajout MF as  
2/3 toluene <HECKMANN96>!

etC6H5+C6H5#=C6H6#+C8H9# 5.27E13 0.0 9.0E3 !test mf

etC6H5+C6H5#=C6H6#+C8H9#-1 5.85E10 0.0 3.83E3 !ajout MF as  
C5H12/4 <Park, Int J. Chem. Kinet.33(2001)64-69>

! Ajout ipso MF

etC6H5+B10=C6H5O#+R11C2H5 1.7E13 0.0 3.6E3 !MF as toluene !  
<TAPPE89>!

etC6H5+R20H=C6H5O#+R11C2H5 1.3E13 0.0 10.6E3 !MF as toluene  
<BAULCH94>as benzene

!etC6H5+R4CH3=toluene+R11C2H5 1.2E12 0.0 1.59E4 !MF as benzene  
<Robaugh, J. Phys. Chem.90(1986)4159 - 4163>

etC6H5+R4CH3=toluene+R11C2H5 1.2E12 0.0 1.24E4 ! MF as benzene-  
kcal <Robaugh, J. Phys. Chem.90(1986)4159 - 4163>

! \*\* Decompositions

C8H9#-1=C2H4Z+C6H5# 2.0E13 0.0 35.5E3 !MF correlation exgas  
C8H9# =R1H+styrene 3.1e13 0.0 50670 !<MULLER88>  
C8H9#-1=R1H+styrene 4.0E13 0.0 33.58E3 !MF <Sirjean,  
J.Phys.Chem.A 2008>

! \*\* Reactions of derived radicals

C8H9#+O2=R300H+styrene 6.90E11 0.0  
15.2E3 !<est (exgas-sylvain)>!

!C8H9#+R300H=R20H+R4CH3+C6H5CHO 3.27E12 0.0  
0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

!C8H9#+R300H=R20H+R1H+C6H5COCH3 7.80E10 0.0  
0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

!C8H9#+R300H=>R20H+C6H5#+CH3CHO 2.54E11 0.0  
0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

C8H9#+R300H=C8H9#00H	3.60E12	0.0	
0.0 !MF KINGAS			
C8H9#00H=R20H+C8H9#0	5.00E15		
0.0 42500 !MF			
C8H9#0=R4CH3+C6H5CHO	2.69E13	0.0	
12117 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>			
C8H9#0=C6H5#+CH3CHO	1.74E14		
0.0 20458 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>			
C8H9#-1+O2=R300H+styrene	2.60E11	0.0	
2.5E3			
C8H9#-1+R300H=R20H+HCHO+benzyl	5.00E12	0.0	
0.0 !<kingas>!			
!*****!			
!*REACTIONS OF STYRENE AND DERIVED RADICALS*!			
!*****!			
styrene+O2=R300H+C6H5C2H2	2.0E13	0.0	57.9E3 !
<asbutadiene/2>!			
!C4H6Z2+O2=iC4H5+R300H	4.0E13	0.0	57.9E3 !
<LEUNG95>!			
!styrene+B10=C6H5#+R13CH2CHO	3.0E08	1.45	0.9E3 !
<asbutadiene/2>! ! ENLEVE PAR BENOIT ET PAG			
styrene+R20H=benzyl+HCHO	1.4E12	0.0	-0.9E3 !<as
butadiene/2!			
styrene+R20H=C6H5CHO+R4CH3	1.4E12	0.0	-0.9E3 !MF
idem rñaction pñcñdente as C3H6Y <TSAnG91>			
!C4H6Z2+B10=C3H5Y+R1H+B2C0	6.0E08	1.45	0.9E3 !
<LEUNG95, BREZINSKY84>!			
!C4H6Z2+R20H=C3H5Y+HCHO	2.8E12	0.0	-0.9E3 !
<LINSTEDT96>!			
!C4H6Z2+R20H=CH3CHO+R10C2H3V	5.6E12	0.0	-0.9E3 !
<fromLINSTEDT96>!			
styrene+R1H=C6H5C2H2+H2	3.3E5	2.53	9.2E3 !MF<as
butadiene/2>!			
styrene+R20H=C6H5C2H2+H2O	1.5E6	2.0	0.4E3 !<as
butadiene/2>!			
styrene+R4CH3=C6H5C2H2+CH4	3.5E13	0.0	15.5E3 !<as
butadiene/2>			
!C4H6Z2+R1H=iC4H5+H2	6.6E5	2.53	9.2E3 !
<WANG97>!			
!C4H6Z2+R20H=iC4H5+H2O	3.1E6	2.0	0.4E3 !
<WANG97>!			
!C4H6Z2+R4CH3=iC4H5+CH4	7.0E13	0.0	15.5E3 !
<WU87-3kcal>!			



C6H5C2H2+O2=C6H5CO+HCHO 4.5E16 -1.39 1.0E3 !  
<asMebel C2H3+O2>! \*\*

!\*Addition Zhenyu\*!

C6H5C2H2+R1H=C6H5#C2H+H2 1.0E13 0.0  
0.0 !in Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and  
Tech. 120 (1996) 119-167.

C6H5C2H2+R2OH=C6H5#C2H+H2O 1.0E13 0.0 0.0 !in  
Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120  
(1996) 119-167.

! ajout d'un amorcage Roda

C6H5#C2H => C6H5# + R9C2H 2.2e16 0.0 98.0e3 ! MF  
as toluene

!\*\*\*\*\*!  
!\*REACTIONS OF C5H5CCH AND DERIVED RADICALS\*!  
!\*\*\*\*\*!

!\*Addition Zhenyu\*!

!C5H5CCH=C5H5#+R9C2H 4.2E15 0.0 125.0E3 !  
<KInGAS1500>! pC3H4=R9C2H+R4CH3  
!C5H5CCH+R1H=C5H5#+C2H2 2.0E10 0.0 0.0  
!Lindstedt96  
!C5H5CCH+R1H=C3H3+C4H4 6.0E10 0.0 0.0  
!Lindstedt96  
!C5H5CCH+R2OH=C5H5#+CH2COZ 4.3E11 0.0 -0.8E3  
!<BOODAGHIANs87>! pC3H4+R2OH=CH2COZ+R4CH3  
!C5H4CCH2=C5H5CCH 2.5E12 0.0 59.0E3 !  
<HIDAKA89>! aC3H4=pC3H4  
!C5H4CCH2+R1H=C5H5CCH+R1H 8.5E12 0.0 2.0E3 !  
<WAGnER72>! aC3H4+R1H(+M)=tC3H5(+M)  
!C5H4CCH2+R2OH=C5H5#+CH2COZ 2.0E12 0.0 -0.2E3 !<LIU88>!  
aC3H4+R2OH=CH2COZ+R4CH3

!\*\*\*\*\*!  
!\*REACTIONS OF BIBENZYL AND DERIVED RADICALS\*!  
!\*\*\*\*\*!

bibenzyl=C14H13#+R1H 1.0E16 0.0 83.66E3 !  
<Oehlschlaeger05>! in Sakai07 Zhenyu  
bibenzyl+O2=C14H13#+R30OH 2.8E12 0.0 35.0E3 !<est  
aaaa!  
bibenzyl+R1H=C14H13#+H2 5.4E4 2.5 -1.9E3 !  
Table A-I-21 Zhenyu

bibenzyl+B10=C14H13#+R2OH 8.4E11 0.0 -2.0 !  
<estimated(t'')>!  
bibenzyl+R2OH=C14H13#+H2O 7.0E9 1.0 -1.13E3 !  
<estimated(t'')>!

```

bibenzyl+R300H=C14H13#+H2O2          5.4E11      0.0  12.0E3  !
<estimated(t'')>!
bibenzyl+R4CH3=C14H13#+CH4          2.2E12      0.0    9.1E3  !
<estimated(t'')>!
bibenzyl+C6H5O#=#C14H13#+C6H5OH#    2.2E12      0.0   13.1e3  !
<estimated(t'')>!
bibenzyl+benzyl=C14H13#+toluene      2.2E12      0.0   9.1E3  !
<Oehlschlaeger05>! in Sakai07 Zhenyu

bibenzyl+C3H5Y=C14H13#+C3H6Y        2.2E12      0.0  13.1E3  !
<estimated(t'')>!
!t'': estimated as toluene with A x(4/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

!Ajout ipso MF
bibenzyl+R1H=C6H6#+C8H9#-1          5.67E8     1.43  5.65E3  !Calcul CBS-
QB3 Fournet as toluene
bibenzyl+R20H=C6H5OH#+C8H9#-1      7.83E2     2.884  3.2193E3 !Seta V
Nakajima V Miyoshi JPCA 2006
C14H13#=stilbene+R1H                7.94E15    0.0   51.864E3 !
<Oehlschlaeger05>! in Sakai07 Zhenyu
C14H13#+O2= stilbene+R300H          1.6E12     0.00  15200  !as allylique
C14H13#+R300H=>R20H+C6H5CHO+benzyl 8.21E4     2.20  -5.13E3 ! as benzyl

!*****!
!*REACTIONS OF STILBENE *!
!*****!

!Ajout Ipso MF
stilbene+R1H=>C6H6#+C2H2+C6H5#      5.67E8     1.43  5.65E3  !Calcul CBS-
QB3 Fournet as toluene
stilbene+R20H=C6H5OH#+C6H5C2H2     7.83E2     2.884  3.2193E3 !Seta V
Nakajima V Miyoshi JPCA 2006

! ajout MF
stilbene+R20H=C6H5CHO+benzyl        1.0E13      0.0    5.94E3  !
<Baulch05> as C2H4

!*****!
!* Reactions of naphthalene *!
!*****!
2C5H5#=naphthalene+H2               4.3E36    -6.3  22.835E3 ! A.M. Dean, J.
Phys. Chem. 94 (1990) 1432-1439.
C6H5#+iC4H3=naphthalene             3.18E23   -3.2  2.13E3  ! H.Y. Zhang, J.T.
McKinnon, CST 107 (1995) 261-300.
C6H5#+C4H4=naphthalene+R1H          3.3E33    -5.7  12.75E3 ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
benzyl+C3H3=>naphthalene+R1H+R1H    6.0E11    0.0  0.0      ! M.B. Colket,
D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.
C6H5C2H2+C2H2=naphthalene+R1H      1.6E16    -1.33  3.3E3   ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.

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naphthalene+O2=R300H+naphthyl like benzene <ALZUETA00>A*8/6!	8.0E13	0.0	63.4E3	!
naphthalene+B10=>indenyl+B2C0+R1H benzene <Nicovich82>A*8/6!	2.7E13	0.0	3.6E3	!like
naphthalene+R1H=naphthyl+H2 benzene <MEBEL97>A*8/6!	8.0E8	1.8	16.8E3	!like
naphthalene+B10=naphthyl+R20H benzene <LINDSTEDT94>A*8/6!	2.7E13	0.0	14.7E3	!like
naphthalene+R20H=naphthyl+H2O benzene <BAULCH92>A*8/6!	2.1E8	1.42	1.45E3	!like
naphthalene+R300H=naphthyl+H2O2 benzene <BAULCH94>A*8/6!	7.3E12	0.0	28.9E3	!like
naphthalene+R4CH3=naphthyl+CH4 benzene <ZHANG89>A*8/6!	2.7E12	0.0	15.0E3	!like

naphthyl+R1H=naphthalene buthylbenzene	1.0E14	0.0	0.0E3	!as n-
naphthyl+O2=>indenyl+B2C0+B10 buthylbenzene	2.6E13	0.0	6.1E3	!as n-
naphthyl+B10=>indenyl+B2C0 buthylbenzene	1.0E14	0.0	0.0	!as n-
naphthyl+R300H=>indenyl+B2C0+R20H buthylbenzene	5.0E12	0.0	0.0	!as n-
naphthyl+R20H=>indenyl+B2C0+R1H buthylbenzene	1.0E13	0.0	0.0	!as n-

!\*\*\*\*\*!  
!\* Reactions of indene and derived radicals \*!  
! Indene C6H4#/CH2/CH//CH/ \*!  
! Indenyl C6H4#/CH/CH//CH/ \*!  
! ph#C3H2 C6H5#/CH(./)/C///CH \*!  
!\*\*\*\*\*!

indene+R20H=>C2H4Z+C6H5C0	1.37E12	0.0	-1.04E3	!Slavinskaya
indene+R20H=>R10C2H3V+B2C0+C6H6#	1.37E12	0.0	-1.04E3	!Est.
!indene+R20H=>o-methylbenzyl+B2C0	1.37E12	0.0	-1.04E3	

indene+O2=R300H+indenyl buthylbenzene mais E = DH de reaction	1.4E12	0.0	31.03E3	! as n-
indene+B10=indenyl+R20H secondary A*2	1.76E11	0.7	3.25E3	! A-I-21
indene+R1H=indenyl+H2 secondary A*2	1.08E5	2.5	-1.9E3	! A-I-21
indene+R20H=indenyl+H2O secondary A*2	6.0E6	2.0	-1.52E3	! A-I-21
indene+R4CH3=indenyl+CH4 secondary A*2	2.0E11	0.0	7.3E3	! A-I-21
indene+R300H=H2O2+indenyl secondary A*2	1.28E4	2.6	12.4E3	! A-I-21

!indene+R1H=ph#C3H4Y	5.8E13	0.0	8.1E3	!ipso-addition
!indene+R1H=ph#C3H4-1	5.8E13	0.0	8.1E3	!ipso-addition
indene+R1H=>C2H2+benzyl	1.16E14	0.0	8.1E3	!mf 2x ipso-addition

indenyl=>C5H5#+C4H2 5.0E13 0.0 75.0E3 !Slavinskaya09  
 5.0E13 0.0 37.5E3  
 indenyl+R1H=indene 1.0E14 0.0 0.0 !as n-buthylbenzene  
 C6H5#+C3H3=indene 6.46E12 0.0 0.0 !Slavinskaya09  
 !indenyl+R300H=>C6H6#+B2C0+R9C2H+R20H 3.0E12 0.0 0.0 ! Est.!  
 similar to C5H5#+H02  
 indenyl+R300H=>C6H5#C2H+R5CHO+R20H 3.0E12 0.0 0.0 ! Est.!  
 similar to C5H5#+H02

indenyl+B10=>C6H6#+B2C0+R9C2H 5.8E13 -0.02 0.02E3 !Est.  
 C5H5#+B10=C5H40#+R1H  
 indenyl+B10=>C6H5#C2H+R5CHO 5.8E13 -0.02 0.02E3 !Est.  
 C5H5#+B10=C5H40#+R1H

indenyl+R20H=>styrene+B2C0 4.0E14 0.0 4.5E3 !Est.  
 C5H5#+0H=C4H6Z2+C0

!C9H70#=C9H60#+R1H 2.0E13 0.0 27.5E3 ! Est.like ph#CH20  
 !C9H70#=>C6H6#+B2C0+R9C2H 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+C0  
 !C9H70#=C6H5#C2H+R5CHO 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+C0

!END

!

!\*\*\*\*\*MPE MECHaNisM\*\*\*\*\*

!

R21CH30C0=R4CH3+C02 4.840E+10 1.11  
 15887.0 !HuyNH aND Vi0li J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 3.570E+04 2.485 37247.0 /  
 R21CH30C0=R7CH30+B2C0 8.020E+11 0.65  
 21123.0 !HuyNH aND Vi0li J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 1.350E+04 2.31 7883.0 /

!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!MEthyl EtHaNOate !

!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!INitiatiONs

ME2j+R1H=ME 1.000E+14 0.00 0.00 !  
 040909  
 ME=MEMj+R1H 7.900E+15 0.00 9.797E+04 !  
 040909

ME=R21CH30C0+R4CH3 1.130E+16 0.00 7.770E+04 !  
 040909

!H-aBstraCtiONs

ME+R1H=ME2j+H2 2.850E+07 2.0 7.700E+03 !  
 3HPalk  
 ME+R1H=MEMj+H2 1.440E+13 0.00 6.095E+03 !MEOH  
 ME+B10=ME2j+R20H 5.100E+13 0.00 7.850E+03 !  
 3HPalk  
 ME+B10=MEMj+R20H 9.650E+04 2.68 3.716E+03 !2  
 aNC7, PriMARIY f  
 ME+R20H=ME2j+H20 2.670E+06 2.00 4.500E+02 !  
 3HPalk  
 ME+R20H=MEMj+H20 7.100E+06 1.80 -5.960E+02 !MEOH

!C-C DECOMPOsitiONs

ME2j=CH2COZ+R7CH3O 1.280E+12 0.6584 49255.0 !  
HuyNH aND ViOli J.Org.CHEM. 73 (2008) 94-101  
rev / 1.060E+02 2.7924 7922.0 /  
MEMj=HCHO+R14CH3CO 1.230E+13 0.375 36714.0 !  
HuyNH aND ViOli J.Org.CHEM. 73 (2008) 94-101  
rev / 1.110E+01 3.14 11198.0 /

!IsOMERisatiONs

ME2j=MEMj 1.500E+08 1.00 1.980E+04 !GlaUDE  
Et al., ENERgy FuELs, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)  
!KETONEs DECOMPOsitiON  
ME2\*O=CH3OH+B2CO+B2CO 1.000E+09 0.00 40000.0 !  
R5CHO+R21CH3OCO=ME2\*O 1.000E+13 0.00 0.0 !9  
ALLARA aND sHaw  
ME2\*O+O2=ME2j\*O+R300H 3.000E+13 0.00 39100.0 !  
ME2\*O+R1H=ME2j\*O+H2 4.000E+13 0.00 4200.0 !26  
aNC7; alDEHyDiC  
ME2\*O+R20H=ME2j\*O+H2O 2.690E+10 0.76 -340.0 !26  
aNC7: alDEHyDiC  
ME2\*O+B10=ME2j\*O+R20H 5.000E+12 0.00 1790.0 !26  
aNC7; alDEHyDiC  
ME2j\*O=R21CH3OCO+B2CO 1.834E+15 -0.73 22910.0 !  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!MEthyl PrOPaNOatE !  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!INitiatiONs

MP=MP3j+R1H 7.900E+15 0.00 9.797E+04 !as N-C4H9 DEaN Et  
al., J.PHyS.CHEM. 89 (1985) 4600-4608  
MP2j+R1H=MP 1.000E+14 0.00 0.00 !1 rNC7\*: H+fragM  
MP=MPMj+R1H 7.900E+15 0.00 9.797E+04 !as N-C4H9 DEaN Et  
al., J.PHyS.CHEM. 89 (1985) 4600-4608

MP=ME2j+R4CH3 7.900E+22 -1.8 8.863E+04 !asC3H8 TsaNg,  
J.PHyS.CHEM.REF.Data 17 (1988) 887-

!H-aBstraCtiONs

MP+R1H=MP3j+H2 9.400E+04 2.75 6.280E+03 !2 aNC7, PriMARY f  
MP+R1H=MP2j+H2 5.400E+04 2.5 -1.900E+03 !  
MP+R1H=MPMj+H2 1.440E+13 0.00 6.095E+03 !(HELD 94)  
MP+B10=MP3j+R20H 9.650E+04 2.68 3.716E+03 !2 aNC7, PriMARY  
f  
MP+B10=MP2j+R20H 8.800E+10 0.70 3.250E+03 !  
MP+B10=MPMj+R20H 9.650E+04 2.68 3.716E+03 !2 aNC7, PriMARY  
f  
MP+R20H=MP3j+H2O 5.250E+09 0.97 1.590E+03 !2 rNC7, PriMARY;  
MP+R20H=MP2j+H2O 3.000E+06 2.00 -1.520E+03 !  
MP+R20H=MPMj+H2O 7.100E+06 1.80 -5.960E+02 !(HELD 98)

!C-C DECOMPOsitiON

MP3j=C2H4Z+R21CH3OCO 3.030E+13 0.27 34667.0 ! HuyNH aND  
ViOli J.Org.CHEM. 73 (2008) 94-101  
rev / 1.660E+02 3.065 4838.0 /  
MP2j=CH3CHCO+R7CH3O 1.460E+12 0.61 53276.0 ! HuyNH aND ViOli  
J.Org.CHEM. 73 (2008) 94-101  
rev / 5.580E+01 2.81 5973.0 /

MPMj=HCHO+R25C2H5CO 1.230E+13 0.375 36714.0 ! HuyNH aND  
 Vi0li J.Org.CHEM. 73 (2008) 94-101  
 rev / 1.110E+01 3.14 11198.0 /

!C-H DECOMPOsitiON  
 MP2D+R1H=MP3j 4.180E+08 1.5576 1697.0 !  
 HuyNH aND Vi0li J.Org.CHEM. 73 (2008) 94-101  
 rev / 1.530E+08 1.5743 38376.0 /

MP2j=MP2D+R1H 3.000E+13 0.00 4.550E+04 !  
 DayMa Et al., Int J CHEM KiNet, 35 (2003) 273-285 (2Hs)-5kCal  
 !OxiDatiONs  
 MP2j+R300H=MP2D+H2O2 2.410E+13 0.0 0.0 !  
 (=NC3H7/TSA88)

!IsOMERisatiON  
 MP3j=MPMj 2.500E+07 1.00 1.450E+04 !GlaUDE  
 Et al., ENERgy FuElS, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)  
 rev/ 2.500E+07 1.00 1.550E+04/ !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC sat a 6 + 3HP + 1kCal /0)  
 MP2j=MPMj 1.500E+08 1.00 1.980E+04 !GlaUDE  
 Et al., ENERgy FuElS, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)  
 rev/ 1.500E+08 1.00 1.830E+04/ !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC sat a 5 + 2Ht + 3kCal /0)  
 MP2D=C2H3CO2+R4CH3 3.160E+16 0.00 8.307E+04 !asDME Batt  
 Et al., PrOC. COMBust. INst. 19 (1982) 81-87  
 !H-aBstraCtiONs  
 MP2D+R1H=MP2DMj+H2 1.440E+13 0.0 6.095E+03 !(HELD 94)  
 MP2D+B10=MP2DMj+R2OH 9.650E+04 2.68 3.716E+03 !2 aNC7,  
 PriMARy f  
 MP2D+R2OH=MP2DMj+H2O 7.100E+06 1.80 -5.960E+02 !(HELD 98)  
 MP2D+R1H=MP2D3j+H2 8.200E+05 2.50 1.228E+04 !TOuCHARD  
 MP2D+R2OH=MP2D3j+H2O 2.200E+06 2.00 2.780E+03 !TOuCHARD  
 MP2D+R4CH3=MP2D3j+CH4 1.360E+00 3.50 1.290E+04 !TOuCHARD  
 MP2D+B10=MP2D3j+R2OH 1.200E+11 0.70 8.960E+03 !TOuCHARD  
 MP2D+R1H=MP2D2j+H2 4.100E+05 2.50 9.790E+03 !TOuCHARD  
 MP2D+R2OH=MP2D2j+H2O 1.100E+06 2.00 1.450E+03 !TOuCHARD  
 MP2D+R4CH3=MP2D2j+CH4 9.800E-01 3.50 1.170E+04 !TOuCHARD  
 MP2D+B10=MP2D2j+R2OH 6.000E+10 0.70 7.630E+03 !TOuCHARD

!BEta-sCiSSIONs  
 MP2D3j=C2H2+R21CH3OCO 2.000E+13 0.00 4.500E+04  
 !MP2D3j=R21CH3OCO+C2H2 5.760E+12 0.8189 38502.0 ! HuyNH aND  
 Vi0li J.Org.CHEM. 73 (2008) 94-101  
 ! rev / 1.860E+04 2.6071 6942.0 /  
 MP2D2j=CH2CCO+R7CH3O 5.030E+12 0.5212 48254.0 ! HuyNH aND  
 Vi0li J.Org.CHEM. 73 (2008) 94-101  
 rev / 1.850E+02 2.8060 3330.0 /  
 MP2DMj=C2H3CO+HCHO 2.830E+11 0.4945 29999.0 ! HuyNH aND Vi0li  
 J.Org.CHEM. 73 (2008) 94-101  
 rev / 3.190E+00 2.9288 7152.0 /  
 !MiB3j=C3H6Y+R21CH3OCO 2.000E+13 0.00 2.400E+04

!IsOMERizatiONs

MP2D3j=MP2DMj 2.500E+07 1.00 1.490E+04 !GlaUDE Et al.,  
 ENergy FuEls, 16 (2002) 1186-1195 (CyC iNsat a 6 + 3HP)  
 ! rev / 1.700E+07 1.00 1.620E+04 / !GlaUDE Et al., ENergy FuEls,  
 16 (2002) 1186-1195 (CyC iNsat a 6 + 2Hs + 0kCal /0)  
 MP2D2j=MP2DMj 1.500E+08 1.00 1.980E+04 !GlaUDE Et al.,  
 ENergy FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)  
 ! rev / 9.900E+07 1.00 2.110E+04 / !GlaUDE Et al., ENergy FuEls,  
 16 (2002) 1186-1195 (CyC sat a 5 + 2Hs + 0kCal /0)  
 MP2D2j=MP2D3j 3.120E+13 0.24 4.214E+04

!ADDITIONs

!\*2

C2H3CO2=>R10C2H3V+CO2 2.200E+11 0.29 4.580E+03 !ZHOu Et  
 al., J.MOl.StruC.THEOCHEM. 854 (2008) 40-45

MP2D3j+O2=R5CHO+ME2\*O 4.600E+16 -1.39 1.010E+03 !ST

!O aND OH DECOMPOsITIONs

MP2D+B10=ME2j+R5CHO 1.580E+07 1.76 -1216.0 !7 MARiNOv  
 Calc fr

MP2D+B10=R21CH3OCO+R13CH2CHO 5.010E+07 1.76 76.0 !7  
 MARiNOv Calc fr

!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!MEthyl ButaNOate !

!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!INItiationS

MB=MB4j+R1H 7.900E+15 0.00 9.797E+04 !as N-C4H9 DEaN Et al.,  
 J.PHys.CHEM. 89 (1985) 4600-4608

MB=MB3j+R1H 5.000E+15 0.00 9.499E+04 !as s-C4H9 DEaN Et al.,  
 J.PHys.CHEM. 89 (1985) 4600-4608

MB2j+R1H=MB 1.000E+14 0.00 0.00 !1 rNC7\*: H+fragM

MB=MBMj+R1H 7.900E+15 0.00 9.797E+04 !as N-C4H9 DEaN Et al.,  
 J.PHys.CHEM. 89 (1985) 4600-4608

MB=MP3j+R4CH3 7.900E+22 -1.8 8.863E+04 !asC3H8 TsaNg,  
 J.PHys.CHEM.REF.Data 17 (1988) 887-

MB=ME2j+R11C2H5 1.580E+17 0.0 8.704E+04 !asC4H10 TsaNg,  
 INT.J.CHEM.KiNEt. 10 (1978) 821-

!MB=R21CH3OCO+NC3H7 1.130E+16 0.00 8.170E+04 !asCH3COCH3 SatO Et  
 al., COMBust. FlaME 122 (2000) 291-311

MB=R21CH3OCO+R19C3H7 1.130E+16 0.00 8.170E+04 !asCH3COCH3 SatO Et  
 al., COMBust. FlaME 122 (2000) 291-311

!H-aBstraCtionS

MB+R1H=MB4j+H2 9.400E+04 2.75 6.280E+03 !2 aNC7, PriMAY f

MB+R1H=MB3j+H2 1.300E+06 2.4 4.471E+03 !2 aNC7, SECONDAry

MB+R1H=MB2j+H2 5.400E+04 2.5 -1.900E+03 !

MB+R1H=MBMj+H2 1.440E+13 0.00 6.095E+03 !(HELD 94)

MB+B10=MB4j+R20H 9.650E+04 2.68 3.716E+03 !2 aNC7, PriMAY f

MB+B10=MB3j+R20H 4.770E+04 2.71 2.106E+03 !2 aNC7, SECONDAry

MB+B10=MB2j+R20H 8.800E+10 0.70 3.250E+03 !

MB+B10=MBMj+R20H 9.650E+04 2.68 3.716E+03 !2 aNC7, PriMAY f

MB+R20H=MB4j+H2 5.250E+09 0.97 1.590E+03 !2 rNC7, PriMAY;

MB+R20H=MB3j+H2 4.680E+07 1.61 -3.500E+01 !2 rNC7, SECONDAry

MB+R20H=MB2j+H2 3.000E+06 2.00 -1.520E+03 !

MB+R4CH3=MB3j+CH4 2.705E+04 2.26 7.287E+03 !2 aNC7, SECONDAry

MB+R4CH3=MB2j+CH4 1.000E+11 0.00 7.300E+03 !  
 !C-C DECOMPOsitiONs  
 MB4j=C2H4Z+ME2j 5.250E+11 0.50 26591.0 ! HuyNH aND  
 Vi0li J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 2.410E+02 2.89 7533.0 /  
 MB3j=C3H6Y+R21CH3OCO 4.530E+12 0.335 34269.0 ! HuyNH aND  
 Vi0li J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 9.550E+01 3.05 4665.0 /  
 MB2j=MP2D+R4CH3 1.330E+11 0.97 34882.0 ! HuyNH aND  
 Vi0li J.Org.CHEM. 73 (2008) 94-101  
 rev / 7.090E+02 2.78 5845.0 /  
 MBMj=HCHO+C3H7CO 1.230E+13 0.375 36714.0 ! HuyNH aND Vi0li  
 J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 1.110E+01 3.14 11198.0 /  
 !C-H DECOMPOsitiONs  
 MB4j=R1H+MB3D 3.000E+13 0.00 3.800E+04 !DayMa Et al.,INT J CHEM  
 KiNEt, 35 (2003) 273-285 (2Hs)  
 MB3j=R1H+MB3D 3.000E+13 0.00 3.900E+04 !TOuCHARD Et al., INT J  
 CHEM KiNEt, 37 (2005) 451-463 (3HP)  
 MB3j=R1H+MB2D 1.500E+13 0.00 3.800E+04 !TOuCHARD (2005) THISE  
 INPL (2Hs)  
 MB3j=R1H+MB2D-z 1.500E+13 0.00 3.800E+04 !TOuCHARD (2005) THISE  
 INPL (2Hs)  
 !IsOMERisatiONs  
 MB4j=MBMj 4.350E+06 1.00 1.990E+04 !GlaUDE Et al., ENERgy  
 FuElS, 16 (2002) 1186-1195 (CyC sat a 7 + 3HP)  
 ! rev/ 4.350E+06 1.00 1.890E+04/ !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC sat a 7 + 3HP - 1kCal /0)  
 MB3j=MBMj 2.500E+07 1.00 1.450E+04 !GlaUDE Et al., ENERgy  
 FuElS, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)  
 rev/ 1.700E+07 1.00 1.400E+04/ !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC sat a 6 + 2Hs + 2kCal /0)  
 MB2j=MBMj 1.500E+08 1.00 1.980E+04 !GlaUDE Et al., ENERgy  
 FuElS, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)  
 rev/ 1.500E+08 1.00 2.030E+04/ !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC sat a 5 + 2Ht + 5kCal /0)  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !MEthyl ButENOatEs !  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !INitiatiONs  
 MB2D=MB3D2j+R1H 2.500E+15 0.0 86640.0  
 MB2D=MP2D3j+R4CH3 1.100E+21 -1.20 97720.0 !  
 (TSANG91)as C3H6=C2H3+R4CH3  
 MB3D2j+R1H=MB3D 1.000E+13 0.00 0.0 !(RTi)  
 !  
 !MB3D=R21CH3OCO+C3H5-a 7.940E+15 0.00 7.074E+04 !TsaNg  
 1978  
 MB3D=R21CH3OCO+C3H5Y 7.940E+15 0.00 7.074E+04 !TsaNg  
 1978  
 !H-abstraCtiONs  
 MB3D+B10=MB3D2j+R2OH 8.800E+10 0.7 3.250E+03 ! TOuCHARD Et  
 al., ProC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)  
 MB3D+B10=MB3DMj+R2OH 9.650E+04 2.68  
 3.716E+03 !2 aNC7, PriMARY f



MB3D+R1H=MB3D2j+H2 5.400E+04 2.5 -1.900E+03 ! TOuCHARD Et  
 al., ProC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)  
 MB3D+R1H=MB3DMj+H2 1.440E+13 0.0 6.095E+03  
 !(HELD 94)  
 MB3D+R20H=MB3D2j+H20 3.000E+06 2.0 -1.520E+03 ! TOuCHARD Et  
 al., ProC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)  
 MB3D+R20H=MB3DMj+H20 7.100E+06 1.80 -5.960E+02  
 !(HELD 98)  
 MB2D+B10=MB2DMj+R20H 9.650E+04 2.68  
 3.716E+03 !2 aNC7, PRIMARY f  
 MB2D+R1H=MB3D2j+H2 5.400E+04 2.5 -1.900E+03 ! TOuCHARD Et  
 al., ProC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)  
 MB2D+R1H=MB2DMj+H2 1.440E+13 0.0 6.095E+03  
 !(HELD 94)  
 MB2D+R20H=MB3D2j+H20 3.000E+06 2.0 -1.520E+03 ! TOuCHARD Et  
 al., ProC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)  
 MB2D+R20H=MB2DMj+H20 7.100E+06 1.80 -5.960E+02  
 !(HELD 98)  
 MB2D-z+B10=MB3D2j+R20H 1.74E+11 0.7  
 5900.0  
 MB2D-z+B10=MB2DMj+R20H 9.650E+04 2.68  
 3.716E+03 !2 aNC7, PRIMARY f  
 MB2D-z+R1H=MB3D2j+H2 1.74E+05 2.5 2510.0  
 MB2D-z+R1H=MB2DMj+H2 1.440E+13 0.0 6.095E+03  
 !(HELD 94)  
 MB2D-z+R20H=MB3D2j+H20 3.00E+06 2.0 -298.0  
 MB2D-z+R20H=MB2DMj+H20 7.100E+06 1.80 -5.960E+02  
 !(HELD 98)  
 MB2D-z+R1H=MB2D3j+H2 8.200E+05 2.50 1.228E+04 !TOuCHARD  
 MB2D-z+R20H=MB2D3j+H20 2.200E+06 2.00 2.780E+03 !TOuCHARD  
 !IsOMERizations  
 MB3D2j=MB3DMj 1.500E+08 1.00 2.780E+04 !GlaUDE Et al.,  
 ENERgy FuElS, 16 (2002) 1186-1195 (X° CyC sat a 5 + 3HP)  
 ! rev / 9.900E+07 1.00 1.180E+04 / !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC sat a 5 + 2Htall + 0kCal /0)  
 MB2D3j=MB2DMj 2.500E+07 1.00 1.490E+04 !GlaUDE Et al.,  
 ENERgy FuElS, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)  
 rev / 8.600E+06 1.00 1.420E+04 / !GlaUDE Et al., ENERgy FuElS,  
 16 (2002) 1186-1195 (CyC iNsat a 6 + 1Ht + 0kCal /0)  
 MB2DMj=sC3H5CO+HCHO 2.830E+11 0.4945 29999.0 ! HuyNH aND  
 Vi0li J.Org.CHEM. 73 (2008) 94-101  
 rev / 3.190E+00 2.9288 7152.0 /  
 MB3DMj=HCHO+aC3H5CO 1.230E+13 0.375 36714.0 ! HuyNH aND Vi0li  
 J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 1.110E+01 3.14 11198.0 /  
 !  
 !MB2D3j=>C3H4-P+R21CH30CO 2.000E+13 0.00 30000.0 !TOuCHARD  
 !  
 MB2D3j=>pC3H4+R21CH30CO 2.000E+13 0.00 30000.0 !TOuCHARD  
 !  
 MB3D2j+R300H=>MB3D20+R20H 2.250E+12 0.00 0.0 !  
 (WALKER 90)  
 MB3D20=>ME2\*0+R10C2H3V 1.700E+14 0.00 22658.0 ! Rauk  
 J. Can. CHEM 2003 v0l. 81

C3H7CO=>R19C3H7+B2CO 1.834E+15 -0.73 1.291E+04 !GlaUDE Et al.,  
 DMC C2H5CO  
 C3H7CO=CH2COZ+R11C2H5 2.745E+09 1.41 3.583E+04  
 rev / 1.000E+04 2.48 6.130E+03 /  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !MEthyl PENTaNOatE !  
 !!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
 !INitiatiONs  
  
 MPE=MB4j+R4CH3 7.900E+22 -1.8 8.863E+04 !asC3H8 TsaNg,  
 J.PHys.CHEM.Ref.Data 17 (1988) 887-  
 MPE=MP3j+R11C2H5 1.580E+17 0.0 8.704E+04 !asC4H10 TsaNg,  
 INT.J.CHEM.KiNEt. 10 (1978) 821-  
 MPE=ME2j+R19C3H7 1.580E+17 0.0 8.704E+04 !asC4H10 TsaNg,  
 INT.J.CHEM.KiNEt. 10 (1978) 821-  
 !  
 !MPE=R21CH3OCO+PC4H9 1.130E+16 0.00 8.170E+04 !asCH3COCH3 Sat0 Et  
 al., COMBust. FlaME 122 (2000) 291-311  
 !  
 NC4H9CO+R7CH3O=MPE 1.500E+13 0.00 0.00 !asDMC GlaUDE Et al.,  
 PrOC.COMBust.INst. 31 (2005) 1111-1118  
 !MPE=PEaOj+R4CH3 3.160E+16 0.00 8.307E+04 !asDME Batt Et al.,  
 PrOC. COMBust. INst. 19 (1982) 81-87  
 !H-aBstraCtiONs  
 MPE+R1H=MPE5j+H2 9.400E+04 2.75 6.280E+03 !2 aNC7, PRIMARY f  
 MPE+R1H=MPE4j+H2 1.300E+06 2.4 4.471E+03 !2 aNC7, SECONDAry  
 MPE+R1H=MPE3j+H2 1.300E+06 2.4 4.471E+03 !2 aNC7, SECONDAry  
 MPE+R1H=MPE2j+H2 5.400E+04 2.5 -1.900E+03 !  
 MPE+R1H=MPEMj+H2 1.440E+13 0.00 6.095E+03 !(HELD 94)  
 MPE+B10=MPE5j+R2OH 9.650E+04 2.68 3.716E+03 !2 aNC7, PRIMARY  
 f  
 MPE+B10=MPE4j+R2OH 4.770E+04 2.71 2.106E+03 !2 aNC7,  
 SECONDAry  
 MPE+B10=MPE3j+R2OH 4.770E+04 2.71 2.106E+03 !2 aNC7,  
 SECONDAry  
 MPE+B10=MPE2j+R2OH 8.800E+10 0.70 3.250E+03 !  
 MPE+B10=MPEMj+R2OH 9.650E+04 2.68 3.716E+03 !2 aNC7, PRIMARY  
 f  
 MPE+R2OH=MPE5j+H2O 5.250E+09 0.97 1.590E+03 !2 rNC7, PRIMARY;  
 MPE+R2OH=MPE4j+H2O 4.680E+07 1.61 -3.500E+01 !2 rNC7, SECONDAry  
 MPE+R2OH=MPE3j+H2O 4.680E+07 1.61 -3.500E+01 !2 rNC7, SECONDAry  
 MPE+R2OH=MPE2j+H2O 3.000E+06 2.00 -1.520E+03 !  
 MPE+R2OH=MPEMj+H2O 7.100E+06 1.80 -5.960E+02 !(HELD 98)  
 MPE+R4CH3=MPE4j+CH4 2.705E+04 2.26 7.287E+03 !2 aNC7,  
 SECONDAry  
 !C-C DECOMPOsitiONs  
 MPE5j=C2H4Z+MP3j 2.000E+13 0.00 2.870E+04 !DayMa Et  
 al., INT J CHEM KiNEt, 35 (2003) 273-285  
 MPE4j=C3H6Y+ME2j 5.250E+11 0.50 26591.0 ! HuyNH aND ViOli  
 J. Org. CHEM. 2008 vOl. 73 PP. 94-101  
 rev / 2.410E+02 2.89 7533.0 /  
 !MPE3j=C4H8-1+R21CH3OCO 4.530E+12 0.335 34269.0 ! HuyNH aND  
 ViOli J. Org. CHEM. 2008 vOl. 73 PP. 94-101

MPE3j=C4H8Y+R21CH30C0 4.530E+13 0.335 34269.0 ! HuyNH aND  
 Vi0li J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 9.550E+01 3.05 4665.0 /  
 MPE3j=R4CH3+MB3D 2.000E+13 0.00 3.200E+04 !  
 MPE2j=R11C2H5+MP2D 2.000E+13 0.00 3.070E+04 !  
 !  
 !MPE2j=C4H8C0+R7CH30 1.460E+12 0.61 53276.0 ! HuyNH aND  
 Vi0li J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 !  
 rev / 5.580E+01 2.81 5973.0 /  
 MPEMj=HCHO+NC4H9C0 1.230E+13 0.375 36714.0 ! HuyNH aND Vi0li  
 J. Org. CHEM. 2008 v0l. 73 PP. 94-101  
 rev / 1.110E+01 3.14 11198.0 /

!C-H DECOMPOsitiONs

MPE5j=R1H+MPE4D 3.000E+13 0.00 3.800E+04 !DayMa Et al.,INT J  
 CHEM KiNET, 35 (2003) 273-285 (2Hs)  
 MPE4j=R1H+MPE4D 3.000E+13 0.00 3.900E+04 !TOuCHARD Et al., INT  
 J CHEM KiNET, 37 (2005) 451-463 (3HP)  
 MPE4j=R1H+MPE3D 3.000E+13 0.00 3.800E+04 !DayMa Et al.,INT J  
 CHEM KiNET, 35 (2003) 273-285 (2Hs)  
 MPE3j=R1H+MPE3D 3.000E+13 0.00 3.800E+04 !DayMa Et al.,INT J  
 CHEM KiNET, 35 (2003) 273-285 (2Hs)  
 MPE3j=R1H+MPE2D 3.200E+13 0.00 3.480E+04 !TOuCHARD (2005) THuSE  
 INPL (2Hs ally)  
 MPE2j=R1H+MPE2D 3.000E+13 0.00 4.500E+04 !DayMa Et al.,INT J  
 CHEM KiNET, 35 (2003) 273-285 (2Hs)

!IsOMERisatiONs

MPE4j=MPEMj 4.350E+06 1.00 1.990E+04 !GlaUDE Et al., ENERgy  
 FuEls, 16 (2002) 1186-1195 (CyC sat a 7 + 3HP)  
 MPE3j=MPEMj 2.500E+07 1.00 1.450E+04 !GlaUDE Et al., ENERgy  
 FuEls, 16 (2002) 1186-1195 (CyC sat a 6 + 3HP)  
 rev/ 1.700E+07 1.00 1.400E+04/ !GlaUDE Et al., ENERgy FuEls,  
 16 (2002) 1186-1195 (CyC sat a 6 + 2Hs + 2kCal /0)  
 MPE2j=MPE5j 1.500E+08 1.00 1.980E+04 !GlaUDE Et al., ENERgy  
 FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)  
 MPE2j=MPEMj 1.500E+08 1.00 1.980E+04 !GlaUDE Et al., ENERgy  
 FuEls, 16 (2002) 1186-1195 (CyC sat a 5 + 3HP)  
 rev/ 1.500E+08 1.00 2.030E+04/ !GlaUDE Et al., ENERgy FuEls,  
 16 (2002) 1186-1195 (CyC sat a 5 + 2Ht + 5kCal /0)

!OxiDatiONs

MPE4j+O2=MPE3D+R300H 1.950E+12 0.00 5.000E+03 !BuDa Et al.,  
 COMBust FlaME, 142 (2005) 170-186  
 MPE3j+O2=MPE3D+R300H 1.950E+12 0.00 5.000E+03 !BuDa Et al.,  
 COMBust FlaME, 142 (2005) 170-186  
 MPE3j+O2=MPE2D+R300H 2.600E+11 0.00 2.500E+03 !BattiN-LEClErC,  
 PrOg ENERgy COMBust SCi, 34 (2008) 440-498  
 MPE2j+O2=MPE2D+R300H 1.580E+12 0.00 1.520E+04 !BattiN-LEClErC,  
 PrOg ENERgy COMBust SCi, 34 (2008) 440-498

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!MEthyl PENTENOatEs !

!!!!!!!!!!!!!!!!!!!!!!!!!!!!

!INitiatiONs

!MPE4D=ME2j+C3H5-a	7.940E+15	0.00	7.074E+04	!TsaNg 1978
MPE4D=ME2j+C3H5Y	7.940E+15	0.00	7.074E+04	!TsaNg 1978
MPE3D+O2=MPE3D2j+R300H	4.000E+12	0.00	37000.0	!EstiMatED
MPE2D+O2=MPE3D2j+R300H	4.000E+12	0.00	40000.0	!as C4H8-1

!H-aBstraCtiONs

MPE4D+B10=MPE4D2j+R20H	8.800E+10	0.7	3.250E+03	! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE3D+B10=MPE4D3j+R20H	8.800E+10	0.7	3.250E+03	! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE3D+B10=MPE3D2j+R20H	8.800E+10	0.7	3.250E+03	! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE2D+B10=MPE3D2j+R20H	8.800E+10	0.7	3.250E+03	! TOuCHARD
Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE4D+R1H=MPE4D3j+H2	5.400E+04	2.5	-1.900E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE4D+R1H=MPE4D2j+H2	5.400E+04	2.5	-1.900E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE3D+R1H=MPE4D3j+H2	5.400E+04	2.5	-1.900E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE3D+R1H=MPE3D2j+H2	5.400E+04	2.5	-1.900E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE2D+R1H=MPE3D2j+H2	5.400E+04	2.5	-1.900E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE4D+R20H=MPE4D3j+H2O	3.000E+06	2.0	-1.520E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE4D+R20H=MPE4D2j+H2O	3.000E+06	2.0	-1.520E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE3D+R20H=MPE4D3j+H2O	3.000E+06	2.0	-1.520E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE3D+R20H=MPE3D2j+H2O	3.000E+06	2.0	-1.520E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				
MPE2D+R20H=MPE3D2j+H2O	3.000E+06	2.0	-1.520E+03	! TOuCHARD Et
al., PrOC COMBust INst, 30 (2005) 1073-1081 (2Hs ally)				

!MPEXDYj raDiCals rEaCtiONs

MPE4D3j=R21CH3OC0+C4H6Z2	1.300E+13	0.00	3.590E+04	!
TOuCHARD Et al., PrOC COMBust INst, 30 (2005) 1073-1081 (Rs+1,3-DiENE)				

!

!MPE4D2j=MP2D+R10C2H3V (02/09/2000)	1.000E+12	0.00	50000.0	!
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!

MPE4D3j=MPE4D2D+R1H	3.000E+13	0.0	51500.0	!tOuCHARD
MPE4D2j=MPE4D2D+R1H	3.160E+13	0.0	34780.0	!Nist

!

NC4H9CO=>R20C4H9+B2CO	1.834e+15	-0.73	1.291e+04	!
Glaude et al., DMC C2H5CO				

CH3CHCO+R20H=R11C2H5+CO2	1.730E+12	0.00	-1.010E+03	
rev /	0.000E+00	0.00	0.000E+00	/

CH3CHCO+R1H=R11C2H5+B2CO	4.400E+12	0.00	1.459E+03	
rev /	0.000E+00	0.00	0.000E+00	/

CH3CHCO+B10=CH3CHO+B2CO	3.200E+12	0.00	-4.370E+02	
rev /	0.000E+00	0.00	0.000E+00	/

C2H3CO+M=>R10C2H3V+B2CO+M	8.600E+15	0.00	23000.0	
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H2O/16.25/ B2CO/1.875/ CO2/3.75/ CH4/16.25/ C2H6/16.25/

C2H3CO+R300H=R10C2H3V+CO2+R20H 2.000E+13 0.00  
0.0

sC3H5CO=sC3H5+B2CO 8.600E+15 0.00 2.300E+04  
rev / 1.000E+11 0.00 6.000E+03 /

!aC3H5CO=C3H5-a+B2CO 6.199E+15 -1.09 -3.300E+02

aC3H5CO=C3H5Y+B2CO 6.199E+15 -1.09 -3.300E+02  
rev / 1.500E+11 0.00 4.810E+03 /

!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
!MEtHyL Hexanoate !  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!

MHX=MHX6j+R1H 7.900e+15 0.0 9.797e+04 !as  
n-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=MHX5j+R1H 5.000e+15 0.0 9.499e+04 !as  
s-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=MHX4j+R1H 5.000e+15 0.0 9.499e+04 !as  
s-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=MHX3j+R1H 5.000e+15 0.0 9.499e+04 !as  
s-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX2j+R1H=MHX 1.000e+14 0.0 0.0 !1  
rnc7\*: h +fragm  
MHX=MHXmj+R1H 7.900e+15 0.0 9.797e+04 !as  
n-C4H9 Dean et al., J.Phys.Chem. 89 (1985) 4600-4608 (-4kcal prox 0)  
MHX=MPE5j+R4CH3 5.000e+16 0.0 8.466e+04 !asC4H10  
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=MB4j+R11C2H5 7.940e+16 0.0 8.028e+04 !asC4H10  
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=MP3j+R19C3H7 7.940e+16 0.0 8.028e+04 !asC4H10  
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=ME2j+R20C4H9 7.940e+16 0.0 8.028e+04 !asC4H10  
Dean et al., J.Phys.Chem. 89 (1985) 4600-4608  
MHX=R21CH30CO+R35C5H11 1.130e+16 0.0 7.770e+04 !  
asCH3COCH3 Sato et al., Combust. Flame 122 (2000) 291-311 (-4kcal prox 0)  
RC6H110+R7CH30=MHX 1.500e+13 0.0 0.000e+00 !  
asDMC Glaude et al., Proc.Combust.Inst. 31 (2005) 1111-1118  
MHX=HXAoj+R4CH3 3.160e+16 0.0 8.307e+04 !asDME Batt  
et al., Proc. Combust. Inst. 19 (1982) 81-87  
MHX+O2=MHX6j+R300H 3.000e+13 0.0 5.280e+04 !2  
anc7, primary f  
MHX+O2=MHX5j+R300H 2.000e+13 0.0 5.105e+04 !2  
anc7, secondary  
MHX+O2=MHX4j+R300H 2.000e+13 0.0 5.105e+04 !2  
anc7, secondary  
MHX+O2=MHX3j+R300H 2.000e+13 0.0 5.105e+04 !2  
anc7, secondary  
MHX+O2=MHX2j+R300H 4.000e+13 0.0 4.130e+04 !2  
rnc7, tertiary

MHX+O2=MHXmj+R300H anc7, primary f !!!	3.000e+13	0.0	5.280e+04	!2	
MHX+R1H=MHX6j+H2 primary f	9.400e+04	2.75	6.280e+03	!2	anc7,
MHX+R1H=MHX5j+H2 secondary	1.300e+06	2.4	4.471e+03	!2	anc7,
MHX+R1H=MHX4j+H2 secondary	1.300e+06	2.4	4.471e+03	!2	anc7,
MHX+R1H=MHX3j+H2 secondary	1.300e+06	2.4	4.471e+03	!2	anc7,
MHX+R1H=MHX2j+H2 anc7, ter	2.520e+14	0.0	7.300e+03	!2	rnc7,
MHX+R1H=MHXmj+H2 primary f	9.400e+04	2.75	6.280e+03	!2	anc7,
MHX+B10=MHX6j+R20H anc7, primary f	9.650e+04	2.68	3.716e+03	!2	
MHX+B10=MHX5j+R20H anc7, secondary	4.770e+04	2.71	2.106e+03	!2	
MHX+B10=MHX4j+R20H anc7, secondary	4.770e+04	2.71	2.106e+03	!2	
MHX+B10=MHX3j+R20H anc7, secondary	4.770e+04	2.71	2.106e+03	!2	
MHX+B10=MHX2j+R20H rnc7, anc7 tert	2.200e+13	0.00	3.280e+03	!2	
MHX+B10=MHXmj+R20H anc7, primary f	9.650e+04	2.68	3.716e+03	!2	
MHX+R20H=MHX6j+H20 rnc7, primary;	5.250e+09	0.97	1.590e+03	!2	
MHX+R20H=MHX5j+H20 rnc7, secondary	4.680e+07	1.61	-3.500e+01	!2	
MHX+R20H=MHX4j+H20 rnc7, secondary	4.680e+07	1.61	-3.500e+01	!2	
MHX+R20H=MHX3j+H20 rnc7, secondary	4.680e+07	1.61	-3.500e+01	!2	
MHX+R20H=MHX2j+H20 rnc7, anc7 tert	1.146e+11	0.51	6.300e+01	!2	
MHX+R20H=MHXmj+H20 rnc7, primary;	5.250e+09	0.97	1.590e+03	!2	
MHX+R300H=MHX6j+H202 primary f	8.400e+12	0.00	2.044e+04	!2	anc7,
MHX+R300H=MHX5j+H202 secondary	5.600e+12	0.00	1.769e+04	!2	anc7,
MHX+R300H=MHX4j+H202 secondary	5.600e+12	0.00	1.769e+04	!2	anc7,
MHX+R300H=MHX3j+H202 secondary	5.600e+12	0.00	1.769e+04	!2	anc7,
MHX+R300H=MHX2j+H202 tertiary	4.320e+12	0.00	1.440e+04	!2	rnc7
MHX+R300H=MHXmj+H202 primary f	8.400e+12	0.00	2.044e+04	!2	anc7,
MHX+R4CH3=MHX6j+CH4 anc7, primary f	4.520e-01	3.65	7.154e+03	!2	

MHX+R4CH3=MHX5j+CH4 anc7, secondary	2.705e+04	2.26	7.287e+03	!2
MHX+R4CH3=MHX4j+CH4 anc7, secondary	2.705e+04	2.26	7.287e+03	!2
MHX+R4CH3=MHX3j+CH4 anc7, secondary	2.705e+04	2.26	7.287e+03	!2
MHX+R4CH3=MHX2j+CH4 rnc7, anc7 tert	2.000e+11	0.00	7.900e+03	!2
MHX+R4CH3=MHXmj+CH4 anc7, primary f	4.520e-01	3.65	7.154e+03	!2
MHX+R7CH30=MHX6j+CH30H rnc7, primary;	1.581e+11	0.00	7.000e+03	!2
MHX+R7CH30=MHX5j+CH30H anc7, secondary	1.095e+11	0.00	5.000e+03	!2
MHX+R7CH30=MHX4j+CH30H anc7, secondary	1.095e+11	0.00	5.000e+03	!2
MHX+R7CH30=MHX3j+CH30H anc7, secondary	1.095e+11	0.00	5.000e+03	!2
MHX+R7CH30=MHX2j+CH30H rnc7, anc7 tert	3.800e+10	0.00	2.800e+03	!2
MHX+R7CH30=MHXmj+CH30H rnc7, primary;	1.581e+11	0.00	7.000e+03	!2
MHX+R8CH300=MHX6j+CH300H corrected to ag	8.400e+12	0.00	2.044e+04	!2
MHX+R8CH300=MHX5j+CH300H corrected to ag	5.600e+12	0.00	1.769e+04	!2
MHX+R8CH300=MHX4j+CH300H corrected to ag	5.600e+12	0.00	1.769e+04	!2
MHX+R8CH300=MHX3j+CH300H corrected to ag	5.600e+12	0.00	1.769e+04	!2
MHX+R8CH300=MHX2j+CH300H same as ho2	4.000e+12	0.00	1.400e+04	!2
MHX+R8CH300=MHXmj+CH300H corrected to ag	8.400e+12	0.00	2.044e+04	!2
MHX+R10C2H3V=MHX6j+C2H4Z rnc7, primary;	5.010e+11	0.00	1.800e+04	!2
MHX+R10C2H3V=MHX5j+C2H4Z rnc7, secondary	4.000e+11	0.00	1.680e+04	!2
MHX+R10C2H3V=MHX4j+C2H4Z rnc7, secondary	4.000e+11	0.00	1.680e+04	!2
MHX+R10C2H3V=MHX3j+C2H4Z rnc7, secondary	4.000e+11	0.00	1.680e+04	!2
MHX+R10C2H3V=MHX2j+C2H4Z rnc7*, tertiary	4.000e+11	0.00	1.430e+04	!2
MHX+R10C2H3V=MHXmj+C2H4Z rnc7**, primary	5.010e+11	0.00	1.800e+04	!2
MHX+R11C2H5=MHX6j+C2H6 rnc7, primary;	5.010e+10	0.00	1.340e+04	!2
MHX+R11C2H5=MHX5j+C2H6 rnc7, secondary	5.000e+10	0.00	1.040e+04	!2
MHX+R11C2H5=MHX4j+C2H6 rnc7, secondary	5.000e+10	0.00	1.040e+04	!2
MHX+R11C2H5=MHX3j+C2H6 rnc7, secondary	5.000e+10	0.00	1.040e+04	!2

MHX+R11C2H5=MHX2j+C2H6 anc7, rnc7*, te	2.000e+11	0.00	7.900e+03	!2
MHX+R11C2H5=MHXmj+C2H6 rnc7**, primary	5.010e+10	0.00	1.340e+04	!2
MHX6j=MHX3j Glaude et al., Energy Fuels, 16 (2002) 1186-1195 + 2Hs)	3.300e+09	1.00	1.730e+04	!
MHX6j=MHX2j Glaude et al., Energy Fuels, 16 (2002) 1186-1195 + 2Ht)	5.700e+08	1.00	1.000e+04	!
MHX5j=MHX2j Glaude et al., Energy Fuels, 16 (2002) 1186-1195 + 2Ht)	3.300e+09	1.00	1.530e+04	!
MHX4j=MHXmj Glaude et al., Energy Fuels, 16 (2002) 1186-1195 + 3Hp)	1.500e+08	1.00	1.990e+04	!
MHX3j=MHXmj radicalc, rs fo	9.256e+10	-0.654	1.390e+04	!5
MHX2j=MHXmj radicalc, rs fo	8.495e+11	-0.507	2.161e+04	!5
MHX6j=C2H4Z+MB4j al., Int J Chem Kinet, 35 (2003) 273-285	2.000e+13	0.00	2.870e+04	!Dayma et
MHX5j=C3H6Y+MP3j al., Int J Chem Kinet, 35 (2003) 273-285	2.000e+13	0.00	2.870e+04	!Dayma et
MHX4j=C4H8Y+ME2j al., Int J Chem Kinet, 35 (2003) 273-285 (Y*+alcene)	3.300e+13	0.00	2.250e+04	!Dayma et
MHX4j=R4CH3+MPE4D et al., Combust Flame, 142 (2005) 170-186	2.000e+13	0.00	3.100e+04	!Buda
MHX3j=R11C2H5+MB3D Dayma et al., Int J Chem Kinet, 35 (2003) 273-285	2.000e+13	0.00	2.870e+04	!
MHX3j=C5H10Z+R21CH3OCO Touchard et al., Int J Chem Kinet, 37 (2005) 451-463 (-4kcal)	2.000e+13	0.00	3.050e+04	!
MHX2j=R19C3H7+MP2D Dayma et al., Int J Chem Kinet, 35 (2003) 273-285	2.000e+13	0.00	2.870e+04	!
C6H10OAY+R7CH3O=MHX2j :oh+c3h6=c	5.000e+11	0.00	-1.000e+03	!3 anc7
RC6H110+HCHO=MHXmj abs val	2.002e+12	0.00	2.400e+04	!3 anist:
CO2+R35C5H11=HXAOj since reaction	1.000e+11	0.00	3.936e+04	!3
MHX6j=R1H+MHX5d al., Int J Chem Kinet, 35 (2003) 273-285 (2Hs)	3.000e+13	0.00	3.800e+04	!Dayma et
MHX5j=R1H+MHX5d et al., Int J Chem Kinet, 37 (2005) 451-463 (3Hp)	3.000e+13	0.00	3.900e+04	!Touchard
MHX5j=R1H+MHX4d al., Int J Chem Kinet, 35 (2003) 273-285 (2Hs)	3.000e+13	0.00	3.800e+04	!Dayma et
MHX4j=R1H+MHX4d al., Int J Chem Kinet, 35 (2003) 273-285 (2Hs)	3.000e+13	0.00	3.800e+04	!Dayma et
MHX4j=R1H+MHX3d al., Int J Chem Kinet, 35 (2003) 273-285 (2Hs)	3.000e+13	0.00	3.800e+04	!Dayma et
MHX3j=R1H+MHX3d al., Int J Chem Kinet, 35 (2003) 273-285 (2Hs)	3.000e+13	0.00	3.800e+04	!Dayma et



MHX2j=R1H+MHX2d	3.000e+13	0.00	3.800e+04	!Dayma et
al., Int J Chem Kinet, 35 (2003)	273-285 (2Hs)			
MHX3j=R1H+MHX2d	3.000e+13	0.00	3.750e+04	!Touchard
(2005) Thise INPL (Ht alk)				
!!!!!!				
MHX5d+B10=MHX5d4j+R20H	8.800e+10	0.70	3.250e+03	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX4d+B10=MHX5d4j+R20H	8.800e+10	0.70	3.250e+03	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX4d+B10=MHX4d3j+R20H	8.800e+10	0.70	3.250e+03	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX3d+B10=MHX4d3j+R20H	8.800e+10	0.70	3.250e+03	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX3d+B10=MHX3d2j+R20H	6.800e+10	0.70	1.330e+03	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Ht)			
MHX2d+B10=MHX3d2j+R20H	8.800e+10	0.70	3.250e+03	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX5d+R1H=MHX5d4j+H2	5.400e+06	2.50	-1.900e+03	!Touchard
et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX4d+R1H=MHX5d4j+H2	1.740e+05	2.50	2.510e+03	!Touchard
et al., Proc Combust Inst, 30 (2005)	1073-1081 (3Hp)			
MHX4d+R1H=MHX4d3j+H2	5.400e+06	2.50	-1.900e+03	!Touchard
et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX3d+R1H=MHX4d3j+H2	5.400e+06	2.50	-1.900e+03	!Touchard
et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX3d+R1H=MHX3d2j+H2	5.000e+04	2.50	-2.790e+03	!Touchard
et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Ht)			
MHX2d+R1H=MHX3d2j+H2	5.400e+06	2.50	-1.900e+03	!Touchard
et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX5d+R20H=MHX5d4j+H2O	3.000e+13	0.00	1.230e+03	!6
anc7				
MHX4d+R20H=MHX5d4j+H2O	3.000e+13	0.00	1.230e+03	!6
anc7				
MHX4d+R20H=MHX4d3j+H2O	3.000e+13	0.00	1.230e+03	!6
anc7				
MHX3d+R20H=MHX4d3j+H2O	3.000e+13	0.00	1.230e+03	!6
anc7				
MHX3d+R20H=MHX3d2j+H2O	3.000e+13	0.00	1.230e+03	!6
anc7				
MHX2d+R20H=MHX3d2j+H2O	3.000e+13	0.00	1.230e+03	!6
anc7				
MHX5d+R300H=MHX5d4j+H2O2	6.400e+03	2.60	1.240e+04	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX4d+R300H=MHX5d4j+H2O2	9.600e+03	2.60	1.390e+04	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (3Hp)			
MHX4d+R300H=MHX4d3j+H2O2	6.400e+03	2.60	1.240e+04	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX3d+R300H=MHX4d3j+H2O2	6.400e+03	2.60	1.240e+04	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
MHX3d+R300H=MHX3d2j+H2O2	3.200e+04	2.60	1.090e+04	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Ht)			
MHX2d+R300H=MHX3d2j+H2O2	6.400e+03	2.60	1.240e+04	!
Touchard et al., Proc Combust Inst, 30 (2005)	1073-1081 (2Hs)			
!!!!!!				

```

MHX5d+R20H=HCHO+MPE5j          1.370e+12   0.00 -1.040e+03   !Heyberger
et al., Combust Flame, 126 (2001) 1780-1802
MHX4d+R20H=CH3CHO+MB4j          1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
MHX3d+R20H=C2H5CHO+MP3j          1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
MHX2d+R20H=C3H8CO+ME2j          1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802
MHX2d+R20H=R20C4H9+ME2*O        1.370e+12   0.00 -1.040e+03   !
Heyberger et al., Combust Flame, 126 (2001) 1780-1802

MHX5d4j=C4H6Z2+ME2j             1.300e+13   0.00  3.490e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (Rs+1,3-diene)
MHX4d3j=C5H8+R21CH30C0          1.300e+13   0.00  3.390e+04   !
Touchard et al., Proc Combust Inst, 30 (2005) 1073-1081 (Rt+1,3-diene)
MHX3d2j=C5H8CO+R7CH30           1.000e+13   0.00  1.500e+04   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (R+cetone/aldehyde)/2
MHX3d2j=MPE4D2D+R4CH3           6.500e+12   0.00  3.820e+04   !Touchard
et al., Proc Combust Inst, 30 (2005) 1073-1081 (CH3+1,3-diene)/2
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!CH2CCO
CH2CCO+R1H=C2H3CO               8.000e+11   0.00   2000.0   !
CH2CCO+R20H=>HCCC0+H20          2.200e+06   2.00  2.780e+03
CH2CCO+R1H=>HCCC0+H2            8.200e+05   2.50  1.228e+04
!HCCC0
HCCC0+O2=>R5CHO+B2CO+B2CO       4.600e+16  -1.39  1.010e+03  !ST
!C2H3CO
!C2H3CO+M=>R10C2H3V+B2CO+M      8.600E+15   0.00  23000.0
END

```

### Механизм окисления смеси этилпентаноат/н-гептан/толуол

```

ELEMENTS
H O C N AR
END
SPECIES

```

! Biradicals :

```

B10
B2CO
B3C
B4CH
B5CH2
B6CH2

```

! Primary molecules :

! Reactants:

```

C7H16-1
C8H18-1
H2
H2O
O2
H2O2
CH4

```

HCHO  
CH3OH  
CO2  
CH3OOH  
C2H2  
C2H4Z  
C2H6  
CH2COZ  
CH3CHO  
C2H5OH  
C2H3OH  
C2H5OOH  
CH3COOOH  
C3H6Y  
C3H8  
C4H8Y  
C4H10  
C2H5CHO  
C3H7OH  
C2H6CO  
C3H8CO  
C4H6Z2  
C2H3CHOZ  
C7H16  
C8H18  
C5H10Z  
C7H14Z  
C6H12Z  
C7H14Y  
C8H16Y  
C8H16Z  
C5H10Y  
C4H100L  
C4H1002P  
C3H802P  
C5H12  
C5H100A  
C4H80A  
C5H120L  
C6H14

! Secondary molecules :

C6H120A  
C7H140A  
!C9H18Z  
!C10H20Z  
!C13H26Z  
!C12H24Z  
!C11H22Z  
!C14H28Z  
C8H160A  
!C9H180A  
!C12H240A  
!C11H220A

!C10H200A  
!C13H260A  
C3H60LY  
C3H602PY  
C4H60AY  
C4H80LY  
C6H10Y2  
C7H12Y2  
C10H18Y2  
C11H20Y2  
C8H14Y2  
C4H802PY  
C5H80AY  
C5H100LY  
!C12H22Y2  
C9H16Y2  
C7H140LY  
C7H1402PY  
C8H140AY  
C8H160LY  
!C14H26Y2  
!C15H28Y2  
C8H1602PY  
!C9H160AY  
!C9H180LY  
!C16H30Y2  
!C13H24Y2  
C5H1002PY  
C6H100AY  
C6H120LY  
C4H60KZ  
C5H80KZ  
C6H100KZ  
C7H120KZ

! Cyclic primary molecules :  
C2H40E#3

! Cyclic secondary molecules :  
C3H60E#3  
C4H80E#3  
C5H100E#3  
C7H140E#3  
C6H120E#3  
C8H160E#3  
!C9H180E#3  
!C10H200E#3  
!C13H260E#3  
!C12H240E#3  
!C11H220E#3  
!C14H280E#3

! Benzenic primary molecules :

! Free radicals :

R1H ! .h  
R2OH ! .oh  
R3OOH ! .o/oh  
R4CH3 ! .ch3  
R5CHO ! .ch//o  
R6CH2OH ! .ch2/oh  
R7CH3O ! .o/ch3  
R8CH3OO ! .o/o/ch3  
R9C2H ! .c///ch  
R10C2H3V ! .ch//ch2  
R11C2H5 ! .ch2/ch3  
R12CHCOZ ! .ch//c//o  
R13CH2CHO ! .ch2/ch//o  
R14CH3CO ! .c(//o)/ch3  
R15C2H5O ! .o/ch2/ch3  
R16C2H4OOH ! .ch2/ch2/o/oh  
R17C2H5OO ! .o/o/ch2/ch3  
R18CH3COOO ! .o/o/c(//o)/ch3  
R19C3H7 ! .ch2/ch2/ch3  
R20C4H9 ! .ch2/ch2/ch2/ch3  
R21CH3OCO ! .c(//o)/o/ch3  
!R22CO2H ! .c(//o)/oh  
!R23C2H3O2B ! .ch2/c(//o)/oh  
!R24C2H4OH ! .ch2/ch2/oh  
!R25C2H4OH ! .ch(/oh)/ch3  
R23C2H4OH ! c.h2-ch2-oh  
R24C2H4OH ! ch3-c.h-oh  
R25C2H5CO ! ch3-ch2-c.o

R26C7H15 ! .ch(/ch2/ch2/ch3)2  
R27C7H15 ! .ch2/ch2/ch2/ch2/ch2/ch2/ch3  
R28C7H15 ! .ch(/ch3)/ch2/ch2/ch2/ch2/ch3  
R29C7H15 ! .ch(/ch2/ch3)/ch2/ch2/ch2/ch3  
R30C8H17 ! .ch2/c(/ch3)2/ch2/ch(/ch3)2  
R31C8H17 ! .ch2/ch(/ch3)/ch2/c(/ch3)3  
R32C8H17 ! .c(/ch3)2/ch2/c(/ch3)3  
R33C8H17 ! .ch(/ch(/ch3)2)/c(/ch3)3  
R34C4H9 ! .ch(/ch3)/ch2/ch3  
R35C5H11 ! .ch2/ch2/ch2/ch2/ch3  
R36C4H9 ! .ch2/ch(/ch3)2  
R37C5H11 ! .ch2/c(/ch3)3  
R38C4H9 ! .c(/ch3)3  
R39C5H11 ! .ch(/ch2/ch3)2  
R40C5H11 ! .ch(/ch3)/ch2/ch2/ch3  
R41C6H13 ! .ch2/ch2/ch2/ch2/ch2/ch3  
R42C7H15 ! .c(/ch3)2/ch2/ch(/ch3)2  
R43C3H7 ! .ch(/ch3)2  
R44C7H15 ! .ch(/ch3)/ch2/c(/ch3)3

!Cyclic free radicals:

!Benzenic free radicals:

! lumped Free radicals :

RC3H5Y

RC4H7Y  
 RC3H50  
 RC7H13Y  
 RC8H15Y  
 RC5H9Y  
 RC5H90  
 RC4H70  
 RC3H503  
 RC6H110  
 RC7H130  
 RC5H903  
 RC4H703  
 RC6H1103  
 RC7H1303  
 RC8H150  
 !RC9H170  
 !RC12H230  
 !RC11H210  
 !RC10H190  
 !RC13H250  
 RC8H1503  
 !RC9H1703  
 RC11H23  
 !RC12H2303  
 RC10H21  
 !RC11H2103  
 RC9H19  
 !RC10H1903  
 RC12H25  
 !RC13H2503  
 RC6H11Y  
 ! lumped Cyclic free radicals :

N2  
AR

!!!!!!!!!!!!Especies rajoutées pour le мйса toлуине

aC3H4	!ch2//ch//ch2	propadiene = allene
pC3H4	!ch///c/ch3	propyne
C4H2	!ch///c/c///ch	butadiyne = diacetylene
C4H4	!ch2//ch/c///ch	1-buten-3-yne ou vinyl
acetylene		
C4H6-12	!ch2//c//ch/ch3	1,2-butadiene ou
мйthyl аллине		
C4H6-1	!ch///c/ch2/ch3	1-butyne
C4H6-2	!ch3/c///c/ch3	2-butyne
iC4H8	!ch2//c(ch3)/ch3	2methyl-propene
C5H8	!ex ch2//ch/ch2/ch//ch2	pentadiene
iC5H8	!ex ch3/c(ch3)//c//ch2	
!iC5H10	!ex ch3/ch(ch3)/ch//ch2	
!C5H10	!ex ch2//ch/ch2/ch2/ch3	pentene
C5H8#	!c(#1)h2/ch2/ch//ch/ch2/1	cyclopentene
C5H6#	!c(#1)h//ch/ch//ch/ch2/1	cyclopentadiene

C6H6# !c(#1)h&ch&ch&ch&ch&ch&1 benzene  
toLuene !c(#1)h&ch&ch&ch&ch&ch&1(/ch3)  
MCP !c(#1)h2/ch2/ch//ch/ch(/ch3)/1 methylcyclopentene  
MCPD !c(#1)h//ch/ch//ch/ch(/ch3)/1 methylcyclopentadiene  
C5H4O# !o//c(#1)/ch//ch/ch//ch/1  
C3H2 !.ch//c//c(.)h  
C2H4O#3 !c(#1)h2/o/ch2/1  
C2H3CHO !ch(/o)/ch//ch2 2-propenal  
cC3H4 !c(#1)h2/ch//ch/1 cyclopropene  
cC3H6 !c(#1)h2/ch2/ch2/1 cyclopropane  
tC4H4 !ch2//c//c//ch2 1,2,3 butatriene  
C6H2 !ch//c/c//c/c//ch hexatriyne  
cC4H6 !c(#1)h2/ch//ch/ch2/1 cyclobutene  
lC6H4 !ch//c/ch//ch/c//ch  
!lC6H6 !ch2//ch/c//c/ch//ch2 !MF car n'intervient plus (une  
rñaction)  
lC6H8 !ch2//ch/ch//ch/ch//ch2  
C6H8# !c(#1)h2/ch//ch/ch2/ch//ch/1 cyclohexadiene  
C6H10# !c(#1)h2/ch//ch/ch2/ch2/ch2/1 cyclohexene  
C8H10# !c(#1)h2/ch//ch/ch//ch/ch//ch/ch2/1 cyclooctatriene  
!Espes excitees  
OHE  
CHE  
iC3H7 !.ch(/ch3)2  
C3H3 !ch//c/ch2(.)  
C3H5Y !.ch2/ch//ch2  
tC3H5 !ch2//c./ch3  
sC3H5 !.ch//ch/ch3  
nC4H3 !.ch//ch/c//ch  
iC4H3 !ch2//c./c//ch  
nC4H5 !.ch//ch/ch//ch2  
iC4H5 !ch2//c./ch//ch2  
C4H5-1s !ch//c/ch./ch3  
C4H5-1p !.ch2/ch2/c//ch  
C4H5-2 !.ch2/c//c/ch3  
lC6H5 !ch//c/ch//ch/ch//ch(.)  
lC6H7 !ex .ch//ch/ch//ch/ch//ch2  
!lC6H9 !ex .ch//ch/ch//ch/ch2/ch3 !MF car n'intervient plus (une  
rñaction)  
C6H4# !.c(#1)&ch&ch&ch&c(.)&1  
C6H5# !.c(#1)&ch&ch&ch&ch&1  
C6H7# !.c(#1)h/ch//ch/ch2/ch//ch/1  
C6H9Z# !.c(#1)h/ch//ch/ch2/ch2/ch2/1  
C4H7-1 !.ch2/ch2/ch//ch2  
C4H7-2 !ch3/c./ch/ch3  
C4H7Y !ch3/c.)h/ch//ch2  
C4H7T !ch2//c./ch2/ch3  
iC4H7 !.ch//c(/ch3)2  
C4H7V !.c(/ch3)//ch/ch3  
!C5H7Y !ch2//ch/ch//ch/c.)h2  
!iC5H7Y !ch2//c(/c.)h2)/ch//ch2  
C5H9Y !ch2//ch/c.)h/ch2/ch3  
iC5H9 !.ch2/ch(/ch3)/ch//ch2  
!iC5H9Y !ch3/c./ch3)/ch//ch2

CH2CHCO !.ch2/ch//c//o  
 cC3H3 !.c(#1)h/ch//ch/1  
 ! MECHANISM OF BENZENE  
 ! Molecules  
 C4H4O !ch2//ch/ch//c//o vinylketene  
 !lC5H6 !ch//c/ch//ch/ch3 !MF car  
 n'intervient plus (une rñaction)  
 C5H5OH# !c(#1)h//ch/ch//ch/ch(/oh)/1 cyclopentadienol  
 C6H5OH# !c(#1)h&ch&ch&ch&c(/oh)&1 phñnol  
 OC6H4O !o//c(#1)/ch//ch/ch//ch/c(/o)/1 orthobenzoquinone  
 C6H5#C2H !ch//c/c(#1)&ch&ch&ch&ch/&1 phenylacetylene  
 etC6H5 !c(#1)h&ch&ch&ch&c(/ch2/ch3)&1 ethylbenzene  
 styrene !c(#1)h&ch&ch&ch&c(/ch//ch2)&1  
 !C6H5C3H3 !c(#1)h&ch&ch&ch&c(/ch//c//ch2)&1 !MF car n'intervient plus  
 (une rñaction)  
 C10H10# !c(#1)h(c(#1)h/ch//ch/ch//ch/1)/ch//ch/ch//ch/1 !  
 bicyclopentadienyl  
 C6H5CHO !c(#1)h&ch&ch&ch&c(/ch//o)&1 benzaldehyde  
 biphenyl !c(#1)h&ch&ch&ch&c(/c(#2)h&ch&ch&ch&c&2)&1  
 C6H5OOH

! Radicals

C5H5# !c(#1)(.)h/ch//ch/ch//ch/1  
 lC5H5 !.c//c/ch//ch/ch3  
 C5H30# !.c(#1)//ch/ch//ch/c(/o)&1  
 C5H50# !c(#1)h//ch/ch//ch/ch(/o(.))&1  
 C5H40H# !.c(#1)//ch/ch//ch/ch(/oh)&1  
 C6H50# !c(#1)h&ch&ch&ch&c(/o(.))&1  
 C6H5O2 !.c(#1)&ch&ch&ch&c(/o/o(.))&1  
 C6H40H# !.c(#1)&ch&ch&ch&c(/oh)&1  
 OC6H4OH !c(#1)h&ch&ch&ch&c(/o(.))&c(/oh)&1

!MECHANISM OF TOLUENE

HOC6H4CH3 !oh/c(#1)&ch&ch&ch&c(/ch3)&1 cresol  
 C6H4OHCHO !oh/c(#1)&ch&ch&ch&c(/ch//o)&1  
 C6H5CH2OH !c(#1)h&ch&ch&ch&c(/ch2/oh)&1  
 C6H5CH2OOH !c(#1)h&ch&ch&ch&c(/ch2/o/oh)&1  
 bibenzyl !ok  
 stilbene !ok  
 benzyl !c(#1)h&ch&ch&ch&c(/c(. )h2)&1  
 C6H4CH3 !c(#1)h&ch&ch&ch&c(/ch3)&1  
 C6H4OHC0 !oh/c(#1)&ch&ch&ch&c(/c(. )//o)&1  
 HOC6H4CH200 !oh/c(#1)&ch&ch&ch&c(/ch2/o/o(.))&1  
 OC6H4CH3 !o(. )/c(#1)&ch&ch&ch&c(/ch3)&1  
 HOC6H4CH2 !oh/c(#1)&ch&ch&ch&c(/c(. )h2)&1  
 C6H5CO !c(#1)h&ch&ch&ch&c(/o(.))&1  
 C6H5CHOH !c(#1)h&ch&ch&ch&c(/c(. )h/oh)&1  
 C6H5CH2O !c(#1)h&ch&ch&ch&c(/ch2/o(.))&1  
 HOC6H4CH2O !oh/c(#1)&ch&ch&ch&c(/ch2/o(.))&1  
 C6H5CH2OO !c(#1)h&ch&ch&ch&c(/ch2/o/o(.))&1  
 C8H9# !c(#1)h&ch&ch&ch&c(/c(. )h2/ch2)&1  
 C8H9#-1 !c(#1)h&ch&ch&ch&c(/ch2/c(. )h2)&1  
 C6H5C2H2 !c(#1)h&ch&ch&ch&c(/ch//c(. )h)&1



C14H13#

!bibenzyl -H

!MECHANISM OF CYCLOPENTENE!

!C5H8-12 !ch2//c//ch/ch2/ch3  
!C5H7# !.c(#1)h/ch2/ch//ch/ch2/1  
!C5H7#Y !c(#1)h2/c(.)h/ch//ch/ch2/1  
!C5H7#V !c(#1)h2/ch2/c(.)//ch/ch2/1  
!C5H7-1s !ch(.)//ch/ch2/ch//ch2  
!C5H7-2t !ch2//ch/ch2/c(.)//ch2  
!C5H7-4t !ch3/c(.)//ch/ch//ch2  
!C5H7-3t !ch3/ch//c(.)//ch//ch2  
!C5H7-5p !ch2(.)//ch2/ch2/c//ch  
!C5H7-12-5p !ch2(.)//ch2/ch//c//ch2  
!C5H9# !.c(#1)h/ch2/ch2/ch2/ch2/1  
!C5H9 !(.)ch2/ch2/ch2/ch//ch2  
!RMCP1 !c(#1)h(.)//ch2/ch//ch/ch(/ch3)/1  
!RMCP2 !c(#1)h2/ch2/ch//ch/ch(/ch2.)/1  
!RMCPY1 !c(#1)h2/ch(.)//ch//ch/ch(/ch3)/1  
!RMCPY2 !c(#1)h2/ch2/ch//ch/c(.)(/ch3)/1  
!RMCPD !c(#1)h//ch/ch//ch/ch(/ch2.)/1  
!RMCPDY !c(#1)h//ch/ch//ch/c(.)(/ch3)/1

!\*Especies ajoutées\*!

!mfC5H5C2H2 !c(#1)h//ch/ch//ch/c(/ch//c(.)h)&1  
!C5H4CCH2 !c(#1)h//ch/ch//ch/c(/c//ch2)/1  
!C5H5CCH !c(#1)h//ch/ch//ch/ch(/c//ch)/1  
!C6H5COCH3 !C6H5x/CO/CH3  
C8H9#00H !C6H5#ch(/ooh)/ch3 ! c(#1)h&ch&ch&ch&c(/ch(/o/o/h)/ch3)&1  
C8H9#0 !C6H5#ch(/o.)/ch3 !  
c(#1)h&ch&ch&ch&c(/ch(/o.)/ch3)&1  
00C6H4CH3 !o(.)//o/c(#1)&ch&ch&ch&c(/ch3)&1  
!C6H5OCH2C6H5 !c(#1)h&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&2)&1  
!To10CH2C6H5 !ch3/c(#1)&ch&ch&ch&c(/o/ch2/c(#2)&ch&ch&ch&ch&2)&1  
!PhenolCH2bz !h/o/c(#1)&ch&ch&ch&c(/ch2/c(#2)&ch&ch&ch&ch&2)&1  
!PhenolC2H4bz !h/o/c(#1)&ch&ch&ch&c(/ch2/ch2/c(#2)&ch&ch&ch&ch&2)&1  
CH3bzOHCH2bz !h/o/c(#1)&ch&ch&c(/ch3)&ch&c(/ch2/c(#2)&ch&ch&ch&ch&2)&1  
!Benzaldtol !  
c(#1)h&ch&ch&ch&c(/c(/o)/o/c(#2)&ch&ch&c(/ch3)&ch&ch&2)&1  
!HOC6H4CHO !h/o/c(#1)&ch&ch&ch&c(/ch//o)&ch&1  
!C6H5C4H7 !c(#1)h&ch&ch&ch&c(/ch2/ch2/ch//ch2)&1  
naphthalene  
!benzofuran  
C8H8O# ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch2/2  
C8H7O# ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch./ch2/2  
C8H7O#-1 ! c(#1)&c(#2)&ch&ch&ch&ch&1,1/o/ch2/ch./2  
naphthyl  
indenyl  
indene  
!cumene  
!CH3styre  
C9H11#-1  
C2H3C6H4CH2

!phenanthrene

!C6H5CH2CHO

!!!!!!!!!!!!!!!!!!!!!!!!!!!!

\*\*\*\*\*

!!!!!!Ethyl esters

EF

HCOOH

C2H5OCO

EFEJ

EFMJ

EFED

CH2OCHO

CH3COOH

EA2J

EA

EA2J

EAEJ

EAMJ

MEMJ

EAEJ

EAMJ

EAED

HOCO

CH2COOH

EP

C2H5COOH

EP3J

EP2J

EPEJ

EPMJ

C2H5CO

MPMJ

CH3CHCO

EP2d

EPED

CH2CH2COOH

CH3CHCOOH

C2H3COOH

EB

C3H7COOH

EB4J

EB3J

EB2J

EBEJ

EBMJ

NC3H7CO

MBMJ

C2H5CHCO

EB3D

EB2D

EBed

PRCOOH-4

PRCOOH-3

PRCOOH-2

C3H5C00H  
 EPE  
 C4H9C00H  
 EPE5J  
 EPE4J  
 EPE3J  
 EPE2J  
 EPEEJ  
 EPEMJ  
 EPE4D  
 EPE3D  
 EPE2D  
 EPEED  
 NC4H9CO  
 MPEMJ  
 C4H8CO  
 BUC00H-5  
 BUC00H-4  
 BUC00H-3  
 BUC00H-2  
 C4H7C00H  
 HC02  
 CH3C02  
 C2H5C02  
 C3H7C02  
 C4H9C02  
 C3H7C0C02  
 CH3C0C02  
 CH3CHCHO  
 NC3H7CHO  
 END

REACTIONS

( $k = A T^{**b} \exp(-E/RT)$ ) A units: mole-cm-sec-K, E units cal/mole)

```

! -----
!   PRIMARY REACTIONS
! -----
!   molecular elimination :
!   unimolecular initiations :
C7H16-1=>R19C3H7+R20C4H9      2.0E+0017  0.000  85750.3  ! UI 1 KB
C7H16-1=>R11C2H5+R35C5H11     1.6E+0017  0.000  85815.5  ! UI 2 KB
C7H16-1=>R4CH3+R41C6H13       3.2E+0017  0.000  87654.8  ! UI 3 KB
C8H18-1=>R4CH3+R42C7H15       1.2E+0018  0.000  81845.9  ! UI 4 KB
C8H18-1=>R36C4H9+R38C4H9      2.4E+0017  0.000  78804.1  ! UI 5 KB
C8H18-1=>R43C3H7+R37C5H11     4.6E+0017  0.000  83562.0  ! UI 6 KB
C8H18-1=>R4CH3+R44C7H15       8.0E+0017  0.000  87665.1  ! UI 7 KB

!   bimolecular initiations :
C7H16-1+O2=>R300H+R26C7H15    1.4E+0013  0.000  50652.5  ! BI 8 CN
C7H16-1+O2=>R300H+R27C7H15    4.2E+0013  0.000  53033.1  ! BI 9 CN
C7H16-1+O2=>R300H+R28C7H15    2.8E+0013  0.000  50588.2  ! BI 10 CN
C7H16-1+O2=>R300H+R29C7H15    2.8E+0013  0.000  50652.5  ! BI 11 CN
  
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C8H18-1+O2=>R300H+R30C8H17	6.3E+0013	0.000	53033.0	!	BI	12	CN
C8H18-1+O2=>R300H+R31C8H17	4.2E+0013	0.000	52333.1	!	BI	13	CN
C8H18-1+O2=>R300H+R32C8H17	7.0E+0012	0.000	47243.3	!	BI	14	CN
C8H18-1+O2=>R300H+R33C8H17	1.4E+0013	0.000	50652.7	!	BI	15	CN

! additions :

! additions with oxygen:

! isomerisations :

R20C4H9=R34C4H9	3.3E+0009	1.000	37000.0	!	IS	16	KB
R26C7H15=R28C7H15	6.7E+0009	1.000	37000.0	!	IS	17	KB
R26C7H15=R27C7H15	1.7E+0009	1.000	19800.0	!	IS	18	KB
R27C7H15=R29C7H15	9.9E+0007	1.000	37000.0	!	IS	19	KB
R27C7H15=R28C7H15	1.7E+0007	1.000	17400.0	!	IS	20	KB
R28C7H15=R29C7H15	5.7E+0008	1.000	17300.0	!	IS	21	KB
R30C8H17=R33C8H17	3.3E+0009	1.000	37000.0	!	IS	22	KB
R30C8H17=R32C8H17	2.9E+0008	1.000	15300.0	!	IS	23	KB
R30C8H17=R31C8H17	3.0E+0008	1.000	14500.0	!	IS	24	KB
R31C8H17=R33C8H17	3.3E+0009	1.000	37000.0	!	IS	25	KB
R35C5H11=R39C5H11	3.3E+0009	1.000	37000.0	!	IS	26	KB
R35C5H11=R40C5H11	5.7E+0008	1.000	17300.0	!	IS	27	KB

! Decomposition of 00Q00H into branching agents:

! beta-scissions :

R19C3H7=>R4CH3+C2H4Z	2.0E+0013	0.000	31000.0	!	DE	28	CN
R19C3H7=>R1H+C3H6Y	3.0E+0013	0.000	38000.0	!	DE	29	CN
R20C4H9=>R11C2H5+C2H4Z	2.0E+0013	0.000	28700.0	!	DE	30	CW
R20C4H9=>R1H+C4H8Y	3.0E+0013	0.000	38000.0	!	DE	31	CN
R26C7H15=>R11C2H5+C5H10Z	4.0E+0013	0.000	28700.0	!	DE	32	CW
R26C7H15=>R1H+C7H14Z	6.0E+0013	0.000	38000.0	!	DE	33	CN
R27C7H15=>R35C5H11+C2H4Z	2.0E+0013	0.000	28700.0	!	DE	34	CW
R27C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	35	CN
R28C7H15=>R20C4H9+C3H6Y	2.0E+0013	0.000	28700.0	!	DE	36	CW
R28C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	37	CN
DUPLICATE							
R28C7H15=>R1H+C7H14Z	3.0E+0013	0.000	39000.0	!	DE	38	CN
DUPLICATE							
R29C7H15=>R19C3H7+C4H8Y	2.0E+0013	0.000	28700.0	!	DE	39	CW
R29C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	40	CN
DUPLICATE							
R29C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	!	DE	41	CN
DUPLICATE							
R29C7H15=>R4CH3+C6H12Z	2.0E+0013	0.000	31000.0	!	DE	42	CN
R30C8H17=>R36C4H9+C4H8Y	2.0E+0013	0.000	28700.0	!	DE	43	CW
R30C8H17=>R4CH3+C7H14Y	4.0E+0013	0.000	31000.0	!	DE	44	CN
R31C8H17=>R37C5H11+C3H6Y	2.0E+0013	0.000	28700.0	!	DE	45	CW
R31C8H17=>R4CH3+C7H14Z	2.0E+0013	0.000	31000.0	!	DE	46	CN
R31C8H17=>R1H+C8H16Y	1.5E+0013	0.000	37500.0	!	DE	47	CN
R32C8H17=>R38C4H9+C4H8Y	2.0E+0013	0.000	26700.0	!	DE	48	
R32C8H17=>R1H+C8H16Y	6.0E+0013	0.000	39000.0	!	DE	49	CN
R32C8H17=>R1H+C8H16Z	3.0E+0013	0.000	38000.0	!	DE	50	CN
R33C8H17=>R4CH3+C7H14Z	4.0E+0013	0.000	31000.0	!	DE	51	CN

R33C8H17=>R4CH3+C7H14Y	6.0E+0013	0.000	31000.0	! DE 52 CN
R33C8H17=>R1H+C8H16Z	3.0E+0013	0.000	37500.0	! DE 53 CN
R34C4H9=>R4CH3+C3H6Y	2.0E+0013	0.000	31000.0	! DE 54 CN
R34C4H9=>R1H+C4H8Y	3.0E+0013	0.000	38000.0	! DE 55 CN
DUPLICATE				
R34C4H9=>R1H+C4H8Y	3.0E+0013	0.000	39000.0	! DE 56 CN
DUPLICATE				
R35C5H11=>R19C3H7+C2H4Z	2.0E+0013	0.000	28700.0	! DE 57 CW
R35C5H11=>R1H+C5H10Z	3.0E+0013	0.000	38000.0	! DE 58 CN
R36C4H9=>R4CH3+C3H6Y	4.0E+0013	0.000	31000.0	! DE 59 CN
R36C4H9=>R1H+C4H8Y	3.0E+0013	0.000	37500.0	! DE 60 CN
R37C5H11=>R4CH3+C4H8Y	6.0E+0013	0.000	31000.0	! DE 61 CN
R38C4H9=>R1H+C4H8Y	9.0E+0013	0.000	39000.0	! DE 62 CN
R39C5H11=>R4CH3+C4H8Y	4.0E+0013	0.000	31000.0	! DE 63 CN
R39C5H11=>R1H+C5H10Y	6.0E+0013	0.000	38000.0	! DE 64 CN
R40C5H11=>R11C2H5+C3H6Y	2.0E+0013	0.000	28700.0	! DE 65 CW
R40C5H11=>R1H+C5H10Z	3.0E+0013	0.000	39000.0	! DE 66 CN
R40C5H11=>R1H+C5H10Y	3.0E+0013	0.000	38000.0	! DE 67 CN
R41C6H13=>R20C4H9+C2H4Z	2.0E+0013	0.000	28700.0	! DE 68 CW
R41C6H13=>R1H+C6H12Z	3.0E+0013	0.000	38000.0	! DE 69 CN
R42C7H15=>R43C3H7+C4H8Y	2.0E+0013	0.000	27700.0	! DE 70
R42C7H15=>R1H+C7H14Y	3.0E+0013	0.000	38000.0	! DE 71 CN
DUPLICATE				
R42C7H15=>R1H+C7H14Y	6.0E+0013	0.000	39000.0	! DE 72 CN
DUPLICATE				
R43C3H7=>R1H+C3H6Y	6.0E+0013	0.000	39000.0	! DE 73 CN
R44C7H15=>R38C4H9+C3H6Y	2.0E+0013	0.000	26700.0	! DE 74
R44C7H15=>R1H+C7H14Z	3.0E+0013	0.000	38000.0	! DE 75 CN
DUPLICATE				
R44C7H15=>R1H+C7H14Z	3.0E+0013	0.000	39000.0	! DE 76 CN
DUPLICATE				

! decomposition of R(.)CO free radicals

! decomposition to o-rings :

! oxidations :

R26C7H15+O2=>C7H14Z+R300H	3.9E+0012	0.000	5000.0	! OX 77 CN
R27C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	! OX 78 CN
R28C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	! OX 79 CN
DUPLICATE				
R28C7H15+O2=>C7H14Z+R300H	8.1E+0011	0.000	5000.0	! OX 80 CN
DUPLICATE				
R29C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	! OX 81 CN
DUPLICATE				
R29C7H15+O2=>C7H14Z+R300H	1.9E+0012	0.000	5000.0	! OX 82 CN
DUPLICATE				
R31C8H17+O2=>C8H16Y+R300H	6.4E+0011	0.000	5000.0	! OX 83 CN
R32C8H17+O2=>C8H16Y+R300H	1.6E+0012	0.000	5000.0	! OX 84 CN
R32C8H17+O2=>C8H16Z+R300H	1.9E+0012	0.000	5000.0	! OX 85 CN
R33C8H17+O2=>C8H16Z+R300H	6.4E+0011	0.000	5000.0	! OX 86 CN
R38C4H9+O2=>C4H8Y+R300H	1.6E+0012	0.000	5000.0	! OX 87 CW
R43C3H7+O2=>C3H6Y+R300H	2.3E+0012	0.000	5000.0	! OX 88 CW

! oxidations of R.)(OH) radicals:

! metathesis :

B10+C7H16-1=>R20H+R26C7H15	2.6E+0013	0.000	5200.0	! ME 89 CW
B10+C7H16-1=>R20H+R27C7H15	1.0E+0014	0.000	7850.0	! ME 90 CW
B10+C7H16-1=>R20H+R28C7H15	5.2E+0013	0.000	5200.0	! ME 91 CW
B10+C7H16-1=>R20H+R29C7H15	5.2E+0013	0.000	5200.0	! ME 92 CW
B10+C8H18-1=>R20H+R30C8H17	1.5E+0014	0.000	7850.0	! ME 93 CW
B10+C8H18-1=>R20H+R31C8H17	1.0E+0014	0.000	7850.0	! ME 94 CW
B10+C8H18-1=>R20H+R32C8H17	1.0E+0013	0.000	3280.0	! ME 95 CW
B10+C8H18-1=>R20H+R33C8H17	2.6E+0013	0.000	5200.0	! ME 96 CW
C7H16-1+R1H=>H2+R26C7H15	9.0E+0006	2.000	5000.0	! ME 97 CW
C7H16-1+R1H=>H2+R27C7H15	5.7E+0007	2.000	7700.0	! ME 98 CW
C7H16-1+R1H=>H2+R28C7H15	1.8E+0007	2.000	5000.0	! ME 99 CW
C7H16-1+R1H=>H2+R29C7H15	1.8E+0007	2.000	5000.0	! ME 100 CW
C8H18-1+R1H=>H2+R30C8H17	8.6E+0007	2.000	7700.0	! ME 101 CW
C8H18-1+R1H=>H2+R31C8H17	5.7E+0007	2.000	7700.0	! ME 102 CW
C8H18-1+R1H=>H2+R32C8H17	4.2E+0006	2.000	2400.0	! ME 103 CN
C8H18-1+R1H=>H2+R33C8H17	9.0E+0006	2.000	5000.0	! ME 104 CW
C7H16-1+R20H=>H20+R26C7H15	2.6E+0006	2.000	-765.0	! ME 105 CW
C7H16-1+R20H=>H20+R27C7H15	5.4E+0006	2.000	450.0	! ME 106 CW
C7H16-1+R20H=>H20+R28C7H15	5.2E+0006	2.000	-765.0	! ME 107 CW
C7H16-1+R20H=>H20+R29C7H15	5.2E+0006	2.000	-765.0	! ME 108 CW
C8H18-1+R20H=>H20+R30C8H17	8.1E+0006	2.000	450.0	! ME 109 CW
C8H18-1+R20H=>H20+R31C8H17	5.4E+0006	2.000	450.0	! ME 110 CW
C8H18-1+R20H=>H20+R32C8H17	1.1E+0006	2.000	-1865.0	! ME 111 CW
C8H18-1+R20H=>H20+R33C8H17	2.6E+0006	2.000	-765.0	! ME 112 CW
C7H16-1+R300H=>H202+R26C7H15	4.0E+0011	0.000	15500.0	! ME 113 CN
C7H16-1+R300H=>H202+R27C7H15	1.2E+0012	0.000	17000.0	! ME 114 CN
C7H16-1+R300H=>H202+R28C7H15	8.0E+0011	0.000	15500.0	! ME 115 CN
C7H16-1+R300H=>H202+R29C7H15	8.0E+0011	0.000	15500.0	! ME 116 CN
C8H18-1+R300H=>H202+R30C8H17	1.8E+0012	0.000	17000.0	! ME 117 CN
C8H18-1+R300H=>H202+R31C8H17	1.2E+0012	0.000	17000.0	! ME 118 CN
C8H18-1+R300H=>H202+R32C8H17	2.0E+0011	0.000	14000.0	! ME 119 CN
C8H18-1+R300H=>H202+R33C8H17	4.0E+0011	0.000	15500.0	! ME 120 CN
C7H16-1+R4CH3=>CH4+R26C7H15	2.0E+0011	0.000	9600.0	! ME 121 CN
C7H16-1+R4CH3=>CH4+R27C7H15	6.0E-0001	4.000	8200.0	! ME 122 CN
C7H16-1+R4CH3=>CH4+R28C7H15	4.0E+0011	0.000	9600.0	! ME 123 CN
C7H16-1+R4CH3=>CH4+R29C7H15	4.0E+0011	0.000	9600.0	! ME 124 CN
C8H18-1+R4CH3=>CH4+R30C8H17	9.0E-0001	4.000	8200.0	! ME 125 CN
C8H18-1+R4CH3=>CH4+R31C8H17	6.0E-0001	4.000	8200.0	! ME 126 CN
C8H18-1+R4CH3=>CH4+R32C8H17	1.0E+0011	0.000	7900.0	! ME 127 CW
C8H18-1+R4CH3=>CH4+R33C8H17	2.0E+0011	0.000	9600.0	! ME 128 CN
C7H16-1+R5CHO=>HCHO+R26C7H15	1.0E+0007	1.900	17000.0	! ME 129 CN
C7H16-1+R5CHO=>HCHO+R27C7H15	2.0E+0005	2.500	18500.0	! ME 130 CN
C7H16-1+R5CHO=>HCHO+R28C7H15	2.2E+0007	1.900	17000.0	! ME 131 CN
C7H16-1+R5CHO=>HCHO+R29C7H15	2.2E+0007	1.900	17000.0	! ME 132 CN
C8H18-1+R5CHO=>HCHO+R30C8H17	3.1E+0005	2.500	18500.0	! ME 133 CN
C8H18-1+R5CHO=>HCHO+R31C8H17	2.0E+0005	2.500	18500.0	! ME 134 CN
C8H18-1+R5CHO=>HCHO+R32C8H17	3.4E+0004	2.500	13500.0	! ME 135 CN
C8H18-1+R5CHO=>HCHO+R33C8H17	1.0E+0007	1.900	17000.0	! ME 136 CN
C7H16-1+R6CH2OH=>CH3OH+R26C7H15	6.0E+0001	2.950	12000.0	! ME 137 CN
C7H16-1+R6CH2OH=>CH3OH+R27C7H15	2.0E+0002	2.950	14000.0	! ME 138 CN
C7H16-1+R6CH2OH=>CH3OH+R28C7H15	1.2E+0002	2.950	12000.0	! ME 139 CN
C7H16-1+R6CH2OH=>CH3OH+R29C7H15	1.2E+0002	2.950	12000.0	! ME 140 CN

C8H18-1+R6CH20H=>CH30H+R30C8H17	3.0E+0002	2.950	14000.0	! ME 141 CN
C8H18-1+R6CH20H=>CH30H+R31C8H17	2.0E+0002	2.950	14000.0	! ME 142 CN
C8H18-1+R6CH20H=>CH30H+R32C8H17	1.2E+0002	2.760	10800.0	! ME 143 CN
C8H18-1+R6CH20H=>CH30H+R33C8H17	6.0E+0001	2.950	12000.0	! ME 144 CN
C7H16-1+R7CH30=>CH30H+R26C7H15	1.5E+0011	0.000	4500.0	! ME 145 CN
C7H16-1+R7CH30=>CH30H+R27C7H15	3.2E+0011	0.000	7300.0	! ME 146 CN
C7H16-1+R7CH30=>CH30H+R28C7H15	2.9E+0011	0.000	4500.0	! ME 147 CN
C7H16-1+R7CH30=>CH30H+R29C7H15	2.9E+0011	0.000	4500.0	! ME 148 CN
C8H18-1+R7CH30=>CH30H+R30C8H17	4.9E+0011	0.000	7300.0	! ME 149 CN
C8H18-1+R7CH30=>CH30H+R31C8H17	3.2E+0011	0.000	7300.0	! ME 150 CN
C8H18-1+R7CH30=>CH30H+R32C8H17	2.3E+0010	0.000	2900.0	! ME 151 CN
C8H18-1+R7CH30=>CH30H+R33C8H17	1.5E+0011	0.000	4500.0	! ME 152 CN
C7H16-1+R8CH300=>CH300H+R26C7H15	3.0E+0012	0.000	17500.0	! ME 153
CN				
C7H16-1+R8CH300=>CH300H+R27C7H15	1.2E+0013	0.000	20000.0	! ME 154
CN				
C7H16-1+R8CH300=>CH300H+R28C7H15	6.0E+0012	0.000	17500.0	! ME 155
CN				
C7H16-1+R8CH300=>CH300H+R29C7H15	6.0E+0012	0.000	17500.0	! ME 156
CN				
C8H18-1+R8CH300=>CH300H+R30C8H17	1.8E+0013	0.000	20000.0	! ME 157
CN				
C8H18-1+R8CH300=>CH300H+R31C8H17	1.2E+0013	0.000	20000.0	! ME 158
CN				
C8H18-1+R8CH300=>CH300H+R32C8H17	1.5E+0012	0.000	15000.0	! ME 159
CN				
C8H18-1+R8CH300=>CH300H+R33C8H17	3.0E+0012	0.000	17500.0	! ME 160
CN				
C7H16-1+R11C2H5=>C2H6+R26C7H15	2.0E+0011	0.000	11000.0	! ME 161 CN
C7H16-1+R11C2H5=>C2H6+R27C7H15	6.0E+0011	0.000	13500.0	! ME 162 CR
C7H16-1+R11C2H5=>C2H6+R28C7H15	4.0E+0011	0.000	11000.0	! ME 163 CN
C7H16-1+R11C2H5=>C2H6+R29C7H15	4.0E+0011	0.000	11000.0	! ME 164 CN
C8H18-1+R11C2H5=>C2H6+R30C8H17	9.0E+0011	0.000	13500.0	! ME 165 CR
C8H18-1+R11C2H5=>C2H6+R31C8H17	6.0E+0011	0.000	13500.0	! ME 166 CR
C8H18-1+R11C2H5=>C2H6+R32C8H17	1.0E+0011	0.000	9200.0	! ME 167 CN
C8H18-1+R11C2H5=>C2H6+R33C8H17	2.0E+0011	0.000	11000.0	! ME 168 CN
C7H16-1+R38C4H9=>C4H10+R26C7H15	1.0E+0011	0.000	12700.0	! ME 169 CR
C7H16-1+R38C4H9=>C4H10+R27C7H15	3.0E+0011	0.000	15000.0	! ME 170 CR
C7H16-1+R38C4H9=>C4H10+R28C7H15	2.0E+0011	0.000	12700.0	! ME 171 CR
C7H16-1+R38C4H9=>C4H10+R29C7H15	2.0E+0011	0.000	12700.0	! ME 172 CR
C8H18-1+R38C4H9=>C4H10+R30C8H17	4.5E+0011	0.000	15000.0	! ME 173 CR
C8H18-1+R38C4H9=>C4H10+R31C8H17	3.0E+0011	0.000	15000.0	! ME 174 CR
C8H18-1+R38C4H9=>C4H10+R32C8H17	5.0E+0010	0.000	11100.0	! ME 175 CR
C8H18-1+R38C4H9=>C4H10+R33C8H17	1.0E+0011	0.000	12700.0	! ME 176 CR

! combinations :

R1H+R38C4H9=>C4H10	8.3E+0012	0.000	0.0	! CO 177 KB
R1H+R43C3H7=>C3H8	8.3E+0012	0.000	0.0	! CO 178 KB
R20H+R38C4H9=>C4H100L	5.7E+0012	0.000	0.0	! CO 179 KB
R20H+R43C3H7=>C3H70H	5.9E+0012	0.000	0.0	! CO 180 KB
R300H+R38C4H9=>C4H1002P	4.5E+0012	0.000	0.0	! CO 181 KB
R300H+R43C3H7=>C3H802P	4.8E+0012	0.000	0.0	! CO 182 KB
R4CH3+R38C4H9=>C5H12	1.5E+0013	0.000	0.0	! CO 183 KB
R4CH3+R43C3H7=>C4H10	1.5E+0013	0.000	0.0	! CO 184 KB

R5CH0+R38C4H9=>C5H100A	4.9E+0012	0.000	0.0	! CO 185 KB
R5CH0+R43C3H7=>C4H80A	5.2E+0012	0.000	0.0	! CO 186 KB
R6CH20H+R38C4H9=>C5H120L	4.8E+0012	0.000	0.0	! CO 187 KB
R6CH20H+R43C3H7=>C4H100L	5.1E+0012	0.000	0.0	! CO 188 KB
R11C2H5+R38C4H9=>C6H14	4.9E+0012	0.000	0.0	! CO 189 KB
R11C2H5+R43C3H7=>C5H12	5.2E+0012	0.000	0.0	! CO 190 KB
R38C4H9+R38C4H9=>C8H18	2.0E+0012	0.000	0.0	! CO 191 KB
R38C4H9+R43C3H7=>C7H16	4.3E+0012	0.000	0.0	! CO 192 KB
R43C3H7+R43C3H7=>C6H14	2.3E+0012	0.000	0.0	! CO 193 KB

! dismutations :

! -----  
! SECONDARY MECHANISM  
! -----

! Peroxide decomposition

! Hydroperoxide decomposition

C4H1002P=>R20H+R11C2H5+CH3CHO	1.5E+0016	0.000	43000.0	! DHP 194
C3H802P=>R20H+R11C2H5+HCHO	1.5E+0016	0.000	43000.0	! DHP 195
C3H602PY=>R20H+R1H+C2H3CHOZ	1.5E+0016	0.000	43000.0	! DHP 196
C4H802PY=>R20H+R4CH3+C2H3CHOZ	1.5E+0016	0.000	43000.0	! DHP 197
C7H1402PY=>R20H+R20C4H9+C2H3CHOZ	1.5E+0016	0.000	43000.0	! DHP 198
C8H1602PY=>R20H+R35C5H11+C2H3CHOZ	1.5E+0016	0.000	43000.0	! DHP 199
C5H1002PY=>R20H+R11C2H5+C2H3CHOZ	1.5E+0016	0.000	43000.0	! DHP 200

! Alcoholhydroperoxide decomposition

! Dihydroperoxide decomposition

! Ketohydroperoxide decomposition

! Aldohydroperoxide decomposition

! Peroxy-ester decomposition

! Hydroperoxy ring decomposition

! Alkane reactions

C3H8+R1H=>H2+R19C3H7	5.7E+0007	2.000	7700.0	! MH 201
DUPLICATE				
C3H8+R1H=>H2+R19C3H7	9.0E+0006	2.000	5000.0	! MH 202
DUPLICATE				
C3H8+R20H=>H20+R19C3H7	5.4E+0006	2.000	450.0	! MH 203
DUPLICATE				
C3H8+R20H=>H20+R19C3H7	2.6E+0006	2.000	-765.0	! MH 204
DUPLICATE				
C3H8+R300H=>H202+R19C3H7	1.2E+0012	0.000	17000.0	! MH 205
DUPLICATE				
C3H8+R300H=>H202+R19C3H7	4.0E+0011	0.000	15500.0	! MH 206
DUPLICATE				
C3H8+R4CH3=>CH4+R19C3H7	6.0E-0001	4.000	8200.0	! MH 207
DUPLICATE				



C3H8+R4CH3=>CH4+R19C3H7	2.0E+0011	0.000	9600.0	! MH 208
DUPLICATE				
C3H8+R8CH300=>CH300H+R19C3H7	1.2E+0013	0.000	20000.0	! MH 209
DUPLICATE				
C3H8+R8CH300=>CH300H+R19C3H7	3.0E+0012	0.000	17500.0	! MH 210
DUPLICATE				
C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	! MH 211
DUPLICATE				
C3H8+R11C2H5=>C2H6+R19C3H7	2.0E+0011	0.000	11000.0	! MH 212
DUPLICATE				
C4H10+R1H=>H2+R20C4H9	5.7E+0007	2.000	7700.0	! MH 213
DUPLICATE				
C4H10+R1H=>H2+R20C4H9	1.8E+0007	2.000	5000.0	! MH 214
DUPLICATE				
C4H10+R20H=>H20+R20C4H9	5.4E+0006	2.000	450.0	! MH 215
DUPLICATE				
C4H10+R20H=>H20+R20C4H9	5.2E+0006	2.000	-765.0	! MH 216
DUPLICATE				
C4H10+R300H=>H202+R20C4H9	1.2E+0012	0.000	17000.0	! MH 217
DUPLICATE				
C4H10+R300H=>H202+R20C4H9	8.0E+0011	0.000	15500.0	! MH 218
DUPLICATE				
C4H10+R4CH3=>CH4+R20C4H9	6.0E-0001	4.000	8200.0	! MH 219
DUPLICATE				
C4H10+R4CH3=>CH4+R20C4H9	4.0E+0011	0.000	9600.0	! MH 220
DUPLICATE				
C4H10+R8CH300=>CH300H+R20C4H9	1.2E+0013	0.000	20000.0	! MH 221
DUPLICATE				
C4H10+R8CH300=>CH300H+R20C4H9	6.0E+0012	0.000	17500.0	! MH 222
DUPLICATE				
C4H10+R11C2H5=>C2H6+R20C4H9	6.0E+0011	0.000	13500.0	! MH 223
DUPLICATE				
C4H10+R11C2H5=>C2H6+R20C4H9	4.0E+0011	0.000	11000.0	! MH 224
DUPLICATE				
C5H12+R1H=>H2+R35C5H11	5.7E+0007	2.000	7700.0	! MH 225
DUPLICATE				
C5H12+R1H=>H2+R35C5H11	2.7E+0007	2.000	5000.0	! MH 226
DUPLICATE				
C5H12+R20H=>H20+R35C5H11	5.4E+0006	2.000	450.0	! MH 227
DUPLICATE				
C5H12+R20H=>H20+R35C5H11	7.8E+0006	2.000	-765.0	! MH 228
DUPLICATE				
C5H12+R300H=>H202+R35C5H11	1.2E+0012	0.000	17000.0	! MH 229
DUPLICATE				
C5H12+R300H=>H202+R35C5H11	1.2E+0012	0.000	15500.0	! MH 230
DUPLICATE				
C5H12+R4CH3=>CH4+R35C5H11	6.0E-0001	4.000	8200.0	! MH 231
DUPLICATE				
C5H12+R4CH3=>CH4+R35C5H11	6.0E+0011	0.000	9600.0	! MH 232
DUPLICATE				
C5H12+R8CH300=>CH300H+R35C5H11	1.2E+0013	0.000	20000.0	! MH 233
DUPLICATE				
C5H12+R8CH300=>CH300H+R35C5H11	9.0E+0012	0.000	17500.0	! MH 234
DUPLICATE				

C5H12+R11C2H5=>C2H6+R35C5H11	6.0E+0011	0.000	13500.0	! MH 235
DUPLICATE				
C5H12+R11C2H5=>C2H6+R35C5H11	6.0E+0011	0.000	11000.0	! MH 236
DUPLICATE				
C6H14+R1H=>H2+R41C6H13	5.7E+0007	2.000	7700.0	! MH 237
DUPLICATE				
C6H14+R1H=>H2+R41C6H13	3.6E+0007	2.000	5000.0	! MH 238
DUPLICATE				
C6H14+R20H=>H2O+R41C6H13	5.4E+0006	2.000	450.0	! MH 239
DUPLICATE				
C6H14+R20H=>H2O+R41C6H13	1.0E+0007	2.000	-765.0	! MH 240
DUPLICATE				
C6H14+R300H=>H2O2+R41C6H13	1.2E+0012	0.000	17000.0	! MH 241
DUPLICATE				
C6H14+R300H=>H2O2+R41C6H13	1.6E+0012	0.000	15500.0	! MH 242
DUPLICATE				
C6H14+R4CH3=>CH4+R41C6H13	6.0E-0001	4.000	8200.0	! MH 243
DUPLICATE				
C6H14+R4CH3=>CH4+R41C6H13	8.0E+0011	0.000	9600.0	! MH 244
DUPLICATE				
C6H14+R8CH300=>CH300H+R41C6H13	1.2E+0013	0.000	20000.0	! MH 245
DUPLICATE				
C6H14+R8CH300=>CH300H+R41C6H13	1.2E+0013	0.000	17500.0	! MH 246
DUPLICATE				
C6H14+R11C2H5=>C2H6+R41C6H13	6.0E+0011	0.000	13500.0	! MH 247
DUPLICATE				
C6H14+R11C2H5=>C2H6+R41C6H13	8.0E+0011	0.000	11000.0	! MH 248
DUPLICATE				
! 0-ring decomposition				
C3H60E#3+R1H=>H2+R4CH3+CH2COZ	2.9E+0007	2.000	7700.0	! DE# 249
DUPLICATE				
C3H60E#3+R1H=>H2+R4CH3+CH2COZ	1.3E+0007	2.000	5000.0	! DE# 250
DUPLICATE				
C3H60E#3+R20H=>H2O+R4CH3+CH2COZ	2.7E+0006	2.000	450.0	! DE# 251
DUPLICATE				
C3H60E#3+R20H=>H2O+R4CH3+CH2COZ	3.9E+0006	2.000	-765.0	! DE# 252
DUPLICATE				
C3H60E#3+R300H=>H2O2+R4CH3+CH2COZ	6.0E+0011	0.000	17000.0	! DE# 253
DUPLICATE				
C3H60E#3+R300H=>H2O2+R4CH3+CH2COZ	6.0E+0011	0.000	15500.0	! DE# 254
DUPLICATE				
C3H60E#3+R4CH3=>CH4+R4CH3+CH2COZ	3.0E-0001	4.000	8200.0	! DE# 255
DUPLICATE				
C3H60E#3+R4CH3=>CH4+R4CH3+CH2COZ	3.0E+0011	0.000	9600.0	! DE# 256
DUPLICATE				
C3H60E#3+R8CH300=>CH300H+R4CH3+CH2COZ	6.0E+0012	0.000	20000.0	! DE#
257				
DUPLICATE				
C3H60E#3+R8CH300=>CH300H+R4CH3+CH2COZ	4.5E+0012	0.000	17500.0	! DE#
258				
DUPLICATE				
C3H60E#3+R11C2H5=>C2H6+R4CH3+CH2COZ	3.0E+0011	0.000	13500.0	! DE#
259				

DUPLICATE  
 C3H60E#3+R11C2H5=>C2H6+R4CH3+CH2COZ 3.0E+0011 0.000 11000.0 ! DE#  
 260  
 DUPLICATE  
 C4H80E#3+R1H=>H2+R11C2H5+CH2COZ 2.9E+0007 2.000 7700.0 ! DE# 261  
 DUPLICATE  
 C4H80E#3+R1H=>H2+R11C2H5+CH2COZ 2.3E+0007 2.000 5000.0 ! DE# 262  
 DUPLICATE  
 C4H80E#3+R20H=>H2O+R11C2H5+CH2COZ 2.7E+0006 2.000 450.0 ! DE# 263  
 DUPLICATE  
 C4H80E#3+R20H=>H2O+R11C2H5+CH2COZ 6.5E+0006 2.000 -765.0 ! DE# 264  
 DUPLICATE  
 C4H80E#3+R300H=>H2O2+R11C2H5+CH2COZ 6.0E+0011 0.000 17000.0 ! DE#  
 265  
 DUPLICATE  
 C4H80E#3+R300H=>H2O2+R11C2H5+CH2COZ 1.0E+0012 0.000 15500.0 ! DE#  
 266  
 DUPLICATE  
 C4H80E#3+R4CH3=>CH4+R11C2H5+CH2COZ 3.0E-0001 4.000 8200.0 ! DE# 267  
 DUPLICATE  
 C4H80E#3+R4CH3=>CH4+R11C2H5+CH2COZ 5.0E+0011 0.000 9600.0 ! DE# 268  
 DUPLICATE  
 C4H80E#3+R8CH300=>CH300H+R11C2H5+CH2COZ 6.0E+0012 0.000 20000.0 !  
 DE# 269  
 DUPLICATE  
 C4H80E#3+R8CH300=>CH300H+R11C2H5+CH2COZ 7.5E+0012 0.000 17500.0 !  
 DE# 270  
 DUPLICATE  
 C4H80E#3+R11C2H5=>C2H6+R11C2H5+CH2COZ 3.0E+0011 0.000 13500.0 ! DE#  
 271  
 DUPLICATE  
 C4H80E#3+R11C2H5=>C2H6+R11C2H5+CH2COZ 5.0E+0011 0.000 11000.0 ! DE#  
 272  
 DUPLICATE  
 C5H100E#3+R1H=>H2+R19C3H7+CH2COZ 2.9E+0007 2.000 7700.0 ! DE# 273  
 DUPLICATE  
 C5H100E#3+R1H=>H2+R19C3H7+CH2COZ 3.2E+0007 2.000 5000.0 ! DE# 274  
 DUPLICATE  
 C5H100E#3+R20H=>H2O+R19C3H7+CH2COZ 2.7E+0006 2.000 450.0 ! DE# 275  
 DUPLICATE  
 C5H100E#3+R20H=>H2O+R19C3H7+CH2COZ 9.1E+0006 2.000 -765.0 ! DE# 276  
 DUPLICATE  
 C5H100E#3+R300H=>H2O2+R19C3H7+CH2COZ 6.0E+0011 0.000 17000.0 ! DE#  
 277  
 DUPLICATE  
 C5H100E#3+R300H=>H2O2+R19C3H7+CH2COZ 1.4E+0012 0.000 15500.0 ! DE#  
 278  
 DUPLICATE  
 C5H100E#3+R4CH3=>CH4+R19C3H7+CH2COZ 3.0E-0001 4.000 8200.0 ! DE#  
 279  
 DUPLICATE  
 C5H100E#3+R4CH3=>CH4+R19C3H7+CH2COZ 7.0E+0011 0.000 9600.0 ! DE#  
 280  
 DUPLICATE

C5H100E#3+R8CH300=>CH300H+R19C3H7+CH2COZ	6.0E+0012	0.000	20000.0	!
DE# 281				
DUPLICATE				
C5H100E#3+R8CH300=>CH300H+R19C3H7+CH2COZ	1.0E+0013	0.000	17500.0	!
DE# 282				
DUPLICATE				
C5H100E#3+R11C2H5=>C2H6+R19C3H7+CH2COZ	3.0E+0011	0.000	13500.0	!
DE# 283				
DUPLICATE				
C5H100E#3+R11C2H5=>C2H6+R19C3H7+CH2COZ	7.0E+0011	0.000	11000.0	!
DE# 284				
DUPLICATE				
C7H140E#3+R1H=>H2+R20C4H9+C2H3CHOZ	2.9E+0007	2.000	7700.0	! DE# 285
DUPLICATE				
C7H140E#3+R1H=>H2+R20C4H9+C2H3CHOZ	5.0E+0007	2.000	5000.0	! DE# 286
DUPLICATE				
C7H140E#3+R20H=>H20+R20C4H9+C2H3CHOZ	2.7E+0006	2.000	450.0	! DE#
287				
DUPLICATE				
C7H140E#3+R20H=>H20+R20C4H9+C2H3CHOZ	1.4E+0007	2.000	-765.0	! DE#
288				
DUPLICATE				
C7H140E#3+R300H=>H202+R20C4H9+C2H3CHOZ	6.0E+0011	0.000	17000.0	!
DE# 289				
DUPLICATE				
C7H140E#3+R300H=>H202+R20C4H9+C2H3CHOZ	2.2E+0012	0.000	15500.0	!
DE# 290				
DUPLICATE				
C7H140E#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ	3.0E-0001	4.000	8200.0	! DE#
291				
DUPLICATE				
C7H140E#3+R4CH3=>CH4+R20C4H9+C2H3CHOZ	1.1E+0012	0.000	9600.0	! DE#
292				
DUPLICATE				
C7H140E#3+R8CH300=>CH300H+R20C4H9+C2H3CHOZ	6.0E+0012	0.000		
20000.0 ! DE# 293				
DUPLICATE				
C7H140E#3+R8CH300=>CH300H+R20C4H9+C2H3CHOZ	1.7E+0013	0.000		
17500.0 ! DE# 294				
DUPLICATE				
C7H140E#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ	3.0E+0011	0.000	13500.0	!
DE# 295				
DUPLICATE				
C7H140E#3+R11C2H5=>C2H6+R20C4H9+C2H3CHOZ	1.1E+0012	0.000	11000.0	!
DE# 296				
DUPLICATE				
C6H120E#3+R1H=>H2+R19C3H7+C2H3CHOZ	2.9E+0007	2.000	7700.0	! DE# 297
DUPLICATE				
C6H120E#3+R1H=>H2+R19C3H7+C2H3CHOZ	4.1E+0007	2.000	5000.0	! DE# 298
DUPLICATE				
C6H120E#3+R20H=>H20+R19C3H7+C2H3CHOZ	2.7E+0006	2.000	450.0	! DE#
299				
DUPLICATE				

C6H120E#3+R20H=>H20+R19C3H7+C2H3CHOZ 300	1.1E+0007	2.000	-765.0	! DE#
DUPLICATE				
C6H120E#3+R300H=>H202+R19C3H7+C2H3CHOZ DE# 301	6.0E+0011	0.000	17000.0	!
DUPLICATE				
C6H120E#3+R300H=>H202+R19C3H7+C2H3CHOZ DE# 302	1.8E+0012	0.000	15500.0	!
DUPLICATE				
C6H120E#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 303	3.0E-0001	4.000	8200.0	! DE#
DUPLICATE				
C6H120E#3+R4CH3=>CH4+R19C3H7+C2H3CHOZ 304	9.0E+0011	0.000	9600.0	! DE#
DUPLICATE				
C6H120E#3+R8CH300=>CH300H+R19C3H7+C2H3CHOZ 20000.0 ! DE# 305	6.0E+0012	0.000		
DUPLICATE				
C6H120E#3+R8CH300=>CH300H+R19C3H7+C2H3CHOZ 17500.0 ! DE# 306	1.3E+0013	0.000		
DUPLICATE				
C6H120E#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ DE# 307	3.0E+0011	0.000	13500.0	!
DUPLICATE				
C6H120E#3+R11C2H5=>C2H6+R19C3H7+C2H3CHOZ DE# 308	9.0E+0011	0.000	11000.0	!
DUPLICATE				
C8H160E#3+R1H=>H2+R20C4H9+C4H60KZ 309	2.9E+0007	2.000	7700.0	! DE#
DUPLICATE				
C8H160E#3+R1H=>H2+R20C4H9+C4H60KZ 310	5.9E+0007	2.000	5000.0	! DE#
DUPLICATE				
C8H160E#3+R20H=>H20+R20C4H9+C4H60KZ 311	2.7E+0006	2.000	450.0	! DE#
DUPLICATE				
C8H160E#3+R20H=>H20+R20C4H9+C4H60KZ 312	1.7E+0007	2.000	-765.0	! DE#
DUPLICATE				
C8H160E#3+R300H=>H202+R20C4H9+C4H60KZ 313	6.0E+0011	0.000	17000.0	! DE#
DUPLICATE				
C8H160E#3+R300H=>H202+R20C4H9+C4H60KZ 314	2.6E+0012	0.000	15500.0	! DE#
DUPLICATE				
C8H160E#3+R4CH3=>CH4+R20C4H9+C4H60KZ 315	3.0E-0001	4.000	8200.0	! DE#
DUPLICATE				
C8H160E#3+R4CH3=>CH4+R20C4H9+C4H60KZ 316	1.3E+0012	0.000	9600.0	! DE#
DUPLICATE				
C8H160E#3+R8CH300=>CH300H+R20C4H9+C4H60KZ DE# 317	6.0E+0012	0.000	20000.0	!
DUPLICATE				
C8H160E#3+R8CH300=>CH300H+R20C4H9+C4H60KZ DE# 318	2.0E+0013	0.000	17500.0	!
DUPLICATE				

C8H160E#3+R11C2H5=>C2H6+R20C4H9+C4H60KZ	3.0E+0011	0.000	13500.0	!
DE# 319				
DUPLICATE				
C8H160E#3+R11C2H5=>C2H6+R20C4H9+C4H60KZ	1.3E+0012	0.000	11000.0	!
DE# 320				
DUPLICATE				
!C9H180E#3+R1H=>H2+R35C5H11+C4H60KZ	2.9E+0007	2.000	7700.0	! DE#
321				
DUPLICATE				
!C9H180E#3+R1H=>H2+R35C5H11+C4H60KZ	6.8E+0007	2.000	5000.0	! DE#
322				
DUPLICATE				
!C9H180E#3+R20H=>H20+R35C5H11+C4H60KZ	2.7E+0006	2.000	450.0	! DE#
323				
DUPLICATE				
!C9H180E#3+R20H=>H20+R35C5H11+C4H60KZ	2.0E+0007	2.000	-765.0	! DE#
324				
DUPLICATE				
!C9H180E#3+R300H=>H202+R35C5H11+C4H60KZ	6.0E+0011	0.000	17000.0	!
DE# 325				
DUPLICATE				
!C9H180E#3+R300H=>H202+R35C5H11+C4H60KZ	3.0E+0012	0.000	15500.0	!
DE# 326				
DUPLICATE				
!C9H180E#3+R4CH3=>CH4+R35C5H11+C4H60KZ	3.0E-0001	4.000	8200.0	! DE#
327				
DUPLICATE				
!C9H180E#3+R4CH3=>CH4+R35C5H11+C4H60KZ	1.5E+0012	0.000	9600.0	! DE#
328				
DUPLICATE				
!C9H180E#3+R8CH300=>CH300H+R35C5H11+C4H60KZ	6.0E+0012	0.000	20000.0	!
! DE# 329				
DUPLICATE				
!C9H180E#3+R8CH300=>CH300H+R35C5H11+C4H60KZ	2.3E+0013	0.000	17500.0	!
! DE# 330				
DUPLICATE				
!C9H180E#3+R11C2H5=>C2H6+R35C5H11+C4H60KZ	3.0E+0011	0.000	13500.0	!
DE# 331				
DUPLICATE				
!C9H180E#3+R11C2H5=>C2H6+R35C5H11+C4H60KZ	1.5E+0012	0.000	11000.0	!
DE# 332				
DUPLICATE				
!C10H200E#3+R1H=>H2+R35C5H11+C5H80KZ	2.9E+0007	2.000	7700.0	! DE#
333				
DUPLICATE				
!C10H200E#3+R1H=>H2+R35C5H11+C5H80KZ	7.7E+0007	2.000	5000.0	! DE#
334				
DUPLICATE				
!C10H200E#3+R20H=>H20+R35C5H11+C5H80KZ	2.7E+0006	2.000	450.0	! DE#
335				
DUPLICATE				
!C10H200E#3+R20H=>H20+R35C5H11+C5H80KZ	2.2E+0007	2.000	-765.0	! DE#
336				
DUPLICATE				

!C10H200E#3+R300H=>H202+R35C5H11+C5H80KZ	6.0E+0011	0.000	17000.0	!
DE# 337				
DUPLICATE				
!C10H200E#3+R300H=>H202+R35C5H11+C5H80KZ	3.4E+0012	0.000	15500.0	!
DE# 338				
DUPLICATE				
!C10H200E#3+R4CH3=>CH4+R35C5H11+C5H80KZ	3.0E-0001	4.000	8200.0	!
DE# 339				
DUPLICATE				
!C10H200E#3+R4CH3=>CH4+R35C5H11+C5H80KZ	1.7E+0012	0.000	9600.0	!
DE# 340				
DUPLICATE				
!C10H200E#3+R8CH300=>CH300H+R35C5H11+C5H80KZ	6.0E+0012	0.000	20000.0	
! DE# 341				
DUPLICATE				
!C10H200E#3+R8CH300=>CH300H+R35C5H11+C5H80KZ	2.6E+0013	0.000	17500.0	
! DE# 342				
DUPLICATE				
!C10H200E#3+R11C2H5=>C2H6+R35C5H11+C5H80KZ	3.0E+0011	0.000		
13500.0 ! DE# 343				
DUPLICATE				
!C10H200E#3+R11C2H5=>C2H6+R35C5H11+C5H80KZ	1.7E+0012	0.000		
11000.0 ! DE# 344				
DUPLICATE				
!C13H260E#3+R1H=>H2+R26C7H15+C6H100KZ	2.9E+0007	2.000	7700.0	! DE#
345				
DUPLICATE				
!C13H260E#3+R1H=>H2+R26C7H15+C6H100KZ	1.0E+0008	2.000	5000.0	! DE#
346				
DUPLICATE				
!C13H260E#3+R20H=>H20+R26C7H15+C6H100KZ	2.7E+0006	2.000	450.0	! DE#
347				
DUPLICATE				
!C13H260E#3+R20H=>H20+R26C7H15+C6H100KZ	3.0E+0007	2.000	-765.0	!
DE# 348				
DUPLICATE				
!C13H260E#3+R300H=>H202+R26C7H15+C6H100KZ	6.0E+0011	0.000	17000.0	!
DE# 349				
DUPLICATE				
!C13H260E#3+R300H=>H202+R26C7H15+C6H100KZ	4.6E+0012	0.000	15500.0	!
DE# 350				
DUPLICATE				
!C13H260E#3+R4CH3=>CH4+R26C7H15+C6H100KZ	3.0E-0001	4.000	8200.0	!
DE# 351				
DUPLICATE				
!C13H260E#3+R4CH3=>CH4+R26C7H15+C6H100KZ	2.3E+0012	0.000	9600.0	!
DE# 352				
DUPLICATE				
!C13H260E#3+R8CH300=>CH300H+R26C7H15+C6H100KZ	6.0E+0012	0.000		
20000.0 ! DE# 353				
DUPLICATE				
!C13H260E#3+R8CH300=>CH300H+R26C7H15+C6H100KZ	3.5E+0013	0.000		
17500.0 ! DE# 354				
DUPLICATE				

!C13H260E#3+R11C2H5=>C2H6+R26C7H15+C6H100KZ	3.0E+0011	0.000	13500.0	
! DE# 355				
DUPLICATE				
!C13H260E#3+R11C2H5=>C2H6+R26C7H15+C6H100KZ	2.3E+0012	0.000	11000.0	
! DE# 356				
DUPLICATE				
!C12H240E#3+R1H=>H2+R41C6H13+C6H100KZ	2.9E+0007	2.000	7700.0	! DE#
357				
DUPLICATE				
!C12H240E#3+R1H=>H2+R41C6H13+C6H100KZ	9.5E+0007	2.000	5000.0	! DE#
358				
DUPLICATE				
!C12H240E#3+R20H=>H20+R41C6H13+C6H100KZ	2.7E+0006	2.000	450.0	! DE#
359				
DUPLICATE				
!C12H240E#3+R20H=>H20+R41C6H13+C6H100KZ	2.7E+0007	2.000	-765.0	!
DE# 360				
DUPLICATE				
!C12H240E#3+R300H=>H202+R41C6H13+C6H100KZ	6.0E+0011	0.000	17000.0	!
DE# 361				
DUPLICATE				
!C12H240E#3+R300H=>H202+R41C6H13+C6H100KZ	4.2E+0012	0.000	15500.0	!
DE# 362				
DUPLICATE				
!C12H240E#3+R4CH3=>CH4+R41C6H13+C6H100KZ	3.0E-0001	4.000	8200.0	!
DE# 363				
DUPLICATE				
!C12H240E#3+R4CH3=>CH4+R41C6H13+C6H100KZ	2.1E+0012	0.000	9600.0	!
DE# 364				
DUPLICATE				
!C12H240E#3+R8CH300=>CH300H+R41C6H13+C6H100KZ	6.0E+0012	0.000		
20000.0 ! DE# 365				
DUPLICATE				
!C12H240E#3+R8CH300=>CH300H+R41C6H13+C6H100KZ	3.2E+0013	0.000		
17500.0 ! DE# 366				
DUPLICATE				
!C12H240E#3+R11C2H5=>C2H6+R41C6H13+C6H100KZ	3.0E+0011	0.000	13500.0	
! DE# 367				
DUPLICATE				
!C12H240E#3+R11C2H5=>C2H6+R41C6H13+C6H100KZ	2.1E+0012	0.000	11000.0	
! DE# 368				
DUPLICATE				
!C11H220E#3+R1H=>H2+R41C6H13+C5H80KZ	2.9E+0007	2.000	7700.0	! DE#
369				
DUPLICATE				
!C11H220E#3+R1H=>H2+R41C6H13+C5H80KZ	8.6E+0007	2.000	5000.0	! DE#
370				
DUPLICATE				
!C11H220E#3+R20H=>H20+R41C6H13+C5H80KZ	2.7E+0006	2.000	450.0	! DE#
371				
DUPLICATE				
!C11H220E#3+R20H=>H20+R41C6H13+C5H80KZ	2.5E+0007	2.000	-765.0	! DE#
372				
DUPLICATE				



!C11H220E#3+R300H=>H202+R41C6H13+C5H80KZ	6.0E+0011	0.000	17000.0	!
DE# 373				
DUPLICATE				
!C11H220E#3+R300H=>H202+R41C6H13+C5H80KZ	3.8E+0012	0.000	15500.0	!
DE# 374				
DUPLICATE				
!C11H220E#3+R4CH3=>CH4+R41C6H13+C5H80KZ	3.0E-0001	4.000	8200.0	!
DE# 375				
DUPLICATE				
!C11H220E#3+R4CH3=>CH4+R41C6H13+C5H80KZ	1.9E+0012	0.000	9600.0	!
DE# 376				
DUPLICATE				
!C11H220E#3+R8CH300=>CH300H+R41C6H13+C5H80KZ	6.0E+0012	0.000	20000.0	
! DE# 377				
DUPLICATE				
!C11H220E#3+R8CH300=>CH300H+R41C6H13+C5H80KZ	2.9E+0013	0.000	17500.0	
! DE# 378				
DUPLICATE				
!C11H220E#3+R11C2H5=>C2H6+R41C6H13+C5H80KZ	3.0E+0011	0.000		
13500.0 ! DE# 379				
DUPLICATE				
!C11H220E#3+R11C2H5=>C2H6+R41C6H13+C5H80KZ	1.9E+0012	0.000		
11000.0 ! DE# 380				
DUPLICATE				
!C14H280E#3+R1H=>H2+R26C7H15+C7H120KZ	2.9E+0007	2.000	7700.0	! DE#
381				
DUPLICATE				
!C14H280E#3+R1H=>H2+R26C7H15+C7H120KZ	1.1E+0008	2.000	5000.0	! DE#
382				
DUPLICATE				
!C14H280E#3+R20H=>H20+R26C7H15+C7H120KZ	2.7E+0006	2.000	450.0	! DE#
383				
DUPLICATE				
!C14H280E#3+R20H=>H20+R26C7H15+C7H120KZ	3.3E+0007	2.000	-765.0	!
DE# 384				
DUPLICATE				
!C14H280E#3+R300H=>H202+R26C7H15+C7H120KZ	6.0E+0011	0.000	17000.0	!
DE# 385				
DUPLICATE				
!C14H280E#3+R300H=>H202+R26C7H15+C7H120KZ	5.0E+0012	0.000	15500.0	!
DE# 386				
DUPLICATE				
!C14H280E#3+R4CH3=>CH4+R26C7H15+C7H120KZ	3.0E-0001	4.000	8200.0	!
DE# 387				
DUPLICATE				
!C14H280E#3+R4CH3=>CH4+R26C7H15+C7H120KZ	2.5E+0012	0.000	9600.0	!
DE# 388				
DUPLICATE				
!C14H280E#3+R8CH300=>CH300H+R26C7H15+C7H120KZ	6.0E+0012	0.000		
20000.0 ! DE# 389				
DUPLICATE				
!C14H280E#3+R8CH300=>CH300H+R26C7H15+C7H120KZ	3.8E+0013	0.000		
17500.0 ! DE# 390				
DUPLICATE				

!C14H280E#3+R11C2H5=>C2H6+R26C7H15+C7H120KZ 3.0E+0011 0.000 13500.0  
! DE# 391  
DUPLICATE  
!C14H280E#3+R11C2H5=>C2H6+R26C7H15+C7H120KZ 2.5E+0012 0.000 11000.0  
! DE# 392  
DUPLICATE

! Metatheses of oxetanes, furanes and pyranes

! decompositions of cyclo-ether radicals

! Addition of oxygen on cyclo-ether radicals

! O2 elimination

! Isomerization

! Cylo-ether keto-hydroperoxide ester formation

! Decomposition of cylo-ether keto-hydroperoxide ester

! Isomerization of peroxy-radicals

!Addition of oxygen on cyclo-peroxy radicals

! Formation of cyclo-ether ketohydroperoxydes

! Decomposition of cyclo-ether ketohydroperoxydes

! Olefin reactions

! addition of H and CH3 on olefins

C3H6Y+R1H=>R19C3H7 1.3E+0013 0.000 1560.0 ! ADZ 393

DUPLICATE

C3H6Y+R1H=>R19C3H7 1.3E+0013 0.000 3260.0 ! ADZ 394

DUPLICATE

C4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 1560.0 ! ADZ 395

DUPLICATE

C4H8Y+R1H=>R20C4H9 1.3E+0013 0.000 3260.0 ! ADZ 396

DUPLICATE

C4H8Y+R4CH3=>C3H6Y+R11C2H5 9.6E+0010 0.000 8000.0 ! ADZ 397

C5H10Z+R1H=>R35C5H11 1.3E+0013 0.000 1560.0 ! ADZ 398

DUPLICATE

C5H10Z+R1H=>R35C5H11 1.3E+0013 0.000 3260.0 ! ADZ 399

DUPLICATE

C5H10Z+R4CH3=>C4H8Y+R11C2H5 1.7E+0011 0.000 7400.0 ! ADZ 400

C5H10Z+R4CH3=>C3H6Y+R19C3H7 9.6E+0010 0.000 8000.0 ! ADZ 401

C7H14Z+R1H=>R26C7H15 1.3E+0013 0.000 1560.0 ! ADZ 402

DUPLICATE

C7H14Z+R1H=>R26C7H15 1.3E+0013 0.000 3260.0 ! ADZ 403

DUPLICATE

C7H14Z+R4CH3=>C4H8Y+R20C4H9 1.7E+0011 0.000 7400.0 ! ADZ 404

C7H14Z+R4CH3=>C3H6Y+R35C5H11 9.6E+0010 0.000 8000.0 ! ADZ 405

C6H12Z+R1H=>R41C6H13 1.3E+0013 0.000 1560.0 ! ADZ 406

DUPLICATE

C6H12Z+R1H=>R41C6H13 1.3E+0013 0.000 3260.0 ! ADZ 407

DUPLICATE

C6H12Z+R4CH3=>C4H8Y+R19C3H7 1.7E+0011 0.000 7400.0 ! ADZ 408

C6H12Z+R4CH3=>C3H6Y+R20C4H9	9.6E+0010	0.000	8000.0	! ADZ 409
C7H14Y+R1H=>R26C7H15	1.3E+0013	0.000	1560.0	! ADZ 410
DUPLICATE				
C7H14Y+R1H=>R26C7H15	1.3E+0013	0.000	3260.0	! ADZ 411
DUPLICATE				
C7H14Y+R4CH3=>C4H8Y+R20C4H9	1.7E+0011	0.000	7400.0	! ADZ 412
C7H14Y+R4CH3=>C3H6Y+R35C5H11	9.6E+0010	0.000	8000.0	! ADZ 413
C8H16Y+R1H=>R30C8H17	1.3E+0013	0.000	1560.0	! ADZ 414
DUPLICATE				
C8H16Y+R1H=>R30C8H17	1.3E+0013	0.000	3260.0	! ADZ 415
DUPLICATE				
C8H16Y+R4CH3=>C4H8Y+R35C5H11	1.7E+0011	0.000	7400.0	! ADZ 416
C8H16Y+R4CH3=>C3H6Y+R41C6H13	9.6E+0010	0.000	8000.0	! ADZ 417
C8H16Z+R1H=>R30C8H17	1.3E+0013	0.000	1560.0	! ADZ 418
DUPLICATE				
C8H16Z+R1H=>R30C8H17	1.3E+0013	0.000	3260.0	! ADZ 419
DUPLICATE				
C8H16Z+R4CH3=>C4H8Y+R35C5H11	1.7E+0011	0.000	7400.0	! ADZ 420
C8H16Z+R4CH3=>C3H6Y+R41C6H13	9.6E+0010	0.000	8000.0	! ADZ 421
C5H10Y+R1H=>R35C5H11	1.3E+0013	0.000	1560.0	! ADZ 422
DUPLICATE				
C5H10Y+R1H=>R35C5H11	1.3E+0013	0.000	3260.0	! ADZ 423
DUPLICATE				
C5H10Y+R4CH3=>C4H8Y+R11C2H5	1.7E+0011	0.000	7400.0	! ADZ 424
C5H10Y+R4CH3=>C3H6Y+R19C3H7	9.6E+0010	0.000	8000.0	! ADZ 425
!C9H18Z+R4CH3=>C4H8Y+R41C6H13	1.7E+0011	0.000	7400.0	! ADZ 426
!C9H18Z+R4CH3=>C3H6Y+R26C7H15	9.6E+0010	0.000	8000.0	! ADZ 427
!C10H20Z+R4CH3=>C4H8Y+R26C7H15	1.7E+0011	0.000	7400.0	! ADZ 428
!C10H20Z+R4CH3=>C3H6Y+R30C8H17	9.6E+0010	0.000	8000.0	! ADZ 429
!C11H22Z+R4CH3=>C4H8Y+R30C8H17	1.7E+0011	0.000	7400.0	! ADZ 430
!C9H18Z+R1H=>4C2H4Z+R4CH3	9.6E+0010	0.000	8000.0	! ADZ 431
!C10H20Z+R1H=>4C2H4Z+R11C2H5	9.6E+0010	0.000	8000.0	! ADZ 432
!C13H26Z+R1H=>6C2H4Z+R4CH3	9.6E+0010	0.000	8000.0	! ADZ 433
!C12H24Z+R1H=>5C2H4Z+R11C2H5	9.6E+0010	0.000	8000.0	! ADZ 434
!C11H22Z+R1H=>5C2H4Z+R4CH3	9.6E+0010	0.000	8000.0	! ADZ 435
!C14H28Z+R1H=>6C2H4Z+R11C2H5	9.6E+0010	0.000	8000.0	! ADZ 436
! addition of OH on olefins				
C3H6Y+R20H=>R4CH3+CH3CHO	1.4E+0012	0.000	-1040.0	! ADZ 437
C3H6Y+R20H=>R11C2H5+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 438
C4H8Y+R20H=>R4CH3+C2H5CHO	1.4E+0012	0.000	-1040.0	! ADZ 439
C4H8Y+R20H=>R19C3H7+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 440
C5H10Z+R20H=>R4CH3+C4H8OA	1.4E+0012	0.000	-1040.0	! ADZ 441
C5H10Z+R20H=>R20C4H9+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 442
C7H14Z+R20H=>R4CH3+C6H12OA	1.4E+0012	0.000	-1040.0	! ADZ 443
C7H14Z+R20H=>R41C6H13+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 444
C6H12Z+R20H=>R4CH3+C5H10OA	1.4E+0012	0.000	-1040.0	! ADZ 445
C6H12Z+R20H=>R35C5H11+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 446
C7H14Y+R20H=>R4CH3+C6H12OA	1.4E+0012	0.000	-1040.0	! ADZ 447
C7H14Y+R20H=>R41C6H13+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 448
C8H16Y+R20H=>R4CH3+C7H14OA	1.4E+0012	0.000	-1040.0	! ADZ 449
C8H16Y+R20H=>R26C7H15+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 450
C8H16Z+R20H=>R4CH3+C7H14OA	1.4E+0012	0.000	-1040.0	! ADZ 451
C8H16Z+R20H=>R26C7H15+HCHO	1.4E+0012	0.000	-1040.0	! ADZ 452

C5H10Y+R20H=>R4CH3+C4H80A 1.4E+0012 0.000 -1040.0 ! ADZ 453  
 C5H10Y+R20H=>R20C4H9+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 454  
 !C9H18Z+R20H=>R4CH3+C8H160A 1.4E+0012 0.000 -1040.0 ! ADZ 455  
 !C9H18Z+R20H=>R30C8H17+HCHO 1.4E+0012 0.000 -1040.0 ! ADZ 456  
 !C10H20Z+R20H=>R4CH3+C9H180A 1.4E+0012 0.000 -1040.0 ! ADZ 457  
 !C13H26Z+R20H=>R4CH3+C12H240A 1.4E+0012 0.000 -1040.0 ! ADZ 458  
 !C12H24Z+R20H=>R4CH3+C11H220A 1.4E+0012 0.000 -1040.0 ! ADZ 459  
 !C11H22Z+R20H=>R4CH3+C10H200A 1.4E+0012 0.000 -1040.0 ! ADZ 460  
 !C14H28Z+R20H=>R4CH3+C13H260A 1.4E+0012 0.000 -1040.0 ! ADZ 461

!C10H20Z+R20H=>HCHO+R4CH3+4C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 462  
 !C13H26Z+R20H=>HCHO+R11C2H5+5C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH  
 463  
 !C12H24Z+R20H=>HCHO+R4CH3+5C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 464  
 !C11H22Z+R20H=>HCHO+R11C2H5+4C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH  
 465  
 !C14H28Z+R20H=>HCHO+R4CH3+6C2H4Z 1.4E+0012 0.000 -1040.0 ! FOH 466

! addition of 0 on olefins

C3H6Y+B10=>CH2COZ+R1H+R4CH3 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C4H8Y+B10=>CH2COZ+R1H+R11C2H5 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C5H10Z+B10=>CH2COZ+R1H+R19C3H7 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C7H14Z+B10=>CH2COZ+R1H+R35C5H11 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C6H12Z+B10=>CH2COZ+R1H+R20C4H9 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C7H14Y+B10=>CH2COZ+R1H+R35C5H11 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C8H16Y+B10=>CH2COZ+R1H+R41C6H13 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C8H16Z+B10=>CH2COZ+R1H+R41C6H13 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 C5H10Y+B10=>CH2COZ+R1H+R19C3H7 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 !C9H18Z+B10=>CH2COZ+R1H+R26C7H15 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 !C10H20Z+B10=>CH2COZ+R1H+R30C8H17 1.2E+0005 2.560 -1130.0 ! AOZ 467  
 !C13H26Z+B10=>CH2COZ+R4CH3+R1H+5C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ  
 467  
 !C12H24Z+B10=>CH2COZ+R11C2H5+R1H+4C2H4Z 7.8E+0013 0.000 5200.0 !  
 AOZ 467  
 !C11H22Z+B10=>CH2COZ+R4CH3+R1H+4C2H4Z 7.8E+0013 0.000 5200.0 ! AOZ  
 467  
 !C14H28Z+B10=>CH2COZ+R11C2H5+R1H+5C2H4Z 7.8E+0013 0.000 5200.0 !  
 AOZ 467

! retroene reactions

C5H10Z=>C3H6Y+C2H4Z 8.0E+0012 0.000 56500.0 ! RTZ 467  
 C7H14Z=>C3H6Y+C4H8Y 8.0E+0012 0.000 56500.0 ! RTZ 468  
 C6H12Z=>C3H6Y+C3H6Y 8.0E+0012 0.000 56500.0 ! RTZ 469  
 C7H14Y=>C3H6Y+C4H8Y 8.0E+0012 0.000 56500.0 ! RTZ 470  
 C8H16Y=>C3H6Y+C5H10Z 8.0E+0012 0.000 56500.0 ! RTZ 471  
 C8H16Z=>C3H6Y+C5H10Z 8.0E+0012 0.000 56500.0 ! RTZ 472  
 C5H10Y=>C3H6Y+C2H4Z 8.0E+0012 0.000 56500.0 ! RTZ 473  
 !C9H18Z=>C3H6Y+C6H12Z 8.0E+0012 0.000 56500.0 ! RTZ 474  
 !C10H20Z=>C3H6Y+C7H14Z 8.0E+0012 0.000 56500.0 ! RTZ 475  
 !C13H26Z=>C3H6Y+C10H20Z 8.0E+0012 0.000 56500.0 ! RTZ 476  
 !C12H24Z=>C3H6Y+C9H18Z 8.0E+0012 0.000 56500.0 ! RTZ 477  
 !C11H22Z=>C3H6Y+C8H16Z 8.0E+0012 0.000 56500.0 ! RTZ 478  
 !C14H28Z=>C3H6Y+C11H22Z 8.0E+0012 0.000 56500.0 ! RTZ 479

! addition of 00H on olefins

C3H6Y+R300H=>R20H+C3H60E#3	1.0E+0012	0.000	14200.0	! ADZ 480
C4H8Y+R300H=>R20H+C4H80E#3	1.0E+0012	0.000	14200.0	! ADZ 481
C5H10Z+R300H=>R20H+C5H100E#3	1.0E+0012	0.000	14200.0	! ADZ 482
C7H14Z+R300H=>R20H+C7H140E#3	1.0E+0012	0.000	14200.0	! ADZ 483
C6H12Z+R300H=>R20H+C6H120E#3	1.0E+0012	0.000	14200.0	! ADZ 484
C7H14Y+R300H=>R20H+C7H140E#3	1.0E+0012	0.000	14200.0	! ADZ 485
C8H16Y+R300H=>R20H+C8H160E#3	1.0E+0012	0.000	14200.0	! ADZ 486
C8H16Z+R300H=>R20H+C8H160E#3	1.0E+0012	0.000	14200.0	! ADZ 487
C5H10Y+R300H=>R20H+C5H100E#3	1.0E+0012	0.000	14200.0	! ADZ 488
!C9H18Z+R300H=>R20H+C9H180E#3	1.0E+0012	0.000	14200.0	! ADZ 489
!C10H20Z+R300H=>R20H+C10H200E#3	1.0E+0012	0.000	14200.0	! ADZ 490
!C13H26Z+R300H=>R20H+C13H260E#3	1.0E+0012	0.000	14200.0	! ADZ 491
!C12H24Z+R300H=>R20H+C12H240E#3	1.0E+0012	0.000	14200.0	! ADZ 492
!C11H22Z+R300H=>R20H+C11H220E#3	1.0E+0012	0.000	14200.0	! ADZ 493
!C14H28Z+R300H=>R20H+C14H280E#3	1.0E+0012	0.000	14200.0	! ADZ 494

! olefin to dienes

C5H10Z+R1H=>H2+C4H6Z2+R4CH3 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 495
C5H10Z+R1H=>H2+C4H6Z2+R4CH3 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 496
C5H10Z+R1H=>H2+C4H6Z2+R4CH3 DUPLICATE	9.0E+0006	2.000	5000.0	! MZ 497
C5H10Z+R20H=>H20+C4H6Z2+R4CH3 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 498
C5H10Z+R20H=>H20+C4H6Z2+R4CH3 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 499
C5H10Z+R20H=>H20+C4H6Z2+R4CH3 DUPLICATE	2.6E+0006	2.000	-765.0	! MZ 500
C5H10Z+R300H=>H202+C4H6Z2+R4CH3 DUPLICATE	6.4E+0003	2.600	12400.0	! MZ 501
C5H10Z+R300H=>H202+C4H6Z2+R4CH3 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 502
C5H10Z+R300H=>H202+C4H6Z2+R4CH3 DUPLICATE	4.0E+0011	0.000	15500.0	! MZ 503
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 504
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 505
C5H10Z+R4CH3=>CH4+C4H6Z2+R4CH3 DUPLICATE	2.0E+0011	0.000	9600.0	! MZ 506
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3 507 DUPLICATE	1.0E+0012	0.000	14550.0	! MZ
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3 508 DUPLICATE	6.0E+0012	0.000	20000.0	! MZ
C5H10Z+R8CH300=>CH300H+C4H6Z2+R4CH3 509 DUPLICATE	3.0E+0012	0.000	17500.0	! MZ
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3 DUPLICATE	1.5E+0000	3.500	4140.0	! MZ 510
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	3.0E+0011	0.000	13500.0	! MZ 511

DUPLICATE					
C5H10Z+R11C2H5=>C2H6+C4H6Z2+R4CH3	2.0E+0011	0.000	11000.0	!	MZ 512
DUPLICATE					
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	5.4E+0004	2.500	-1900.0	!	MZ 513
DUPLICATE					
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	2.9E+0007	2.000	7700.0	!	MZ 514
DUPLICATE					
C7H14Z+R1H=>H2+C4H6Z2+R19C3H7	2.7E+0007	2.000	5000.0	!	MZ 515
DUPLICATE					
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7	3.0E+0006	2.000	-1520.0	!	MZ 516
DUPLICATE					
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7	2.7E+0006	2.000	450.0	!	MZ 517
DUPLICATE					
C7H14Z+R20H=>H20+C4H6Z2+R19C3H7	7.8E+0006	2.000	-765.0	!	MZ 518
DUPLICATE					
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7	6.4E+0003	2.600	12400.0	!	MZ 519
DUPLICATE					
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7	6.0E+0011	0.000	17000.0	!	MZ 520
DUPLICATE					
C7H14Z+R300H=>H202+C4H6Z2+R19C3H7	1.2E+0012	0.000	15500.0	!	MZ 521
DUPLICATE					
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	1.0E+0011	0.000	7300.0	!	MZ 522
DUPLICATE					
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	3.0E-0001	4.000	8200.0	!	MZ 523
DUPLICATE					
C7H14Z+R4CH3=>CH4+C4H6Z2+R19C3H7	6.0E+0011	0.000	9600.0	!	MZ 524
DUPLICATE					
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7	1.0E+0012	0.000	14550.0	!	MZ 525
DUPLICATE					
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7	6.0E+0012	0.000	20000.0	!	MZ 526
DUPLICATE					
C7H14Z+R8CH300=>CH300H+C4H6Z2+R19C3H7	9.0E+0012	0.000	17500.0	!	MZ 527
DUPLICATE					
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	1.5E+0000	3.500	4140.0	!	MZ 528
DUPLICATE					
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	3.0E+0011	0.000	13500.0	!	MZ 529
DUPLICATE					
C7H14Z+R11C2H5=>C2H6+C4H6Z2+R19C3H7	6.0E+0011	0.000	11000.0	!	MZ 530
DUPLICATE					
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5	5.4E+0004	2.500	-1900.0	!	MZ 531
DUPLICATE					
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5	2.9E+0007	2.000	7700.0	!	MZ 532
DUPLICATE					
C6H12Z+R1H=>H2+C4H6Z2+R11C2H5	1.8E+0007	2.000	5000.0	!	MZ 533
DUPLICATE					
C6H12Z+R20H=>H20+C4H6Z2+R11C2H5	3.0E+0006	2.000	-1520.0	!	MZ 534
DUPLICATE					
C6H12Z+R20H=>H20+C4H6Z2+R11C2H5	2.7E+0006	2.000	450.0	!	MZ 535
DUPLICATE					

C6H12Z+R20H=>H2O+C4H6Z2+R11C2H5 DUPLICATE	5.2E+0006	2.000	-765.0	! MZ 536
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5 DUPLICATE	6.4E+0003	2.600	12400.0	! MZ 537
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 538
C6H12Z+R300H=>H2O2+C4H6Z2+R11C2H5 DUPLICATE	8.0E+0011	0.000	15500.0	! MZ 539
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 540
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 541
C6H12Z+R4CH3=>CH4+C4H6Z2+R11C2H5 DUPLICATE	4.0E+0011	0.000	9600.0	! MZ 542
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5 543 DUPLICATE	1.0E+0012	0.000	14550.0	! MZ
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5 544 DUPLICATE	6.0E+0012	0.000	20000.0	! MZ
C6H12Z+R8CH300=>CH300H+C4H6Z2+R11C2H5 545 DUPLICATE	6.0E+0012	0.000	17500.0	! MZ
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5 DUPLICATE	1.5E+0000	3.500	4140.0	! MZ 546
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5 547 DUPLICATE	3.0E+0011	0.000	13500.0	! MZ
C6H12Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5 548 DUPLICATE	4.0E+0011	0.000	11000.0	! MZ
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 549
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 550
C8H16Z+R1H=>H2+C4H6Z2+R20C4H9 DUPLICATE	3.6E+0007	2.000	5000.0	! MZ 551
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 552
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 553
C8H16Z+R20H=>H2O+C4H6Z2+R20C4H9 DUPLICATE	1.0E+0007	2.000	-765.0	! MZ 554
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9 DUPLICATE	6.4E+0003	2.600	12400.0	! MZ 555
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9 DUPLICATE	6.0E+0011	0.000	17000.0	! MZ 556
C8H16Z+R300H=>H2O2+C4H6Z2+R20C4H9 DUPLICATE	1.6E+0012	0.000	15500.0	! MZ 557
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 558
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 559
C8H16Z+R4CH3=>CH4+C4H6Z2+R20C4H9	8.0E+0011	0.000	9600.0	! MZ 560

DUPLICATE				
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 561	1.0E+0012	0.000	14550.0	! MZ
DUPLICATE				
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 562	6.0E+0012	0.000	20000.0	! MZ
DUPLICATE				
C8H16Z+R8CH300=>CH300H+C4H6Z2+R20C4H9 563	1.2E+0013	0.000	17500.0	! MZ
DUPLICATE				
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9	1.5E+0000	3.500	4140.0	! MZ 564
DUPLICATE				
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 565	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
C8H16Z+R11C2H5=>C2H6+C4H6Z2+R20C4H9 566	8.0E+0011	0.000	11000.0	! MZ
DUPLICATE				
!C9H18Z+R1H=>H2+C4H6Z2+R35C5H11	5.4E+0004	2.500	-1900.0	! MZ 567
DUPLICATE				
!C9H18Z+R1H=>H2+C4H6Z2+R35C5H11	2.9E+0007	2.000	7700.0	! MZ 568
DUPLICATE				
!C9H18Z+R1H=>H2+C4H6Z2+R35C5H11	4.5E+0007	2.000	5000.0	! MZ 569
DUPLICATE				
!C9H18Z+R20H=>H20+C4H6Z2+R35C5H11	3.0E+0006	2.000	-1520.0	! MZ 570
DUPLICATE				
!C9H18Z+R20H=>H20+C4H6Z2+R35C5H11	2.7E+0006	2.000	450.0	! MZ 571
DUPLICATE				
!C9H18Z+R20H=>H20+C4H6Z2+R35C5H11	1.3E+0007	2.000	-765.0	! MZ 572
DUPLICATE				
!C9H18Z+R300H=>H202+C4H6Z2+R35C5H11 573	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
!C9H18Z+R300H=>H202+C4H6Z2+R35C5H11 574	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
!C9H18Z+R300H=>H202+C4H6Z2+R35C5H11 575	2.0E+0012	0.000	15500.0	! MZ
DUPLICATE				
!C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11	1.0E+0011	0.000	7300.0	! MZ 576
DUPLICATE				
!C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11	3.0E-0001	4.000	8200.0	! MZ 577
DUPLICATE				
!C9H18Z+R4CH3=>CH4+C4H6Z2+R35C5H11	1.0E+0012	0.000	9600.0	! MZ 578
DUPLICATE				
!C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 MZ 579	1.0E+0012	0.000	14550.0	!
DUPLICATE				
!C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 MZ 580	6.0E+0012	0.000	20000.0	!
DUPLICATE				
!C9H18Z+R8CH300=>CH300H+C4H6Z2+R35C5H11 MZ 581	1.5E+0013	0.000	17500.0	!
DUPLICATE				



!C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 582	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
!C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 583	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
!C9H18Z+R11C2H5=>C2H6+C4H6Z2+R35C5H11 584	1.0E+0012	0.000	11000.0	! MZ
DUPLICATE				
!C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 585
!C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 586
!C10H20Z+R1H=>H2+C4H6Z2+R41C6H13 DUPLICATE	5.4E+0007	2.000	5000.0	! MZ 587
!C10H20Z+R20H=>H2O+C4H6Z2+R41C6H13 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 588
!C10H20Z+R20H=>H2O+C4H6Z2+R41C6H13 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 589
!C10H20Z+R20H=>H2O+C4H6Z2+R41C6H13 DUPLICATE	1.5E+0007	2.000	-765.0	! MZ 590
!C10H20Z+R300H=>H2O2+C4H6Z2+R41C6H13 591	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
!C10H20Z+R300H=>H2O2+C4H6Z2+R41C6H13 592	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
!C10H20Z+R300H=>H2O2+C4H6Z2+R41C6H13 593	2.4E+0012	0.000	15500.0	! MZ
DUPLICATE				
!C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 594
!C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 595
!C10H20Z+R4CH3=>CH4+C4H6Z2+R41C6H13 DUPLICATE	1.2E+0012	0.000	9600.0	! MZ 596
!C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 597	1.0E+0012	0.000	14550.0	!
DUPLICATE				
!C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 598	6.0E+0012	0.000	20000.0	!
DUPLICATE				
!C10H20Z+R8CH300=>CH300H+C4H6Z2+R41C6H13 MZ 599	1.8E+0013	0.000	17500.0	!
DUPLICATE				
!C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 600	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
!C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 601	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
!C10H20Z+R11C2H5=>C2H6+C4H6Z2+R41C6H13 602	1.2E+0012	0.000	11000.0	! MZ
DUPLICATE				

!C13H26Z+R1H=>H2+C4H6Z2+R4CH3+4C2H4Z	5.4E+0004	2.500	-1900.0	! MZ
603				
!C13H26Z+R20H=>H20+C4H6Z2+R4CH3+4C2H4Z	3.0E+0006	2.000	-1520.0	! MZ
604				
!C13H26Z+R300H=>H202+C4H6Z2+R4CH3+4C2H4Z	6.4E+0003	2.600	12400.0	!
MZ 605				
!C13H26Z+R4CH3=>CH4+C4H6Z2+R4CH3+4C2H4Z	1.0E+0011	0.000	7300.0	! MZ
606				
!C13H26Z+R8CH300=>CH300H+C4H6Z2+R4CH3+4C2H4Z	1.0E+0011	0.000	7300.0	
! MZ 607				
!C13H26Z+R11C2H5=>C2H6+C4H6Z2+R4CH3+4C2H4Z	1.5E+0000	3.500	4140.0	!
MZ 608				
!C12H24Z+R1H=>H2+C4H6Z2+R30C8H17	5.4E+0004	2.500	-1900.0	! MZ 609
DUPLICATE				
!C12H24Z+R1H=>H2+C4H6Z2+R30C8H17	2.9E+0007	2.000	7700.0	! MZ 610
DUPLICATE				
!C12H24Z+R1H=>H2+C4H6Z2+R30C8H17	7.2E+0007	2.000	5000.0	! MZ 611
DUPLICATE				
!C12H24Z+R20H=>H20+C4H6Z2+R30C8H17	3.0E+0006	2.000	-1520.0	! MZ 612
DUPLICATE				
!C12H24Z+R20H=>H20+C4H6Z2+R30C8H17	2.7E+0006	2.000	450.0	! MZ 613
DUPLICATE				
!C12H24Z+R20H=>H20+C4H6Z2+R30C8H17	2.1E+0007	2.000	-765.0	! MZ 614
DUPLICATE				
!C12H24Z+R300H=>H202+C4H6Z2+R30C8H17	6.4E+0003	2.600	12400.0	! MZ
615				
DUPLICATE				
!C12H24Z+R300H=>H202+C4H6Z2+R30C8H17	6.0E+0011	0.000	17000.0	! MZ
616				
DUPLICATE				
!C12H24Z+R300H=>H202+C4H6Z2+R30C8H17	3.2E+0012	0.000	15500.0	! MZ
617				
DUPLICATE				
!C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17	1.0E+0011	0.000	7300.0	! MZ 618
DUPLICATE				
!C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17	3.0E-0001	4.000	8200.0	! MZ 619
DUPLICATE				
!C12H24Z+R4CH3=>CH4+C4H6Z2+R30C8H17	1.6E+0012	0.000	9600.0	! MZ 620
DUPLICATE				
!C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17	1.0E+0012	0.000	14550.0	!
MZ 621				
DUPLICATE				
!C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17	6.0E+0012	0.000	20000.0	!
MZ 622				
DUPLICATE				
!C12H24Z+R8CH300=>CH300H+C4H6Z2+R30C8H17	2.4E+0013	0.000	17500.0	!
MZ 623				
DUPLICATE				
!C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17	1.5E+0000	3.500	4140.0	! MZ
624				
DUPLICATE				
!C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17	3.0E+0011	0.000	13500.0	! MZ
625				
DUPLICATE				

!C12H24Z+R11C2H5=>C2H6+C4H6Z2+R30C8H17 626	1.6E+0012	0.000	11000.0	! MZ
DUPLICATE				
!C11H22Z+R1H=>H2+C4H6Z2+R26C7H15 DUPLICATE	5.4E+0004	2.500	-1900.0	! MZ 627
!C11H22Z+R1H=>H2+C4H6Z2+R26C7H15 DUPLICATE	2.9E+0007	2.000	7700.0	! MZ 628
!C11H22Z+R1H=>H2+C4H6Z2+R26C7H15 DUPLICATE	6.3E+0007	2.000	5000.0	! MZ 629
!C11H22Z+R20H=>H2O+C4H6Z2+R26C7H15 DUPLICATE	3.0E+0006	2.000	-1520.0	! MZ 630
!C11H22Z+R20H=>H2O+C4H6Z2+R26C7H15 DUPLICATE	2.7E+0006	2.000	450.0	! MZ 631
!C11H22Z+R20H=>H2O+C4H6Z2+R26C7H15 DUPLICATE	1.8E+0007	2.000	-765.0	! MZ 632
!C11H22Z+R300H=>H2O2+C4H6Z2+R26C7H15 633	6.4E+0003	2.600	12400.0	! MZ
DUPLICATE				
!C11H22Z+R300H=>H2O2+C4H6Z2+R26C7H15 634	6.0E+0011	0.000	17000.0	! MZ
DUPLICATE				
!C11H22Z+R300H=>H2O2+C4H6Z2+R26C7H15 635	2.8E+0012	0.000	15500.0	! MZ
DUPLICATE				
!C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15 DUPLICATE	1.0E+0011	0.000	7300.0	! MZ 636
!C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15 DUPLICATE	3.0E-0001	4.000	8200.0	! MZ 637
!C11H22Z+R4CH3=>CH4+C4H6Z2+R26C7H15 DUPLICATE	1.4E+0012	0.000	9600.0	! MZ 638
!C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15 MZ 639	1.0E+0012	0.000	14550.0	!
DUPLICATE				
!C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15 MZ 640	6.0E+0012	0.000	20000.0	!
DUPLICATE				
!C11H22Z+R8CH300=>CH300H+C4H6Z2+R26C7H15 MZ 641	2.1E+0013	0.000	17500.0	!
DUPLICATE				
!C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15 642	1.5E+0000	3.500	4140.0	! MZ
DUPLICATE				
!C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15 643	3.0E+0011	0.000	13500.0	! MZ
DUPLICATE				
!C11H22Z+R11C2H5=>C2H6+C4H6Z2+R26C7H15 644	1.4E+0012	0.000	11000.0	! MZ
DUPLICATE				
!C14H28Z+R1H=>H2+C4H6Z2+R11C2H5+4C2H4Z 645	5.4E+0004	2.500	-1900.0	! MZ
!C14H28Z+R20H=>H2O+C4H6Z2+R11C2H5+4C2H4Z MZ 646	3.0E+0006	2.000	-1520.0	!
!C14H28Z+R300H=>H2O2+C4H6Z2+R11C2H5+4C2H4Z 12400.0 ! MZ 647	6.4E+0003	2.600		

!C14H28Z+R4CH3=>CH4+C4H6Z2+R11C2H5+4C2H4Z	1.0E+0011	0.000	7300.0	!
MZ 648				
!C14H28Z+R8CH300=>CH300H+C4H6Z2+R11C2H5+4C2H4Z	1.0E+0011	0.000		
7300.0 ! MZ 649				
!C14H28Z+R11C2H5=>C2H6+C4H6Z2+R11C2H5+4C2H4Z	1.5E+0000	3.500	4140.0	
! MZ 650				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	8.8E+0010	0.700	3250.0	! MZ 651
DUPLICATE				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	5.1E+0013	0.000	7850.0	! MZ 652
DUPLICATE				
C5H10Z+B10=>R20H+C4H6Z2+R4CH3	2.6E+0013	0.000	5200.0	! MZ 653
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	8.8E+0010	0.700	3250.0	! MZ 654
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	5.1E+0013	0.000	7850.0	! MZ 655
DUPLICATE				
C7H14Z+B10=>R20H+C4H6Z2+R19C3H7	7.8E+0013	0.000	5200.0	! MZ 656
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	8.8E+0010	0.700	3250.0	! MZ 657
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	5.1E+0013	0.000	7850.0	! MZ 658
DUPLICATE				
C6H12Z+B10=>R20H+C4H6Z2+R11C2H5	5.2E+0013	0.000	5200.0	! MZ 659
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	8.8E+0010	0.700	3250.0	! MZ 660
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	5.1E+0013	0.000	7850.0	! MZ 661
DUPLICATE				
C8H16Z+B10=>R20H+C4H6Z2+R20C4H9	1.0E+0014	0.000	5200.0	! MZ 662
DUPLICATE				
!C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	8.8E+0010	0.700	3250.0	! MZ 663
DUPLICATE				
!C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	5.1E+0013	0.000	7850.0	! MZ 664
DUPLICATE				
!C9H18Z+B10=>R20H+C4H6Z2+R35C5H11	1.3E+0014	0.000	5200.0	! MZ 665
DUPLICATE				
!C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	8.8E+0010	0.700	3250.0	! MZ 666
DUPLICATE				
!C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	5.1E+0013	0.000	7850.0	! MZ 667
DUPLICATE				
!C10H20Z+B10=>R20H+C4H6Z2+R41C6H13	1.6E+0014	0.000	5200.0	! MZ 668
DUPLICATE				
!C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	8.8E+0010	0.700	3250.0	! MZ 669
DUPLICATE				
!C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	5.1E+0013	0.000	7850.0	! MZ 670
DUPLICATE				
!C12H24Z+B10=>R20H+C4H6Z2+R30C8H17	2.1E+0014	0.000	5200.0	! MZ 671
DUPLICATE				
!C11H22Z+B10=>R20H+C4H6Z2+R26C7H15	8.8E+0010	0.700	3250.0	! MZ 672
DUPLICATE				
!C11H22Z+B10=>R20H+C4H6Z2+R26C7H15	5.1E+0013	0.000	7850.0	! MZ 673
DUPLICATE				
!C11H22Z+B10=>R20H+C4H6Z2+R26C7H15	1.8E+0014	0.000	5200.0	! MZ 674
DUPLICATE				

! Metathesis with YH

C3H6Y+R1H=>RC3H5Y+H2	1.7E+0005	2.500	2510.0	! MES 675
C3H6Y+R20H=>RC3H5Y+H20	3.0E+0006	2.000	-298.0	! MES 676
C3H6Y+R300H=>RC3H5Y+H202	9.6E+0003	2.600	13900.0	! MES 677
C3H6Y+R4CH3=>RC3H5Y+CH4	2.2E+0000	3.500	5670.0	! MES 678
C3H6Y+R8CH300=>RC3H5Y+CH300H	2.0E+0012	0.000	17050.0	! MES 679
C3H6Y+R11C2H5=>RC3H5Y+C2H6	2.2E+0000	3.500	6640.0	! MES 680
C4H8Y+R1H=>RC4H7Y+H2	5.4E+0004	2.500	-1900.0	! MES 681
DUPLICATE				
C4H8Y+R1H=>RC4H7Y+H2	2.9E+0007	2.000	7700.0	! MES 682
DUPLICATE				
C4H8Y+R20H=>RC4H7Y+H20	3.0E+0006	2.000	-1520.0	! MES 683
DUPLICATE				
C4H8Y+R20H=>RC4H7Y+H20	2.7E+0006	2.000	450.0	! MES 684
DUPLICATE				
C4H8Y+R300H=>RC4H7Y+H202	6.4E+0003	2.600	12400.0	! MES 685
DUPLICATE				
C4H8Y+R300H=>RC4H7Y+H202	6.0E+0011	0.000	17000.0	! MES 686
DUPLICATE				
C4H8Y+R4CH3=>RC4H7Y+CH4	1.0E+0011	0.000	7300.0	! MES 687
DUPLICATE				
C4H8Y+R4CH3=>RC4H7Y+CH4	3.0E-0001	4.000	8200.0	! MES 688
DUPLICATE				
C4H8Y+R8CH300=>RC4H7Y+CH300H	1.0E+0012	0.000	14550.0	! MES 689
DUPLICATE				
C4H8Y+R8CH300=>RC4H7Y+CH300H	6.0E+0012	0.000	20000.0	! MES 690
DUPLICATE				
C4H8Y+R11C2H5=>RC4H7Y+C2H6	1.5E+0000	3.500	4140.0	! MES 691
DUPLICATE				
C4H8Y+R11C2H5=>RC4H7Y+C2H6	3.0E+0011	0.000	13500.0	! MES 692
DUPLICATE				
C7H14Y+R1H=>RC7H13Y+H2	5.4E+0004	2.500	-1900.0	! MES 693
DUPLICATE				
C7H14Y+R1H=>RC7H13Y+H2	2.9E+0007	2.000	7700.0	! MES 694
DUPLICATE				
C7H14Y+R1H=>RC7H13Y+H2	2.7E+0007	2.000	5000.0	! MES 695
DUPLICATE				
C7H14Y+R20H=>RC7H13Y+H20	3.0E+0006	2.000	-1520.0	! MES 696
DUPLICATE				
C7H14Y+R20H=>RC7H13Y+H20	2.7E+0006	2.000	450.0	! MES 697
DUPLICATE				
C7H14Y+R20H=>RC7H13Y+H20	7.8E+0006	2.000	-765.0	! MES 698
DUPLICATE				
C7H14Y+R300H=>RC7H13Y+H202	6.4E+0003	2.600	12400.0	! MES 699
DUPLICATE				
C7H14Y+R300H=>RC7H13Y+H202	6.0E+0011	0.000	17000.0	! MES 700
DUPLICATE				
C7H14Y+R300H=>RC7H13Y+H202	1.2E+0012	0.000	15500.0	! MES 701
DUPLICATE				
C7H14Y+R4CH3=>RC7H13Y+CH4	1.0E+0011	0.000	7300.0	! MES 702
DUPLICATE				
C7H14Y+R4CH3=>RC7H13Y+CH4	3.0E-0001	4.000	8200.0	! MES 703
DUPLICATE				

C7H14Y+R4CH3=>RC7H13Y+CH4	6.0E+0011	0.000	9600.0	! MES 704
DUPLICATE				
C7H14Y+R8CH300=>RC7H13Y+CH300H	1.0E+0012	0.000	14550.0	! MES 705
DUPLICATE				
C7H14Y+R8CH300=>RC7H13Y+CH300H	6.0E+0012	0.000	20000.0	! MES 706
DUPLICATE				
C7H14Y+R8CH300=>RC7H13Y+CH300H	9.0E+0012	0.000	17500.0	! MES 707
DUPLICATE				
C7H14Y+R11C2H5=>RC7H13Y+C2H6	1.5E+0000	3.500	4140.0	! MES 708
DUPLICATE				
C7H14Y+R11C2H5=>RC7H13Y+C2H6	3.0E+0011	0.000	13500.0	! MES 709
DUPLICATE				
C7H14Y+R11C2H5=>RC7H13Y+C2H6	6.0E+0011	0.000	11000.0	! MES 710
DUPLICATE				
C8H16Y+R1H=>RC8H15Y+H2	5.4E+0004	2.500	-1900.0	! MES 711
DUPLICATE				
C8H16Y+R1H=>RC8H15Y+H2	2.9E+0007	2.000	7700.0	! MES 712
DUPLICATE				
C8H16Y+R1H=>RC8H15Y+H2	3.6E+0007	2.000	5000.0	! MES 713
DUPLICATE				
C8H16Y+R20H=>RC8H15Y+H20	3.0E+0006	2.000	-1520.0	! MES 714
DUPLICATE				
C8H16Y+R20H=>RC8H15Y+H20	2.7E+0006	2.000	450.0	! MES 715
DUPLICATE				
C8H16Y+R20H=>RC8H15Y+H20	1.0E+0007	2.000	-765.0	! MES 716
DUPLICATE				
C8H16Y+R300H=>RC8H15Y+H202	6.4E+0003	2.600	12400.0	! MES 717
DUPLICATE				
C8H16Y+R300H=>RC8H15Y+H202	6.0E+0011	0.000	17000.0	! MES 718
DUPLICATE				
C8H16Y+R300H=>RC8H15Y+H202	1.6E+0012	0.000	15500.0	! MES 719
DUPLICATE				
C8H16Y+R4CH3=>RC8H15Y+CH4	1.0E+0011	0.000	7300.0	! MES 720
DUPLICATE				
C8H16Y+R4CH3=>RC8H15Y+CH4	3.0E-0001	4.000	8200.0	! MES 721
DUPLICATE				
C8H16Y+R4CH3=>RC8H15Y+CH4	8.0E+0011	0.000	9600.0	! MES 722
DUPLICATE				
C8H16Y+R8CH300=>RC8H15Y+CH300H	1.0E+0012	0.000	14550.0	! MES 723
DUPLICATE				
C8H16Y+R8CH300=>RC8H15Y+CH300H	6.0E+0012	0.000	20000.0	! MES 724
DUPLICATE				
C8H16Y+R8CH300=>RC8H15Y+CH300H	1.2E+0013	0.000	17500.0	! MES 725
DUPLICATE				
C8H16Y+R11C2H5=>RC8H15Y+C2H6	1.5E+0000	3.500	4140.0	! MES 726
DUPLICATE				
C8H16Y+R11C2H5=>RC8H15Y+C2H6	3.0E+0011	0.000	13500.0	! MES 727
DUPLICATE				
C8H16Y+R11C2H5=>RC8H15Y+C2H6	8.0E+0011	0.000	11000.0	! MES 728
DUPLICATE				
C5H10Y+R1H=>RC5H9Y+H2	5.4E+0004	2.500	-1900.0	! MES 729
DUPLICATE				
C5H10Y+R1H=>RC5H9Y+H2	2.9E+0007	2.000	7700.0	! MES 730
DUPLICATE				

C5H10Y+R1H=>RC5H9Y+H2 DUPLICATE	9.0E+0006	2.000	5000.0	! MES 731
C5H10Y+R20H=>RC5H9Y+H20 DUPLICATE	3.0E+0006	2.000	-1520.0	! MES 732
C5H10Y+R20H=>RC5H9Y+H20 DUPLICATE	2.7E+0006	2.000	450.0	! MES 733
C5H10Y+R20H=>RC5H9Y+H20 DUPLICATE	2.6E+0006	2.000	-765.0	! MES 734
C5H10Y+R300H=>RC5H9Y+H202 DUPLICATE	6.4E+0003	2.600	12400.0	! MES 735
C5H10Y+R300H=>RC5H9Y+H202 DUPLICATE	6.0E+0011	0.000	17000.0	! MES 736
C5H10Y+R300H=>RC5H9Y+H202 DUPLICATE	4.0E+0011	0.000	15500.0	! MES 737
C5H10Y+R4CH3=>RC5H9Y+CH4 DUPLICATE	1.0E+0011	0.000	7300.0	! MES 738
C5H10Y+R4CH3=>RC5H9Y+CH4 DUPLICATE	3.0E-0001	4.000	8200.0	! MES 739
C5H10Y+R4CH3=>RC5H9Y+CH4 DUPLICATE	2.0E+0011	0.000	9600.0	! MES 740
C5H10Y+R8CH300=>RC5H9Y+CH300H DUPLICATE	1.0E+0012	0.000	14550.0	! MES 741
C5H10Y+R8CH300=>RC5H9Y+CH300H DUPLICATE	6.0E+0012	0.000	20000.0	! MES 742
C5H10Y+R8CH300=>RC5H9Y+CH300H DUPLICATE	3.0E+0012	0.000	17500.0	! MES 743
C5H10Y+R11C2H5=>RC5H9Y+C2H6 DUPLICATE	1.5E+0000	3.500	4140.0	! MES 744
C5H10Y+R11C2H5=>RC5H9Y+C2H6 DUPLICATE	3.0E+0011	0.000	13500.0	! MES 745
C5H10Y+R11C2H5=>RC5H9Y+C2H6 DUPLICATE	2.0E+0011	0.000	11000.0	! MES 746
C3H6Y+B10=>RC3H5Y+R20H	1.7E+0011	0.700	5900.0	! MES 747
C4H8Y+B10=>RC4H7Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 748
C4H8Y+B10=>RC4H7Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 749
C7H14Y+B10=>RC7H13Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 750
C7H14Y+B10=>RC7H13Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 751
C7H14Y+B10=>RC7H13Y+R20H DUPLICATE	7.8E+0013	0.000	5200.0	! MES 752
C8H16Y+B10=>RC8H15Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 753
C8H16Y+B10=>RC8H15Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 754
C8H16Y+B10=>RC8H15Y+R20H DUPLICATE	1.0E+0014	0.000	5200.0	! MES 755
C5H10Y+B10=>RC5H9Y+R20H DUPLICATE	8.8E+0010	0.700	3250.0	! MES 756
C5H10Y+B10=>RC5H9Y+R20H DUPLICATE	5.1E+0013	0.000	7850.0	! MES 757
C5H10Y+B10=>RC5H9Y+R20H	2.6E+0013	0.000	5200.0	! MES 758

DUPLICATE

! Addition of .Y on YH

RC3H5Y+C5H10Y=>R10C2H3V+C6H12Z	6.0E+0009	0.000	11400.0	! ADY 759
!RC3H5Y+C8H16Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 760
RC3H5Y+C7H14Y=>R10C2H3V+C8H16Z	6.0E+0009	0.000	11400.0	! ADY 761
RC3H5Y+C4H8Y=>R10C2H3V+C5H10Z	6.0E+0009	0.000	11400.0	! ADY 762
RC3H5Y+C3H6Y=>R10C2H3V+C4H8Y	6.0E+0009	0.000	11400.0	! ADY 763
RC4H7Y+C5H10Y=>R10C2H3V+C7H14Z	6.0E+0009	0.000	11400.0	! ADY 764
!RC4H7Y+C8H16Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 765
!RC4H7Y+C7H14Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 766
RC4H7Y+C4H8Y=>R10C2H3V+C6H12Z	6.0E+0009	0.000	11400.0	! ADY 767
RC4H7Y+C3H6Y=>R10C2H3V+C5H10Z	6.0E+0009	0.000	11400.0	! ADY 768
!RC7H13Y+C5H10Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 769
!RC7H13Y+C8H16Y=>R10C2H3V+C13H26Z	6.0E+0009	0.000	11400.0	! ADY 770
!RC7H13Y+C7H14Y=>R10C2H3V+C12H24Z	6.0E+0009	0.000	11400.0	! ADY 771
!RC7H13Y+C4H8Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 772
RC7H13Y+C3H6Y=>R10C2H3V+C8H16Z	6.0E+0009	0.000	11400.0	! ADY 773
!RC8H15Y+C5H10Y=>R10C2H3V+C11H22Z	6.0E+0009	0.000	11400.0	! ADY 774
!RC8H15Y+C8H16Y=>R10C2H3V+C14H28Z	6.0E+0009	0.000	11400.0	! ADY 775
!RC8H15Y+C7H14Y=>R10C2H3V+C13H26Z	6.0E+0009	0.000	11400.0	! ADY 776
!RC8H15Y+C4H8Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 777
!RC8H15Y+C3H6Y=>R10C2H3V+C9H18Z	6.0E+0009	0.000	11400.0	! ADY 778
RC5H9Y+C5H10Y=>R10C2H3V+C8H16Z	6.0E+0009	0.000	11400.0	! ADY 779
!RC5H9Y+C8H16Y=>R10C2H3V+C11H22Z	6.0E+0009	0.000	11400.0	! ADY 780
!RC5H9Y+C7H14Y=>R10C2H3V+C10H20Z	6.0E+0009	0.000	11400.0	! ADY 781
RC5H9Y+C4H8Y=>R10C2H3V+C7H14Z	6.0E+0009	0.000	11400.0	! ADY 782
RC5H9Y+C3H6Y=>R10C2H3V+C6H12Z	6.0E+0009	0.000	11400.0	! ADY 783

! Alkohol reactions

C3H7OH+R1H=>H2+R2OH+C3H6Y	2.9E+0007	2.000	7700.0	! MOL 784
DUPLICATE				
C3H7OH+R1H=>H2+R2OH+C3H6Y	1.8E+0007	2.000	5000.0	! MOL 785
DUPLICATE				
C3H7OH+R1H=>H2+R11C2H5+HCHO	2.4E+0006	2.000	6525.0	! MOL 786
C3H7OH+R2OH=>H2O+R2OH+C3H6Y	2.7E+0006	2.000	450.0	! MOL 787
DUPLICATE				
C3H7OH+R2OH=>H2O+R2OH+C3H6Y	5.2E+0006	2.000	-765.0	! MOL 788
DUPLICATE				
C3H7OH+R2OH=>H2O+R11C2H5+HCHO	4.0E+0005	2.000	-475.0	! MOL 789
C3H7OH+R300H=>H2O2+R2OH+C3H6Y	6.0E+0011	0.000	17000.0	! MOL 790
DUPLICATE				
C3H7OH+R300H=>H2O2+R2OH+C3H6Y	8.0E+0011	0.000	15500.0	! MOL 791
DUPLICATE				
C3H7OH+R300H=>H2O2+R11C2H5+HCHO	5.4E+0004	2.000	15025.0	! MOL 792
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y	3.0E-0001	4.000	8200.0	! MOL 793
DUPLICATE				
C3H7OH+R4CH3=>CH4+R2OH+C3H6Y	4.0E+0011	0.000	9600.0	! MOL 794
DUPLICATE				
C3H7OH+R4CH3=>CH4+R11C2H5+HCHO	3.9E+0004	2.000	7525.0	! MOL 795
C3H7OH+R8CH300=>CH300H+R2OH+C3H6Y	1.6E+0011	0.000	7300.0	! MOL 796
DUPLICATE				
C3H7OH+R8CH300=>CH300H+R2OH+C3H6Y	2.9E+0011	0.000	4500.0	! MOL 797
DUPLICATE				



C3H70H+R8CH300=>CH300H+R11C2H5+HCHO	0.0E+0000	0.000	0.0	! MOL 798
C3H70H+R11C2H5=>C2H6+R20H+C3H6Y	3.0E+0011	0.000	13500.0	! MOL 799
DUPLICATE				
C3H70H+R11C2H5=>C2H6+R20H+C3H6Y	4.0E+0011	0.000	11000.0	! MOL 800
DUPLICATE				
C3H70H+R11C2H5=>C2H6+R11C2H5+HCHO	2.3E+0004	2.000	10525.0	! MOL 801
C4H100L+R1H=>H2+R20H+C4H8Y	2.9E+0007	2.000	7700.0	! MOL 802
DUPLICATE				
C4H100L+R1H=>H2+R20H+C4H8Y	2.7E+0007	2.000	5000.0	! MOL 803
DUPLICATE				
C4H100L+R1H=>H2+R19C3H7+HCHO	2.4E+0006	2.000	6525.0	! MOL 804
C4H100L+R20H=>H20+R20H+C4H8Y	2.7E+0006	2.000	450.0	! MOL 805
DUPLICATE				
C4H100L+R20H=>H20+R20H+C4H8Y	7.8E+0006	2.000	-765.0	! MOL 806
DUPLICATE				
C4H100L+R20H=>H20+R19C3H7+HCHO	4.0E+0005	2.000	-475.0	! MOL 807
C4H100L+R300H=>H202+R20H+C4H8Y	6.0E+0011	0.000	17000.0	! MOL 808
DUPLICATE				
C4H100L+R300H=>H202+R20H+C4H8Y	1.2E+0012	0.000	15500.0	! MOL 809
DUPLICATE				
C4H100L+R300H=>H202+R19C3H7+HCHO	5.4E+0004	2.000	15025.0	! MOL 810
C4H100L+R4CH3=>CH4+R20H+C4H8Y	3.0E-0001	4.000	8200.0	! MOL 811
DUPLICATE				
C4H100L+R4CH3=>CH4+R20H+C4H8Y	6.0E+0011	0.000	9600.0	! MOL 812
DUPLICATE				
C4H100L+R4CH3=>CH4+R19C3H7+HCHO	3.9E+0004	2.000	7525.0	! MOL 813
C4H100L+R8CH300=>CH300H+R20H+C4H8Y	1.6E+0011	0.000	7300.0	! MOL 814
DUPLICATE				
C4H100L+R8CH300=>CH300H+R20H+C4H8Y	4.4E+0011	0.000	4500.0	! MOL 815
DUPLICATE				
C4H100L+R8CH300=>CH300H+R19C3H7+HCHO	0.0E+0000	0.000	0.0	! MOL 816
C4H100L+R11C2H5=>C2H6+R20H+C4H8Y	3.0E+0011	0.000	13500.0	! MOL 817
DUPLICATE				
C4H100L+R11C2H5=>C2H6+R20H+C4H8Y	6.0E+0011	0.000	11000.0	! MOL 818
DUPLICATE				
C4H100L+R11C2H5=>C2H6+R19C3H7+HCHO	2.3E+0004	2.000	10525.0	! MOL 819
C5H120L+R1H=>H2+R20H+C5H10Z	2.9E+0007	2.000	7700.0	! MOL 820
DUPLICATE				
C5H120L+R1H=>H2+R20H+C5H10Z	3.6E+0007	2.000	5000.0	! MOL 821
DUPLICATE				
C5H120L+R1H=>H2+R20C4H9+HCHO	2.4E+0006	2.000	6525.0	! MOL 822
C5H120L+R20H=>H20+R20H+C5H10Z	2.7E+0006	2.000	450.0	! MOL 823
DUPLICATE				
C5H120L+R20H=>H20+R20H+C5H10Z	1.0E+0007	2.000	-765.0	! MOL 824
DUPLICATE				
C5H120L+R20H=>H20+R20C4H9+HCHO	4.0E+0005	2.000	-475.0	! MOL 825
C5H120L+R300H=>H202+R20H+C5H10Z	6.0E+0011	0.000	17000.0	! MOL 826
DUPLICATE				
C5H120L+R300H=>H202+R20H+C5H10Z	1.6E+0012	0.000	15500.0	! MOL 827
DUPLICATE				
C5H120L+R300H=>H202+R20C4H9+HCHO	5.4E+0004	2.000	15025.0	! MOL 828
C5H120L+R4CH3=>CH4+R20H+C5H10Z	3.0E-0001	4.000	8200.0	! MOL 829
DUPLICATE				

C5H120L+R4CH3=>CH4+R20H+C5H10Z 8.0E+0011 0.000 9600.0 ! MOL 830  
 DUPLICATE  
 C5H120L+R4CH3=>CH4+R20C4H9+HCHO 3.9E+0004 2.000 7525.0 ! MOL 831  
 C5H120L+R8CH300=>CH300H+R20H+C5H10Z 1.6E+0011 0.000 7300.0 ! MOL 832  
 DUPLICATE  
 C5H120L+R8CH300=>CH300H+R20H+C5H10Z 5.8E+0011 0.000 4500.0 ! MOL 833  
 DUPLICATE  
 C5H120L+R8CH300=>CH300H+R20C4H9+HCHO 0.0E+0000 0.000 0.0 ! MOL 834  
 C5H120L+R11C2H5=>C2H6+R20H+C5H10Z 3.0E+0011 0.000 13500.0 ! MOL 835  
 DUPLICATE  
 C5H120L+R11C2H5=>C2H6+R20H+C5H10Z 8.0E+0011 0.000 11000.0 ! MOL 836  
 DUPLICATE  
 C5H120L+R11C2H5=>C2H6+R20C4H9+HCHO 2.3E+0004 2.000 10525.0 ! MOL 837  
 C3H70H+B10=>R20H+R20H+C3H6Y 3.9E+0013 0.000 5200.0 ! MOL 838  
 DUPLICATE  
 C3H70H+B10=>R20H+R20H+C3H6Y 4.0E+0013 0.000 5200.0 ! MOL 839  
 DUPLICATE  
 C3H70H+B10=>R20H+R11C2H5+HCHO 1.3E+0006 2.000 5025.0 ! MOL 840  
 C4H100L+B10=>R20H+R20H+C4H8Y 3.9E+0013 0.000 5200.0 ! MOL 841  
 DUPLICATE  
 C4H100L+B10=>R20H+R20H+C4H8Y 6.0E+0013 0.000 5200.0 ! MOL 842  
 DUPLICATE  
 C4H100L+B10=>R20H+R19C3H7+HCHO 1.3E+0006 2.000 5025.0 ! MOL 843  
 C5H120L+B10=>R20H+R20H+C5H10Z 3.9E+0013 0.000 5200.0 ! MOL 844  
 DUPLICATE  
 C5H120L+B10=>R20H+R20H+C5H10Z 8.0E+0013 0.000 5200.0 ! MOL 845  
 DUPLICATE  
 C5H120L+B10=>R20H+R20C4H9+HCHO 1.3E+0006 2.000 5025.0 ! MOL 846

! Aldehydes metathesis

C2H5CHO+R1H=>H2+RC3H50 4.0E+0013 0.000 4200.0 ! ADZ 847  
 C2H5CHO+R20H=>H20+RC3H50 4.2E+0012 0.000 500.0 ! ADZ 848  
 C2H5CHO+R300H=>H202+RC3H50 1.0E+0012 0.000 10000.0 ! ADZ 849  
 C2H5CHO+R4CH3=>CH4+RC3H50 2.0E-0006 5.600 2500.0 ! ADZ 850  
 C2H5CHO+R11C2H5=>C2H6+RC3H50 1.3E+0012 0.000 8500.0 ! ADZ 851  
 C5H100A+R1H=>H2+RC5H90 4.0E+0013 0.000 4200.0 ! ADZ 852  
 C5H100A+R20H=>H20+RC5H90 4.2E+0012 0.000 500.0 ! ADZ 853  
 C5H100A+R300H=>H202+RC5H90 1.0E+0012 0.000 10000.0 ! ADZ 854  
 C5H100A+R4CH3=>CH4+RC5H90 2.0E-0006 5.600 2500.0 ! ADZ 855  
 C5H100A+R11C2H5=>C2H6+RC5H90 1.3E+0012 0.000 8500.0 ! ADZ 856  
 C4H80A+R1H=>H2+RC4H70 4.0E+0013 0.000 4200.0 ! ADZ 857  
 C4H80A+R20H=>H20+RC4H70 4.2E+0012 0.000 500.0 ! ADZ 858  
 C4H80A+R300H=>H202+RC4H70 1.0E+0012 0.000 10000.0 ! ADZ 859  
 C4H80A+R4CH3=>CH4+RC4H70 2.0E-0006 5.600 2500.0 ! ADZ 860  
 C4H80A+R11C2H5=>C2H6+RC4H70 1.3E+0012 0.000 8500.0 ! ADZ 861  
 C6H120A+R1H=>H2+RC6H110 4.0E+0013 0.000 4200.0 ! ADZ 862  
 C6H120A+R20H=>H20+RC6H110 4.2E+0012 0.000 500.0 ! ADZ 863  
 C6H120A+R300H=>H202+RC6H110 1.0E+0012 0.000 10000.0 ! ADZ 864  
 C6H120A+R4CH3=>CH4+RC6H110 2.0E-0006 5.600 2500.0 ! ADZ 865  
 C6H120A+R11C2H5=>C2H6+RC6H110 1.3E+0012 0.000 8500.0 ! ADZ 866  
 C7H140A+R1H=>H2+RC7H130 4.0E+0013 0.000 4200.0 ! ADZ 867

C7H140A+R20H=>H20+RC7H130 4.2E+0012 0.000 500.0 ! ADZ 868  
C7H140A+R300H=>H202+RC7H130 1.0E+0012 0.000 10000.0 ! ADZ 869  
C7H140A+R4CH3=>CH4+RC7H130 2.0E-0006 5.600 2500.0 ! ADZ 870  
C7H140A+R11C2H5=>C2H6+RC7H130 1.3E+0012 0.000 8500.0 ! ADZ 871  
C8H160A+R1H=>H2+RC8H150 4.0E+0013 0.000 4200.0 ! ADZ 872  
C8H160A+R20H=>H20+RC8H150 4.2E+0012 0.000 500.0 ! ADZ 873  
C8H160A+R300H=>H202+RC8H150 1.0E+0012 0.000 10000.0 ! ADZ 874  
C8H160A+R4CH3=>CH4+RC8H150 2.0E-0006 5.600 2500.0 ! ADZ 875  
C8H160A+R11C2H5=>C2H6+RC8H150 1.3E+0012 0.000 8500.0 ! ADZ 876  
!C9H180A+R1H=>H2+RC9H170 4.0E+0013 0.000 4200.0 ! ADZ 877  
!C9H180A+R20H=>H20+RC9H170 4.2E+0012 0.000 500.0 ! ADZ 878  
!C9H180A+R300H=>H202+RC9H170 1.0E+0012 0.000 10000.0 ! ADZ 879  
!C9H180A+R4CH3=>CH4+RC9H170 2.0E-0006 5.600 2500.0 ! ADZ 880  
!C9H180A+R11C2H5=>C2H6+RC9H170 1.3E+0012 0.000 8500.0 ! ADZ 881  
!C12H240A+R1H=>H2+RC12H230 4.0E+0013 0.000 4200.0 ! ADZ 882  
!C12H240A+R20H=>H20+RC12H230 4.2E+0012 0.000 500.0 ! ADZ 883  
!C12H240A+R300H=>H202+RC12H230 1.0E+0012 0.000 10000.0 ! ADZ 884  
!C12H240A+R4CH3=>CH4+RC12H230 2.0E-0006 5.600 2500.0 ! ADZ 885  
!C12H240A+R11C2H5=>C2H6+RC12H230 1.3E+0012 0.000 8500.0 ! ADZ 886  
!C11H220A+R1H=>H2+RC11H210 4.0E+0013 0.000 4200.0 ! ADZ 887  
!C11H220A+R20H=>H20+RC11H210 4.2E+0012 0.000 500.0 ! ADZ 888  
!C11H220A+R300H=>H202+RC11H210 1.0E+0012 0.000 10000.0 ! ADZ 889  
!C11H220A+R4CH3=>CH4+RC11H210 2.0E-0006 5.600 2500.0 ! ADZ 890  
!C11H220A+R11C2H5=>C2H6+RC11H210 1.3E+0012 0.000 8500.0 ! ADZ 891  
!C10H200A+R1H=>H2+RC10H190 4.0E+0013 0.000 4200.0 ! ADZ 892  
!C10H200A+R20H=>H20+RC10H190 4.2E+0012 0.000 500.0 ! ADZ 893  
!C10H200A+R300H=>H202+RC10H190 1.0E+0012 0.000 10000.0 ! ADZ 894  
!C10H200A+R4CH3=>CH4+RC10H190 2.0E-0006 5.600 2500.0 ! ADZ 895  
!C10H200A+R11C2H5=>C2H6+RC10H190 1.3E+0012 0.000 8500.0 ! ADZ 896  
!C13H260A+R1H=>H2+RC13H250 4.0E+0013 0.000 4200.0 ! ADZ 897  
!C13H260A+R20H=>H20+RC13H250 4.2E+0012 0.000 500.0 ! ADZ 898  
!C13H260A+R300H=>H202+RC13H250 1.0E+0012 0.000 10000.0 ! ADZ 899  
!C13H260A+R4CH3=>CH4+RC13H250 2.0E-0006 5.600 2500.0 ! ADZ 900  
!C13H260A+R11C2H5=>C2H6+RC13H250 1.3E+0012 0.000 8500.0 ! ADZ 901  
  
C4H60AY+R1H=>H2+R10C2H3V+CH2COZ 4.0E+0013 0.000 4200.0 ! ADZ 902  
C4H60AY+R20H=>H20+R10C2H3V+CH2COZ 4.0E+0012 0.000 500.0 ! ADZ 903  
C4H60AY+R300H=>H202+R10C2H3V+CH2COZ 1.0E+0012 0.000 10000.0 ! ADZ  
904  
C4H60AY+R4CH3=>CH4+R10C2H3V+CH2COZ 2.0E-0006 0.000 2500.0 ! ADZ 905  
C4H60AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ 1.3E+0012 0.000 8500.0 ! ADZ  
906  
C5H80AY+R1H=>H2+RC3H5Y+CH2COZ 4.0E+0013 0.000 4200.0 ! ADZ 907  
C5H80AY+R20H=>H20+RC3H5Y+CH2COZ 4.0E+0012 0.000 500.0 ! ADZ 908  
C5H80AY+R300H=>H202+RC3H5Y+CH2COZ 1.0E+0012 0.000 10000.0 ! ADZ 909  
C5H80AY+R4CH3=>CH4+RC3H5Y+CH2COZ 2.0E-0006 0.000 2500.0 ! ADZ 910  
C5H80AY+R11C2H5=>C2H6+RC3H5Y+CH2COZ 1.3E+0012 0.000 8500.0 ! ADZ  
911  
!C8H140AY+R1H=>H2+R10C2H3V+CH2COZ+2C2H4Z 4.0E+0013 0.000 4200.0 !  
ADZ 912  
!C8H140AY+R20H=>H20+R10C2H3V+CH2COZ+2C2H4Z 4.0E+0012 0.000 500.0 !  
ADZ 913  
!C8H140AY+R300H=>H202+R10C2H3V+CH2COZ+2C2H4Z 1.0E+0012 0.000 10000.0  
! ADZ 914

!C8H140AY+R4CH3=>CH4+R10C2H3V+CH2COZ+2C2H4Z 2.0E-0006 0.000  
 2500.0 ! ADZ 915  
 !C8H140AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+2C2H4Z 1.3E+0012 0.000  
 8500.0 ! ADZ 916  
 !C9H160AY+R1H=>H2+RC3H5Y+CH2COZ+2C2H4Z 4.0E+0013 0.000 4200.0 ! ADZ  
 917  
 !C9H160AY+R20H=>H20+RC3H5Y+CH2COZ+2C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 918  
 !C9H160AY+R300H=>H202+RC3H5Y+CH2COZ+2C2H4Z 1.0E+0012 0.000  
 10000.0 ! ADZ 919  
 !C9H160AY+R4CH3=>CH4+RC3H5Y+CH2COZ+2C2H4Z 2.0E-0006 0.000 2500.0 !  
 ADZ 920  
 !C9H160AY+R11C2H5=>C2H6+RC3H5Y+CH2COZ+2C2H4Z 1.3E+0012 0.000 8500.0  
 ! ADZ 921  
 !C6H100AY+R1H=>H2+R10C2H3V+CH2COZ+C2H4Z 4.0E+0013 0.000 4200.0 !  
 ADZ 922  
 !C6H100AY+R20H=>H20+R10C2H3V+CH2COZ+C2H4Z 4.0E+0012 0.000 500.0 !  
 ADZ 923  
 !C6H100AY+R300H=>H202+R10C2H3V+CH2COZ+C2H4Z 1.0E+0012 0.000 10000.0  
 ! ADZ 924  
 !C6H100AY+R4CH3=>CH4+R10C2H3V+CH2COZ+C2H4Z 2.0E-0006 0.000 2500.0 !  
 ADZ 925  
 !C6H100AY+R11C2H5=>C2H6+R10C2H3V+CH2COZ+C2H4Z 1.3E+0012 0.000 8500.0  
 ! ADZ 926

! Keto radicals decomposition

RC3H50=>B2C0+R11C2H5 1.8E+0014 0.000 15600.0 ! COR 927  
 RC5H90=>B2C0+R20C4H9 1.8E+0014 0.000 15600.0 ! COR 928  
 RC4H70=>B2C0+R19C3H7 1.8E+0014 0.000 15600.0 ! COR 929  
 RC6H110=>B2C0+R35C5H11 1.8E+0014 0.000 15600.0 ! COR 930  
 RC7H130=>B2C0+R41C6H13 1.8E+0014 0.000 15600.0 ! COR 931  
 RC8H150=>B2C0+R26C7H15 1.8E+0014 0.000 15600.0 ! COR 932  
 !RC9H170=>B2C0+R30C8H17 1.8E+0014 0.000 15600.0 ! COR 933  
 !RC12H230=>B2C0+R4CH3+5C2H4Z 1.8E+0014 0.000 15600.0 ! COR 934  
 !RC11H210=>B2C0+R11C2H5+4C2H4Z 1.8E+0014 0.000 15600.0 ! COR 935  
 !RC10H190=>B2C0+R4CH3+4C2H4Z 1.8E+0014 0.000 15600.0 ! COR 936  
 !RC13H250=>B2C0+R11C2H5+5C2H4Z 1.8E+0014 0.000 15600.0 ! COR 937

! keto radicals addition to O2

RC3H50+O2=>RC3H503 3.0E+0019 -2.500 0.0 ! COR 938  
 RC5H90+O2=>RC5H903 3.0E+0019 -2.500 0.0 ! COR 939  
 RC4H70+O2=>RC4H703 3.0E+0019 -2.500 0.0 ! COR 940  
 RC6H110+O2=>RC6H1103 3.0E+0019 -2.500 0.0 ! COR 941  
 RC7H130+O2=>RC7H1303 3.0E+0019 -2.500 0.0 ! COR 942  
 RC8H150+O2=>RC8H1503 3.0E+0019 -2.500 0.0 ! COR 943  
 !RC9H170+O2=>RC9H1703 3.0E+0019 -2.500 0.0 ! COR 944  
 !RC12H230+O2=>RC12H2303 3.0E+0019 -2.500 0.0 ! COR 945  
 !RC11H210+O2=>RC11H2103 3.0E+0019 -2.500 0.0 ! COR 946  
 !RC10H190+O2=>RC10H1903 3.0E+0019 -2.500 0.0 ! COR 947  
 !RC13H250+O2=>RC13H2503 3.0E+0019 -2.500 0.0 ! COR 948

! Peroxide radical decomposition

RC3H503=>C2H4Z+R20H+C02 4.5E+0011 0.000 25000.0 ! PER 949

RC5H903=>C4H8Y+R20H+C02	4.5E+0011	0.000	25000.0	! PER 950
RC4H703=>C3H6Y+R20H+C02	4.5E+0011	0.000	25000.0	! PER 951
RC6H1103=>C5H10Y+R20H+C02	4.5E+0011	0.000	25000.0	! PER 952
RC7H1303=>C6H12Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 953
RC8H1503=>C7H14Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 954
!RC9H1703=>C8H16Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 955
!RC12H2303=>C11H22Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 956
!RC11H2103=>C10H20Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 957
!RC10H1903=>C9H18Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 958
!RC13H2503=>C12H24Z+R20H+C02	4.5E+0011	0.000	25000.0	! PER 959

! Ketones reactions

!C2H6CO+R1H=>H2+CH2COZ+R4CH3	5.7E+0007	2.000	7700.0	! MK 960
!C2H6CO+R20H=>H2O+CH2COZ+R4CH3	5.4E+0006	2.000	450.0	! MK 961
!C2H6CO+R300H=>H2O2+CH2COZ+R4CH3	1.2E+0012	0.000	17000.0	! MK 962
!C2H6CO+R4CH3=>CH4+CH2COZ+R4CH3	6.0E-0001	4.000	8200.0	! MK 963
!C2H6CO+R8CH300=>CH300H+CH2COZ+R4CH3	1.2E+0013	0.000	20000.0	! MK 964
!C2H6CO+R11C2H5=>C2H6+CH2COZ+R4CH3	6.0E+0011	0.000	13500.0	! MK 965
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	5.7E+0007	2.000	7700.0	! MK 966
DUPLICATE				
C3H8CO+R1H=>H2+CH2COZ+R11C2H5	9.0E+0006	2.000	5000.0	! MK 967
DUPLICATE				
C3H8CO+R20H=>H2O+CH2COZ+R11C2H5	5.4E+0006	2.000	450.0	! MK 968
DUPLICATE				
C3H8CO+R20H=>H2O+CH2COZ+R11C2H5	2.6E+0006	2.000	-765.0	! MK 969
DUPLICATE				
C3H8CO+R300H=>H2O2+CH2COZ+R11C2H5	1.2E+0012	0.000	17000.0	! MK 970
DUPLICATE				
C3H8CO+R300H=>H2O2+CH2COZ+R11C2H5	4.0E+0011	0.000	15500.0	! MK 971
DUPLICATE				
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	6.0E-0001	4.000	8200.0	! MK 972
DUPLICATE				
C3H8CO+R4CH3=>CH4+CH2COZ+R11C2H5	2.0E+0011	0.000	9600.0	! MK 973
DUPLICATE				
C3H8CO+R8CH300=>CH300H+CH2COZ+R11C2H5	1.2E+0013	0.000	20000.0	! MK 974
DUPLICATE				
C3H8CO+R8CH300=>CH300H+CH2COZ+R11C2H5	3.0E+0012	0.000	17500.0	! MK 975
DUPLICATE				
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	6.0E+0011	0.000	13500.0	! MK 976
DUPLICATE				
C3H8CO+R11C2H5=>C2H6+CH2COZ+R11C2H5	2.0E+0011	0.000	11000.0	! MK 977
DUPLICATE				

! Unsaturated ester reactions

! Esters metatesis

! Ester with aldehyde function metathesis

! Ester with ceton function metathesis  
! Addition on unsaturated esters

! Carboxylic acid reactions  
! Carboxylic acid metathesis

! Carboxylic acid decomposition

! Alkohol ene to dienes

C3H60LY+R1H=>H2+HCHO+R10C2H3V 5.4E+0004 2.500 -1900.0 ! ROH 978  
C3H60LY+R20H=>H2O+HCHO+R10C2H3V 3.0E+0006 2.000 -1520.0 ! ROH 979  
C3H60LY+R300H=>H2O2+HCHO+R10C2H3V 6.4E+0003 2.600 12400.0 ! ROH 980  
C3H60LY+R4CH3=>CH4+HCHO+R10C2H3V 1.0E+0011 0.000 7300.0 ! ROH 981  
C3H60LY+R8CH300=>CH300H+HCHO+R10C2H3V 1.0E+0012 0.000 14550.0 ! ROH  
982  
C3H60LY+R11C2H5=>C2H6+HCHO+R10C2H3V 1.5E+0000 3.500 4140.0 ! ROH  
983  
C4H80LY+R1H=>H2+HCHO+RC3H5Y 5.4E+0004 2.500 -1900.0 ! ROH 984  
C4H80LY+R20H=>H2O+HCHO+RC3H5Y 3.0E+0006 2.000 -1520.0 ! ROH 985  
C4H80LY+R300H=>H2O2+HCHO+RC3H5Y 6.4E+0003 2.600 12400.0 ! ROH 986  
C4H80LY+R4CH3=>CH4+HCHO+RC3H5Y 1.0E+0011 0.000 7300.0 ! ROH 987  
C4H80LY+R8CH300=>CH300H+HCHO+RC3H5Y 1.0E+0012 0.000 14550.0 ! ROH  
988  
C4H80LY+R11C2H5=>C2H6+HCHO+RC3H5Y 1.5E+0000 3.500 4140.0 ! ROH 989  
C5H100LY+R1H=>H2+HCHO+RC4H7Y 5.4E+0004 2.500 -1900.0 ! ROH 990  
C5H100LY+R20H=>H2O+HCHO+RC4H7Y 3.0E+0006 2.000 -1520.0 ! ROH 991  
C5H100LY+R300H=>H2O2+HCHO+RC4H7Y 6.4E+0003 2.600 12400.0 ! ROH 992  
C5H100LY+R4CH3=>CH4+HCHO+RC4H7Y 1.0E+0011 0.000 7300.0 ! ROH 993  
C5H100LY+R8CH300=>CH300H+HCHO+RC4H7Y 1.0E+0012 0.000 14550.0 ! ROH  
994  
C5H100LY+R11C2H5=>C2H6+HCHO+RC4H7Y 1.5E+0000 3.500 4140.0 ! ROH 995  
C7H140LY+R1H=>H2+HCHO+RC6H11Y 5.4E+0004 2.500 -1900.0 ! ROH 996  
C7H140LY+R20H=>H2O+HCHO+RC6H11Y 3.0E+0006 2.000 -1520.0 ! ROH 997  
C7H140LY+R300H=>H2O2+HCHO+RC6H11Y 6.4E+0003 2.600 12400.0 ! ROH 998  
C7H140LY+R4CH3=>CH4+HCHO+RC6H11Y 1.0E+0011 0.000 7300.0 ! ROH 999  
C7H140LY+R8CH300=>CH300H+HCHO+RC6H11Y 1.0E+0012 0.000 14550.0 ! ROH  
1000  
C7H140LY+R11C2H5=>C2H6+HCHO+RC6H11Y 1.5E+0000 3.500 4140.0 ! ROH  
1001  
C8H160LY+R1H=>H2+HCHO+RC7H13Y 5.4E+0004 2.500 -1900.0 ! ROH 1002  
C8H160LY+R20H=>H2O+HCHO+RC7H13Y 3.0E+0006 2.000 -1520.0 ! ROH 1003  
C8H160LY+R300H=>H2O2+HCHO+RC7H13Y 6.4E+0003 2.600 12400.0 ! ROH  
1004  
C8H160LY+R4CH3=>CH4+HCHO+RC7H13Y 1.0E+0011 0.000 7300.0 ! ROH 1005  
C8H160LY+R8CH300=>CH300H+HCHO+RC7H13Y 1.0E+0012 0.000 14550.0 ! ROH  
1006  
C8H160LY+R11C2H5=>C2H6+HCHO+RC7H13Y 1.5E+0000 3.500 4140.0 ! ROH  
1007  
! C9H180LY+R1H=>H2+HCHO+RC8H15Y 5.4E+0004 2.500 -1900.0 ! ROH 1008  
! C9H180LY+R20H=>H2O+HCHO+RC8H15Y 3.0E+0006 2.000 -1520.0 ! ROH 1009  
! C9H180LY+R300H=>H2O2+HCHO+RC8H15Y 6.4E+0003 2.600 12400.0 ! ROH  
1010  
! C9H180LY+R4CH3=>CH4+HCHO+RC8H15Y 1.0E+0011 0.000 7300.0 ! ROH 1011

!C9H180LY+R8CH300=>CH300H+HCHO+RC8H15Y 1.0E+0012 0.000 14550.0 !  
 ROH 1012  
 !C9H180LY+R11C2H5=>C2H6+HCHO+RC8H15Y 1.5E+0000 3.500 4140.0 ! ROH  
 1013  
 C6H120LY+R1H=>H2+HCHO+RC5H9Y 5.4E+0004 2.500 -1900.0 ! ROH 1014  
 C6H120LY+R20H=>H2O+HCHO+RC5H9Y 3.0E+0006 2.000 -1520.0 ! ROH 1015  
 C6H120LY+R300H=>H2O2+HCHO+RC5H9Y 6.4E+0003 2.600 12400.0 ! ROH 1016  
 C6H120LY+R4CH3=>CH4+HCHO+RC5H9Y 1.0E+0011 0.000 7300.0 ! ROH 1017  
 C6H120LY+R8CH300=>CH300H+HCHO+RC5H9Y 1.0E+0012 0.000 14550.0 ! ROH  
 1018  
 C6H120LY+R11C2H5=>C2H6+HCHO+RC5H9Y 1.5E+0000 3.500 4140.0 ! ROH  
 1019

! Additions on dienes

C4H6Z2+R20H=>RC3H5Y+HCHO 1.4E+0012 0.000 -1040.0 ! AD 1020!!!!!!!ds  
 мйса toлуине

!

!C4H6Z2+R20H=>RC3H5Y+HCHO 3.0E+0012 0.000 -1040.0 !

!

C6H10Y2+R1H=>H2+C4H6Z2+R10C2H3V 1.0E+0005 2.500 -1900.0 ! AD 1021  
 C6H10Y2+R20H=>H2O+C4H6Z2+R10C2H3V 6.0E+0006 2.000 -1520.0 ! AD 1022  
 C6H10Y2+R300H=>H2O2+C4H6Z2+R10C2H3V 1.2E+0004 2.600 12400.0 ! AD  
 1023  
 C6H10Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD 1024  
 C6H10Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V 2.0E+0011 0.000 7300.0 ! AD  
 1025  
 C6H10Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V 3.0E+0000 3.500 4140.0 ! AD  
 1026  
 C7H12Y2+R1H=>H2+C4H6Z2+RC3H5Y 1.0E+0005 2.500 -1900.0 ! AD 1027  
 C7H12Y2+R20H=>H2O+C4H6Z2+RC3H5Y 6.0E+0006 2.000 -1520.0 ! AD 1028  
 C7H12Y2+R300H=>H2O2+C4H6Z2+RC3H5Y 1.2E+0004 2.600 12400.0 ! AD 1029  
 C7H12Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD 1030  
 C7H12Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y 2.0E+0011 0.000 7300.0 ! AD  
 1031  
 C7H12Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y 3.0E+0000 3.500 4140.0 ! AD  
 1032  
 !C10H18Y2+R1H=>H2+C4H6Z2+R10C2H3V+2C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1033  
 !C10H18Y2+R20H=>H2O+C4H6Z2+R10C2H3V+2C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1034  
 !C10H18Y2+R300H=>H2O2+C4H6Z2+R10C2H3V+2C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1035  
 !C10H18Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1036  
 !C10H18Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1037  
 !C10H18Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+2C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1038  
 !C11H20Y2+R1H=>H2+C4H6Z2+RC3H5Y+2C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1039  
 !C11H20Y2+R20H=>H2O+C4H6Z2+RC3H5Y+2C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1040  
 !C11H20Y2+R300H=>H2O2+C4H6Z2+RC3H5Y+2C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1041

!C11H20Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+2C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1042  
 !C11H20Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+2C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1043  
 !C11H20Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+2C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1044  
 !C8H14Y2+R1H=>H2+C4H6Z2+R10C2H3V+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1045  
 !C8H14Y2+R20H=>H20+C4H6Z2+R10C2H3V+C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1046  
 !C8H14Y2+R300H=>H202+C4H6Z2+R10C2H3V+C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1047  
 !C8H14Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1048  
 !C8H14Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1049  
 !C8H14Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1050  
 !C12H22Y2+R1H=>H2+C4H6Z2+R10C2H3V+3C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1051  
 !C12H22Y2+R20H=>H20+C4H6Z2+R10C2H3V+3C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1052  
 !C12H22Y2+R300H=>H202+C4H6Z2+R10C2H3V+3C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1053  
 !C12H22Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1054  
 !C12H22Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1055  
 !C12H22Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+3C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1056  
 !C9H16Y2+R1H=>H2+C4H6Z2+RC3H5Y+C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1057  
 !C9H16Y2+R20H=>H20+C4H6Z2+RC3H5Y+C2H4Z 6.0E+0006 2.000 -1520.0 ! AD  
 1058  
 !C9H16Y2+R300H=>H202+C4H6Z2+RC3H5Y+C2H4Z 1.2E+0004 2.600 12400.0 !  
 AD 1059  
 !C9H16Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0 ! AD  
 1060  
 !C9H16Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+C2H4Z 2.0E+0011 0.000 7300.0  
 ! AD 1061  
 !C9H16Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+C2H4Z 3.0E+0000 3.500 4140.0 !  
 AD 1062  
 !C14H26Y2+R1H=>H2+C4H6Z2+R10C2H3V+4C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1063  
 !C14H26Y2+R20H=>H20+C4H6Z2+R10C2H3V+4C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1064  
 !C14H26Y2+R300H=>H202+C4H6Z2+R10C2H3V+4C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1065  
 !C14H26Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+4C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1066  
 !C14H26Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+4C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1067  
 !C14H26Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+4C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1068



!C15H28Y2+R1H=>H2+C4H6Z2+RC3H5Y+4C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1069  
 !C15H28Y2+R20H=>H20+C4H6Z2+RC3H5Y+4C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1070  
 !C15H28Y2+R300H=>H202+C4H6Z2+RC3H5Y+4C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1071  
 !C15H28Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+4C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1072  
 !C15H28Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+4C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1073  
 !C15H28Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+4C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1074  
 !C16H30Y2+R1H=>H2+C4H6Z2+R10C2H3V+5C2H4Z 1.0E+0005 2.500 -1900.0 !  
 AD 1075  
 !C16H30Y2+R20H=>H20+C4H6Z2+R10C2H3V+5C2H4Z 6.0E+0006 2.000  
 -1520.0 ! AD 1076  
 !C16H30Y2+R300H=>H202+C4H6Z2+R10C2H3V+5C2H4Z 1.2E+0004 2.600 12400.0  
 ! AD 1077  
 !C16H30Y2+R4CH3=>CH4+C4H6Z2+R10C2H3V+5C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1078  
 !C16H30Y2+R8CH300=>CH300H+C4H6Z2+R10C2H3V+5C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1079  
 !C16H30Y2+R11C2H5=>C2H6+C4H6Z2+R10C2H3V+5C2H4Z 3.0E+0000 3.500  
 4140.0 ! AD 1080  
 !C13H24Y2+R1H=>H2+C4H6Z2+RC3H5Y+3C2H4Z 1.0E+0005 2.500 -1900.0 ! AD  
 1081  
 !C13H24Y2+R20H=>H20+C4H6Z2+RC3H5Y+3C2H4Z 6.0E+0006 2.000 -1520.0 !  
 AD 1082  
 !C13H24Y2+R300H=>H202+C4H6Z2+RC3H5Y+3C2H4Z 1.2E+0004 2.600  
 12400.0 ! AD 1083  
 !C13H24Y2+R4CH3=>CH4+C4H6Z2+RC3H5Y+3C2H4Z 2.0E+0011 0.000 7300.0 !  
 AD 1084  
 !C13H24Y2+R8CH300=>CH300H+C4H6Z2+RC3H5Y+3C2H4Z 2.0E+0011 0.000  
 7300.0 ! AD 1085  
 !C13H24Y2+R11C2H5=>C2H6+C4H6Z2+RC3H5Y+3C2H4Z 3.0E+0000 3.500 4140.0  
 ! AD 1086

! Diels Alder

! .Y termination

RC3H5Y+R1H=>C3H6Y 1.0E+0014 0.000 0.0 ! TER  
 1087 !!!multipliй x10  
 RC3H5Y+R20H=>C3H60LY 1.0E+0013 0.000 0.0 ! TER 1088  
 RC3H5Y+R300H=>C3H602PY 5.0E+0012 0.000 0.0 ! TER 1089  
 RC3H5Y+R4CH3=>C4H8Y 1.0E+0013 0.000 0.0 ! TER 1090  
 RC3H5Y+R5CH0=>C4H60AY 1.0E+0013 0.000 0.0 ! TER 1091  
 RC3H5Y+R6CH20H=>C4H80LY 1.0E+0013 0.000 0.0 ! TER 1092  
 RC3H5Y+R8CH300=>HCH0+R7CH30+R10C2H3V 1.0E+0013 0.000 0.0 ! TER 1093  
 RC3H5Y+R11C2H5=>C5H10Y 1.0E+0013 0.000 0.0 ! TER 1094  
 RC4H7Y+R1H=>C4H8Y 1.0E+0014 0.000 0.0 ! TER  
 1095!!multipliй x10  
 RC4H7Y+R20H=>C4H80LY 1.0E+0013 0.000 0.0 ! TER 1096  
 RC4H7Y+R300H=>C4H802PY 5.0E+0012 0.000 0.0 ! TER 1097  
 RC4H7Y+R4CH3=>C5H10Y 1.0E+0013 0.000 0.0 ! TER 1098

RC4H7Y+R5CHO=>C5H80AY 1.0E+0013 0.000 0.0 ! TER 1099  
RC4H7Y+R6CH20H=>C5H100LY 1.0E+0013 0.000 0.0 ! TER 1100  
RC4H7Y+R8CH300=>HCHO+R7CH30+RC3H5Y 1.0E+0013 0.000 0.0 ! TER 1101  
RC4H7Y+R11C2H5=>C6H12Z 1.0E+0013 0.000 0.0 ! TER 1102  
RC7H13Y+R1H=>C7H14Y 1.0E+0014 0.000 0.0 ! TER  
1103!!multipliй x10  
RC7H13Y+R20H=>C7H140LY 1.0E+0013 0.000 0.0 ! TER 1104  
RC7H13Y+R300H=>C7H1402PY 5.0E+0012 0.000 0.0 ! TER 1105  
RC7H13Y+R4CH3=>C8H16Y 1.0E+0013 0.000 0.0 ! TER 1106  
RC7H13Y+R5CHO=>C8H140AY 1.0E+0013 0.000 0.0 ! TER 1107  
RC7H13Y+R6CH20H=>C8H160LY 1.0E+0013 0.000 0.0 ! TER 1108  
RC7H13Y+R8CH300=>HCHO+R7CH30+RC6H11Y 1.0E+0013 0.000 0.0 ! TER 1109  
!RC7H13Y+R11C2H5=>C9H18Z 1.0E+0013 0.000 0.0 ! TER 1110  
RC8H15Y+R1H=>C8H16Y 1.0E+0014 0.000 0.0 ! TER  
1111!!multipliй x10  
RC8H15Y+R20H=>C8H160LY 1.0E+0013 0.000 0.0 ! TER 1112  
RC8H15Y+R300H=>C8H1602PY 5.0E+0012 0.000 0.0 ! TER 1113  
!RC8H15Y+R4CH3=>C9H18Z 1.0E+0013 0.000 0.0 ! TER 1114  
!RC8H15Y+R5CHO=>C9H160AY 1.0E+0013 0.000 0.0 ! TER 1115  
!RC8H15Y+R6CH20H=>C9H180LY 1.0E+0013 0.000 0.0 ! TER 1116  
RC8H15Y+R8CH300=>HCHO+R7CH30+RC7H13Y 1.0E+0013 0.000 0.0 ! TER 1117  
!RC8H15Y+R11C2H5=>C10H20Z 1.0E+0013 0.000 0.0 ! TER 1118  
RC5H9Y+R1H=>C5H10Y 1.0E+0014 0.000 0.0 ! TER  
1119!!multipliй x10  
RC5H9Y+R20H=>C5H100LY 1.0E+0013 0.000 0.0 ! TER 1120  
RC5H9Y+R300H=>C5H1002PY 5.0E+0012 0.000 0.0 ! TER 1121  
RC5H9Y+R4CH3=>C6H12Z 1.0E+0013 0.000 0.0 ! TER 1122  
RC5H9Y+R5CHO=>C6H100AY 1.0E+0013 0.000 0.0 ! TER 1123  
RC5H9Y+R6CH20H=>C6H120LY 1.0E+0013 0.000 0.0 ! TER 1124  
RC5H9Y+R8CH300=>HCHO+R7CH30+RC4H7Y 1.0E+0013 0.000 0.0 ! TER 1125  
RC5H9Y+R11C2H5=>C7H14Y 1.0E+0013 0.000 0.0 ! TER 1126  
RC3H5Y+RC3H5Y=>C6H10Y2 1.0E+0013 0.000 0.0 ! TER 1127  
RC3H5Y+RC4H7Y=>C7H12Y2 1.0E+0013 0.000 0.0 ! TER 1128  
RC3H5Y+RC7H13Y=>C10H18Y2 1.0E+0013 0.000 0.0 ! TER 1129  
RC3H5Y+RC8H15Y=>C11H20Y2 1.0E+0013 0.000 0.0 ! TER 1130  
RC3H5Y+RC5H9Y=>C8H14Y2 1.0E+0013 0.000 0.0 ! TER 1131  
RC4H7Y+RC4H7Y=>C8H14Y2 1.0E+0013 0.000 0.0 ! TER 1132  
RC4H7Y+RC7H13Y=>C11H20Y2 1.0E+0013 0.000 0.0 ! TER 1133  
!RC4H7Y+RC8H15Y=>C12H22Y2 1.0E+0013 0.000 0.0 ! TER 1134  
RC4H7Y+RC5H9Y=>C9H16Y2 1.0E+0013 0.000 0.0 ! TER 1135  
!RC7H13Y+RC7H13Y=>C14H26Y2 1.0E+0013 0.000 0.0 ! TER 1136  
!RC7H13Y+RC8H15Y=>C15H28Y2 1.0E+0013 0.000 0.0 ! TER 1137  
!RC7H13Y+RC5H9Y=>C12H22Y2 1.0E+0013 0.000 0.0 ! TER 1138  
!RC8H15Y+RC8H15Y=>C16H30Y2 1.0E+0013 0.000 0.0 ! TER 1139  
!RC8H15Y+RC5H9Y=>C13H24Y2 1.0E+0013 0.000 0.0 ! TER 1140  
!RC8H15Y+RC6H11Y=>C14H26Y2 1.0E+0013 0.000 0.0 ! TER 1141  
RC5H9Y+RC5H9Y=>C10H18Y2 1.0E+0013 0.000 0.0 ! TER 1142  
RC5H9Y+RC6H11Y=>C11H20Y2 1.0E+0013 0.000 0.0 ! TER 1143

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!especes excitees!

R1H+B10+M=OHE+M <HALL05>!	6.0E14	0.0	6.94E3	!
B4CH+O2=B2CO+OHE <HALL05>!	4.0E13	0.0	0.0	!
OHE+AR=R20H+AR <HALL05>!	5.2E10	0.5	0.0	!
OHE+H2O=R20H+H2O <HALL05>!	8.6E12	0.5	0.0	!
OHE+H2=R20H+H2 <HALL05>!	1.5E12	0.5	0.0	!
OHE+R1H=R20H+R1H <HALL05>!	1.5E12	0.5	0.0	!
OHE+O2=R20H+O2 <HALL05>!	1.5E12	0.5	0.0	!
OHE+B10=R20H+B10 <HALL05>!	1.5E12	0.5	0.0	!
OHE+R20H=R20H+R20H <HALL05>!	1.5E12	0.5	0.0	!
OHE=>R20H <HALL05>!	1.4E6	0.0	0.0	!
OHE+CO2=R20H+CO2 <HALL05>!	2.75E12	0.5	-968.	!
OHE+B2CO=R20H+B2CO <HALL05>!	3.23E12	0.5	-787.	!
OHE+CH4=R20H+CH4 <HALL05>!	3.36E12	0.5	-635.	!
R9C2H+B10=B2CO+CHE <HALL05>!	6.2E12	0.0	0.0	!
R9C2H+O2=CO2+CHE <HALL05>!	2.17E10	0.0	0.0	!
CHE+AR=B4CH+AR <HALL05>!	4.0E10	0.5	0.0	!
CHE+O2=B4CH+O2 <HALL05>!	2.48E6	2.14	0.0	!
CHE+H2O=B4CH+H2O <HALL05>!	5.3E13	0.0	0.0	!
CHE+H2=B4CH+H2 <HALL05>!	1.47E14	0.0	1360.	!
CHE+CO2=B4CH+CO2 <HALL05>!	2.41E-1	4.3	-1694.	!
CHE+B2CO=B4CH+B2CO <HALL05>!	2.44E12	0.5	0.0	!
CHE+CH4=B4CH+CH4 <HALL05>!	1.73E13	0.0	167.	!
CHE=>B4CH <HALL05>!	1.86E6	0.0	0.0	!

!\*\*\*\*\*!  
! REACTIONS DE LA MATRICE O(θ)C(y)H(z) !  
!\*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE H2\*\*\*\*\*!

R1H+R1H+M=H2+M	1.87E18	-1.00	0.00
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02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ H2/0.0/ C2H6/3.0/  
AR/0.35/  
! N2/0.4/ HE/0.35/

!\*\*\*\*\* REACTIONS DE B4CH \*\*\*\*\*!

B4CH+R1H=B3C+H2 7.8E13 0. 0. !(2, -  
2)<PEETERS97>!

!\*\*\*\*\* REACTIONS DE B6CH2 \*\*\*\*\*!

B6CH2+M=B5CH2+M 1.51E13 0.0 0.0  
02/.4/ B2C0/.75/ C02/1.5/ H20/6.5/ CH4/.48/ C2H4Z/1.6/  
AR/.24/  
B6CH2+R1H=B4CH+H2 3.0E13 0. 0. !(4, -  
4)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE B5CH2 \*\*\*\*\*!

B5CH2+R1H=B4CH+H2 6.0E12 0. -1.8E3 !(5, -  
5)<BAULCH94>!  
B5CH2+B3C=R9C2H+R1H 5.0E13 0. 0. !(6, -  
6)<RAnZI94>!  
B5CH2+B5CH2=>C2H2+R1H+R1H 1.2E14 0. 0.8E3 !  
(7)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE R4CH3 \*\*\*\*\*!

R4CH3+M=B5CH2+R1H+M 2.91E16 0.0 90.7E3  
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
R4CH3+R1H=B6CH2+H2 6.0E13 0. 15.0E3 !  
(9, -9)<BAULCH94>!  
R4CH3+B4CH=R10C2H3V+R1H 3.0E13 0. 0. !(10, -  
10)<DAGAUT91>  
R4CH3+B6CH2=C2H4Z+R1H 1.8E13 0. 0. !(11, -  
11)<TSAnG86>!  
R4CH3+B5CH2=C2H4Z+R1H 4.2E13 0. 0. !(12, -  
12)<BAULCH94>!  
R4CH3+B3C=C2H2+R1H 5.0E13 0. 0. !(13, -  
13)<RAnZI94>!  
R4CH3+R4CH3(+M)=>C2H6(+M) 3.61E13 0. 0. !  
(14)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
LOW / 3.63E41 -7.0 2.76E3 /  
TROE / 0.62 73 1180 /  
C2H6(+M)=>R4CH3+R4CH3(+M) 1.8E21 -1.24 90.9E3 !(-  
14)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/  
LOW / 1.89E49 -8.24 93.7E3/  
TROE / 0.62 73 1180 /

R4CH3+R4CH3=R11C2H5+R1H 3.0E13 0. 13.5E3 !(15, -  
15)<BAULCH94>!  
R4CH3+R4CH3=C2H4Z+H2 2.1E14 0. 19.3E3 !(16, -  
16)<FRAnK86nIST>!

!\*\*\*\*\* REACTIONS DE CH4 \*\*\*\*\*!

R1H+R4CH3(+M)=>CH4(+M) 1.67E14 0. 0. !  
(17)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/

! N2/0.4/ HE/0.35/  
LOW / 1.408E24 -1.8 0.0 /  
TROE / 0.37 3315 61 /

CH4(+M)=>R4CH3+R1H(+M) 2.4E16 0. 105.0E3 !(-  
17)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/0.0/ C2H6/3.0/ AR/0.35/

! N2/0.4/ HE/0.35/  
LOW / 1.29E18 0.00 90.9E3 /  
TROE / 0 1350 1 7830 /

CH4(+CH4)=>R4CH3+R1H(+CH4) 2.4E16 0. 105.0E3 !(-  
17')<BAULCH94>!

LOW / 8.43E17 0.00 90.9E3 /  
TROE / 0.69 90 2210 /

CH4+R1H=R4CH3+H2 1.3E04 3. 8.0E3 !(18, -  
18)<BAULCH94>!

CH4+B4CH=C2H4Z+R1H 3.0E13 0. -0.4E3 !(19, -  
19)<DAGAUT91BAULCH94>!

CH4+B6CH2=R4CH3+R4CH3 4.2E13 0. 0. !(20, -  
20)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE R9C2H \*\*\*\*\*!

R9C2H+B6CH2=C2H2+B4CH 1.8E13 0. 0. !(21, -  
21)<TSAnG86>!

R9C2H+B5CH2=C2H2+B4CH 1.8E13 0. 0. !(22, -  
22)<TSAnG86>!

R9C2H+CH4=C2H2+R4CH3 1.2E12 0. 0. !(23, -  
23)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE C2H2 \*\*\*\*\*!

C2H2+M=R9C2H+R1H+M 1.14E17 0. 107.0E3 !(24, -  
24)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/

! N2/0.4/ HE/0.35/  
C2H2+R1H=R9C2H+H2 6.6E13 0. 27.7E3 !(25, -  
25)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE R10C2H3V \*\*\*\*\*!

R10C2H3V(+M)=C2H2+R1H(+M) 2.0E14 0. 39.8E3 !(26, -  
26)<BAULCH94>!

02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ AR/0.35/

! N2/0.4/ HE/0.35/  
LOW / 1.19E42 -7.50 45.55E3 /  
TROE / 0.35 1.0 1.E8/

R10C2H3V+R1H=C2H2+H2 1.2E13 0. 0. !(27, -  
27)<BAULCH94>!

R10C2H3V+B6CH2=C2H2+R4CH3 1.8E13 0. 0. !(28, -  
28)<TSAnG86>!

R10C2H3V+B5CH2=C2H2+R4CH3 1.8E13 0. 0. !(29, -  
29)<TSAnG86>!

R10C2H3V+R4CH3=CH4+C2H2 3.9E11 0. 0. !(30, -  
 30)<TSAnG86>!  
 R10C2H3V+R9C2H=2C2H2 9.6E11 0. 0. !(31, -  
 31)<TSAnG86>!  
 R10C2H3V+R10C2H3V=C2H4Z+C2H2 9.6E11 0. 0. !(32, -  
 32)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE C2H4Z \*\*\*\*\*!

C2H4Z+M=C2H2+H2+M 9.97E16 0. 71.6E3 !(33, -  
 33)<BAULCH94>!  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 C2H4Z+M=R10C2H3V+R1H+M 7.40E17 0. 96.7E3 !(34, -  
 34)<BAULCH94>!  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 !C2H4Z+R1H=R10C2H3V+H2 5.4E14 0. 14.8E3 !(35, -  
 35)<BAULCH94>!  
 C2H4Z+R1H=R10C2H3V+H2 5.0E7 1.93 13.0E3 !(35, -  
 35)SLAGLE96!  
 !C2H4Z+R4CH3=CH4+R10C2H3V 4.1E12 0. 11.1E3 !(36, -  
 36)<BAULCH94>!  
 C2H4Z+R4CH3=CH4+R10C2H3V 6.3E11 0. 16.0E3 !(36, -  
 36)BACK89!

!\*\*\*\*\* REACTIONS DE R11C2H5 \*\*\*\*\*!

!C2H4Z+R1H(+M)=>R11C2H5(+M) 3.97E09 1.28 1.3E3  
 ! 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 ! LOW / 1.35E19 0.00 0.76E3 /  
 ! TROE / 0.76 40 1025/  
 R11C2H5(+M)=C2H4Z+R1H(+M) 8.2E13 0. 40.0E3  
 02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 ! N2/0.4/ HE/0.35/  
 ! LOW / 3.40E17 0.00 33.4E3 /  
 ! TROE / 0.75 97 1379/  
 R11C2H5+R1H=C2H4Z+H2 1.8E12 0. 0. !(38, -  
 38)<TSAnG86>!  
 R11C2H5+R1H=C2H6 3.6E13 0. 0. !(39, -  
 39)<TSAnG86>!  
 R11C2H5+B6CH2=C2H4Z+R4CH3 9.0E12 0. 0. !(40, -  
 40)<TSAnG86>!  
 R11C2H5+B5CH2=C2H4Z+R4CH3 1.8E13 0. 0. !(41, -  
 41)<TSAnG86>!  
 R11C2H5+R4CH3=C2H4Z+CH4 1.1E12 0. 0. !(42, -  
 42)<BAULCH94>!  
 R11C2H5+R9C2H=C2H2+C2H4Z 1.8E12 0. 0. !(43, -  
 43)<TSAnG86>!  
 R11C2H5+R10C2H3V=2C2H4Z 4.8E11 0. 0. !(44, -  
 44)<TSAnG86>!  
 R11C2H5+R10C2H3V=C2H2+C2H6 4.8E11 0. 0. !(45, -  
 45)<TSAnG86>!  
 R11C2H5+R11C2H5=C2H4Z+C2H6 1.4E12 0. 0. !(46, -  
 46)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE C2H6 \*\*\*\*\*!

C2H6+M=C2H4Z+H2+M 47)<SCHULTZ85nIST>!	2.3E17	0.	67.4E3	!(47, -
C2H6+R1H=R11C2H5+H2 48)<BAULCH94>!	1.4E9	1.5	7.4E3	!(48, -
C2H6+B6CH2=R4CH3+R11C2H5 49)<TSAnG86>!	1.1E14	0.	0.	!(49, -
C2H6+R4CH3=R11C2H5+CH4 50)<BAULCH94>!	1.5E-7	6.0	5.8E3	!(50, -
C2H6+R9C2H=C2H2+R11C2H5 51)<TSAnG86>!	3.6E12	0.	0.	!(51, -
C2H6+R10C2H3V=R11C2H5+C2H4Z 52)<TSAnG86>!	6.0E2	3.3	10.5E3	!(52, -

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!\*\*\*\*\* REACTIONS DE LA MATRICE O(x)C(y)H(z) x>0 !

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!\*\*\*\*\* REACTIONS DE B10 \*\*\*\*\*!

B10+H2=R20H+R1H 53)<BAULCH94>!	5.1E4	2.67	6.2E3	!(53, -
B10+B4CH=B2C0+R1H 54)<BAULCH94>!	3.9E13	0.	0.	!(54, -
B10+B4CH=B3C+R20H 55)<MUR86nIS>!	1.5E13	0.	4.7E3	!(55, -
B10+B6CH2=>B2C0+2R1H <TSAnG86>!	1.5E13	0.	0.	!(56)
B10+B6CH2=B2C0+H2 <TSAnG86>!	1.5E13	0.	0.	!(57, -57)
B10+B5CH2=>B2C0+2R1H <BAULCH94>!	7.2E13	0.	0.	!(58)
B10+B5CH2=B2C0+H2 59)<BAULCH94>!	4.8E13	0.	0.	!(59, -
B10+R4CH3=HCHO+R1H 60)<BAULCH94>!	8.4E13	0.	0.	!(60, -
B10+R4CH3=R7CH30 61)<DEAn87nIS>!	8.0E15	-2.12	0.6E3	!(61, -
B10+CH4=R4CH3+R20H 62)<BAULCH94>!	7.2E8	1.56	8.4E3	!(62, -
B10+R9C2H=B4CH+B2C0 63)<DAGAUT91>!	1.0E13	0.	0.	!(63, -
B10+C2H2=B5CH2+B2C0 64)<BAULCH LEEDS>!	2.17E06	2.1	1.6E3	!(64, -

B10+C2H2=R12CHCOZ+R1H 65)<BAULCH LEEDS>!	5.06E06	2.1	1.6E3	!(65, -
R20H+R9C2H=C2H2+B10 89)<TSANG86>! modif MF	1.8E13	0.	0.	!(89, -
B10+R10C2H3V=R4CH3+B2CO 66)<DAGAUT91>!	3.0E13	0.	0.	!(66, -
B10+R10C2H3V=CH2COZ+R1H 67)<TSAnG86>!	9.6E13	0.	0.	!(67, -
B10+C2H4Z=R4CH3+R5CHO 68)<BAULCH94>!	8.1E6	1.88	0.2E3	!(68, -
B10+C2H4Z=HCHO+B5CH2 69)<BAULCH94>!	4.00E5	1.88	0.2E3	!(69, -
B10+C2H4Z=CH2COZ+H2 70)<BAULCH94>!	6.6E5	1.88	0.2E3	!(70, -
B10+C2H4Z=R13CH2CHO+R1H 71)<BAULCH94>!	4.7E6	1.88	0.2E3	!(71, -
B10+C2H4Z=R20H+R10C2H3V 72)<MAHMUD87nIST>!	1.5E7	1.91	3.7E3	!(72, -
B10+R11C2H5=HCHO+R4CH3 73)<BAULCH94>!	1.1E13	0.	0.	!(73, -
B10+R11C2H5=CH3CHO+R1H 74)<BAULCH94>!	5.5e13	0.	0.	!(74, -
B10+R11C2H5=C2H4Z+R20H 75)<DAGAUT91>!	3.0E13	0.	0.	!(75, -
B10+C2H6=R11C2H5+R20H 76)<BAULCH94>!	1.0E9	1.5	5.8E3	!(76, -

!\*\*\*\*\* REACTIONS DE R20H \*\*\*\*\*!

R1H+B10+M=R20H+M	1.18E19	-1.0	0.0	
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
R1H+R20H+M=H2O+M	5.53E+22	-2.0	0.0	
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/2.55/ CH4/3.0/ C2H6/3.0/ AR/0.15/				
! N2/0.4/ HE/0.35/				
R20H+H2=R1H+H2O 79)<BAULCH94>!	1.0E8	1.6	3.3E3	!(79, -
R20H+B3C=B2CO+R1H 80)<RAnZI94>!	5.0E13	0.	0.	!(80, -
R20H+B4CH=R5CHO+R1H 81)<DAGAUT91>!	3.0E13	0.	0.	!(81, -
R20H+B6CH2=HCHO+R1H 82)<TSAnG86>!	3.0E13	0.	0.	!(82, -
R20H+B5CH2=HCHO+R1H 83)<TSAnG86>!	1.8E13	0.	0.	!(83, -
R20H+R4CH3=B6CH2+H2O 84)<BAULCH94>!	7.2E13	0.	2.7E3	!(84, -
R20H+R4CH3(+M)=CH3OH(+M) 85)<BAULCH94>!	6.0E13	0.	0.	!(85, -
LOW /1.4E44	-8.2	0./		
TROE /0.82	200.	1438./		
R20H+R4CH3=HCHO+H2 86)<DAGAUT91>!	3.2E12	-0.53	10.8E3	!(86, -
R20H+R4CH3=R7CH30+R1H 87)<DAGAUT91>!	5.7E12	-0.23	13.9E3	!(87, -



R20H+CH4=R4CH3+H2O 88)<BAULCH94>!	1.6E7	1.83	2.7E3	!(88, -
!R20H+R9C2H=C2H2+B10 89)<TSAnG86>!	1.8E13	0.	0.	!(89, -
R20H+R9C2H=B5CH2+B2C0 90)<TSAnG86>!	1.8E13	0.	0.	!(90, -
R20H+R9C2H=R12CHCOZ+R1H 91)<DAGAUT91>!	2.0E13	0.	0.	!(91, -
R20H+C2H2=R9C2H+H2O 92)<KONNOV00>!	3.385E+07	2.0	14000.0	!(92, -
R20H+C2H2=CH2COZ+R1H 93)<KONNOV00>!	1.100E+13	0.0	7170.0	!(93, -
R20H+C2H2=R4CH3+B2C0 94)<DAGAUT91>!	4.8E-4	4.	-2.0E3	!(94, -
R20H+R10C2H3V=C2H2+H2O 95)<TSAnG86>!	3.0E13	0.	0.	!(95, -
R20H+R10C2H3V=CH3CHO 96)<TSAnG86>!	3.0E13	0.	0.	!(96, -
R20H+C2H4Z=R10C2H3V+H2O 97)<BAULCH94>!	2.0E13	0.	5.9E3	!(97, -
R20H+C2H4Z=R4CH3+HCHO 98)<GLARBORG86>!	2.0E12	0.	0.9E3	!(98, -
R20H+R11C2H5=C2H4Z+H2O 99)<TSAnG86>!	2.4E13	0.	0.	!(99, -
R20H+R11C2H5=>R4CH3+R1H+HCHO <TSAnG86>!	2.4E13	0.	0.	!(100)
R20H+C2H6=R11C2H5+H2O 101)<BAULCH94>!	7.2E6	2.	0.9E3	!(101, -
R20H+R20H=H2O+B10 102)<BAULCH94>!	1.5E9	1.14	0.1E3	!(102, -
!***** REACTIONS DE H2O *****!				
H2O+B4CH=R6CH2OH 103)<BAULCH94>!	5.7E12	0.	-0.8E3	!(103, -
H2O+B6CH2=CH3OH 104)<TSAnG86>!	1.8E13	0.	0.	!(104, -
!REACTIOnS DE B2C0!				
B2C0+R4CH3(+M)=R14CH3C0(+M) 105)<BAULCH94>!	5.0E11	0.	6.9E3	!(105, -
LOW /1.1E14	0.	3.8E3/		
TR0E /0.5	1.0	1.0E8/		
B2C0+B10+M=C02+M 106)<TSAnG86>!	1.54E15	0.0	3.0E3	!(106, -
02/0.4/ B2C0/0.75/ C02/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
B2C0+R20H=C02+R1H 107)<BAULCH94>!	6.3E6	1.5	-0.5E3	!(107, -
!REACTIOnS DE R5CHO!				
R5CHO+M=R1H+B2C0+M 108)<WAnG97>!	1.9E17	-1.	17.0E3	!(108, -
H2/2.0/ B2C0/1.5/ C02/2.0/ H2O/6.0/				

R5CHO+R1H=H2+B2CO 109)<BAULCH94>!	9.0E13	0.	0.	!(109, -
R5CHO+R1H=B10+B5CH2 110)<TSUB0I81nIST>!	4.0E13	0.	102.5E3	!(110, -
R5CHO+B6CH2=R4CH3+B2CO 111)<TSAnG86>!	1.8E13	0.	0.	!(111, -
R5CHO+B5CH2=R4CH3+B2CO 112)<TSAnG86>!	1.8E13	0.	0.	!(112, -
R5CHO+R4CH3=CH4+B2CO 113)<TSAnG86>!	1.2E14	0.	0.	!(113, -
R5CHO+R4CH3=CH3CHO 114)<TSAnG86>!	1.8E13	0.	0.	!(114, -
R4CH3+HCHO=R5CHO+CH4 115)<BAULCH94>!	7.7E-8	6.1	1.97E3	!(115, -
R5CHO+R9C2H=C2H2+B2CO 116)<TSAnG86>!	6.0E13	0.	0.	!(116, -
R5CHO+R10C2H3V=C2H4Z+B2CO 117)<TSAnG86>!	9.0E13	0.	0.	!(117, -
R10C2H3V+HCHO=R5CHO+C2H4Z 118)<TSAnG86>!	5.4E3	2.81	5.9E3	!(118, -
R5CHO+R11C2H5=C2H6+B2CO 119)<TSAnG86>!	1.2E14	0.	0.	!(119, -
R11C2H5+HCHO=R5CHO+C2H6 120)<TSAnG86>!	5.57E3	2.81	5.86E3	!(120, -
R5CHO+B10=R1H+C02 121)<BAULCH94>!	3.0E13	0.	0.	!(121, -
R5CHO+B10=R20H+B2CO 122)<BAULCH94>!	3.0E13	0.	0.	!(122, -
R5CHO+R20H=H20+B2CO 123)<BAULCH94>!	1.1E14	0.	0.	!(123, -
R5CHO+R5CHO=HCHO+B2CO 124)<BAULCH94>!	3.0E13	0.	0.	!(124, -

!\*\*\*\*\* REACTIONS DE HCHO \*\*\*\*\*!

HCHO+M=R5CHO+R1H+M 125)<BAULCH94>!	1.40E36	-5.54	96.8E3	!(125, -
02/0.4/ B2CO/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
HCHO+M=H2+B2CO+M 126)<BAULCH94>!	3.26E36	-5.54	96.8E3	!(126, -
02/0.4/ B2CO/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
HCHO+R1H=R5CHO+H2 127)<BAULCH94>!	1.3E8	1.62	2.1E3	!(127, -
HCHO+B4CH=R13CH2CHO 128)<BAULCH94average>!	9.6E13	0.	-0.5E3	!(128, -
HCHO+B6CH2=R4CH3+R5CHO 129)<TSAnG86>!	1.2E12	0.	0.	!(129, -
HCHO+B10=R5CHO+R20H 130)<BAULCH94>!	4.1E11	0.57	2.7E3	!(130, -
HCHO+R20H=R5CHO+H20	7.82E07	1.63	-1.06E3	!MF

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!\*\*\*\*\* REACTIONS DE R7CH3O \*\*\*\*\*!

R7CH30+M=HCHO+R1H+M	1.55E14	0.00	13.5E3	
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
R7CH30+R1H=HCHO+H2	1.8E13	0.	0.	!(133, -
133)<BAULCH94>!				
R7CH30+B6CH2=R4CH3+HCHO	1.8E13	0.	0.	!(134, -
134)<TSAng86>!				
R7CH30+B5CH2=R4CH3+HCHO	1.8E13	0.	0.	!(135, -
135)<TSAng86>!				
R7CH30+R4CH3=HCHO+CH4	2.4E13	0.	0.	!(136, -
136)<TSAng86>!				
R7CH30+CH4=R4CH3+CH30H	1.6E11	0.	8.8E3	!(137, -
137)<TSAng86>!				
R7CH30+R9C2H=HCHO+C2H2	2.4E13	0.	0.	!(138, -
138)<TSAng86>!				
R7CH30+R10C2H3V=HCHO+C2H4Z	2.4E13	0.	0.	!(139, -
139)<TSAng86>!				
R7CH30+C2H4Z=HCHO+R11C2H5	1.2E11	0.	6.7E3	!(140, -
140)<TSAng86>!				
R7CH30+R11C2H5=HCHO+C2H6	2.4E13	0.	0.	!(141, -
141)<TSAng86>!				
R7CH30+C2H6=R11C2H5+CH30H	2.4E11	0.	7.0E3	!(142, -
142)<TSAng86>!				
R7CH30+B10=HCHO+R20H	1.8E12	0.	0.	!(143, -
143)<BAULCH94>!				
R7CH30+R20H=HCHO+H20	1.8E13	0.	0.	!(144, -
144)<TSAng86>!				
R7CH30+B2C0=R4CH3+C02	1.6E13	0.	11.7E3	!(145, -
145)<TSAng86>!				
R7CH30+R5CHO=CH30H+B2C0	9.1E13	0.	0.	!(146, -
146)<TSAng86>!				
R7CH30+HCHO=CH30H+R5CHO	1.0E11	0.	3.0E3	!(147, -
147)<TSAng86>!				
R7CH30+R7CH30=CH30H+HCHO	6.0E13	0.	0.	!(148, -
148)<TSAng86>!				

!\*\*\*\*\* REACTIONS DE R6CH20H \*\*\*\*\*!

R6CH20H+M=HCHO+R1H+M	1.26E16	0.00	30.0E3	!(149, -
149)<BAULCHLEEDS>!				
02/0.4/ B2C0/0.75/ C02/1.5/ H20/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
R6CH20H+R1H=R4CH3+R20H	9.6E13	0.	0.	!(150, -
150)<TSAng87>!				
R6CH20H+R1H=HCHO+H2	6.0E12	0.	0.	!(151, -
151)<TSAng87>!				
R6CH20H+H2=CH30H+R1H	6.7E5	2.	13.4E3	!(152, -
152)<TSAng87>!				
R6CH20H+B6CH2=CH3CHO+R1H	1.8E13	0.	0.	!(153, -
153)<TSAng87>!				
R6CH20H+B5CH2=C2H4Z+R20H	2.4E13	0.	0.	!(154, -
154)<TSAng87>!				
R6CH20H+B5CH2=R4CH3+HCHO	1.2E12	0.	0.	!(155, -
155)<TSAng87>!				

R6CH2OH+R4CH3=C2H5OH 156)<TSAnG87>!	1.2E13	0.	0.	!(156, -
R6CH2OH+R4CH3=CH4+HCHO 157)<TSAnG87>!	2.4E12	0.	0.	!(157, -
R6CH2OH+CH4=CH3OH+R4CH3 158)<TSAnG87>!	21.7	3.1	16.2E3	!(158, -
R6CH2OH+R9C2H=C2H2+HCHO 159)<TSAnG87>!	4.8E13	0.	0.	!(159, -
!la constante de vitesse du processus 159 est globalisee!				
!R6CH2OH+R9C2H=C3H3+R2OH 159a)<TSAnG87>!	1.2E13	0.	0.	!(159a, -
!R6CH2OH+R9C2H=C2H2+HCHO 159b)<TSAnG87>!	3.6E13	0.	0.	!(159b, -
R6CH2OH+C2H2=R10C2H3V+HCHO 160)<TSAnG87>!	7.2E11	0.	9.0E3	!(160, -
R6CH2OH+R10C2H3V=C2H4Z+HCHO 161)<TSAnG87>!	4.2E13	0.	0.	!(161, -
!La constante de vitesse du processus 161 est globalisee!				
R6CH2OH+R11C2H5=C2H4Z+CH3OH 162)<TSAnG87>!	2.4E12	0.	0.	!(162, -
R6CH2OH+R11C2H5=C2H6+HCHO 163)<TSAnG87>!	2.4E12	0.	0.	!(163, -
R6CH2OH+C2H6=CH3OH+R11C2H5 164)<TSAnG87>!	199.	3.	14.0E3	!(164, -
R6CH2OH+B10=HCHO+R2OH 165)<TSAnG87>!	4.2E13	0.	0.	!(165, -
R6CH2OH+R2OH=H2O+HCHO 166)<TSAnG87>!	2.4E13	0.	0.	!(166, -
!attention (167) metatheses dans les reactions de CH3OH!				
!R6CH2OH+H2O=CH3OH+R2OH 167)<TSUB0I81nIST>!	1.6E14	0.	26.3E3	!(167, -
R6CH2OH+R5CHO=CH3OH+B2CO 168)<TSAnG87>!	1.2E14	0.	0.	!(168, -
R6CH2OH+R5CHO=HCHO+HCHO 169)<TSAnG87>!	1.8E14	0.	0.	!(169, -
R6CH2OH+HCHO=CH3OH+R5CHO 170)<TSAnG87>!	5.5E3	2.8	5.9E3	!(170, -
R6CH2OH+R7CH30=CH3OH+HCHO 171)<TSAnG87>!	2.4E13	0.	0.	!(171, -
R6CH2OH+R6CH2OH=CH3OH+HCHO 172)<TSAnG87>!	1.4E13	0.	0.	!(172, -
!la constante de vitesse du processus 172 est globalisee!				
!R6CH2OH+R6CH2OH=CH3OH+HCHO 172a)<TSAnG87>!	4.8E12	0.	0.	!(172a, -
!R6CH2OH+R6CH2OH=HOCH2CH2OH 172b)<TSAnG87>!	9.6E12	0.	0.	!(172b, -
!***** REACTIONS DE CH3OH *****!				
CH3OH+R1H=R4CH3+H2O 173)<HIDAKA89nIST>!	2.0E14	0.	5.3E3	!(173, -
CH3OH+R1H=R7CH30+H2 174)<TSAnG87>!	4.2E6	2.1	4.9E3	!(174, -
CH3OH+B6CH2=R6CH2OH+R4CH3 175)<TSAnG87>!	1.5E12	0.	0.	!(175, -

CH3OH+B5CH2=R4CH3+R6CH2OH 176)<TSAnG87>!	31.9	3.2	7.2E3	!(176, -
CH3OH+B5CH2=R4CH3+R7CH30 177)<TSAnG87>!	14.4	3.1	6.9E3	!(177, -
CH3OH+R9C2H=C2H2+R6CH2OH 178)<TSAnG87>!	6.0E12	0.	0.	!(178, -
CH3OH+R9C2H=C2H2+R7CH30 179)<TSAnG87>!	1.2E12	0.	0.	!(179, -
CH3OH+R10C2H3V=C2H4Z+R6CH2OH 180)<TSAnG87>!	31.9	3.2	7.2E3	!(180, -
CH3OH+R10C2H3V=C2H4Z+R7CH30 181)<TSAnG87>!	14.4	3.1	6.9E3	!(181, -
CH3OH+B10=R6CH2OH+R20H 182)<GROTHEER81nIST>!	3.4E13	0.	5.5E3	!(182, -
CH3OH+B10=R7CH30+R20H 183)<WARnATZ84>!	1.0E13	0.	4.7E3	!(183, -
!modification des metatheses avec OH!				
!CH3OH+R20H=R7CH30+H2O 184)<WARnATZ84>!	1.0E13	0.	1.7E3	!(184, -
CH3OH+R20H=R6CH2OH+H2O 184a)<Atkinson86>85%!	3.1E06	2.	-3.4E2	!(184a, -
CH3OH+R20H=R7CH30+H2O 184b)<Atkinson86>15%!	5.4E05	2.	-3.4E2	!(184b, -
CH3OH+R7CH30=CH3OH+R6CH2OH 185)<TSAnG87>!	3.0E11	0.	4.1E3	!(185, -
!***** REACTIONS DE R12CHCOD *****!				
R12CHCOZ+M=B4CH+B2CO+M 186)<DAGAUT91>!	6.0E15	0.	58.8E3	!(186, -
R12CHCOZ+R1H=B5CH2+B2CO 187a)<BAULCH94>!	1.5E14	0.	0.	!(187a, -
R12CHCOZ+R1H=B6CH2+B2CO 187b)<PEETERS97>!	1.3E14	0.	0.	!(187b, -
R12CHCOZ+B5CH2=R9C2H+HCHO 188)<DAGAUT91>!	1.0E13	0.	2.0E3	!(188, -
R12CHCOZ+B5CH2=R10C2H3V+B2CO 189)<DAGAUT91>!	3.0E13	0.	0.	!(189, -
R12CHCOZ+B10=>B2CO+B2CO+R1H (190)<BAULCH94>!	9.6E13	0.	0.	!
R12CHCOZ+R20H=>R5CHO+B2CO+R1H (191)<DAGAUT91>!	1.0E13	0.	0.	!
!***** REACTIONS DE CH2COD *****!				
CH2COZ+M=B6CH2+B2CO+M 192)<FRAnK86nIST>!	6.57E15	0.0	57.6E3	!(192, -
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
CH2COZ+M=R12CHCOZ+R1H+M 193)<FRAnK86nIST>!	2.7E17	0.	87.0E3	!(193, -
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/				
! N2/0.4/ HE/0.35/				
CH2COZ+R1H=R4CH3+B2CO 194)<BAULCH94>!	1.8E13	0.	3.4E3	!(194, -

CH2COZ+R1H=R12CHCOZ+H2 195)<DAGAUT91>!	5.0E13	0.	8.0E3	!(195, -
CH2COZ+B5CH2=C2H4Z+B2CO 196)<CAnOSA-MAS84nIST>!	1.3E14	0.	0.	!(196, -
CH2COZ+B10=B5CH2+C02 197)<DAGAUT91>!	1.8E12	0.	1.3E3	!(197, -
CH2COZ+B10=R12CHCOZ+R20H 198)<DAGAUT91>!	1.0E13	0.	8.0E3	!(198, -
CH2COZ+R20H=R12CHCOZ+H2O 199)<DAGAUT91>!	7.5E12	0.	2.0E3	!(199, -
!CH2COZ+R20H=R5CHO+HCHO 200)<VAnD00REn77nIST>!	2.8E13	0.	0.	!(200, -
CH2COZ+R20H=R4CH3+C02 200a)<BAULCH LEEDS>!	2.52E12	0.	0.	!(200a, -
CH2COZ+R20H=R6CH20H+B2CO 200b)<BAULCH LEEDS>!	4.68E12	0.	0.	!(200b, -

!\*\*\*\*\* REACTIONS DE R14CH3CO \*\*\*\*\*!

R14CH3CO+R1H=R4CH3+R5CHO 201)<TSAnG86>!	9.6E13	0.	0.	!(201, -
R14CH3CO+B6CH2=R4CH3+CH2COZ 202)<TSAnG86>!	1.8E13	0.	0.	!(202, -
R14CH3CO+B5CH2=R4CH3+CH2COZ 203)<TSAnG86>!	1.8E13	0.	0.	!(203, -
R14CH3CO+B10=R4CH3+C02 204)<TSAnG86>!	9.6E12	0.	0.	!(204, -
R14CH3CO+R20H=CH2COZ+H2O 205)<TSAnG86>!	1.2E13	0.	0.	!(205, -
R14CH3CO+R20H=>R4CH3+B2CO+R20H (206)<TSAnG86>!	3.0E13	0.	0.	!
R14CH3CO+R5CHO=CH3CHO+B2CO 207)<TSAnG86>!	9.0E12	0.	0.	!(207, -
R14CH3CO+HCHO=CH3CHO+R5CHO 208)<TSAnG86>!	1.8E11	0.	12.9E3	!(208, -
R14CH3CO+R7CH3O=CH3OH+CH2COZ 209)<TSAnG86>!	6.0E12	0.	0.	!(209, -
R14CH3CO+R7CH3O=HCHO+CH3CHO 210)<TSAnG86>!	6.0E12	0.	0.	!(210, -
R14CH3CO+CH3OH=CH3CHO+R6CH20H 211)<TSAnG87>!	4.85E3	3.	12.3E3	!(211, -
R14CH3CO+R14CH3CO=CH2COZ+CH3CHO 212)<TSAnG86>!	1.2E13	0.	0.	!(212, -

!\*\*\*\*\* REACTIONS DE R13CH2CHO \*\*\*\*\*!

!R13CH2CHO=R14CH3CO (213, -213)<COLKET75nIST>!	1.0E13	0.	47.0E3	!
!R13CH2CHO=R1H+CH2COZ (214, -214)<COLKET75nIST>!	1.6E13	0.	35.0E3	!
R13CH2CHO=R4CH3+B2CO	2.93E12	0.29	40.3E3	!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.				
R13CH2CHO=R1H+CH2COZ	1.43E15	-0.15	45.6E3	!at
infinite, ref: J.phys.Chem A 2006,110,5772-5781, Klippenstein et al.				

!\*\*\*\*\* REACTIONS DE CH3CHO \*\*\*\*\*!

!CH3CHO+R1H=H2+R14CH3CO (215, -215)<WARnATZ84>!	4.0E13	0.	4.2E3	!
!CH3CHO+R4CH3=R14CH3CO+CH4 (216, -216)<BAULCH94>!	2.0E-6	5.6	2.5E3	!
!CH3CHO+R10C2H3V=C2H4Z+R14CH3CO (217, -217)<SCHERZER87>!	8.1E10	0.	3.7E3	!
!CH3CHO+R11C2H5=C2H6+R14CH3CO (218, -218)<HOHLEIn70>!	1.3E12	0.	8.5E3	!
!CH3CHO+B10=R14CH3CO+R20H (219, -219)<CAVAnAGH90>!	1.4E13	0.	2.3E3	!
!CH3CHO+R20H=R14CH3CO+H2O (220, -220)<CAVAnAGH90>!	4.2E12	0.	0.5E3	!
!CH3CHO+R7CH30=R14CH3CO+CH3OH (221, -221)<CAVAnAGH90>!	2.4E11	0.	1.8E3	!
!CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO (222, -222)<SCHUCHMAnn70nIST>!	2.5E7	0.	0.	!

!\*\*\*\*\* REACTIONS DE C2H4O# \*\*\*\*\*!

C2H4O#3=CH4+B2CO 223)<LIFSHITZ83nIST>!	1.2E13	0.	57.2E3	!(223, -
C2H4O#3=CH3CHO 224)<LIFSHITZ83nIST>!	7.3E13	0.	57.2E3	!(224, -
C2H4O#3=R4CH3+R5CHO 225)<LIFSHITZ83nIST>!	3.6E13	0.	57.2E3	!(225, -
C2H4O#3+R1H=H2+R13CH2CHO 226)<LIFSHITZ83nIST*>!	2.0E13	0.	8.3E3	!(226, -
C2H4O#3+R1H=H2O+R10C2H3V 227)<LIFSHITZ83nIST>!	5.0E9	0.	5.0E3	!(227, -
C2H4O#3+R1H=C2H4Z+R20H 228)<LIFSHITZ83nIST>!	9.5E10	0.	5.0E3	!(228, -
C2H4O#3+R4CH3=CH4+R13CH2CHO 229)<BALDWIn84nIST*>!	1.1E12	0.	11.8E3	!(229, -
C2H4O#3+R4CH3=R11C2H5+HCHO 230)<RAnZI94>!	1.4E11	0.	7.6E3	!(230, -
C2H4O#3+R4CH3=C2H4Z+R7CH3O 231)<RAnZI94>!	1.5E10	0.	7.6E3	!(231, -
C2H4O#3+R9C2H=C2H2+R13CH2CHO 232)<RAnZI94>!	1.2E12	0.	9.8E3	!(232, -
C2H4O#3+R10C2H3V=C2H4Z+R13CH2CHO 233)<RAnZI94>!	2.0E12	0.	9.3E3	!(233, -
C2H4O#3+R11C2H5=C2H6+R13CH2CHO 234)<RAnZI94>!	6.8E11	0.	11.4E3	!(234, -
C2H4O#3+B10=R20H+R13CH2CHO 235)<BOGAn78nIST>!	1.9E12	0.	5.2E3	!(235, -
C2H4O#3+R20H=H2O+R13CH2CHO 236)<BALDWIn84nIST*>!	1.8E13	0.	3.6E3	!(236, -
C2H4O#3+R5CHO=HCHO+R13CH2CHO 237)<RAnZI94>!	3.7E12	0.	15.8E3	!(237, -
C2H4O#3+R7CH30=CH3OH+R13CH2CHO 238)<RAnZI94>!	1.3E12	0.	5.8E3	!(238, -
C2H4O#3+R6CH2OH=CH3OH+R13CH2CHO 239)<RAnZI94>!	8.4E11	0.	13.4E3	!(239, -

C2H4O#3+R14CH3CO=CH3CHO+R13CH2CHO 4.0E12 0. 17.5E3 !(240, -  
240)<RAnZI94>!

C2H4O#3+R13CH2CHO=CH3CHO+R13CH2CHO 6.8E11 0. 15.4E3 !(241, -  
241)<RAnZI94>!

!\* assuming that C2H3O decompose rapidly to R13CH2CHO!

!\*\*\*\*\* REACTIONS DE R15C2H5O \*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C2H5OH \*\*\*\*\*!

!Voir Plus bas meca 10a Luc Sy Tran

!\*\*\*\*\* REACTIONS DE O2 \*\*\*\*\*!

B10+B10+M=O2+M 5.40E13 0. -1.79E3 !(244, -  
244)<BAULCH94>!

02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
! N2/0.4/ HE/0.35/

O2+R1H=R2OH+B10 9.8E13 0. 14.8E3 !(245, -  
245)<BAULCH94>!

!O2+R1H+M=R300H+M 2.10E18 -0.8 0.00 !(246, -  
246)<baseLeeds>!

! 02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/  
! N2/0.4/ HE/0.35/

!O2+R1H+H2O=R300H+H2O 6.90E15 0.0 -2.10E3 !(246, -  
246bis)<base Leeds>!

O2+R1H(+M)=R300H(+M) 4.52E13 0. 0. !(246, -  
246)<COBOS85>!

LOW /1.8E18 -0.8 0.00/ !k0

BAULCH94!

TROE /0.5 1.0 1.0E8/  
02/0.4/ B2CO/0.75/ CO2/1.5/ H2O/0.0/ CH4/3.0/ C2H6/3.0/ AR/0.29/  
! N2/0.4/ HE/0.35/

!O2+R1H(+H2O)=R300H(+H2O) 1.63E14 0. 761. !(246b, -  
246b)<COBOS85>!

O2+R1H(+H2O)=R300H(+H2O) 4.52E13 0. 0. !(246b, -  
246b)<BAULCH94>!

LOW /6.9E15 0.0 -2080/  
TROE /0.45 1.0 1.0E8/

O2+B3C=B2CO+B10 1.2E14 0. 0. !(247, -  
247)<RAnZI94>!

O2+B4CH=R5CHO+B10 3.3E13 0. 0. !(248, -  
248)<DAGAUT91>!

O2+B4CH=B2CO+R2OH 3.2E13 0. 0. !(249, -  
249)<PEETERS97>!

O2+B6CH2=>B2CO+R2OH+R1H 3.1E12 0. 0. !  
(250)<BAULCH94>!

O2+B5CH2=R5CHO+R2OH 4.3E10 0. -0.5E3 !(251, -  
251)<DAGAUT91>!

O2+B5CH2=CO2+H2 6.9E11 0. 0.5E3 !(252, -  
252)<DAGAUT91>!

O2+B5CH2=>CO2+R1H+R1H 1.6E12 0. 1.0E3 !  
(253)<DAGAUT91>!



02+B5CH2=B2CO+H2O 254)<DAGAUT91>!	1.9E10	0.	-1.0E3	!(254, -
02+B5CH2=>B2CO+R20H+R1H (255)<DAGAUT91>!	8.6E10	0.	-0.5E3	!
02+B5CH2=HCHO+B10 256)<DAGAUT91>!	1.0E14	0.	4.5E3	!(256, -
02+R4CH3(+M)=R8CH300(+M) 257)<BAULCH94>!	7.8E8	1.2	0.	!(257, -
	LOW /5.6E25	-3.3	0./	
	TROE /0.36	1.0	1.0E8/	
02+R4CH3=R7CH30+B10 258)<BAULCH94>!	1.3E14	0.	31.3E3	!(258, -
!02+R4CH3=R7CH30+B10 258)<HWAnG&RABInOVITCH99>!	1.6E13	0.	31.4E3	!(258, -
02+R4CH3=HCHO+R20H 259)<DAGAUT91>!	3.0E30	-4.69	36.6E3	!(259, -
02+CH4=R4CH3+R300H 260)<BAULCH94>!	4.0E13	0.	56.7E3	!(260, -
02+R9C2H=B2CO+R5CHO 261)<TIESEMAAnn97/TSAnG86>!	3.8E13	-0.16	0.	!(261, -
02+R9C2H=R12CHCOZ+B10 262)<TIESEMAAnn97/TSAnG86>!	9.0E12	-0.16	0.	!(262, -
02+C2H2=R9C2H+R300H 263)<TSAnG86>!	1.2E13	0.	74.5E3	!(263, -
!02+C2H2=R12CHCOZ+R20H 264)<DAGAUT91>!	2.0E8	1.5	30.1E3	!(264, -
02+C2H2=R5CHO+R5CHO 264)<BEEnS0n95>!	7.0E7	1.8	30.6E3	!(264, -
!02+R10C2H3V=C2H2+R300H 265)<TSAnG86>!	1.2E11	0.	0.	!(265, -
!02+R10C2H3V=C2H2+R300H 265)<WAnG97>!	1.6E14	-0.83	2.5E3	!(265, -
!at 760 Torr				
!02+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	8.6E21	-2.97	3.3E3	!(266a, -
!02+R10C2H3V=B10+R13CH2CHO 266b)<WAnG97>!	1.2E13	-0.12	1.7E3	!(266b, -
!at 20-90 Torr				
!02+R10C2H3V=HCHO+R5CHO 266a)<WAnG97>!	1.6E21	-2.78	2.5E3	!(266a, -
!02+R10C2H3V=B10+R13CH2CHO 266b)<WAnG97>!	2.5E12	0.057	0.9E3	!(266b, -
02+R10C2H3V=C2H2+R300H 265)<MEBEL nIST>!	1.34E6	1.61	-0.4E3	!(265, -
02+R10C2H3V=HCHO+R5CHO 266a)<MEBEL nIST>!	4.5E16	-1.39	1.0E3	!(266a, -
02+R10C2H3V=B10+R13CH2CHO 266b)<MEBEL nIST>!	3.3E11	-0.29	10.	!(266b, -

02+C2H4Z=R10C2H3V+R300H 267)<TSAnG86>!	4.2E13	0.	57.4E3	!(267, -
02+R11C2H5=R17C2H500 268)<WAGnER90>!	2.2E10	0.77	-0.6E3	!(268, -
02+R11C2H5=C2H4Z+R300H 269)<TSAnG86>!	8.4E11	0.	3.9E3	!(269, -
02+R11C2H5=R15C2H50+B10 270)<BOZZELLI90nIST>!	1.2E13	-0.2	27.9E3	!(270, -
02+R11C2H5=CH3CHO+R20H 271)<TSAnG86>!	6.0E10	0.	6.9E3	!(271, -
02+C2H6=R11C2H5+R300H 272)<BAULCH94>!	6.0E13	0.	51.7E3	!(272, -
02+R20H=R300H+B10 273)<TSAnG86>!	2.2E13	0.	52.5E3	!(273, -
02+B2CO=C02+B10 274)<TSAnG86>!	2.5E12	0.	47.7E3	!(274, -
!02+R5CHO=B2CO+R300H 275)<TSAnG86>!	5.1E13	0.	1.7E3	!(275, -
02+R5CHO=B2CO+R300H 275)<TIM0nEn88>!	7.6E12	0.	0.41E3	!(275, -
02+HCHO=R5CHO+R300H 276)<TSAnG86>!	2.0E13	0.	38.8E3	!(276, -
02+R7CH30=HCHO+R300H 277)<BAULCH94>!	2.2E10	0.	1.7E3	!(277, -
02+R6CH20H=HCHO+R300H 278)<TSAnG87>!	1.2E12	0.	0.	!(278, -
02+CH30H=R6CH20H+R300H 279)<TSAnG87>!	2.0E13	0.	44.9E3	!(279, -
02+R12CHCOZ=>B2CO+B2CO+R20H <DAGAUT91>!	1.5E12	0.	2.5E3	!(280)
!02+CH2COZ=HCHO+C02 281)<DAGAUT91>!bizarre	1.0E8	0.	0.	!(281, -
02+R14CH3CO=R18CH3C000 282)<COX90>!	2.4E12	0.	0.	!(282, -
02+R13CH2CHO=>HCHO+R20H+B2CO <COX90>!	5.9E9	0.	-1.4E3	!(283)
02+R13CH2CHO=CH2COZ+R300H 284)<COX90>!	1.0E10	0.	-1.4E3	!(284, -
02+CH3CHO=R14CH3CO+R300H 285)<COX90>!	5.0E13	0.	36.4E3	!(285, -
! ajout demande par Laetitia le 25 Avril 95				
02+CH3CHO=R13CH2CHO+R300H 285)<Ranzi94>!	1.0E13	0.5	46.0E3	!(285', -
02+C2H40#3=R300H+R13CH2CHO 286)<RAnZI94>!	5.0E13	0.	48.0E3	!(286, -
!02+R15C2H50=CH3CHO+R300H 287)<BAULCH94>!	6.0E10	0.	1.7E3	!(287, -
!***** REACTIONS DE R300H *****!				
R300H+R1H=H2+O2 288)<BAULCH94>!	4.3E13	0.	1.4E3	!(288, -
R300H+R1H=2R20H 289)<BAULCH94>!	1.7E14	0.	0.9E3	!(289, -

R300H+R1H=H2O+B10 290)<BAULCH94>!	3.0E13	0.	1.7E3	!(290, -
R300H+B6CH2=HCHO+R20H 291)<TSAnG86>!	3.0E13	0.	0.	!(291, -
R300H+B5CH2=HCHO+R20H 292)<TSAnG86>!	1.8E13	0.	0.	!(292, -
R300H+R4CH3=R7CH30+R20H 293)<BAULCH94>!	1.8E13	0.	0.	!(293, -
!R300H+R4CH3=R7CH30+R20H 293)<DAGAUT>	4.0E13	0.	5.0E3	!(293, -
R300H+CH4=R4CH3+H2O2 294)<BAULCH94>!	9.0E12	0.	24.6E3	!(294, -
R300H+R9C2H=R12CHCOZ+R20H 295)<TSAnG86>!	1.8E13	0.	0.	!(295, -
R300H+C2H2=CH2COZ+R20H 296)<TSAnG86>!	6.0E9	0.	8.0E3	!(296, -
!incertitude au moins un facteur 10				
R300H+R10C2H3V=>R20H+R4CH3+B2CO <TSAnG86>!	3.0E13	0.	0.	!(297)
R300H+C2H4Z=CH3CHO+R20H 298)<TSAnG86>!	6.0E9	0.	7.9E3	!(298, -
R300H+C2H4Z=C2H4O#3+R20H 299)<BAULCH94>!	2.2E12	0.	17.2E3	!(299, -
R300H+R11C2H5=>R4CH3+HCHO+R20H <TSAnG86>!	2.4E13	0.	0.	!(300)
R300H+R11C2H5=C2H4Z+H2O2 301)<TSAnG86>!	3.0E11	0.	0.	!(301, -
R300H+C2H6=R11C2H5+H2O2 302)<BAULCH94>!	1.3E13	0.	20.4E3	!(302, -
R300H+R20H=H2O+O2 303)<BAULCH94>!	2.9E13	0.	-0.5E3	!(303, -
R300H+B2CO=CO2+R20H Phys. Chem. A 111(2007)4031 - 4042	1.57E05	2.18	17.9E3	!MF Wang, J.
R300H+R5CHO=>R20H+R1H+CO2 <TSAnG86>!	3.0E13	0.	0.	!(305)
R300H+HCHO=R5CHO+H2O2 306)<BAULCH94>!	3.0E12	0.	13.0E3	!(306, -
R300H+R7CH30=HCHO+H2O2 307)<TSAnG86>!	3.0E11	0.	0.	!(307, -
R300H+R6CH20H=HCHO+H2O2 308)<TSAnG87>!	1.2E13	0.	0.	!(308, -
R300H+CH30H=R6CH20H+H2O2 309)<TSAnG87>!	9.6E10	0.	12.6E3	!(309, -
R300H+R14CH3CO=>R4CH3+CO2+R20H (310)<TSAnG86>!	3.0E13	0.	0.	!
R300H+CH3CHO=R14CH3CO+H2O2 311)<CAVAnAGH90>!	1.0E12	0.	10.0E3	!(311, -
R300H+C2H4O#3=H2O2+R13CH2CHO 312)<RAnZI94>	1.6E12	0.	15.0E3	!(312, -
R300H+R300H=H2O2+O2 313)<BAULCH 94>!	1.3E11	0.	-1.63E3	!(313, -
DUPLICATE				
R300H+R300H=H2O2+O2 313)<BAULCH 94>!	4.2E14	0.	11.98E3	!(313, -

DUPLICATE

!\*\*\*\*\* REACTIONS DE H2O2 \*\*\*\*\*!

!R2OH+R2OH(+ M)=>H2O2 (+ M) 7.23E13 -0.37 0.00  
 ! O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 !! N2/0.4/ HE/0.35/  
 ! LOW /5.53E19 -0.76 0.00 /  
 ! TROE /0.5 1 1.E8/  
 !H2O2(+M)=>R2OH+R2OH(+M) 3.00E14 0.00 48.5E3  
 ! O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ CH4/3.0/ C2H6/3.0/ AR/0.35/  
 !! N2/0.4/ HE/0.35/  
 ! LOW /3.0E17 0.0 45.5E3/  
 ! TROE /0.5 1 1.E8/

! MF Troe, Comb.Flam. 158(2011)594-601

H2O2(+M)=R2OH+R2OH(+M) 1.99E12 0.9 4.8749E4 !<BAULCH94>!  
 AR/0.68/ O2/0.79/ N2/1.00/ CO2/1.06/ H2O/5.1/ H2O2/5.2/  
 LOW /3.65e24 -2.3 4.8749E4/  
 TROE /0.43 1 1.E8/

H2O2+R1H=H2+R300H 1.7E12 0. 3.7E3 !(315, -  
 315)<BAULCH94>!  
 H2O2+R1H=H2O+R2OH 1.0E13 0. 3.6E3 !(316, -  
 316)<BAULCH94>!  
 H2O2+B6CH2=R7CH30+R2OH 3.0E13 0. 0. !(317, -  
 317)<TSAnG86>!  
 H2O2+R10C2H3V=C2H4Z+R300H 1.2E10 0. -0.6E3 !(318, -  
 318)<TSAnG86>!  
 H2O2+B10=R2OH+R300H 6.6E11 0. 4.0E3 !(319, -  
 319)<BAULCH94>!  
 H2O2+R2OH=H2O+R300H 7.8E12 0. 1.3E3 !(320, -  
 320)<BAULCH94>!

!\*\*\*\*\* REACTIONS DE CO2 \*\*\*\*\*!

CO2+B5CH2=HCHO+B2CO 2.3E10 0. 0. !(321, -  
 321)<TSAnG86>!

!\*\*\*\*\* REACTIONS DE R8CH300 \*\*\*\*\*!

R8CH300=HCHO+R2OH 1.5E13 0. 47.0E3 !(322, -  
 322)<RAnZI94>!  
 R8CH300+R1H=R7CH30+R2OH 9.6E13 0. 0. !(323, -  
 323)<TSAnG86>!  
 R8CH300+H2=CH300H+R1H 3.0E13 0. 26.0E3 !(324, -  
 324)<TSAnG86>!  
 R8CH300+B6CH2=HCHO+R7CH30 1.8E13 0. 0. !(325, -  
 325)<TSAnG86>!  
 R8CH300+B5CH2=HCHO+R7CH30 1.8E13 0. 0. !(326, -  
 326)<TSAnG86>!  
 R8CH300+R4CH3=R7CH30+R7CH30 5.0E12 0. -1.4E3 !(327, -  
 327)<CAVAnAGH90>!  
 R8CH300+CH4=CH300H+R4CH3 1.8E11 0. 18.5E3 !(328, -  
 328)<TSAnG86>!  
 R8CH300+R9C2H=R7CH30+R12CHCOZ 2.4E13 0. 0. !(329, -  
 329)<TSAnG86>!

!R8CH300+C2H2=CH300H+R9C2H	5.6E11	0.	24.5E3	!(330, -
330)<RAnZI94>! MF car i<<0				
R8CH300+R10C2H3V=R7CH30+R13CH2CHO	2.4E13	0.	0.	!(331, -
331)<TSAnG86*>!				
!* assuming that C2H3O decompose rapidly to R13CH2CHO!				
R8CH300+C2H4Z=R7CH30+C2H4O#3	1.1E15	0.	20.0E3	!(332, -
332)<nIKISHA81/MOSHKInA80nIST>!				
R8CH300+C2H4Z=CH300H+R10C2H3V	3.9E12	0.	24.5E3	!(333, -
333)<RAnZI94>!				
R8CH300+R11C2H5=R7CH30+R15C2H5O	2.4E13	0.	0.	!(334, -
334)<TSAnG86>!				
R8CH300+C2H6=CH300H+R11C2H5	2.9E11	0.	14.9E3	!(335, -
335)<TSAnG86>!				
R8CH300+B10=R7CH30+O2	3.6E13	0.	0.	!(336, -
336)<TSAnG86>!				
R8CH300+R20H=CH30H+O2	6.0E13	0.	0.	!(337, -
337)<TSAnG86>!				
R8CH300+R20H=R7CH30+R300H	3.0E12	0.	0.	!(338, -
338)<RAnZI94>!				
R8CH300+B2C0=R7CH30+C02	1.0E14	0.	24.0E3	!(339, -
339)<RAnZI94>!				
R8CH300+R5CHO=>R7CH30+R1H+C02	3.0E13	0.	0.	!(340)
<TSAnG86>!				
R8CH300+HCHO=CH300H+R5CHO	1.0E12	0.	12.1E3	!(341, -
341)<CAVAnAGH90>!				
R8CH300+R7CH30=HCHO+CH300H	3.0E11	0.	0.	!(342, -
342)<TSAnG86>!				
R8CH300+R6CH20H=>R7CH30+R20H+HCHO	1.2E13	0.	0.	!
(343)<TSAnG87>!				
R8CH300+CH30H=CH300H+R6CH20H	1.8E12	0.	13.7E3	!(344, -
344)<TSAnG87>!				
R8CH300+CH30H=CH300H+R7CH30	2.8E11	0.	18.8E3	!(345, -
345)<RAnZI94>!				
R8CH300+CH2COZ=CH300H+R12CHCOZ	1.7E12	0.	27.0E3	!(346, -
346)<RAnZI94>!				
R8CH300+R14CH3C0=R4CH3+C02+R7CH30	2.4E13	0.	0.	!(347, -
347)<TSAnG86>!				
R8CH300+CH3CHO=CH300H+R14CH3C0	1.0E12	0.	12.1E3	!(348, -
348)<CAVAnAGH90>!				
R8CH300+CH3CHO=CH300H+R13CH2CHO	1.7E12	0.	19.2E3	!(349, -
349)<RAnZI94>!				
R8CH300+C2H4O#3=CH300H+R13CH2CHO	2.2E12	0.	16.0E3	!(350, -
350)<RAnZI94>!				
R8CH300+R300H=CH300H+O2	2.5E11	0.	-1.6E3	!(351, -
351)<BAULCH94>!				
R8CH300+R300H=>O2+HCHO+H2O	5.0E10	0.	0.	!
(352)<RAnZI94>!				
R8CH300+H2O2=CH300H+R300H	2.4E12	0.	9.9E3	!(353, -
353)<TSAnG86>!				
R8CH300+R8CH300=CH30H+HCHO+O2	2.5E10	0.	-0.8E3	!(354, -
354)<BAULCH94>!				
R8CH300+R8CH300=R7CH30+R7CH30+O2	2.5E10	0.	-0.8E3	!(355, -
355)<BAULCH94>!				

!\*\*\*\*\* REACTIOns DE CH300H \*\*\*\*\*!

CH300H=R7CH30+R20H	6.0E14	0.	42.3E3 !(356, -
356)<BAULCH94>!			
CH300H+B10=R8CH300+R20H	2.0E13	0.	4.8E3 !(357, -
357)<BAULCH94average>!			
CH300H+R20H=H2O+R8CH300	1.8E12	0.	-0.37E3 !(358, -
358)<BAULCH94average>!			
CH300H+R7CH30=>CH30H+R20H+HCHO	1.5E11	0.	6.5E3 !
(359)<RAnZI94>!			

!\*\*\*\*\* REACTIOns DE R17C2H500 \*\*\*\*\*!

R17C2H500=R16C2H400H	4.2E12	0.	36.9E3 !(360, -
360)<HUGHES93>!			
R17C2H500+H2=C2H500H+R1H	7.9E12	0.	21.0E3 !(361, -
361)<RAnZI94>!			
R17C2H500+R4CH3=R15C2H50+R7CH30	2.0E12	0.	-1.2E3 !(362, -
362)<RAnZI94>!			
R17C2H500+CH4=C2H500H+R4CH3	3.9E12	0.	24.0E3 !(363, -
363)<RAnZI94>!			
R17C2H500+C2H2=C2H500H+R9C2H	5.6E11	0.	24.4E3 !(364, -
364)<RAnZI94>!			
R17C2H500+C2H4Z=C2H500H+R10C2H3V	3.9E12	0.	24.4E3 !(365, -
365)<RAnZI94>!			
R17C2H500+C2H4Z=R15C2H50+C2H40#3	2.3E16	0.	21.9E3 !(366, -
366)<MOSHkinA80nIST>!			
R17C2H500+C2H6=C2H500H+R11C2H5	5.1E12	0.	19.5E3 !(367, -
367)<RAnZI94>!			
R17C2H500+H2O=C2H500H+R20H	5.6E12	0.	30.6E3 !(368, -
368)<RAnZI94>!			
R17C2H500+B2C0=C02+R15C2H50	1.0E14	0.	24.0E3 !(369, -
369)<RAnZI94>!			
R17C2H500+HCHO=C2H500H+R5CHO	4.5E12	0.	14.4E3 !(370, -
370)<RAnZI94>!			
R17C2H500+CH30H=C2H500H+R7CH30	2.8E11	0.	18.4E3 !(371, -
371)<RAnZI94>!			
R17C2H500+CH30H=C2H500H+R6CH20H	2.8E12	0.	19.5E3 !(372, -
372)<RAnZI94>!			
R17C2H500+CH2C0Z=C2H500H+R12CHC0Z	1.7E12	0.	24.4E3 !(373, -
373)<RAnZI94>!			
R17C2H500+CH3CHO=C2H500H+R14CH3C0	3.9E12	0.	14.4E3 !(374, -
374)<RAnZI94>!			
R17C2H500+CH3CHO=C2H500H+R13CH2CHO	1.7E12	0.	19.5E3 !(375, -
375)<RAnZI94>!			
R17C2H500+C2H40#3=C2H500H+R13CH2CHO	2.2E12	0.	16.3E3 !(376, -
376)<RAnZI94>!			
R17C2H500+R300H=02+C2H500H	3.9E11	0.	-1.3E3 !(377, -
377)<BAULCH89>!			
!Rate constant measured between 240 and 380K!			
R17C2H500+H202=C2H500H+R300H	4.5E11	0.	10.8E3 !(378, -
378)<RAnZI94>!			
R17C2H500+R8CH300=>R15C2H50+R7CH30+02	2.0E11	0.	0. !
(379)<RAnZI94>!			
R17C2H500+CH300H=C2H500H+R8CH300	1.1E12	0.	16.3E3 !(380, -
380)<RAnZI94>!			

R17C2H500+R17C2H500=2R15C2H50+02 4.1E10 0. 0.2E3 !(381, -  
 381)<LIGHTFOOT92>!  
 R17C2H500+R17C2H500=C2H50H+CH3CHO+02 1.8E10 0. 0.2E3 !(382, -  
 382)<LIGHTFOOT92>!

!\*\*\*\*\* REACTIONS DE R16C2H400H \*\*\*\*\*!

R16C2H400H=C2H40#3+R20H 1.5E11 0. 20.0E3 !(383, -  
 383)<RAnZI94>!  
 R16C2H400H=R6CH20H+HCHO 2.5E13 0. 27.5E3 !(384, -  
 384)<RAnZI94>!  
 R16C2H400H=C2H4Z+R300H 2.0E13 0. 23.5E3 !(385, -  
 385)<RAnZI94>!

!\*\*\*\*\* REACTIONS DE C2H500H \*\*\*\*\*!

C2H500H=R15C2H50+R20H 4.0E15 0. 42.9E3 !(386, -  
 386)<BAULCH94>!  
 C2H500H+R1H=>CH3CHO+R20H+H2 3.2E13 0. 7.7E3 !  
 (387)<RAnZI94>!  
 C2H500H+R4CH3=>CH3CHO+R20H+CH4 5.7E11 0. 8.7E3 !  
 (388)<RAnZI94>!  
 C2H500H+R9C2H=>CH3CHO+R20H+C2H2 6.0E11 0. 9.2E3 !  
 (389)<RAnZI94>!  
 C2H500H+R10C2H3V=>CH3CHO+R20H+C2H4Z 1.0E12 0. 8.7E3 !  
 (390)<RAnZI94>!  
 C2H500H+R11C2H5=>CH3CHO+R20H+C2H6 3.4E11 0. 11.4E3 !  
 (391)<RAnZI94>!  
 C2H500H+R20H=>CH3CHO+R20H+H2O 5.9E12 0. 0.9E3 !  
 (392)<RAnZI94>!  
 C2H500H+R5CHO=>CH3CHO+R20H+HCHO 1.8E12 0. 16.7E3 !  
 (393)<RAnZI94>!  
 C2H500H+R7CH3O=>CH3CHO+R20H+CH3OH 6.3E11 0. 5.5E3 !  
 (394)<RAnZI94>!  
 C2H500H+R6CH20H=>CH3CHO+R20H+CH3OH 4.2E11 0. 13.6E3 !  
 (395)<RAnZI94>!  
 C2H500H+R14CH3CO=>2CH3CHO+R20H 2.0E12 0. 18.5E3 !  
 (396)<RAnZI94>!  
 C2H500H+R13CH2CHO=>2CH3CHO+R20H 3.4E11 0. 15.7E3 !  
 (397)<RAnZI94>!  
 C2H500H+R300H=>CH3CHO+R20H+H2O2 8.0E11 0. 16.2E3 !  
 (398)<RAnZI94>!  
 C2H500H+R8CH300=>CH3CHO+R20H+CH300H 1.1E12 0. 16.7E3 !  
 (399)<RAnZI94>!  
 C2H500H+R17C2H500=>CH3CHO+R20H+C2H500H 1.1E12 0. 16.7E3 !  
 (400)<RAnZI94>!

!\*\*\*\*\* REACTIONS DE R18CH3C000 \*\*\*\*\*!

R18CH3C000+C2H40#3=CH3C000H+R13CH2CHO 1.0E12 0. 9.3E3 !  
 (401, -402)<RAnZI94>!  
 R18CH3C000+R300H=CH3C000H+02 5.5E10 0. -2.6E3 !  
 (402, -402)<COX90>!  
 R18CH3C000+C2H500H=CH3C000H+R17C2H500 5.0E11 0. 9.2E3 !  
 (403, -403)<RAnZI94>!  
 R18CH3C000+C2H500H=>CH3CHO+R20H+CH3C000H 5.0E11 0. 9.2E3 !  
 (404)<RAnZI94>!

R18CH3C000+R18CH3C000=>2R4CH3+O2+2C02          1.7E12          0.          -1.0E3 !  
 (405)<CAVAnAGH90>!

!\*\*\*\*\* REACTIONS DE CH3C000H \*\*\*\*\*!  
 CH3C000H=>R4CH3+C02+R20H                    1.0E16          0.          40.0E3 !  
 (406)<CAVAnAGH90>!

!\*\*\*\*\*  
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 !\*    Primary mechanism of the  
 oxidation of Ethanol    \*!  
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!\*\*\*\*\*!  
 !\*    REACTIONS OF ETHANOL                        \*!  
 !\*\*\*\*\*!

!Unimolecular initiation

C2H5OH(+M)=R11C2H5+R20H(+M)                  2.95E+22          -2.16          96.6E+3  
 !Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!  
     LOW          /3.80E+88          -19.70          114.5E+3/  
     TROE          /2.094          16539          1.114          161.36/

C2H5OH(+M)=C2H4Z+H20(+M)                    4.90E+9            1.36          65.8E+3  
 !Tsang, J Chem Kinet 36,436-63,2004!T=800-1800K!  
     LOW          /2.404+8            -17.9          84.8E+3/  
     TROE          /2.126            13568          0.969          160.4/

C2H5OH(+M)=R4CH3+R6CH20H(+M)              6.61E+23          -2.16          88.04E+3  
 !Tsang, J Chem Kinet 36,436-63,2004!  
     LOW          /1.99E+85          -18.9          104.8E+3/  
     TROE          /2.058            16911          1.071          135.3/

C2H5OH(+M)=R23C2H40H+R1H(+M)              2.01E+17          -0.149          101.8E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!  
     LOW          /4.902E+94          -21.65          123.1E+3/  
 !Reaction (c5),T=500-1800K  
     !LOW          /2.716E+83          -21.47          38.44E+3/  
 !Reaction (c5),T=1800-3000K



C2H50H(+M)=R24C2H40H+R1H(+M) 7.54E+16 -0.275 94.05E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011!  
 LOW /7.708E+96 -22.47 116.9E+3/  
 !T=500-1800K  
 !LOW /5.58E+82 -21.20 37824.5/  
 !T=1800-3000K

DUPLICATE

C2H50H(+M)=R15C2H50+R1H(+M) 2.70E+15 0.305 101.3E+3  
 !T=500-3000K, Lin et al, J chem phys A, 115,3509-22, 2011b!  
 LOW /2.794E+88 -19.76 121.0E+3/  
 !T=500-1800K;  
 !LOW /4.246E+91 -23.49 49435.8/  
 !T=1800-3000K,

DUPLICATE

!Bimolecular initiation

C2H50H+O2=R23C2H40H+R300H 2.100E+13 0.0 52400.0  
 C2H50H+O2=R24C2H40H+R300H 1.400E+13 0.0 46300.0  
 C2H50H+O2=R15C2H50+R300H 7.000E+12 0.0 55730.0

!Metatheses with abstraction of H-atom

!C2H50H+R20H=R23C2H40H+H2O 6.203E+03 2.68 -576.3  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!  
 C2H50H+R20H=R23C2H40H+H2O 3.60E+06 2.0 950.0  
 !Nancy, correlation Bozzelli 1999!

!C2H50H+R20H=R24C2H40H+H2O 1.307E+05 2.43 -1456.6  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!  
 C2H50H+R20H=R24C2H40H+H2O 2.40E+06 2.00 -2100.0  
 !Nancy, correlation Bozzelli 1999!

C2H50H+R20H=R15C2H50+H2O 2.812E+02 2.97 -580.3  
 !T=200-3000K, Lin et al, proc combust inst, 31, 159-166, 2007!

C2H50H+B10=R23C2H40H+R20H 9.69E+02 3.23 4658.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007

C2H50H+B10=R24C2H40H+R20H 1.45E+05 2.47 876.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H50H+B10=R15C2H50+R20H 1.46E-03 4.73 1727.0  
 !T=300-3000K, Lin et al, J phys chem A, 111, 6693-703, 2007!

C2H50H+R1H=R23C2H40H+H2 1.88E+03 3.20 7150.0  
 !T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H50H+R1H=R24C2H40H+H2 1.79E+05 2.53 3420.0  
 !T=300-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

C2H50H+R1H=R15C2H50+H2 5.33E-23 10.58 -4459.0  
 !T=300-1000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).

!C2H50H+R1H=R15C2H50+H2	5.36E+4	2.53	8753.6	
!T=1000-3000K, Park,Zhu,Lin, J chem Phys 118, 9990-9996 (2003).				
!C2H50H+R4CH3=R23C2H40H+CH4	6.99E-83	30.14	-15663.0	
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
C2H50H+R4CH3=R23C2H40H+CH4	3.30E+02	3.30	12291.0	
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
!C2H50H+R4CH3=R24C2H40H+CH4	1.02E-47	18.51	-9409.4	
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
C2H50H+R4CH3=R24C2H40H+CH4	1.99E+01	3.37	7635.0	
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)				
!C2H50H+R4CH3=R15C2H50+CH4	1.01E-51	19.68	-10323.5	
!T=300-600K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004).				
C2H50H+R4CH3=R15C2H50+CH4	2.035E+0	3.57	7722.0	
!T=600-3000K, Xu,Park,Lin, JchemPhys 120, 6593-6599 (2004)				
C2H50H+R300H=R23C2H40H+H2O2	4.2E+04	2.69	19080	
!correlation (Dean and Bozzelli 2000)				
C2H50H+R300H=R24C2H40H+H2O2	2.80E+04	2.69	15420	
!correlation (Dean and Bozzelli 2000)				
C2H50H+R300H=R15C2H50+H2O2	5.400E+04	2.0	15025.0	!
Grana et al.2010				
C2H50H+R11C2H5=R23C2H40H+C2H6	1.500E+12	0.0	11700.0	!
Konnov 2005!				
C2H50H+R11C2H5=R24C2H40H+C2H6	4.000E+13	0.0	10000.0	!
Konnov 2005!				
C2H50H+R11C2H5=R15C2H50+C2H6	2.300E+04	2.0	10525.0	!
Grana et al.2010!				
C2H50H+R6CH2OH=R24C2H40H+CH3OH	4.000E+11	0.0	9700.0	!
Konnov 2005!				
C2H50H+R7CH3O=R24C2H40H+CH3OH	2.000E+11	0.0	7000.0	!
Konnov 2005!				
C2H50H+R15C2H5O=C2H50H+R24C2H40H	2.000E+11	0.0	7000.0	!
Konnov 2005!				

!\*\*\*\*\*!  
!\* REACTIONs OF R23C2H40H \*!  
!\*\*\*\*\*!

R23C2H40H=C2H4Z+R2OH	3.52E-34	11.84	-18737.4	
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.				
!	1.35E+43	-10.29	28035.5	
!at 1 atm, T=300-1000K				

!		7.93E+2	1.51	15180.3
!at 1 Torr, T=300-3000K				
!		1.51E+33	-6.54	26960.4
!at 100 atm, T=300-1000K				
!		4.90E-24	9.44	-12183.6
!at 100 atm, T=1000-3000K				
R23C2H40H=R1H+C2H30H		3.33E+28	-5.26	35586.9
!at 1 atm, T=300-3000K.ref: Lin et al 2009, chemphyschem, 10(6),972-81.				
!		2.67E+15	-1.92	29386.8
!at 1 Torr, T=300-3000K.				
!		2.67E+27	-4.44	37208.5
!at 100 atm, T=300-3000K				
R23C2H40H=R24C2H40H		1.000E+11	0.0	39500.0
! A=Konnov 2005; Ea=Lin et al 2009, chemphyschem, 10(6),972-81				
R23C2H40H+O2=C2H30H+R300H		1.600E+12	0.0	5000.0
!*****!				
!* REACTIONs OF R24C2H40H *				
!*****!				
R24C2H40H=CH3CHO+R1H		8.34E+27	-5.19	35576.9
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.				
!!		8.96E+13	-1.61	28844.3
!at 1 Torr, T=300-3000K				
!!		5.47E+27	-4.67	37685.4
!at 100 atm, T=300-3000K				
R24C2H40H=R1H+C2H30H		2.00E+28	-5.08	39380.5
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81				
!!		4.44E+21	-3.23	36570.6
!at 1 Torr, T=300-3000K				
!!		1.22E+30	-5.17	41916.2
!at 100 atm, T=300-3000K				
R24C2H40H=R4CH3+HCHO		1.14E+22	-3.59	34662.9
!at 1 atm, T=300-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81				
!!		5.92E+11	-1.04	28739.0
!at 1 Torr, T=300-3000K				
!!		4.36E+23	-3.55	38679.0
!at 100 atm, T=300-3000K				
R24C2H40H+O2=CH3CHO+R300H		5.26E+17	-1.637	838.0
!at 0.1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.				
!!R24C2H40H+O2=CH3CHO+R300H		5.28E+17	-1.637	839.0
!at 1 atm, Ref: DaSilva et al 2009, JphyschemA, 113,31.				
R24C2H40H+O2=C2H30H+R300H		5.33E+2	2.490	-402
!at 0.1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.				
!!R24C2H40H+O2=C2H30H+R300H		7.62E+2	2.446	-296
!at 1 atm, T=300-2000K, Ref: DaSilva et al 2009, JphyschemA, 113,31.				

R24C2H40H+R1H=CH3CHO+H2	1.361E+09	1.29	2823.8
! T=100-2000K! ref: Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H=R6CH20H+R4CH3	8.67E+16	-0.891	2903.3
!Reaction (b2), Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H=C2H30H+H2	4.896E+08	1.70	588.2
!Reaction (b11), T=100-2000K! Ref: Lin et al 2011b, JphyschemA,115,3509-22.			
R24C2H40H+R1H(+M)=C2H50H(+M)	3.607E+13	0.06	437.2
!Reaction (b1), T=500-2000K!Ref: Lin et al 2011b, JphyschemA,115,3509-22,			
	LOW /2.767E+56	-15.72	
10.7E+03/			
	Duplicate		
R24C2H40H+R20H=CH3CHO+H2O	1.500E+13	0.0	0.0
!Konnov 2005			
R24C2H40H+B10=CH3CHO+R20H	9.040E+13	0.0	0.0
!Konnov 2005			
!*****!			
!* REACTIOnS OF R15C2H50 *!			
!*****!			
R15C2H50=R4CH3+HCHO	4.4E-29	10.69	-16245.4
!at 1 atm, T=1000-3000K, ref: Lin et al 2009, chemphyschem, 10(6),972-81.			
!!	1.03E+23	-3.82	19303.7
!at 1 atm, T=300-1000K,			
!!	2.71E+24	-4.50	21018.7
!at 1 Torr, T=300-1000K,			
!!	1.87E-28	10.39	-12910.9
!at 1 Torr, T=1000-3000K,			
!!	5.31E+21	-2.97	19560.1
!at 100 atm, T=300-1000K,			
!!	9.56E-17	7.66	-7408.3
!at 100 atm, T=1000-3000K,			
R15C2H50=R1H+CH3CHO	4.25E-32	11.49	-16541.5
!at 1 atm,T=1000-3000K ref: Lin et al 2009, chemphyschem, 10(6),972-81			
!!	1.33E+38	-8.61	25513.8
!at 1 atm,T=300-1000K			
!!	7.25E+31	-7.58	21370.4
!at 1 Torr,T=300-1000K			
!!	2.14E-34	11.63	-15651.2
!at 1 Torr,T=1000-3000K			
!!	2.61E+19	-2.15	21996.4
!at 100 atm,T=300-1000K			
!!	1.64E-27	10.5	-15315.4
!at 100 atm,T=1000-3000K			

R15C2H50+O2=CH3CHO+R300H 6.0E+10 0.0 1.7E+3  
!(287, -287)<BAULCH94>!

R15C2H50+R20H=CH3CHO+H2O 1.0E+13 0.0 0.0  
!Marinov 1998

R15C2H50+R1H=CH3CHO+H2 7.47E+09 1.15 673.7  
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22

R15C2H50+R1H(+M)=C2H5OH(+M) 3.08E+11 0.894 12.9  
!T=100-2000K! Lin et al 2011b, JphyschemA,115,3509-22  
LOW / 3.772E+51 -15.55  
11.1E+3/

DUPLICATE

R15C2H50+B10=CH3CHO+R20H 1.210E+14 0.0 0.0  
!Konnov 2005

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!\* Secondary mechanism of the  
oxidation of Ethanol \*!

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!\* REACTIONS OF C2H3OH \*!

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

!C2H3OH+B10=R13CH2CHO+R20H 4.4E+10 0.7 3250.0  
!<PAG,Ulisier paras. des m̃tathises d'atome H allylique secondaire>!  
C2H3OH+B10=R13CH2CHO+R20H 1.4E+13 0.0 2.3E3  
!Ac̃tald̃hyde! (219, -219)<CAVAnAGH90>

!C2H3OH+R1H=R13CH2CHO+H2 2.700E+04 2.5  
-1900.0 !<PAG,Ulisier paras. des m̃tathises d'atome H allylique  
secondaire>!

!C2H3OH+R1H=R13CH2CHO+H2 1477.2 3.077  
7230 !T=300-3000!RAO 2011! J Phys Chem 2011,115  
! REV /1.41 3.721 24600/  
C2H3OH+R1H=R13CH2CHO+H2 1.31E+5 2.58 1220.0  
!Ac̃tald̃hyde! T=200-2500K!Klippenstein et al.2010. J Phys Chem  
A,114,755-764.

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!C2H3OH+R2OH=R13CH2CHO+H2O          1.500E+06      2.0
-1520.0      !<PAG,Ulisier paras. des m̃tathises d'atome H allylique
secondaire>!
C2H3OH+R2OH=R13CH2CHO+H2O          2.300E+10      0.73      -1100.0
!Ac̃tald̃hyde! Konnov 2005

!C2H3OH+R3OOH=R13CH2CHO+H2O2        3.200E+03      2.6
12400.0     !<PAG,Ulisier paras. des m̃tathises d'atome H allylique
secondaire>!
!C2H3OH+R3OOH=R13CH2CHO+H2O2        1.626E+12      0.0
16295.1     !Syn_CH2H3OH! ajout̃ le 20/10/2011 !Altarawneh et al 2011!
T=700-1300K!
C2H3OH+R3OOH=R13CH2CHO+H2O2        1.0E12         0.0         10.0E3
!Ac̃tald̃hyde! (311, -311)<CAVANAGH90>!

!C2H3OH+R4CH3=R13CH2CHO+CH4         5.000E+10      0.0
7300.0      !<PAG,Ulisier paras. des m̃tathises d'atome H allylique
secondaire>!
C2H3OH+R4CH3=R13CH2CHO+CH4         2.0E-6         5.6         2.5E+3
!Ac̃tald̃hyde! (216, -216)<BAULCH94>!Nancy! T=300-125

!C2H3OH+R11C2H5=R13CH2CHO+C2H6      0.740          3.5         4140.0
!<PAG,Ulisier paras. des m̃tathises d'atome H allylique secondaire>!
C2H3OH+R11C2H5=R13CH2CHO+C2H6      1.3E12         0.0         8.5E3
!Ac̃tald̃hyde! (218, -218)<HOHLEIn70>

C2H3OH=CH3CHO                        4.5E+06        1.8         5.1E+4
!Prof. Fournet
!!C2H3OH=CH3CHO                       8.590E+11      0.318      55900.00
! DaSilva 2006!
!!                                     REV/  1.050E+09    1.202
66300.00 /

!C2H3OH+R3OOH=CH3CHO+R3OOH          1.49E+05        1.67        6810.0
!P=1atm, T=300-2000K!Da silva 2009, Chem Phys Letters 483, 25-29
C2H3OH+R1H=CH3CHO+R1H                1.00E+13        0.00        1506.0
!T=300-2000K!form observation in Huynh et al 2009, j phys chem A
113,3177-3185:

!"The rate of this reaction is close to that of the H addition to C2H4:
C2H4 + H=C2H5, ref: Warnatz 1984

C2H3OH+R2OH=R4CH3+C02+H2             1.40E+12        0.00        -1040.0
!Nancy, tableau A-I-5
!C2H3OH+R2OH=HCHO+R6CH2OH           1.40E+12        0.00        -1040.0
!Nancy, tableau A-I-5

!C2H4+OH<=>C2H3OH+H                 1.070E+04        2.600      4133.00
!Senosiain et al 2006
C2H4Z+R2OH=C2H3OH+R1H                4.000E+12        0.000      4880.00
!Hippler et al 2000

!*****!
!*          REACTIONs OF CH3CHO          *!

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

CH3CHO+R20H=R14CH3CO+H2O 2.300E+10 0.73  
-1100.0 ! Konnov 2005!  
CH3CHO+R1H=H2+R14CH3CO 1.31E+5 2.58  
1220.0 !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-  
764.  
CH3CHO+R4CH3=R14CH3CO+CH4 2.0E-6 5.6  
2.5E+3 !(216, -216)<BAULCH94>! T=300-1250K  
CH3CHO+B10=R14CH3CO+R20H 1.4E+13 0.  
2.3E3 !(219, -219)<CAVAnAGH90>!  
CH3CHO+R10C2H3V=C2H4Z+R14CH3CO 8.1E10 0.  
3.7E3 !(217, -217)<SCHERZER87>T=480-520K!NIST  
CH3CHO+R11C2H5=C2H6+R14CH3CO 1.3E12 0.  
8.5E3 !(218, -218)<HOHLEIn70>!  
CH3CHO+R7CH3O=R14CH3CO+CH3OH 5.000E+12 0.0  
0.0 !Konnov 2005!  
CH3CHO+R13CH2CHO=CH3CHO+R14CH3CO 3.000E+12 0.0  
11200.0 !Konnov 2005!

!CH3CHO+R20H=R13CH2CHO+H2O 1.600E+13 0.0  
2000.0 !T=1000-1700K, P=1.2-2.8 atm. ref: Yasunaga et al 2008, J  
Chem Kin 2008,40,73-102  
CH3CHO+R20H=R13CH2CHO+H2O 3.370e+11 0.0  
-619.98 !Mech Sandiego=ref:Juan Li's PhD thesis!  
!CH3CHO+R1H=R13CH2CHO+H2 4.40E+14 0.0  
10.0E+3 !NIST! 2008YAS/KUB73-102! T=1000-1700K, P=1.2-2.8 atm  
CH3CHO+R1H=R13CH2CHO+H2 2.72E+03 3.1  
5206.5 !T=200-2500K!Klippenstein et al.2010. J Phys Chem A,114,755-  
764.  
!CH3CHO+R4CH3=R13CH2CHO+CH4 6.00E+12 0.0  
11000.0 !2008YAS/KUB73-102!T=1000-1700K, P=1.2-2.8 atm  
CH3CHO+R4CH3=R13CH2CHO+CH4 2.45E+1 3.15  
5727.0 !Marinov 1998  
CH3CHO+B10=R13CH2CHO+R20H 3.720E+13 -0.2  
3556.0 !Marinov 1998

!\*\*\*\*\* REACTIONS DE C2H5 \*\*\*\*\*!

R11C2H5+R10C2H3V=>C4H8Y 1.5E13 0. 0. !  
(61, -61)<TSAng86>!  
!R11C2H5+R11C2H5=>C4H10 1.1E13 0. 0. !  
(65, -65)<BAULCH94>!

!\*\*\*\*\* REACTIONS RAJOUTEES POUR TENIR COMPTE DE L ACROLEINE \*\*\*\*\*!

C2H3CHO+R20H=CH2CHCO+H2O 1.0E13 0.0 0.0 !  
<MARInOV>!  
C2H3CHO+B10=CH2CHCO+R20H 7.2E12 0.0 2.0E3 !  
<MARInOV>!

C2H3CHO+B10=CH2COZ+R5CHO+R1H <MARInOV>!	5.0E7	1.76	0.08E3 !
C2H3CHO+R1H=CH2CHCO+H2 <MARInOV>!	4.0E13	0.0	4.2E3 !
C2H3CHO+R1H=C2H4Z+R5CHO <MARInOV>!	2.0E13	0.0	3.5E3 !
C2H3CHO+O2=CH2CHCO+R3OOH <MARInOV99>+ MF correlation Baptiste	3.0E13	0.0	38.5E3 !
CH2CHCO=R10C2H3V+B2CO <MARInOV>!	1.0E14	0.0	34.0E3 !
CH2CHCO+B10=R10C2H3V+CO2 <MARInOV>!	1.0E14	0.0	0.0 !
C3H5Y+R300H=>C2H3CHO+R1H+R20H <TSAng91>!	7.0E18	-2.0	0.0 !
C3H5Y+O2=C2H3CHO+R20H <BOZELLI93>!	1.8E13	-0.41	22.9E3 !
C3H5Y+B10=C2H3CHO+R1H <SLAGLE92>!	1.8E14	0.0	0.0 !

!\*\*\*\*\*!  
! REACTIONS DES ESPECES NON OXYGENNS EN C3 !  
!\*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C3H2 \*\*\*\*\* (CHCCH(..))\*\*\*\*\*!

B4CH+C2H2=C3H2+R1H <MILLER92/BAULCH94>!	2.1E14	0.0	-0.5E3 !
C3H2+B10=R9C2H+R1H+B2CO <PEETERS97>!	3.0E13	0.0	0.0 !
C3H2+R20H=C2H2+R5CHO <MILLER92>!	5.0E13	0.0	0.0 !
C3H2+O2=R12CHCOZ+B2CO+R1H <MILLER92>!	5.0E13	0.0	0.0 !

!\*\*\*\*\* REACTIONS DE C3H3 \*\*\*\*\* (CHCCH2(..)) Propargyl\*\*\*\*\*stabilise par resonance !

B6CH2+C2H2=C3H3+R1H <MILLER87/BAULCH94>!	1.8E14	0.0	0.0 !
C3H3+R1H=C3H2+H2 <MILLER92/BRAUn89>!	2.0E13	0.0	0.0 !
C3H3+B10=R9C2H+HCHO <MILLER92/SLAGUE91>!	1.4E14	0.0	0.0 !
C3H3+R20H=C3H2+H2O <MILLER92>!	2.0E13	0.0	0.0 !
C3H3+R20H=R10C2H3V+R5CHO <WAnG97>!	4.0E13	0.0	0.0 !
C2H2+R12CHCOZ=C3H3+B2CO <MILLER92>!	1.0E11	0.0	3.0E3 !
C3H3+O2=CH2COZ+R5CHO <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3 !
C3H2+R1H=C3H3 <est>!	1.0E14	0.0	0.0 !



C3H3+R300H=>R20H+R9C2H+HCHO <Heyberger>!	1.0E15	-0.8	0.0	!
C3H3+C3H3=C6H6# <STEIn90>shocktube!	1.0E12	0.0	0.0	!
C3H3+C3H3=C6H5#+R1H <STEIn90>flame!	1.0E12	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE pC3H4 \*\*\*\*\* (CH3CCH) Propyne \*\*\*\*\*!

!pC3H4=>aC3H4 !<HIDAKA89>!	2.1E12	0.0	60.0E3	
pC3H4+M=C3H3+R1H+M !<HIDAKA89>!	4.7E18	0.0	80.0E3	
C2H2+B5CH2=pC3H4 !<TSAnG86>!	3.5E12	0.0	0.0	
pC3H4=R9C2H+R4CH3 <KInGAS1500>!	4.2E15	0.0	125.0E3	!
pC3H4+O2=C3H3+R300H <est Ingham>!	2.1E12	0.0	40.8E3	!
pC3H4+R1H=C2H2+R4CH3 <hidaka89> !	1.3E5	2.5	1.00E3	!
pC3H4+R1H(+M)=tC3H5(+M) <WAGnER72>!	8.5E12	0.0	1.7E3	!
LOW /5.6E25	-7.27	6.58E3/		
!<Marinov97>!				
pC3H4+R1H(+M)=sC3H5(+M) <WAGnER72>!	5.8E12	0.0	3.1E3	!
LOW /3.8E25	-7.27	7.98E3/		
!<estimated>!				
pC3H4+R4CH3=C3H3+CH4 <asTSAnG91>!	2.2E0	3.5	5.7E3	!
pC3H4+R1H=C3H3+H2 <asTSAnG91>	1.7E5	2.5	2.5E3	!
pC3H4+R9C2H=C3H3+C2H2 !<asTSAnG91>!	3.6E12	0.0	0.0	
pC3H4+R10C2H3V=C3H3+C2H4Z <asTSAnG91>!	2.2E0	3.5	4.7E3	!
pC3H4+R11C2H5=C3H3+C2H6 <asTSAnG91>!	2.2E0	3.5	6.6E3	!
pC3H4+B10=R12CHCOZ+R4CH3 <WARnATZ84>!	1.5E13	0.0	2.1E3	!
pC3H4+B10=R20H+C3H3 <<ADUSEI, G.Y, 1996>>!	3.4E4	2.16	4.8E3	!
pC3H4+R20H=CH2COZ+R4CH3 <BOODAGHIANs87>!	4.3E11	0.0	-0.8E3	!
pC3H4+R20H=R1H+C2H3CHO <asBOODAGHIANs87>!	4.3E11	0.0	-0.8E3	!
pC3H4+R20H=C3H3+H2O <asTSAnG91>!	3.1E6	2.0	-0.3E3	!

pC3H4+R300H=C2H4Z+B2C0+R20H as296<TSAnG86>!	6.0E9	0.0	8.0E3	!
pC3H4+R300H=C3H3+H202 <asTSAnG91>!	9.6E3	2.6	13.9E3	!
pC3H4+R7CH30=CH30H+C3H3 <Heyberger>!	2.0E12	0.0	4.0E3	!

!\*\*\*\*\* REACTIONS DE aC3H4 \*\*\*\*\* (CH2CCH2) Allene \*\*\*\*\*!

aC3H4=pC3H4 <HIDAKA89>!	2.5E12	0.0	59.0E3	!
aC3H4+M=C3H3+R1H+M <HIDAKA89>!	2.0E18	0.0	80.0E3	!
aC3H4+O2=C3H3+R300H <Estimation Ingham>!	2.8E13	0.0	39.0E3	!
aC3H4+R1H(+M)=C3H5Y(+M) 2.7E3 !<WAGnER72>!		4.0E12	0.0	
LOW /5.6E33 -5.0 4.44E3/ !<Marinov97> !				
aC3H4+R1H(+M)=tC3H5(+M) <WAGnER72>!	8.5E12	0.0	2.0E3	!
LOW /1.1E34 -5.0 4.44E3/ !<Marinov97>!				
C2H4Z+B4CH=aC3H4+R1H <BAULCH94base>!	1.3E14	0.0	-0.3E3	!
R10C2H3V+B5CH2=aC3H4+R1H <MILLER92>!	3.0E13	0.0	0.0	!
iC4H3+B5CH2=aC3H4+R9C2H <MILLER92>!	2.0E13	0.0	0.0	!
aC3H4+B10=R1H+B2C0+R10C2H3V <Aleksandrev nist>!	6.6E12	0.0	3.0E3	!
aC3H4+R20H=CH2COZ+R4CH3 <LIU88>!	2.0E12	0.0	-0.2E3	!
aC3H4+R20H=HCHO+R10C2H3V <LIU88>!	2.0E12	0.0	-0.2E3	!
aC3H4+R1H=C3H3+H2 <est.butatiene>!	1.3E6	2.53	9.2E3	!
aC3H4+B10=C3H3+R20H <fromAleksandrev nist>!	6.2E12	0.0	1.9E3	!
!d'après leur vitesse de réaction total et d'addition !				
aC3H4+R20H=C3H3+H20 <est.butadiene>!	6.2E6	2.0	0.4E3	!
aC3H4+R4CH3=C3H3+CH4 <WU87>!	2.0E12	0.0	7.7E3	!
aC3H4+R9C2H=C3H3+C2H2 <WU87>!	1.0E13	0.0	0.0	!
aC3H4+C3H5Y=C3H3+C3H6Y <DAGAUT92>	2.0E12	0.0	7.7E3	!
aC3H4+R7CH30=CH30H+C3H3 9.6E3 !<correlations a partir de Heyberger>!		4.0E12	0.0	
aC3H4+R11C2H5=C2H6+C3H3 !<asbutadiene>!	5.0E14	0.0	19.8E3	

aC3H4+R10C2H3V=C2H4Z+C3H3 <asbutadiene>!	5.0E14	0.0	19.8E3	!
!aC3H4+R4CH3=C4H7T <Scherzer>!	5.7E10	0.0	6.8E3	!
!aC3H4+R4CH3=C4H7T !<Tsang91x2>!	3.4E11	0.0	7.4E3	
!aC3H4+R4CH3=iC4H7 !<Tsang73>!	1.6E11	0.0	5.0E3	
!aC3H4+R4CH3=C4H7T 7.4E3 !<Tsang91x2/4>!	0.8E11	0.0		
aC3H4+R4CH3=iC4H7 !<Tsang73/3>!	0.4E11	0.0	5.0E3	

!fort effet de fall off, environ un facteur 4 pour 6.7 kPa et 1100 K (Tsang91)!

!aC3H4+C3H3=C6H6#+R1H <HIDAKA89>!	1.4E12	0.0	10.0E3	!
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!\*\*\*\*\* REACTIONS DE cC3H4 \*\*\*\*\* cyclopropene \*\*\*\*\*!

cC3H4=aC3H4 <Karni>	1.5E14	0.0	50.5E3	!
cC3H4=pC3H4 <Karni>	7.1E13	0.0	47.8E3	!
cC3H4+R1H=cC3H3+H2 <Heyberger>!	5.4E4	2.5	-1.9E3	!
cC3H4+R20H=cC3H3+H2O <Heyberger>!	3.0E6	2.0	-1.5E3	!
cC3H4+R20H=C2H4Z+R5CHO <Heyberger>!	2.8E12	0.0	-1.0E3	!
cC3H3+R300H=R20H+C2H2+R5CHO <Heyberger>!	1.0E15	-0.8	0.0	!
cC3H3+R4CH3=cC4H6 <estimation>!	1.0E13	0.0	0.0	!
cC3H3+R1H=cC3H4 <estimation>!	1.0E14	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE C3H5Y \*\*\*\*\* (CH2CHCH2(.)) Allyl \*\*\*\*\*stabilise par resonance !

!C3H5Y+R1H=C3H6Y <TSAnG91>!	2.0E13	0.0	0.0	!
C3H5Y+R1H=aC3H4+H2 TSANG 91!* C3H5Y+R1H=C3H6Y <allara>!!	1.8E13	0.0	0.0	!
	1.0E14	0.0	0.0	!

!rñaction importante pour la formation de propine!

C3H5Y+R4CH3=aC3H4+CH4 <TSAnG91>!	3.0E12	-0.32	-0.1E3	!
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C3H5Y+R4CH3=C4H8Y <TSAnG91>!	1.0E14	-0.32	-0.1E3	!
C3H5Y+R20H=aC3H4+H2O Tsang 91! !peu d'effet de fall off!	6.03E12	0.0	0.0	!
C3H5Y+R10C2H3V=aC3H4+C2H4Z <TSAnG91>!	2.4E12	0.0	0.0	!
!C3H5Y+R11C2H5=aC3H4+C2H6 <TSAnG91>!	9.6E11	0.0	-0.1E3	!
C3H5Y+R11C2H5=aC3H4+C2H6 <TSAnG91>MODIF!!!!	2.0E13	0.0	-0.1E3	!
C3H5Y+B10=R10C2H3V+HCHO <SLAGLE90,LEUnG95>!	1.8E14	0.0	0.0	!
!processus non elementaire impliquant la formation-decomposition de l'hydroperoxyde				
!C3H5Y+C3H3=C6H6#+2R1H <MARInOV97>!	5.6E20	-2.535	1.7E3	!
C3H5Y+C3H5Y=aC3H4+C3H6Y <TSAnG91>!	8.4E10	0.0	-0.3E3	!

!\*\*\*\*\* REACTIONS DE sC3H5 \*\*\*\*\* (CH3CHCH(.)) 2-methyl vinyl \*\*\*\*\*!

sC3H5=C3H5Y <WEISSMAN89>!	5.0E13	0.0	37.0E3	!
R4CH3+C2H2=sC3H5 <BAULCH94>!	6.0E11	0.0	7.7E3	!

!\*\*\*\*\* REACTIONS DE tC3H5 \*\*\*\*\* (CH3C(.)CH2) 1-methyl vinyl \*\*\*\*\*!

tC3H5+R1H=aC3H4+H2 <DAGAUT90>!	3.3E12	0.0	0.0	!
tC3H5+R4CH3=aC3H4+CH4 <DAGAUT90>!	1.0E11	0.0	0.0	!
tC3H5+R10C2H3V=aC3H4+C2H4Z <LEUnG95>!	1.0E12	0.0	0.0	!
tC3H5+R11C2H5=aC3H4+C2H6 <LEUnG95>!	1.0E12	0.0	0.0	!
tC3H5+B10=CH2COZ+R4CH3 <LEUnG95>!	1.8E14	0.0	0.0	!
tC3H5+O2=R4CH3+B2CO+HCHO <DAGAUT90>!	4.3E12	0.0	0.0	!
tC3H5=C3H5Y <Weissman89>!	2.0E13	0.0	47.0E3	!

!\*\*\*\*\* REACTIONS DE C3H6Y \*\*\*\*\* (CH3CHCH2) propene \*\*\*\*\*!

C2H4Z+B6CH2=C3H6Y <BAULCH94>!	9.6E13	0.0	0.0	!
C2H4Z+B5CH2=C3H6Y <BAULCH94>!	3.2E12	0.0	5.1E3	!
!duplicate R10C2H3V+R4CH3=C3H6Y <TSAnG86>!	2.5E13	0.0	0.0	!

C2H4Z+R4CH3=C3H6Y+R1H <TSAnG86>!	6.6E11	0.0	15.9E3	!
R11C2H5+B6CH2=C3H6Y+R1H <TSAnG86>!	9.0E12	0.0	0.0	!
C2H6+B4CH=C3H6Y+R1H <BAULCH94>!	1.1E14	0.0	-0.3E3	!
C3H6Y+R1H=sC3H5+H2 <TSAnG92>!	7.83E5	2.5	12.28E3	!
C3H6Y+R1H=tC3H5+H2 <TSAnG92>!	3.9E5	2.5	5.82E3	!
C3H6Y+R1H=C3H5Y+H2 <TSAnG91>!	1.7E5	2.5	2.5E3	!
C3H6Y+R4CH3=C3H5Y+CH4 <TSAnG91>!	2.2E0	3.5	5.7E3	!
C3H6Y+R4CH3=sC3H5+CH4 <TSAnG91>!	8.4E-1	3.5	11.7E3	!
C3H6Y+R4CH3=tC3H5+CH4 <TSAnG91>!	1.3E0	3.5	12.9E3	!
C3H6Y+R11C2H5=C3H5Y+C2H6 <TSAnG91>!	2.2E0	3.5	6.6E3	!
!C3H6Y+B10=>CH2COZ+R1H+R4CH3 <TSAnG91>! MF!!ds мйса PRF	1.2E+5	2.56	-1130.0	!
C3H6Y+B10=C3H5Y+R20H <TSAnG91>!	1.7E11	0.7	5.9E3	!
!C3H6Y+R20H=HCHO+R11C2H5 <TSAnG91>! MF!!ds мйса PRF	1.45E12	0.0	-0.9E3	!
!C3H6Y+R20H=R4CH3+CH3CHO <TSAnG91>! MF!!ds мйса PRF	1.45E12	0.0	-0.9E3	!
C3H6Y+R20H=C3H5Y+H20 <TSAnG91>!	3.1E6	2.0	-0.3E3	!
C3H6Y+R20H=sC3H5+H20 <TSAnG91>!	1.1E6	2.0	1.45E3	!
C3H6Y+R20H=tC3H5+H20 <TSAnG91>!	2.1E6	2.0	2.8E3	!
C3H6Y+O2=C3H5Y+R300H <WALKER93>!	1.9E12	0.0	39.0E3	!
C3H6Y+R300H=C3H5Y+H202 <TSAnG91>!	9.6E3	2.6	13.9E3	!
C3H6Y+R9C2H=pC3H4+R10C2H3V 91 mehdi!	1.2E13	0.0	0.0	!TSANG

!\*\*\*\*\* REACTIONS DE cC3H6 \*\*\*\*\* cyclopropane \*\*\*\*\*!

cC3H6=C3H6Y <Hidaka87>!	4.6E14	0.0	62.6E3	!
cC3H6+R1H=C3H5Y+H2 <Marshall86>!	1.6E14	0.0	11.7E3	!
cC3H6+R20H=C3H5Y+H20 <Dobe82>!	7.0E7	1.5	1.0E3	!
cC3H6+R4CH3=C3H5Y+CH4 <Exgas>!	2.0E11	0.0	9.6E3	!

!\*\*\*\*\* REACTIONS DE R19C3H7 et iC3H7 \*\*\*\*\* CH3CH2CH2(.) et CH3CH(.)CH3  
 \*\*\*\*\* !

!R19C3H7 = R4CH3+C2H4Z	6.400E+12	0.00	31000.0!!
ds мйса PRF			
!R19C3H7 = R1H+C3H6Y	3.000E+13	0.00	38000.00!!
ds мйса PRF			
iC3H7 = R1H+C3H6Y	6.000E+13	0.00	39000.00
R19C3H7 = iC3H7	1.960E+10	1.00	38600.00
!R19C3H7+O2 =R300H+C3H6Y	1.600E+12	0.00	5000.00
R19C3H7+O2 =R300H+C3H6Y	3.7e16	-1.63	3420 !
2003DES/KLI4415-4427			
iC3H7+O2 = R300H+C3H6Y	1.400E+12	0.00	5000.00

!\*\*\*\*\* Propane (C3H8) chemistry \*\*\*\*\*!

R11C2H5+R4CH3=C3H8	3.4E13	0.	0.	!(59, -
59)<BAULCH94>!				
C3H8+O2=>R300H+iC3H7	1.4E+0013	0.000	50323.7	! BI 2 CN
C3H8+O2=>R300H+R19C3H7	4.2E+0013	0.000	53033.0	! BI 3 CN
B10+C3H8=>R20H+iC3H7	2.6E+0013	0.000	5200.0	! ME 15 CW
B10+C3H8=>R20H+R19C3H7	1.0E+0014	0.000	7850.0	! ME 16 CW
C3H8+R1H=>H2+iC3H7	9.0E+0006	2.000	5000.0	! ME 17 CW
!C3H8+R1H=>H2+R19C3H7	5.7E+0007	2.000	7700.0	! ME 18 CW!!ds
мйса PRF				
C3H8+R20H=>H2O+iC3H7	2.6E+0006	2.000	-765.0	! ME 19 CW
!C3H8+R20H=>H2O+R19C3H7	5.4E+0006	2.000	450.0	! ME 20 CW!!ds
мйса PRF				
C3H8+R300H=>H2O2+iC3H7	4.0E+0011	0.000	15500.0	! ME 21 CN
!C3H8+R300H=>H2O2+R19C3H7	1.2E+0012	0.000	17000.0	! ME 22 CN!!ds
мйса PRF				
C3H8+R4CH3=>CH4+iC3H7	2.0E+0011	0.000	9600.0	! ME 23 CN
!C3H8+R4CH3=>CH4+R19C3H7	6.0E-0001	4.000	8200.0	! ME 24 CN!!ds
мйса PRF				
C3H8+R5CH0=>HCHO+iC3H7	1.0E+0007	1.900	17000.0	! ME 25 CN
C3H8+R5CH0=>HCHO+R19C3H7	2.0E+0005	2.500	18500.0	! ME 26 CN
C3H8+R11C2H5=>C2H6+iC3H7	2.0E+0011	0.000	11000.0	! ME 33 CN
!C3H8+R11C2H5=>C2H6+R19C3H7	6.0E+0011	0.000	13500.0	! ME 34 CR!!ds
мйса PRF				
C3H8+iC3H7=>C3H8+R19C3H7	8.4E-0003	4.200	8700.0	! ME 35 CN
R1H+iC3H7=>C3H8	8.3E+0012	0.000	0.0	! CO 36 K

!\*\*\*\*\*Reactions of Acetone\*\*\*\*\*!

!R14CH3CO+R4CH3=>C2H6CO	4.0E15	-0.8	0. !
(231, -231)<TSAnG86>!			
R14CH3CO+R4CH3=>C2H6CO	2.7E15	-0.8	0. !
(231, -231)<TSAnG86>! A/1.5 to improve the agreement simu/exp at low pressure.			
iC3H7+B10=>C2H6CO+R1H	1.0	0.0	0.0 !
Tsang88 (Nist)			
C2H6CO+O2=>R300H+CH2COZ+R4CH3	4.2E12	0.0	49.28E3 !
Kingas!			
C2H6CO+B10=>CH2COZ+R4CH3+R20H	1.02E14	0.0	7.85E3 !
Buda!			

C2H6CO+R1H=>CH2COZ+R4CH3+H2	5.70E07	2.0	7.70E3
C2H6CO+R20H=>CH2COZ+R4CH3+H2O	5.34E06	2.0	0.45E3
C2H6CO+R4CH3=>CH2COZ+R4CH3+CH4	6.00E-1	4.0	8.20E3
C2H6CO+R300H=>CH2COZ+R4CH3+H2O2	1.20E12	0.0	17.0E3

!\*\*\*\*\*Reactions of Propanal\*\*\*\*\*!

!R5CHO+R11C2H5=>C2H5CHO	1.8E13	0.	0.
!(141, -141)<TSAng86>!			
!C2H5CHO=R5CHO+R11C2H5	1.07E+14	0.0	62600
!Decottignies et al.COMBT.FLAME 2002, 130, 225-240			
R5CHO+R11C2H5=C2H5CHO	3.4E+13	0.0	0.0
!= "CH3+C2H5=C3H8".			
!C2H5CHO=R5CHO+R11C2H5	2.45E+15	0.0	72864.5
!Lifshitz et al.J. Phys. Chem., 94 (1990)			
R13CH2CHO+R4CH3=C2H5CHO	3.4E+13	0.0	0.0
!= "CH3+C2H5=C3H8".			
!C2H5CHO=R13CH2CHO+R4CH3	1.000e+17	0.0	8.465e+04 !
asC4H10 Dean, J.Phys.Chem. 89 (1985) 4600-4608			
!C2H5CHO=R4CH3+R13CH2CHO	7.00E+15	0	81703
!Baulch et al 1992, J. Phys.Chem.Ref.Data 21 411-429.			
B10+C3H6Y=>C2H5CHO	1.000E+12	0	5000.0
!Mech Franssoldati			
!C2H5CHO+R1H=H2+B2CO+R11C2H5	4.0E13	0.0	4.2E3
!<Heyberger>! ADZ 714			
!C2H5CHO+R20H=H2O+B2CO+R11C2H5	4.0E12	0.0	0.5E3
!<Heyberger>! ADZ 715			
!C2H5CHO=R4CH3+R13CH2CHO	2.00E+16	0	83800.
!Mech Franssoldati			
C2H5CHO+R1H=H2+R25C2H5CO	1.17E+11	0.0	6000
!Decottignies et al.2002.			
!C2H5CHO+R1H=R25C2H5CO+H2	1.200E+14	0.00	7000.0 !
Yasunaga et			
C2H5CHO+B10=R20H+R25C2H5CO	5.000e+12	0.0	
1.790e+03 !Curran et al. Fuel (2011) 90(1) 331-338.			
C2H5CHO+R20H=H2O+R25C2H5CO	2.690e+10	0.760	
-3.400e+02 !Curran et al. Fuel (2011) 90(1) 331-338.			
!C2H5CHO+R20H=R25C2H5CO+H2O	2.650E+12	0.00	-730.0 !
Atkinson et			
R25C2H5CO=B2CO+R11C2H5	2.95E+12	0.0	11100.0
!Decottignies et al.2002.			
!R25C2H5CO=>R11C2H5+B2CO	1.834e+15	-0.73	1.291e+04
!Glaude et a			

!\*\*\*\*\*

!\*\*\*\*\*

!\*\*\*\*\*!  
! REACTIONS DES ESPECES NON OXYGENES EN C4 !  
!\*\*\*\*\*!

!\*\*\*\*\* REACTIONS DE C4H2 \*\*\*\*\* (CH//CC//CH) diacetylene \*\*\*\*\* !

R9C2H+R9C2H=C4H2 <TSAng86>!	1.8E13	0.0	0.0	!
2C2H2=C4H2+H2 <LEUnG95>!	1.5E13	0.0	42.7E3	!
C2H2+R9C2H=C4H2+R1H BAULCH94!	9.0E13	0.0	0.0	!
!C4H2+R1H=C2H2+R9C2H <MEREDITH86>!	6.0E14	0.0	15.4E3	!
C4H2+R20H=>R5CHO+C3H2 <LEEDS-website>!	6.7E12	0.0	-0.4E3	!
C4H2+O2=R12CHCOZ+R12CHCOZ <HIDAKA02>!!!	9.6E12	0.0	31.1E3	!
C4H2+R9C2H=>C6H2+R1H <MEREDITH86>!	4.0E13	0.0	0.0	!
C6H2+R1H=>C4H2+R9C2H <MEREDITH86>!	9.3E14	0.0	15.1E3	!

!\*\*\*\*\* REACTIONS DE nC4H3 \*\*\*\*\* (ΓCH//CHC//CH) \*\*\*\*\*!

nC4H3(+M)=C4H2+R1H(+M) <MILLER92>!	1.0E14	0.0	36.0E3	!
LOW /1.0E14 0.0 30E3/ TROE / 1.0 1.0 1.0E8/				
C3H3+B4CH=nC4H3+R1H <MILLER92>!	7.0E13	0.0	0.0	!
!C3H3+B4CH=nC4H3+R1H <MILLER92>!	5.0E13	0.0	0.0	!
R9C2H+R10C2H3V=nC4H3+R1H <TSAng86>!	1.8E13	0.0	0.0	!
nC4H3+R1H=iC4H3+R1H <WAnG97>20Torr!	2.4E11	0.79	2.41E3	!
nC4H3+R1H=C4H2+H2 <0.5* la cst de la react(c2h3+h)>!	0.6E13	0.0	0.0	!
2C2H2=nC4H3+R1H <LEUnG95>!	1.0E12	0.0	64.1E3	!
nC4H3+R20H=C4H2+H2O <0.5* la cst de la react(c2h3+oh)>!	1.5E13	0.0	0.0	!
!***				
!nC4H3+C2H2=C6H4#+R1H <WESTMORELANd89, p=2.6kPa>!	1.64E9	0.73	12.2E3	!
nC4H3+C2H2=C6H4#+R1H <WESTMORELANd89, p=101kPa>!	3.0E-11	6.48	6.6E3	!
!***				
!nC4H3+C2H2=1C6H4+R1H <WESTMORELANd89, p=2.6kPa>!	29.6	3.33	9.6E3	!
nC4H3+C2H2=1C6H4+R1H <WESTMORELANd89, p=101kPa>!	2.77E-7	5.59	6.0E3	!
!***				
!nC4H3+C2H2=1C6H5 <WESTMORELANd89, p=2.6kPa>!	1.73E11	-0.41	4.0E3	!



nC4H3+C2H2=1C6H5 <WESTMORELANd89, p=101kPa>! !***	6.17E15	-1.51	4.8E3	!
!nC4H3+C2H2=C6H5# <WESTMORELANd89, p=2.6kPa>! nC4H3+C2H2=C6H5# <WESTMORELANd89, p=101kPa>! !***	3.33E24	-3.89	9.2E3	!
	7.0E14	-0.86	6.4E3	!

!\*\*\*\*\* REACTIONS DE iC4H3 \*\*\*\*\* (CH2//CΓC///CH) \*\*\*\*\*

iC4H3=nC4H3 <LEUnG95>!	1.5E13	0.0	67.8E3	!
iC4H3(+M)=C4H2+R1H(+M) <MILLER92>!	1.0E14	0.0	55.0E3	!
LOW /2.0E15 0.0 48E3/ TROE /1.0 1.0 1.0E8/				
C3H2+B5CH2=iC4H3+R1H as(7)<BAULCH94>!	1.2E14	0.0	0.8E3	!
iC4H3+R1H=2C2H2 <WAnG97>20Torr! !	2.40E19	-1.6	2800	!
C3H3+B4CH=iC4H3+R1H <MILLER92>!	7.0E13	0.0	0.0	!
iC4H3+R1H=C4H2+H2 <equiv a la cst de la react(c2h3+h)>!	1.2E13	0.0	0.0	!
iC4H3+B10=CH2COZ+R9C2H <MILLER92>!	2.0E13	0.0	0.0	!
iC4H3+R20H=C4H2+H2O <equiv a la cst de la react(c2h3+oh)>!	3.0E13	0.0	0.0	!<
iC4H3+O2=CH2COZ+R12CHCOZ <MILLER92>!	1.0E12	0.0	0.0	!
*				
iC4H3+R10C2H3V=2C3H3 MILLER 92 !	4.0E12	0.0	0.0	!
iC4H3+R10C2H3V=>1C6H5+R1H MILLER 92!	6.0E12	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE C4H4 \*\*\*\*\* (CH2//CHC///CH) vinylacetylene \*\*\*\*\*!

C3H3+B5CH2=C4H4+R1H <MILLER92>!	4.0E13	0.0	0.0	!
R10C2H3V+C2H2=>C4H4+R1H (40, -40)<DOUTE95>!	2.0E13	0.0	25.1E3	!
C4H4+R1H=>R10C2H3V+C2H2 <DOUTE95>	2.0E13	0.0	12.4E3	!
C2H4Z+R9C2H=C4H4+R1H (50, -50)<TSAnG86>!	1.2E13	0.0	0.0	!
C4H4+R1H=nC4H3+H2 <Miller 92>!	2.0E7	2.0	15.E3	!
C4H4+R1H=iC4H3+H2 <Miller 92>!	3.0E7	2.0	5.E3	!
R9C2H+C4H4=>C2H2+iC4H3 <MEREDITH86>!	4.0E13	0.0	0.0	!

C2H2+iC4H3=>R9C2H+C4H4 <MEREDITH86>!	3.0E13	0.0	27.9E3 !
R10C2H3V+C4H4=>C2H4Z+nC4H3 <MEREDITH86>!	5.0E11	0.0	16.3E3 !
nC4H3+C2H4Z=>R10C2H3V+C4H4 <MEREDITH86>!	3.5E11	0.0	13.4E3 !
R10C2H3V+C4H4=>C2H4Z+iC4H3 <MEREDITH86>!	5.0E11	0.0	16.3E3 !
iC4H3+C2H4Z=>R10C2H3V+C4H4 <MEREDITH86>!	1.3E11	0.0	24.1E3 !
C4H4+C2H2=C6H5#+R1H BENSON !MF	1.0E09	0.0	30.02E3 !
C4H4+R10C2H3V=C6H6#+R1H <LInSTEDT96>!	1.9E12	0.0	2.5E3 !
C4H4+B10=aC3H4+B2C0 <LEUnG95>!	3.0E13	0.0	1.8E3 !
C4H4+B10=pC3H4+B2C0 <MILLER>!	2.7E13	0.0	1.8E3 !
C4H4+R20H=nC4H3+H20 <MILLER92>!	7.5E6	2.0	5.0E3 !
C4H4+R20H=iC4H3+H20 <MILLER92>!	1.0E7	2.0	2.0E3 !
aC3H4+aC3H4=C2H4Z+C4H4 <HIDAKA89>!	1.0E15	0.0	48.0E3 !

!\*\*\*\*\* REACTIONS DE tC4H4 \*\*\*\*\* (CH2//C//C//CH2) \*\*\*\*\*!

tC4H4+R20H=iC4H3+H20 <Marinov>!	2.0E7	2.0	2.0E3 !
tC4H4+R1H=iC4H3+H2 <Marinov>!	3.0E7	2.0	6.0E3 !

!\*\*\*\*\* REACTIONS DE nC4H5 \*\*\*\*\* (ΓCH//CHCH//CH2) \*\*\*\*\*

nC4H5(+M)=R1H+C4H4(+M) <MILLER92>!	1.0E14	0.0	37.0E3 !
LOW /1.00e+14 0.0 30000/			
nC4H5+R1H=C4H4+H2 <WAnG97>!	1.5E13	0.0	0.0 !
nC4H5+R1H=iC4H5+R1H <MILLER92>!	1.0E14	0.0	0.0 !
nC4H5+R4CH3=C5H8 <estimated> !	1.0E13	0.0	0.0 !
nC4H5=C2H2+R10C2H3V <HIDAKA96>!	1.0E14	0.0	43.9E3 !
!*** !MF car lC6H6 n'intervient qu'ici			
!nC4H5+C2H2=lC6H6+R1H <WESTMORELANd89, p=2.6kPa>!	1.17E-15	7.84	2.0E3 !
!nC4H5+C2H2=lC6H6+R1H <WESTMORELANd89, p=101kPa>!	3.47E-15	7.73	2.5E3 !
!***			

!nC4H5+C2H2=C6H6#+R1H	1.90E7	1.47	4.2E3 !
<WESTMORELANd89, p=2.6kPa>!			
nC4H5+C2H2=C6H6#+R1H	2.38E8	1.18	3.7E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
!nC4H5+C2H2=1C6H7	8.74E12	-1.27	3.6E3 !
<WESTMORELANd89, p=2.6kPa>!			
nC4H5+C2H2=1C6H7	7.24E14	-1.38	4.0E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
!nC4H5+C2H2=C6H7#	1.96E19	-3.35	5.2E3 !
<WESTMORELANd89, p=2.6kPa>!			
nC4H5+C2H2=C6H7#	7.12E21	-3.64	6.3E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
!R10C2H3V+nC4H5=1C6H7+R1H	8.28E-28	11.89	5.0E3 !
<WESTMORELANd89, p=2.6kPa>!			
R10C2H3V+nC4H5=1C6H7+R1H	3.55E-43	16.16	-0.2E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
!R10C2H3V+nC4H5=1C6H8	2.90E15	-0.78	1.0E3 !
<WESTMORELANd89, p=2.6kPa>!			
R10C2H3V+nC4H5=1C6H8	1.50E13	-0.075	0.1E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
!R10C2H3V+nC4H5=C6H8#	5.50E15	-1.67	1.5E3 !
<WESTMORELANd89, p=2.6kPa>!			
R10C2H3V+nC4H5=C6H8#	8.53E13	-1.11	0.8E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
!R10C2H3V+nC4H5=C6H6#+H2	2.80E-7	5.63	-1.9E3 !
<WESTMORELANd89, p=2.6kPa>!			
R10C2H3V+nC4H5=C6H6#+H2	1.84E-13	7.07	-3.6E3 !
<WESTMORELANd89, p=101kPa>!			
!***			
nC4H5+R20H=C4H4+H2O	2.5E12	0.0	0.0 !
<WAnG97>!			
!nC4H5+O2=R5CHO+C2H3CHO	1.7e29	-5.31	6.5E3 !MF
as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>			
nC4H5+O2=R5CHO+C2H3CHO	5.67E28	-5.31	6.5E3 !MF
nC4H5+O2=C2H4Z+B2CO+R5CHO	1.13e29	-5.31	6.5E3 !MF
nC4H5+O2=C4H4+R300H	5.19E15	-1.26	3.31e3 !
MF as O2+C2H3=HCHO+CHO <Marinov Combust. Flame114(1998)192 - 213>			
!***** REACTIONS DE iC4H5 ***** (CH2//CHCΓ//CH2) *****stabilise par			
resonnance			
iC4H5=nC4H5	1.5E13	0.0	67.8E3 !
<LEUnG95>!			
iC4H5(+M)=R1H+C4H4(+M)	1.0E14	0.0	50.0E3 !
<MILLER92>!			
LOW /2.0E15 0.0 42000/			

iC4H5+R1H=C4H4+H2 <WAnG97>!	3.0E13	0.0	0.0	!
iC4H5+R4CH3=iC5H8 <estimated> !	1.0E13	0.0	0.0	!
2R10C2H3V=iC4H5+R1H <WAnG97>20Torr!	1.5E30	-4.95	13.0E3	!
!***2R10C2H3V=iC4H5+R1H <WAnG97>760Torr!	1.2E22	-2.44	13.7E3	!
iC4H5+R20H=C4H4+H20 <WAnG97>!	5.50E12	0.0	0.0	!
iC4H5+O2=HCHO+CH2CHCO estimй par {O2+C2H3=HCHO+CHO}!	4.5E16	-1.39	1.0E3	!
iC4H5+O2=C4H4+R300H estimй par {O2+C2H3=C2H2+O0H}!	1.34E6	1.61	-400	!

!\*\*\*\*\* REACTIONS DE C4H5-1s \*\*\*\*\* (CH3/CH<sup>Г</sup>/C///CH) \*\*\*\*\*stabililise par resonance

!C4H5-1s=R1H+C4H4 <HIDAKA96>!	3.0E13	0.0	45.0E3	!
C4H5-1s=R1H+C4H4 add inverse!	6.0E13	0.0	50.4E3	!
! Les rйactions suivantes sont deduites de celles de C3H3				
C4H5-1s+R1H=C4H4+H2 <MILLER92/BRAUn89>!	2.0E13	0.0	0.0	!
C4H5-1s+B10=R9C2H+CH3CHO <MILLER92/SLAGUE91>!	1.4E14	0.0	0.0	!
C4H5-1s+R20H=C4H4+H20 <MILLER92>!	2.0E13	0.0	0.0	!
C4H5-1s+R20H=R5CHO+sC3H5 <WAnG97>!	4.0E13	0.0	0.0	!
C4H5-1s+O2=R5CHO+B2CO+C2H4Z <MILLER92/SLAGUE88>!	3.0E10	0.0	2.9E3	!
C4H5-1s+C4H5-1s=C8H10# <STEIn90>shocktube!	1.0E12	0.0	0.0	!

!\*\*\*\*\* REACTIONS DE C4H5-1p \*\*\*\*\* (CH2<sup>Г</sup>/CH2/C///CH) \*\*\*\*\*

!C4H5-1p=R1H+C4H4 <HIDAKA96>!	3.0E13	0.0	45.0E3	!
!C4H5-1p=R1H+C4H4 <HIDAKA96>!	4.0E13	0.0	38.8E3	!
C4H5-1p=R9C2H+C2H4Z <HIDAKA96>!	2.0E14	0.0	57.0E3	!
C4H5-1p+O2=C4H4+R300H PAG00!	1.6E12	0.0	5.0E3	!
C4H5-1p=C4H5-1s PAG00!	5.0E12	0.0	37.4E3	!

!\*\*\*\*\* REACTIONS DE C4H5-2 \*\*\*\*\* (CH3/C///C/CH2<sup>Г</sup>) \*\*\*\*\*stabililise par resonance

!C4H5-2=R1H+tC4H4	3.0E13	0.0	50.0E3 !
<fromHIDAKA96>!			
C4H5-2=R1H+tC4H4	6.0E13	0.0	54.3E3 !
toto!			

!C4H5-2=iC4H5	3.0E13	0.0	50.0E3 !
<fromHIDAKA96>!			
C4H5-2=iC4H5	5.0E12	0.0	50.5E3 !
PAG00!			
C4H5-2+C4H5-2=C8H10#	1.0E12	0.0	0.0 !
<STEIn90>shocktube!			

! Les rñactions suivantes sont deduities de celles de C3H3

C4H5-2+B10=C3H3+HCHO	1.4E14	0.0	0.0 !
<MILLER92/SLAGUE91>!			
C4H5-2+R20H=R10C2H3V+B2CO+R4CH3	4.0E13	0.0	0.0 !
<WAnG97>!			
C4H5-2+O2=CH2COZ+B2CO+R4CH3	3.0E10	0.0	2.9E3 !
<MILLER92/SLAGUE88>!			

!***** REACTIONS DE C4H6Z2 ***** 1,3 Butadiene (CH2CHCHCH2) *****!			
!R10C2H3V+R10C2H3V=C4H6Z2	6.8E12	0.0	0.0 !
<TSAnG86 P=2.6KPa T=1500>!			
R10C2H3V+R10C2H3V=C4H6Z2	9.8E14	-0.5	0.0 !
<HIDAKA96shocktube>!			
!			
C4H6Z2=C4H4+H2	2.5E15	0.0	94.7E3 !
<HIDAKA96>			
C4H6Z2=iC4H5+R1H	1.4E15	0.0	98.0E3 !
<HIDAKA96>!			
!			
C2H4Z+R10C2H3V=C4H6Z2+R1H	5.0E11	0.0	7.3E3 !
<TSAnG86>!			
!			
C4H6Z2+R1H=nC4H5+H2	1.3E6	2.53	12.2E3 !
<WAnG97>!			
C4H6Z2+R1H=iC4H5+H2	6.6E5	2.53	9.2E3 !
<WAnG97>!			
!			
!C4H6Z2+R1H=C4H7-1	2.6E13	0	3.2E3 !
ESTIMATED *2!			
!C4H6Z2+R1H=C4H7Y	2.6E13	0	1.56E3 !
ESTIMATED *2!			
C4H6Z2+R1H=C4H7-1	1.3E13	0	3.2E3 !
ESTIMATED			
C4H6Z2+R1H=C4H7Y	1.3E13	0	1.56E3 !
ESTIMATED !			
!			
C4H6Z2+R4CH3=nC4H5+CH4	7.0E13	0.0	18.5E3 !
<WU87>!			
C4H6Z2+R4CH3=iC4H5+CH4	7.0E13	0.0	15.5E3 !
<WU87-3kcal>!			

!C4H6Z2+R4CH3=C5H9Y 88 nist!	6.3E10	0.0	7.49E3	! PERRIN
!C4H6Z2+R4CH3=iC5H9 Estimated*2!	1.8E11	0.0	8.0E3	!
C4H6Z2+R4CH3=C5H9Y PERRIN 88 nist!	6.31E10	0.0	7.49E3	!
C4H6Z2+R4CH3=iC5H9 Estimated!	9.64E10	0.0	8.0E3	!
!				
!C4H6Z2+R10C2H3V=nC4H5+C2H4Z <HIDAKA96>!	5.0E14	0.0	22.8E3	!
C4H6Z2+R10C2H3V=iC4H5+C2H4Z <HIDAKA96-3kcal>!	5.0E14	0.0	19.8E3	!
!				
C4H6Z2+B10=C3H5Y+R1H+B2C0 <LEUnG95, BREZInSKY84>!	6.0E08	1.45	0.9E3	!
!				
R10C2H3V+C4H6Z2=C6H8#+R1H <frenklach >!	7.4E014	-0.66	8.42E3	!
!R10C2H3V+C4H6Z2=C6H8#+R1H <WESTMORELANd89, p=2.6kPa>!	2.28E12	-0.24	9.9E3	!
!R10C2H3V+C4H6Z2=C6H8#+R1H <WESTMORELANd89, p=101kPa>!	4.15E-11	6.39	2.4E3	!
!***				
!R10C2H3V+C4H6Z2=lC6H8+R1H <WESTMORELANd89, p=2.6kPa>!	1.0E10	1.05	14.0E3	!
!R10C2H3V+C4H6Z2=lC6H8+R1H <WESTMORELANd89, p=101kPa>!	2.48E-15	8.20	6.3E3	!
!***				
C4H6Z2+C2H2=C6H8# <WESTMORELANd89>!	2.3E12	0.0	35.0E3	!
!***				
!MF car lC6H9 n'intervient qu'ici				
!R10C2H3V+C4H6Z2=lC6H9 <WESTMORELANd89, p=2.6kPa>!	5.48E28	-5.31	9.3E3	!
!R10C2H3V+C4H6Z2=lC6H9 <WESTMORELANd89, p=101kPa>!	1.48E12	-0.17	3.2E3	!
!***				
R10C2H3V+C4H6Z2=C6H9Z# <WESTMORELANd89, p=2.6kPa>!	1.64E29	-6.12	9.6E3	!
!R10C2H3V+C4H6Z2=C6H9Z# <WESTMORELANd89, p=101kPa>!	7.06E13	-1.35	4.0E3	!
!***				
C4H6Z2+C2H4Z=C6H10# <WESTMORELANd89>!	2.3E10	0.0	27.0E3	!
C4H6Z2+R20H=nC4H5+H2O <WAnG97>!	6.2E6	2.0	3.4E3	!
C4H6Z2+R20H=iC4H5+H2O <WAnG97>!	3.1E6	2.0	0.4E3	!
C4H6Z2+R20H=C3H5Y+HCHO <LInSTEDT96>!	2.8E12	0.0	-0.9E3	!
C4H6Z2+R20H=CH3CHO+R10C2H3V <fromLInSTEDT96>!	5.6E12	0.0	-0.9E3	!

C4H6Z2+O2=iC4H5+R300H <LEUnG95>!	4.0E13	0.0	57.9E3	!
C4H6Z2+C3H3=nC4H5+aC3H4 <HIDAKA96>!	1.0E13	0.0	22.5E3	!
C4H6Z2+C3H3=iC4H5+aC3H4 <HIDAKA96-3kcal>!	1.0E13	0.0	19.5E3	!

!\*\*\*\*\* REACTIONS DE C4H6-12 \*\*\*\*\* (1,2) Butadiene (CH2CCHCH3) \*\*\*\*\*

!C4H6-12=C4H6Z2 <HIDAKA96>!	3.0E13	0.0	65.0E3	!
!C4H6-12=iC4H5+R1H <LEUnG95>!	4.2E15	0.0	92.6E3	!
!C4H6-12+R1H=R10C2H3V+C2H4Z <LEUnG95>!	4.0E11	0.0	0.0	!
!C4H6-12=C3H3+R4CH3 <kingas1500K>!	7.3E14	0.0	75.4E3	!
!C4H6-12+R1H=C4H7-2 <heyberger> !	1.3E13	0.0	1.6E3	!
!C4H6-12+R1H=C4H7Y <heyberger>!	1.2E11	0.69	3.0E3	!
!C4H6-12+R1H=C4H7T <heyberger> !	1.3E13	0.0	3.2E3	!
!C4H6-12+R1H=iC4H5+H2 <asTSAnG91>!	1.7E5	2.5	2.5E3	!
!C4H6-12+R4CH3=iC4H5+CH4 <asTSAnG91>!	2.2E0	3.5	5.7E3	!
!C4H6-12+R11C2H5=iC4H5+C2H6 <asTSAnG91>!	2.2E0	3.5	6.6E3	!
!C4H6-12+B10=iC4H5+R20H <asTSAnG91>!	1.7E11	0.7	5.9E3	!
!C4H6-12+R20H=iC4H5+H2O <asTSAnG91>!	3.1E6	2.0	-0.3E3	!
!C4H6-12+R300H=iC4H5+H2O2 <asTSAnG91>!	9.6E3	2.6	13.9E3	!

!\*\*\*\*\* REACTIONS DE (c-C4H6) \*\*\*\*\* methyl-cyclopropene \*\*\*\*\*

!B6CH2+pC3H4=cC4H6 <LEUnG95>!	1.8E14	0.0	0.0	!
!cC4H6=C4H6Z2 <LEUnG95>!	3.0E13	0.0	42.3E3	!
!cC4H6=C4H6-12 <LEUnG95>!	3.0E13	0.0	43.8E3	!

!\*\*\*\*\* REACTIONS DE (C4H6-1) \*\*\*\*\* 1 Butyne \*\*\*\*\*

!C4H6-1=C4H6-12 <HIDAKA96>!	2.5E13	0.0	65.0E3	!
!C4H6-1=C4H5-1s+R1H Kinga&dH Melius!	7.7E14	0.0	87.9E3	!
!C4H6-1=C4H5-1p+R1H Kingas!	9.1E14	0.0	99.6E3	!

!C4H6-1=>C3H3+R4CH3	3.0E15	0.0	75.8E3 !
<HIDAKA96>!			
!C4H6-1+R1H=R4CH3+aC3H4	1.3E5	2.5	1.0E3 !
<HIDAKA96>!			
!C4H6-1+R1H=R11C2H5+C2H2	6.5E4	2.5	1.0E3 !
<HIDAKA96>!			
!C4H6-1+R1H=R4CH3+aC3H4	3.2E12	0.0	1.7E3 !
<asWAGnER72>!			
!C4H6-1+R1H=R11C2H5+C2H2	3.2E12	0.0	1.7E3 !
<asWAGnER72>!			
! Les rñactions suivantes sont deduites de celles de 1-C4H8 generes par EXGAS			
!C4H6-1+R1H=H2+C4H5-1s	5.4E4	2.5	-1.9E3 !
<EXGAS>!			
!C4H6-1+R4CH3=CH4+C4H5-1s	1.5E12	0.0	7.1E3 !
<EXGAS>!			
!C4H6-1+B10=R20H+C4H5-1s	8.8E10	0.7	3.2E3 !
<EXGAS>!			
!C4H6-1+R20H=H2O+C4H5-1s	3.0E6	2.0	-1.5E3 !
<EXGAS>!			
!C4H6-1+O2=>R300H+C4H5-1s	1.4E12	0.0	36.0E3 !
<InGHAM95sec>!			
!C4H6-1+O2=>R300H+C4H5-1s	1.4E12	0.0	41.4E3 !
<InGHAM95sec>!			
!C4H6-1+O2=>R300H+C4H5-1s	4.2E12	0.0	49.5E3 !
<DAGAUT90sec>!			
!C4H6-1+R300H=>H2O2+C4H5-1s	6.4E3	2.6	12.4E3 !
<EXGAS>!			
! Les rñactions suivantes sont deduites de celles generes par EXGAS pour H primaires			
!C4H6-1+R1H=H2+C4H5-1p	2.9E7	2.0	7.7E3 !
<EXGAS>!			
!C4H6-1+R4CH3=CH4+C4H5-1p	3.7	4.0	8.2E3 !
<EXGAS>!MF			
!C4H6-1+B10=R20H+C4H5-1p	5.1E13	0.0	7.8E3 !
<EXGAS>!			
!C4H6-1+R20H=>H2O+C4H5-1p	2.7E6	2.0	-0.4E3 !
<EXGAS>!			
!C4H6-1+O2=>R300H+C4H5-1p	1.2E13	0.0	49.0E3 !
<EXGAS>!			
!C4H6-1+R300H=>H2O2+C4H5-1p	6.0E11	0.0	17.0E3 !
<EXGAS>!			
! Les rñactions d'addition suivantes sont deduites de celles de pC3H4			
!C4H6-1+B10=R12CHCOZ+R11C2H5	1.5E13	0.0	2.1E3 !
<asWARnATZ84>!			
!C4H6-1+R20H=CH2COZ+R11C2H5	4.3E11	0.0	-0.8E3 !
<asB00DAGHIANs87>!			
!***** REACTIONS DE (C4H6-2)***** 2 Butyne *****			
!C4H6-2=C4H6Z2	3.0E13	0.0	65.0E3 !
<HIDAKA96>!			
!C4H6-2=C4H6-12	3.0E13	0.0	67.0E3 !
<HIDAKA96>!			



!C4H6-2=C4H5-2+R1H <HIDAKA96>!	2.0E14	0.0	87.3E3 !
!C4H6-2+R1H=R4CH3+pC3H4 <HIDAKA96>!	2.6E5	2.5	1.0E3 !
!C4H6-2+R1H=R4CH3+pC3H4 <asWAGnER72>	6.5E12	0.0	1.7E3 !

! Les rñactions suivantes sont deduites de celles de pC3H4

!C4H6-2+R1H=C4H5-2+H2 <asTSAnG91*2>!	3.4E5	2.5	2.5E3 !
!C4H6-2+R4CH3=C4H5-2+CH4 <asTSAnG91*2>!	4.4E0	3.5	5.7E3 !
!C4H6-2+B10=B2C0+R10C2H3V+R4CH3 <asWARnATZ84>!	1.5E13	0.0	2.1E3 !
!C4H6-2+B10=R20H+C4H5-2 <asTSAnG91*2>!	1.2E11	0.7	7.6E3 !
!C4H6-2+R20H=B2C0+C2H4Z+R4CH3 <asBOODAGHIANs87>!	4.3E11	0.0	-0.8E3 !
!C4H6-2+R20H=C4H5-2+H2O <asTSAnG91*2>!	6.2E6	2.0	-0.3E3 !
!C4H6-2+O2=C4H5-2+R300H <InGHAM95*2>+4!	4.2E12	0.0	44.0E3 !
!C4H6-2+R300H=C4H5-2+H2O2 <asTSAnG91*2>!	1.9E4	2.6	13.9E3 !

!\*\*\*\*\* Reactions de C4H7-1 (CH2=CH-CH2-CH2.)!

!C4H7-1=C4H7Y ESTIMATED !	3.34E09	1.0	39.1E3 !
!C4H7-1=C4H7V Estimated!	3.3E9	1.0	20.7E3 !
!C4H7-1=C2H4Z+R10C2H3V Estimated!	2.0E13	0.0	35.5E3 !
!C4H7-1+R4CH3=C5H10 Estimated !	2.0E13	0.0	0.0 !
!C4H7-1+R1H=C4H8Y Estimated!	1.0E14	0.0	0.0 !

!\*\*\*\*\* Reactions de C4H7Y (CH3-CH.-CH=CH2)!\*\*\*\*\*stabililise par resonance

!C4H7Y+R1H=C4H8Y asTSANG 91!!	2.0E13	0.0	0.0 !
!C4H7Y+R1H=H2+C4H6Z2 asTSANG 91!!	0.9E13	0.0	0.0 !
!C4H7Y+R1H=H2+C4H6-12 asTSANG 91!	0.9E13	0.0	0.0 !
!C4H7Y+R300H=R20H+C2H3CHO+R4CH3 <Heyberger>!	1.0E15	-0.8	0.0 !
!C4H7Y+R4CH3=iC5H10 Estimated !	0.5E13	0.0	0.0 !

!\*\*\*\*\*Reactions de C4H7V (CH3-CH2-CH=CH.)\*\*\*\*\*!

!C4H7V=C4H7Y Heyberger!	1.9E10	1.0	36.3E3	!
!C4H7V=R11C2H5+C2H2 Heyberger!	2.0E13	0.0	33.0E3	!

!\*\*\*\*\*Reactions de C4H7-2 (CH3-C.=CH-CH3)\*\*\*\*\*!

!C4H7-2=C4H7Y ESTIMATED !	2.9E10	1.0	37.8E3	!
!C4H7-2=R4CH3+pC3H4 ESTIMATED !	2.0E13	0.0	31.5E3	!

!\*\*\*\*\*Reactions de C4H7T (CH2=C.-CH2-CH3)\*\*\*\*\*!

!C4H7T=C4H7-1 ESTIMATED !	3.34E09	1.0	40.6E3	!
!C4H7T=C4H7Y <Heyberger>!	2.0E13	0.0	47.0E3	!
!C4H7T=R4CH3+aC3H4 ESTIMATED !	2.0E13	0.0	32.5E3	!

!\*\*\*\*\*Reactions du 1-butene!

!C4H8Y+O2=C4H7Y+R300H <Heyberger>!	3.6E12	0.0	38.2E3	!
!C4H8Y+R1H=C4H7Y+H2 <Heyberger>!	5.4E4	2.5	-1.9E3	!
!C4H8Y+R20H=>HCHO+R4CH3+C2H4Z <Heyberger>!	1.4E12	0.0	-1.0E3	!
!C4H8Y+R20H=R4CH3+C2H5CHO <Heyberger>!!ds мйса PRF	1.4E12	0.0	-1.0E3	!
!C4H8Y+R20H=R4CH3+C2H5CHO	6.800E+11	0.0	-928.0	!(89ATK*RTi)
!C4H8Y+R20H=C4H7Y+H2O <Heyberger>!	3.0E6	2.0	-1.52E3	!
!C4H8Y+R4CH3=C4H7Y+CH4 <Heyberger>!	1.0E11	0.0	7.3E3	!
!C2H5CHO+R1H=H2+B2C0+R11C2H5 <Heyberger>!	4.0E13	0.0	4.2E3	!
!C2H5CHO+R20H=H2O+B2C0+R11C2H5 <Heyberger>!	4.0E12	0.0	0.5E3	!

!\*\*\*\*\*reactions de iC4H8\*\*\*\*\*!

!iC4H8+R20H=iC3H7+HCHO (idem RF)	1.4E12	0.0	-1040.0	!
!iC4H8+R1H=>iC4H7+H2 (idem RF)	3.5E5	2.5	2510	!
!iC4H8+R20H=>iC4H7+H2O MES 878<C.M.>!(idem RF)	6.0D+06	2.000	-298.0	!
!iC4H7+R1H=iC4H8 <estimation>!	1.0E14	0.0	0.0	!
!iC4H7+R300H=>R20H+HCHO+tC3H5 <Heyberger>!	1.0E15	-0.8	0.0	!

```

!
*****
**!
!
*****
*****!
!*          MECHANISM FOR THE GAS PHASE OXIDATION OF BENZENE
*!
!*
*!
!*      efficiency coefficients for O2, CO, CO2, H2O, AR, C6H6#
*!
!
*****
*****!
!*          PRIMARY MECHANISM OF THE OXIDATION OF BENZENE
*!
!
*****
*****!

```

!REACTIONS OF BENZENE MOLECULES!

!\*\*\*Umimolecular inititiation!

C6H5#+R1H(+M)=C6H6#(+M)                    1.0E14            0.0            0.0            !  
<WANG97>!

LOW /6.6E75 -16.3 7.0E3/  
TROE /1.0 0.1 585 6113/

O2/0.4/ B2C0/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/

!\*\*\*Bimolecular inititiation!

C6H6#+O2=C6H5#+R300H                    6.0E13            0.0            63.4E3        !  
<ALZUETA00>!

!\*\*\*additions!

C6H6#+R1H=C6H7#                        3.2E13            0.0            3.2E3        !  
<MEBEL97>!

C6H6#+B10=C6H50#+R1H                    2.8E13            0.0            4.91E3        !  
<EMDEE92>!

C6H6#+R20H=C6H50H#+R1H                    1.3E13            0.0            10.6E3        !  
<BAULCH94>!

C6H6#+R9C2H=C6H5#C2H+R1H                    5.0E13            0.0            0.0            !  
<WANG97>!

C6H6#+R10C2H3V=styrene+R1H                    7.9E11            0.0            6.4E3        !  
<WANG97>!

!\*\*\*Metatheses!

!\*modif Zhenyu\*!

!C6H6#+R1H=C6H5#+H2                    6.0E8            1.8            16.8E3        !  
<MEBEL97>!

C6H6#+R1H=C6H5#+H2                    1.22E8            2.031            15.88E3        !  
calcul CBS-QB3 Fournet

C6H6#+B10=C6H5#+R20H                    2.0E13            0.0            14.7E3        !  
<LINDSTEDT94>!

```

!*modif Zhenyu*!
!C6H6#+R20H=C6H5#+H2O          1.6E8      1.42      1.45E3    !
<BAULCH92>!
C6H6#+R20H=C6H5#+H2O          1.36E4      2.7      0.6196E3  !as
toluene+R20H=C6H4CH3+H2O

!*modif Zhenyu*!
!C6H6#+R300H=C6H5#+H2O2       5.5E12      0.0      28.9E3    !
<BAULCH94>!
C6H6#+R300H=C6H5#+H2O2       9.2E12      0.0      28.81E3   !as
toluene+R300H=C6H4CH3+H2O2

!*modif Zhenyu*!
!C6H6#+R4CH3=C6H5#+CH4        2.0E12      0.0      15.0E3    !
<ZHANG89>!
C6H6#+R4CH3=C6H5#+CH4        2.07E0      3.861     13.3E3    !
calcul CBS-QB3 Fournet

C6H6#+R11C2H5=C6H5#+C2H6      6.3E11      0.0      15.0E3    !
<ZHANG89>!
C6H5#+C3H6Y=C6H6#+C3H5Y      7.94E13     0.0      11.94E3   !MF
<Heckmann,Hippler,Troe(1996)>
C6H6#+nC4H5=C6H5#+C4H6Z2     6.3E11      0.0      15.0E3    !
estimated!
C6H6#+iC4H5=C6H5#+C4H6Z2     6.3E11      0.0      20.0E3    !
estimated!

!REACTIONS OF C6H7# RADICALS!
!***Isomerization!
C6H7#=lC6H7                    2.5E14      0.7      41.8E3    !
<WEISSMAN89!

!***Decomposition by beta-scission!
!C6H7#=>C2H2+nC4H5            2.0E13      0.0      50.0E3    !
estimated!
!Breaking of a Csp3-Csp2 bond in an allylic radical as proposed by
HEYBERGER02!
!***Oxidation!
C6H7#+O2=C6H6#+R300H          7.9E11      0.0      9.9E3     !
estimated!
!Oxidation of an allylic radical as proposed by HEYBERGER02!
!combinations!
C6H7#+R1H=C6H8#                1.0E14      0.0      0.0       !
estimated!
!***Disproportionnations!
C6H7#+R1H=C6H6#+H2            3.3E12      0.0      0.0       !
<RISTORI01>!
C6H7#+R20H=C6H6#+H2O          1.0E13      0.0      0.0       !
estimated!
C6H7#+R4CH3=C6H6#+CH4         3.0E12     -0.32     -0.1E3    !
estimated!
C6H7#+C6H7#=C6H6#+C6H8#      8.4E10      0.0      -0.3E3    !
estimated!
!analogy with the disproportionnations ofC3H5Y proposed by TSANG91!

```

!REACTIONS OF C6H5# RADICALS!

!\*\*\*Isomerization!

C6H5#=1C6H5 5.0E13 0.0 72.5E3 !  
<BRAUN89>!

!1C6H5 = ch///c/ch//ch/ch//ch(.)!

1C6H5=>2C2H2+R9C2H 2.0E13 0.0 51.0E3 !  
estimated!

!DH298 =44kcal/mol, Eadd=7 kcal/mol!

1C6H5=1C6H4+R1H 2.0E12 0.0  
41.0E3 !estimated!

!1C6H4 = ch///c/ch//ch/c///ch , DH298 =38kcal/mol, Eadd=3 kcal/mol!

!from BRAUN89 at 1500 K!

!\*\*\*Reactions with O2!

C6H5#+O2=C6H5O2 2.2E19 -2.5 0.0 !  
estimated!

C6H5#+O2=C6H5O##+B10 2.6E13 0.0 6.1E3 !  
<FRANK94>!

C6H5#+O2=OC6H4O+R1H 3.0E13 0.0 9.0E3 !  
<FRANK94>!

!as the addition of oxygen to alkyl radicals proposed by GLAUDE99!

!\*\*\*Additions!

C6H5#+C2H2=C6H5#C2H+R1H 4.0E13 0.0 10.1E3 !  
<MARINOV97>!

C6H5#+C6H6#=biphenyl+R1H 5.6E12 -0.074 7.5E3 !  
<WANG97>!

!\*\*\*Combinations!

C6H5#+B10=C5H5##+B2C0 1.0E14 0.0 0.0 !  
<FRANK94>!

C6H5#+R20H=C6H5OH# 1.0E13 0.0 0.0  
!calculated!

!toluene=C6H5#+R4CH3 1.0E16 0.0 97.0E3  
!<COLKET94>!

!calculation by KINGAS!

C6H5#+R5CHO=C6H5CHO 5.0E12 0.0 0.0 !  
estimated!

C6H5#+R10C2H3V=styrene 5.0E12 0.0 0.0 !  
estimated!

C6H5#+R11C2H5=etC6H5 5.0E12 0.0 0.0 !  
estimated!

C6H5#+R300H=C6H5O##+R20H 5.0E12 0.0 0.0 !  
estimated!

!C6H5C3H3 n'intervient qu'ici

!C6H5#+C3H3=C6H5C3H3 3.0E12 0.0 0.0 !  
<D'ANNA98>!

C6H5#+C6H5#=biphenyl 3.8E31 -5.75 7.9E3 !  
<WANG97>!

!\*\*\*disproportionations!

C6H5#+R20H=C6H5O##+R1H 5.0E13 0.0 0.0 !  
<ALZUETA00>!

C6H5#+C6H7#=C6H6#+C6H6# 1.0E12 0.0 0.0 !  
<SHANDROSS96>!

!REACTIONS OF PHENYLPEROXY RADICALS!

!\*\*\*Decomposition by beta-scission!

!mfC6H5O2=OC6H4O+R1H 2.0E13 0.0 30.0E3 !  
estimated!

C6H5O2=C5H4O#+R5CHO 2.0E13 0.0 30.0E3 !  
estimated!

!see DA COSTA01!

!MF

C6H5O2+R300H=C6H500H+O2 2.0E11 0.00 -1300  
C6H500H=C6H50#+R20H 1.5E16 0.00 43000

!REACTIONS OF PHENOXY RADICALS!

!\*\*\*CO elimination!

C6H5O#=B2CO+C5H5# 2.5E11 0.0 43.8E3 !  
<BAULCH92>!

!\*\*\*Combinations!

! --C6H5O#+R1H(+M)=C6H5OH#(+M) 2.5E14 0.0 0.0 !  
<FRENKLACH>!

C6H5O#+R1H(+M)=C6H5OH#(+M) 1.0E14 0.0 0.0 !  
estimated!

LOW /1.0E94 -21.84 13.9E3/ !

<FRENKLACH>!

TROE /0.043 304 60000 5896/

O2/0.4/ B2CO/0.75/ CO2/1.5/ H2O/6.5/ AR/0.35/ C6H6#/3.0/  
C6H5O#+R1H=C5H6#+B2CO 1.1E53 -10.7 41.4E3 !

<TAN96>!

C6H5O#+B10=OC6H4OH 2.6E10 0.47 0.8E3 !  
<LIN95>!

C6H5O#+B10=OC6H4O+R1H 8.5E13 0.0 0.0 !  
<FRANCK94>!

C6H5O#+B10=C5H5#+CO2 1.0E13 0.0 0.0 !  
<FRANCK94>!

!REACTIONS OF HYDROXYPHENOXY RADICALS!

!\*\*\*CO elimination!

OC6H4OH=B2CO+C5H4OH# 7.4E11 0.0 43.8E3 !  
estimated!

!as for phenoxy radicals!

!REACTIONS OF CYCLOPENTADIENYL RADICALS!

!\*\*\*Isomerization!

C5H5#=1C5H5 1.0E14 0.0 45.5E3 !  
<BRAUN89>!

!1C5H5 = ch///c/ch//ch/ch2(.), DH298 =31kcal/mol!

!MF car 1C5H6 n'intervient qu'ici

!1C5H5+R1H=1C5H6 1.0E14 0.0 0.0 !  
estimated!

1C5H5=C3H3+C2H2 estimated! !DH298 =43kcal/mol, Eadd=7 kcal/mol!	2.0E13	0.0	50.0E3	!
!***Reactions with O2!				
C5H5#+O2=R5CHO+C4H4O <ZHONG98>!	1.2E19	-2.48	11.0E3	!
!***Combinations!				
C5H6# = C5H5# + R1H ! MF<Burcat, Int.J.Chem.Kinet.29(1997)505>	5.0E15		0.00	7.87E4
C5H5#+B10=C5H40#+R1H <ZHONG98>!	5.8E13	-0.02	0.02E3	!
C5H5#+B10=>2C2H2+R5CHO <ZHONG98>!	3.2E13	-0.17	0.44E3	!
C5H5#+R20H=>C4H6Z2+B2CO [PENGLAN- RODA]	4e14	0.0	4500	!
C5H5#+R20H=C5H50H# calculated!	1.0E13	0.0	0.0	!
C5H5#+R300H=C5H50#+R20H calculated!	3.0E12	0.0	0.0	!
!calculation by KINGAS!				
C5H5#+C5H5#=>C10H10# estimated!	2.0E12	0.0	0.0	!
C10H10#=>C5H5#+C5H5# calculated!	3.2E15	0.0	57.5E3	!
!***disproportionations!				
C5H5#+R300H=>C5H6#+O2 estimated!	2.5E9	1.0	3.5E3	!
!estimated as for allylic radicals (HEYBERGER02)/10!				
!REACTIONS OF CYCLOPENTADIONYL RADICALS!				
!***Decompositions by beta-scission!				
C5H50#=>2C2H2+R5CHO estimated!	2.0E13	0.0	30.0E3	!
C5H50#=C5H40#+R1H estimated!	2.0E13	0.0	30.0E3	!
!see DA COSTA01!				
!***Combinations!				
C5H50#+R1H=C5H50H# estimated!	1.0E14	0.0	0.0	!
!***no disproportionations considered!				
!REACTIONS OF HYDROXYCYCLOPENTADIENYL RADICALS!				
C5H40H#+O2=C5H40#+R300H estimated!	1.0E13	0.0	5.0E3	!
C5H40H#+R1H=C5H50H# estimated!	1.0E14	0.0	0.0	!
C5H40H#+B10=C02+C2H2+R10C2H3V estimated!	3.2E13	-0.17	0.44E3	!

!C5H40H##+R300H=>R20H+C02+R10C2H3V+C2H2 3.0E12 0.0 0.0 !  
 estimated!  
 C5H40H##+R300H=>R20H+R20H+C5H40# 3.0E12 0.0 0.0 ! mf  
 C5H40H##+R300H=>C5H50H##+O2 2.5E9 1.0 3.5E3 !  
 estimated!  
 !Reactions derived from those of cyclopentadienyl radicals!  
 C5H40H##+C6H50#=C5H40##+C6H50H# 1.0E12 0.0 0.0 !  
 estimated!

!  
 \*\*\*\*\*  
 \*\*\*\*\*!  
 !\*  
 !\* SECONDARY MECHANISM OF THE OXIDATION OF BENZENE!!\*  
 !  
 \*\*\*\*\*  
 \*\*\*\*\*!

!REACTIONS OF ORTHOBENZOQUINONE!  
 OC6H40=>C5H40##+B2C0 1.0E12 0.0 40.0E3 !  
 <ALZUETA00>!  
 OC6H40+R1H=>2B2C0+C2H2+R10C2H3V 5.2E13 0.0 3.2E3 !  
 estimated!  
 !estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!  
 !OC6H40+R1H=>H2+2B2C0+C2H2+R9C2H 1.6E6 2.5 9.8E3 !  
 estimated!  
 !OC6H40+R20H=>H2O+2B2C0+C2H2+R9C2H 4.4E6 2.0 1.4E3 !  
 estimated!  
 !estimated as the metathesis of 4 tertiary vinylic H-atoms (HEYBERGER02)!

!REACTIONS OF PHENOL AND DERIVED RADICALS!  
 C6H50H##=C5H6##+B2C0 1.0E12 0.0 61.2E3 !  
 <HORN98>!

C6H50H##+O2=R300H+C6H50# 1.0E13 0.0 38.9E3 !  
 <ALZUETA00>!

C6H50H##+B10=OC6H40H+R1H 1.6E13 0.0 3.4E3 !  
 estimated!

!as the addition of O-atoms to toluene (DACOSTA01)!  
 C6H50H##+R1H=C6H50##+H2 1.2E14 0.0 12.4E3 !  
 <ALZUETA00>!  
 C6H50H##+B10=C6H50##+R20H 1.3E13 0.0 2.9E3 !  
 <ALZUETA00>!  
 C6H50H##+R20H=C6H50##+H2O 1.4E8 1.4 -0.96E3 !  
 <SHANDROSS96>!  
 C6H50H##+R300H=C6H50##+H2O2 1.0E12 0.0 10.0E3 !  
 <ALZUETA00>!



C6H50H##+R4CH3=C6H50##+CH4 <MULCAHY65>!	1.8E11	0.0	7.7E3	!
C6H50H##+C6H5#=C6H50##+C6H6# <ALZUETA00>!	4.9E12	0.0	4.4E3	!
!C6H50H##+C5H5#=C6H50##+C5H6# estimated!	4.9E11	0.0	9.4E3	!
!C6H50H##+C3H5Y=C6H50##+C3H6Y estimated!	4.9E11	0.0	9.4E3	!
!C6H50H##+iC4H5=C6H50##+C4H6Z2 estimated!	4.9E11	0.0	9.4E3	!
C6H50H##+C5H5#=C6H50##+C5H6#	2.67e14	0.0	25.238e3	
!mf <Lovell Int. J. Chem. Kinet.21(1989)547>				
C6H50H##+C3H5Y=C6H50##+C3H6Y <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	!mf
C6H50H##+iC4H5=C6H50##+C4H6Z2 !mf <Lovell Int. J. Chem. Kinet.21(1989)547>	2.67e14	0.0	25.238e3	

!A/10 and 5 kcal/mol more than C6H5# because of the stabilization!

C6H50H##+R1H=C6H40H##+H2 <SHANDROSS96>!	1.7E14	0.0	16.0E3	!
C6H50H##+B10=C6H40H##+R20H estimated!	2.0E13	0.0	14.7E3	!
C6H50H##+R20H=C6H40H##+H20 <SHANDROSS96>!	1.4E13	0.0	4.6E3	!
C6H50H##+R300H=C6H40H##+H202 estimated!	4.0E11	0.0	28.9E3	!
C6H50H##+R4CH3=C6H40H##+CH4 estimated!	2.0E12	0.0	15.0E3	!
!as the H-abstractions from benzene!				
C6H40H##+O2=OC6H40H+B10 estimated!	2.1E13	0.0	6.1E3	!
!as for phenyl radicals (FRANCK94)!				
C6H40H##+R1H=C6H50H## estimated!	1.0E14	0.0	0.0	!
C6H40H##+R4CH3=HOC6H4CH3	5.0E12	0.0	0.0	!mf

!REACTIONS OF CYCLOPENTADIENE AND DERIVED RADICALS!

C5H6##+O2=>C5H5##+R300H <INGHAM94>!	1.4E12	0.0	31.6E3	!
!C5H6##+R1H=C5H7# estimated!	5.2E13	0.0	3.2E3	!
!estimated as the addition of H-atoms to four tertiary C (HEYBERGER02)!				
C5H6##+B10=>C5H50##+R1H <ZHONG98>!	8.9E12	-0.15	590.0	!
C5H6##+R1H=C5H5##+H2 <ROY97>!	2.8E13	0.0	2.0E3	!
C5H6##+B10=C5H5##+R20H <ZHONG98>!	4.8E4	2.7	1.1E3	!
C5H6##+R20H=C5H5##+H20 <ZHONG98>!	3.1E6	2.0	0.0	!

C5H6#+R300H=C5H5#+H2O2 <ZHONG98>!	1.1E4	2.6	12.9E3	!
C5H6#+R4CH3=C5H5#+CH4 <ZHONG98>!	1.8E-1	4.0	0.0	!
C5H6#+C3H5Y=C5H5#+C3H6Y astoluene!	1.6E12	0.0	15.1E3	!
C5H6#+nC4H5=C5H5#+C4H6Z2 astoluene!	1.6E12	0.0	11.1E3	!
C5H6#+iC4H5=C5H5#+C4H6Z2 astoluene!	1.6E12	0.0	15.1E3	!
!C5H6#+C3H5Y=C5H5#+C3H6Y estimated!	6.0E12	0.0	0.0	!
!C5H6#+nC4H5=C5H5#+C4H6Z2 estimated!	6.0E12	0.0	0.0	!
!C5H6#+iC4H5=C5H5#+C4H6Z2 <EMDEE92>!	6.0E12	0.0	0.0	!
!C5H7#=>C2H2+C3H5Y estimated!	2.0E13	0.0	35.5E3	!
!Breaking of a Csp3-Csp2 bond in an alkenyl radical as proposed by HEYBERGER02!				
!C5H7#+O2=C5H6#+R300H estimated!	7.9E11	0.0	5.0E3	!
!oxidation of an alkylic radical!				
!REACTIONS OF CYCLOPENTADIONE AND DERIVED RADICALS!				
C5H40#=>2C2H2+B2C0 <ALZUETA00>!	5.7E32	-6.76	68.5E3	!
!C5H40#=B2C0+C4H4 roda PENGLOAN!	1.00e12	0.0	53000	!
C5H40#+R1H=B2C0+nC4H5 estimated!	2.6E13	0.0	3.2E3	!
!estimated as the addition of H-atoms to two tertiary C (HEYBERGER02)!				
C5H40#+B10=C4H4+C02 <ALZUETA00>!	1.0E13	0.0	2.0E3	!
C5H40#+R1H=C5H30#+H2 idem C6H6#+R1H=C6H5#+H2	8.13E7	2.031	15.88E3	!MF
C5H40#+B10=C5H30#+R20H <ALZUETA00>!	1.4E13	0.0	14.7E3	!
C5H40#+R20H=C5H30#+H2O <ALZUETA00>!	1.1E8	1.42	1.4E3	!
C5H30#=>C2H2+B2C0+R9C2H estimated!	2.0E13	0.0	51.0E3	!
!estimated as the decomposition of lC6H5!				
C5H30#+O2=>C02+C2H2+R12CHCOZ <ALZUETA00>!	9.7E58	-13.47	38.2E3	!
C5H50H#+R1H=C5H50#+H2 <ALZUETA00>!	4.0E13	0.0	6.1E3	!
C5H50H#+B10=C5H50#+R20H <ALZUETA00>!	1.0E13	0.0	4.6E3	!

C5H5OH#+R2OH=C5H5O#+H2O 1.0E13 0.0 1.7E3 !  
<ALZUETA00>!

!Estimated from the same reaction for CH3OH!

C5H5OH#+R1H=C5H4OH#+H2 1.4E13 0.0 2.0E3 !  
estimated!  
C5H5OH#+B10=C5H4OH#+R2OH 4.8E4 2.7 1.1E3 !  
estimated!  
C5H5OH#+R2OH=C5H4OH#+H2O 1.5E6 2.0 0.0E3 !  
estimated!

!estimated from the same reaction for cyclopentadiene!

!REACTIONS OF VINYLKETENE!

!additions decomposition

C4H4O+R1H=>R10C2H3V+CH2COZ 1.3E13 0.0 3.0E3 !  
estimated!  
C4H4O+R1H=>C2H4Z+R12CHCOZ 1.3E13 0.0 3.0E3 !  
estimated!  
C4H4O+R1H=>sC3H5+B2CO 1.3E13 0.0 1.5E3 !  
estimated!  
C4H4O+R2OH=>C2H3CHO+R5CHO 1.4E12 0.0 -1.0E3 !  
estimated!  
C4H4O+R2OH=>CO2+C3H5Y 1.4E12 0.0 -1.0E3 !  
estimated!  
C4H4O+B10=>R13CH2CHO+R12CHCOZ 6.0E4 2.56 -1.1E3 !  
estimated!  
C4H4O+B10=>2CH2COZ 6.0E4 2.56 -1.1E3 !  
estimated!

!estimated as the addition of radicals to a double bond (HEYBERGER02)!

!metatheses/decomposition

C4H4O+R1H=>C2H2+R12CHCOZ+H2 8.2E5 2.5 12.3E3 !  
estimated!  
C4H4O+R1H=>C3H3+B2CO+H2 4.1E5 2.5 9.8E3 !  
estimated!  
C4H4O+R2OH=>C2H2+R12CHCOZ+H2O 2.2E6 2.0 2.8E3 !  
estimated!  
C4H4O+R2OH=>C3H3+B2CO+H2O 1.1E6 2.0 1.5E3 !  
estimated!  
C4H4O+B10=>C2H2+R12CHCOZ+R2OH 1.2E11 0.7 8.7E3 !  
estimated!  
C4H4O+B10=>C3H3+B2CO+R2OH 6.0E10 0.7 8.7E3 !  
estimated!

!estimated as the metatheses of vinylic H-atoms (HEYBERGER02)!

!

\*\*\*\*\*

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!\* \*!

!\* \*!

\*!

MECHANISM FOR THE GAS PHASE OXIDATION OF TOLUENE

```

!*                                     *!
!* efficiency coefficients for O2, CO, CO2, H2O, N2, AR, HE, C6H6#
and toluene*!
!*                                     *!
!
*****!
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!*                                     *!
!* PRIMARY MECHANISM OF THE OXIDATION OF TOLUENE
*!
!*                                     *!
!
*****!
*****!

```

```

!*****!
!*REACTIONS OF TOLUENE MOLECULES*!
!*****!

```

!\*\*UMIMOLECULAR INITIATIONS

```

toluene=benzyl+R1H          2.09E15  0.0  87.51E3  !
<Oehlschlaeger07>! Zhenyu
toluene=C6H5#+R4CH3        2.66E16  0.0  97.88E3  !
<Oehlschlaeger07> Zhenyu

```

!\*\*BIMOLECULAR INITIATION

```

toluene+O2=benzyl+R300H    1.8E12  0.0  39.7E3  !<BAULCH94>!
!toluene+O2=benzyl+R300H  2.18e7  2.50  46045  !
mf<Oehlschlaeger06>!

```

!\*\*ADDITIONS

```

toluene+R1H=C6H6#+R4CH3    5.67E8  1.43  5.65E3  !Calcul CBS-
QB3 Fournet Zhenyu

```

```

toluene+B10=OC6H4CH3+R1H   1.7E13  0.0  3.6E3  !<TAPPE89>!
!toluene+R20H=HOC6H4CH3+R1H 2.3E12  0.0  -0.36E3 !<BAULCH92>!
toluene+R20H=HOC6H4CH3+R1H 1.3E13  0.0  10.6E3 !<BAULCH94>as
benzene!

```

```

toluene+R20H=C6H50H#+R4CH3 7.83E2  2.884  3.2193E3 !Seta V Nakajima
V Miyoshi JPCA 2006 Zhenyu
!toluene+R20H=C6H50H#+R4CH3 1E5  2.58  1134.0 !Olive as
benzene+OH

```

!\*\*METATHESES

!\*\*METATHESES WITH ABSTRACTION OF BENZYLIC H-ATOM

```

toluene+R1H=benzyl+H2          2.92E6   2.372   5.81E3   !Calcul CBS-QB3
Fournet Zhenyu
toluene+B10=benzyl+R20H        6.3E11   0.0      0.0      !
<HOFFMANN90>!

toluene+R20H=benzyl+H20        5.2E09   1.0      0.87E3   !<BAULCH94>!

toluene+R300H=benzyl+H202      4.0E11   0.0      14.0E3   !<BAULCH94>!
toluene+R4CH3=benzyl+CH4       3.91E0   3.76     6.98E3   !Calcul CBS-QB3
Fournet Zhenyu

! ajout MF
toluene+R7CH30=benzyl+CH30H    2.12E+10 0.0 3000.0      !PITZ2001
toluene+R8CH300=benzyl+CH300H  1.02E+04 2.5 12339.3 !PITZ2001

!toluene+R5CHO=benzyl+HCHO     3.77E13  0.0 23.7874E3   !MEHL 09 Zhenyu
benzyl+HCHO = toluene+R5CHO     1.26e8   1.9  18.183E3
benzyl+CH3CHO = toluene+R14CH3CO 1.26e8   1.9  18.183E3

toluene+R10C2H3V=benzyl+C2H4Z  4.0e12   0.0      8.0e3     !<COLKET94>!

toluene+C3H5Y=benzyl+C3H6Y     1.6E12   0.0      15.1E3   !<estimated(a)>!
toluene+C3H3=benzyl+pC3H4      1.6E12   0.0      15.1E3   !<estimated(a)>!
toluene+iC4H5=benzyl+C4H6Z2    1.6E12   0.0      15.1E3   !
<estimated(a)>!
toluene+nC4H5=benzyl+C4H6Z2    1.6E12   0.0      11.1E3   !
<estimated(a)>!
toluene+C5H5#=benzyl+C5H6#     1.6E11   0.0      15.1E3   !<estimated(a)>!
!(a) :Rate constant taken equal to that of the H-abstraction with methyl
radicals proposed !
!by COLKETT94 with A divided by 10 for cyclic radicals !
! and with an activation energy 4 kcal/mol higher for resonance
stabilised radicals!

!ajout MF
toluene+C6H502=benzyl+C6H500H   1.02E+04 2.5 12339.3   !
PITZ2001

toluene+C6H5#=benzyl+C6H6#      7.9E13   0.0      12.0E3   !<HECKMANN96>!

toluene+C6H50#=benzyl+C6H50H#   1.6E11   0.0      15.1E3   !
<estimated(a)>! peut etre trop rapide
toluene+C6H4CH3=benzyl+toluene  7.9E13   0.0      12.0E3   !
<estimated(b)>!
toluene+OC6H4CH3=benzyl+HOC6H4CH3 1.6E11   0.0      15.1E3   !
<estimated(a)>!
toluene+C6H5CH200=benzyl+C6H5CH200H 4.0E11   0.0      14.0E3   !
<estimated(c)>!

```

toluene+C6H5CH2O=benzyl+C6H5CH2OH 1.6E11 0.0 11.1E3 !  
 <estimated(a)>!  
 toluene+HOC6H4CH2=benzyl+HOC6H4CH3 1.6E11 0.0 15.1E3 !  
 <estimated(a)>!  
 !(b) :Rate constant taken equal to that of the H-abstraction with phenyl  
 radicals proposed !  
 !by HECKMANN96!  
 !(c) :Rate constant taken equal to that of the H-abstraction with HO2  
 radicals proposed !  
 !by BAULCH94!

!\*\*METATHESSES WITH ABSTRACTION OF PHENYLIC H-ATOM!

toluene+R1H=C6H4CH3+H2 1.22E08 2.031 15.88E3 !as  
 C6H6#+R1H=C6H5#+H2 CBS-QB3 Fournet Zhenyu  
 toluene+B10=C6H4CH3+R2OH 2.0E13 0.0 14.7E3 !<estimated(d)>!  
 toluene+R2OH=C6H4CH3+H2O 1.36E4 2.7 0.6196E3 !<Seta06>! in  
 Sakai07 Zhenyu  
 toluene+R300H=C6H4CH3+H2O2 9.2E12 0.0 28.81E3 !<Baulch94>! in  
 Sakai07 Zhenyu  
 toluene+R4CH3=C6H4CH3+CH4 2.07E0 3.861 13.3E3 !as  
 C6H6#+R4CH3=C6H5#+CH4 CBS-QB3 Fournet Zhenyu

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYL RADICALS\*!  
 !\*\*\*\*\*!

!\*\*DECOMPOSITION BY BETA-SCISSION

benzyl=>C5H5#+C2H2 6.0E13 0.0 70.0E3 !<Colket94>!  
 benzyl=>C3H3+C4H4 2.0E14 0.0 83.6E3 !<Colket94>!

!\*\*REACTIONS WITH OXYGEN

benzyl+O2=C6H5CH2OO 4.6E11 0.0 -377.0 !<FENTER94>!  
 benzyl+O2=C6H5CH2O+B10 6.3E12 0.0 40.0E3 !<BREZYNSKY84>!

!\*\*TERMINATION REACTIONS

benzyl+B10=C6H5#+HCHO 3.5E13 0.0 0.0 !<EMDEE92>!  
 benzyl+B10=C6H5CHO+R1H 1.0E14 0.0 0.0 !  
 <estimated(e)>!

!(e) : This rate constant is that proposed by <HIPPLER90-2> divided by 4  
 !(LINSTEDT96?? has used 3.5E13)!

benzyl+R8CH3OO=>C6H5CH2O+R7CH3O 5.0E12 0.0 0.0  
 benzyl+R17C2H5OO=>C6H5CH2O+R15C2H5O 5.0E12 0.0 0.0

benzyl+R2OH=C6H5CH2OH 2.0E13 0.0 0.0 !<HIPLER91>!

!MFbenzyl+R300H=C6H5CH2OOH 5.0E12 0.0 0.0 !<HIPPLER92>!  
 benzyl+R300H=C6H5CH2OOH 8.21E4 2.20 -5.13E3 !MF<da  
 silva-bozzelli- proceedings comb inst 32(2009)287-294>!

```

2benzyl=bibenzyl          5.01E12  0.0 0.454E3  !
<Oehlschlaeger05>! in Sakai07 Zhenyu

etC6H5 = benzyl + R4CH3      6.1e15  0.0  75120  !<BAULCH94>!

!*****!
!*REACTIONS OF METHYL PHENYL RADICALS*!
!*****!

!**reactions with oxygen
!mfC6H4CH3+O2=OC6H4CH3+B10      2.6E13  0.0  6.1E3  !
<estimated(f)>!
!mfC6H4CH3+O2=OC6H4O+R4CH3      3.0E13  0.0  9.0E3  !
<estimated(f)>!
!(f) : Rate constant taken equal to that of the similar reaction in the
case of phenyl!
!radicals!

!ajout mf
C6H4CH3+O2=>OOC6H4CH3          3.72E13      -0.22      -711
      !2008DAS/BOZ3566-3575
OOC6H4CH3=>C6H4CH3+O2          6.36E19      -1.372      48.74E3
      !2008DAS/BOZ3566-3575
OOC6H4CH3=>OC6H4CH3+B10        1.27E15      -0.25
      3.85E4      !2008DAS/BOZ3566-3575

OOC6H4CH3=>OC6H4O+R4CH3        5.0E11      0.00
      46400      !

!***termination reactions!
C6H4CH3+R1H=toluene            1.0E14  0.0  0.0  !
<estimated(g)>!
!(g) : Rate constant taken equal to that of the recombination of H atoms
with alkyl !
!radicals as proposed by Allara!

C6H4CH3+B10=OC6H4CH3          1.0E14  0.0  0.0  !
<estimated(f)>!
C6H4CH3+R2OH=HOC6H4CH3        1.0E13  0.0  0.0  !
<estimated(f)>!
C6H4CH3+R4CH3=C8H10#           1.2E06  1.96  -3.7E3  !
<estimation(fbis)>!
!(fbis) : Rate constant taken equal to that of the similar reaction in
the case of phenyl!
!radicals: Rao, skinner, 1989 J.P.C. (93,1864)!

C6H4CH3+R3OOH=OC6H4CH3+R2OH    5.0E12  0.0  0.0  !
<estimated(f)>!
C6H4CH3 +R1H = benzyl + R1H     1.0E13  0.0  0.0  !<MILLER92>!

!*****!

```

!\*REACTIONS OF BENZYL PEROXY RADICALS\*!  
!\*\*\*\*\*!

!\*\*isomerisation-decomposition reactions

C6H5CH2OO=C6H5CHO+R2OH 3.4E9 1.0 37.5E3 !

<estimated(h)>!

!(h) : Rate constant of the isomerisation :!

!A =  $ekbT/h \times rpd \times \exp((Dnirot \times 3.5)/R)$ , Ea = 23 (4 membered transition ring)!

!+ 14.5 (secondary allylic H-atom)!

!\*\*Combination reactions

!MF C6H5CH2OO+R1H=C6H5CH2OOH 1.0E14 0.0 0.0E3 !

<estimated(g)>!

!\*\*dispropotionnation reactions!

C6H5CH2OO+R3OOH=C6H5CH2OOH+O2 2.0E11 0.0 -1.3E3 !

<estimated(i)>!

2C6H5CH2OO=C6H5CH2OH+C6H5CHO+O2 1.4E10 0.0 -725.0 !

<estimated(i)>!

C6H5CH2OO+C6H5CH2OO=2C6H5CH2O+O2 6.3E10 0.0 -725.0 !

<estimated(i)>!

!(i) : Rate constant taken equal to that the disproportionnation of peroxyalkyl radicals !

!as proposed by Warth!

! ajout MF

C6H5CH2OO+R1H=C6H5CH2O+R2OH 3.80E14 -0.19

1.89E3 !<da silva J Chem Theory Comput 2009>

C6H5CH2OO+R1H=C6H5CH2OOH 4.35e60 -15.92 11.40E3

!<da silva J Chem Theory Comput 2009>

C6H5CH2OO+R1H=benzyl+R3OOH 1.96E4 2.47 1.43E3

!<da silva J Chem Theory Comput 2009>

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

!\*REACTIONS OF BENZYL ALCOXY RADICALS\*!

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

!\*\*Decomposition by beta-scission \*\*\*\*\*

C6H5CH2O=R1H+C6H5CHO 2.0E13 0.0 27.5E3 !

<estimated(j)>! INHIBE

C6H5CH2O=C6H5#+HCHO 2.0E13 0.0 27.5E3 !

<estimated(j)>! ACCELERE

!DH = 23.59 kcal/mol!

!(j) For these beta-scissions involving the breaking of a C-C or a C-H bond, A-factor !

!is an average value for beta-scissions [Heyberger] and activation energies have been!

! estimated from thermochemistry and to obtain the best results!



!C6H5CH2O=R1H+C6H5CHO 5.26E28 -5.081 22.25E3 !  
mf<Da silva-bozzelli J phys chem 25(2009)6979>!  
!C6H5CH2O=C6H6#+R5CHO 2.37E32 -6.095 28.81E3 !  
mf<Da silva-bozzelli J phys chem 25(2009)6979>!  
!C6H5CH2O=C6H5#+HCHO 7.21E33 -6.21 36.85E3 !  
mf<Da silva-bozzelli J phys chem 25(2009)6979>!

!C6H5CH2O=R1H+C6H5CHO 1.00e14 0.00 2.91e4 !  
mf<Mehl Proc comb inst 33(2011)193>!  
!C6H5CH2O=C6H5#+HCHO 1.46e20 -2.00 3.51e4 !  
mf<Mehl Proc comb inst 33(2011)193>!

!\*\*\*reactions with oxygen  
C6H5CH2O+O2=R300H+C6H5CHO 6.0E10 0.0 1.6E3 !  
<estimated(k)>!  
!(k) : Rate constant taken equal to that of the similar reaction in the  
case of ethoxy!  
!radicals as proposed by BAULCH92!

!\*\*\*\*\*!  
!\*REACTIONS OF CRESOXY RADICALS\*!  
!\*\*\*\*\*!

!\*\*OC6H4CH3=HOC6H4CH2 2.9E9 1.0 3.2E3 !<estimated(h')>!  
!(h') : Rate constant of the isomerisation :!  
!A =  $k_bT/h \times rpd \times \exp((Dnirot \times 3.5)/R)$ , Ea = 5.9 + 5 (5 membered  
transition ring)!  
!+ 7.3 (primary alkyllic H-atom by CH3O)!

!OC6H4CH3=HOC6H4CH2 1.1E9 1.0 22.9E3 !  
! A x2/5 only for ortho isomere, Ea= 5.9(RSE)+17 (H allylique p by R00.  
close bde)

!\*\*CO elimination with rearrangement  
!OC6H4CH3=>R1H+C6H6#+B2CO 7.5E11 0.0 43.8E3 !  
<FRANCK94>!  
OC6H4CH3=>R1H+C6H6#+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
!OC6H4CH3=>R10C2H3V+C4H4+B2CO 3.0E11 0.0 43.8E3!<FRANCK94>!  
!OC6H4CH3=>C2H2+iC4H5+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
!OC6H4CH3=>C2H2+C4H4+R1H+B2CO 3.0E11 0.0 43.8E3 !  
<FRANCK94>!  
OC6H4CH3=>C3H3+aC3H4+B2CO 1.5E11 0.0 43.8E3 !  
<FRANCK94>!

!\*\*termination reactions!  
OC6H4CH3+R1H=HOC6H4CH3 1.0E14 0.0 0.0E3 !  
<estimated(g)>!

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!*****!
!*REACTIONS OF BENZALDEHYDE AND DERIVED RADICALS*!
!*****!

```

```

! Amorcage
!C6H5CHO+O2=C6H5CO+R300H      2.0E13   0.0   38.9E3      !<EMDEE92>!
C6H5CHO+O2=C6H5CO+R300H      7.0E11   0.0   39.5E3      !RODA RODA
C6H5CHO = C6H5CO + R1H      3.98E15  0.0  83.74E3     !NIST GRELA86!

```

```

! Addition
C6H5CHO+R1H=C6H6#+R5CHO      5.8E13   0.0   8.1E3      !
<estimated(m)>!
!(m) : Rate constant taken equal to that of the same reaction in the case
of toluene!

```

```

! Metatheses
C6H5CHO+R1H=C6H5CO+H2      4.0E13   0.0     3.2E3      !
<estimated(n)>!
!(n) : Rate constant estimated from the parameters proposed by WARNATZ84
for acetaldehyde!
!with an activation energy 1 kcal/mol lower due to the resonance
stabilisation of the!
! obtained radical!

```

```

C6H5CHO+B10=C6H5CO+R20H      6.0E12   0.0   1.8E3      !<BAULCH94>!
C6H5CHO+R20H=C6H5CO+H2O      7.8E12   0.0   0.0        !<BAULCH94>!
C6H5CHO+R300H=C6H5CO+H2O2   3.0E12   0.0  11.0E3     !<estimated(o)>!
C6H5CHO+R4CH3=C6H5CO+CH4    2.0E-6   5.6   2.5E3      !MF <BAULCH94>!

```

```

C6H5CHO+R11C2H5=C6H5CO+C2H6  1.3E12   0.0   7.5E3      !<estimated(o)>!
!(o) : Rate constant estimated from the parameters proposed by BAULCH94
(HO2, CH3) and by !
!HOLHEIN70 (C2H5) for acetaldehyde with an activation energy 1 kcal/mol
lower due to the !
!resonance stabilisation of the obtained radical!

```

```

C6H5CHO+C3H5Y=C6H5CO+C3H6Y  1.3E12   0.0   11.5E3     !
<estimated(p)>!
C6H5CHO+iC4H5=C6H5CO+C4H6Z2  1.3E12   0.0   11.5E3     !
<estimated(p)>!

```

$C_6H_5CHO+nC_4H_5=C_6H_5CO+C_4H_6Z_2$       1.3E12      0.0      7.5E3      !  
 <estimated(p)>!  
 $C_6H_5CHO+benzyl=toluene+C_6H_5CO$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+C_6H_5O\# =C_6H_5CO+C_6H_5OH\#$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+OC_6H_4CH_3=C_6H_5CO+HOC_6H_4CH_3$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+C_5H_5\# =C_6H_5CO+C_5H_6\#$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>

!(p) :Rate constant taken equal to that of the H-abstraction with ethyl radicals !  
 ! with A divided by 10 for cyclic radicals and with an activation energy !  
 !4 kcal/mol higher for resonance stabilised radicals!

$C_6H_5CHO+HOC_6H_4CH_2=C_6H_5CO+HOC_6H_4CH_3$       1.3E11      0.0      11.5E3      !  
 <estimated(p)>  
 $C_6H_5CHO+C_6H_5\# =C_6H_5CO+C_6H_6\#$       1.3E11      0.0      11.5E3      !<estimated(p)>

$C_6H_5CO=C_6H_5\#+B_2CO$       4E14      0.0      29.5e3      !  
 <SOLLY71>!

!Author(s): Solly, R.K.; Benson, S.W.  
 !Title: Kinetics of the gas-phase unimolecular decomposition of the benzoyl radical  
 !Journal: J. Am. Chem. Soc.  
 !Volume: 93  
 !Page(s): 2127  
 !Year: 1971

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYL HYDROPEROXYDE\*!  
 !\*\*\*\*\*!

$!MFC_6H_5CH_2OOH=C_6H_5CH_2O+R_2OH$       1.5E16      0.0      42.0E3      !  
 <estimated(r)>!  
 !(r) : Rate constant taken equal to that the decomposition of hydroperoxide species !  
 ! proposed by Bounaceur <SAHETCHIAN>!  
 $!MFC_6H_5CH_2OOH=C_6H_5CH_2O+R_2OH$       2.03E47      -10.27  
           50.71E3      !<da silva J Chem Theory Comput 2009>  
 $C_6H_5CH_2OOH=C_6H_5CH_2O+R_2OH$       3.29E13      0.42      39.89E3      !  
 MF<da silva Proc comb inst 32(2009)287-294>  
 $C_6H_5CH_2OOH=C_6H_5CHO+H_2O$       7.45E8      1.19  
           46.04E3      !MF<da silva Proc comb inst 32(2009)287-294>

!\*\*\*\*\*!  
 !\*REACTIONS OF CRESOL AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

! amorcage  
 $HOC_6H_4CH_3+O_2=OC_6H_4CH_3+R_3OOH$       1.0E13      0.0      38.9E3      !  
 <estimated(s)>! ralenti

!A=1E13 pour phenol!  
 !(s) : Rate constant taken equal to that of the same reaction for phenol !

!HOC6H4CH3+O2=HOC6H4CH2+R300H 2.1E13 0.0 38.0E3 !  
 <EMDEE92\*2>!  
 HOC6H4CH3+O2=HOC6H4CH2+R300H 2.1E12 0.0 38.6E3 !  
 RODA <estimated(aaa)>!

! addition  
 HOC6H4CH3+R1H=C6H5OH#+R4CH3 5.8E13 0.0 8.1E3  
 !<estimated(t)>!  
 !(t) : Rate constant taken equal to that of the same reaction for toluene  
 !

!HOC6H4CH2+B10=C6H4OH#+HCHO 8E13 0.0 0.0

! metatheses  
 HOC6H4CH3+R1H=OC6H4CH3+H2 1.2E14 0.0 12.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+B10=OC6H4CH3+R20H 1.3E13 0.0 2.9E3 !  
 <estimated(s)>!  
 HOC6H4CH3+R20H=OC6H4CH3+H2O 1.4E8 1.4 -0.96E3 !  
 <estimated(s)>!  
 HOC6H4CH3+R300H=OC6H4CH3+H2O2 1.0E12 0.0 10.0E3 !  
 <estimated(s)>!  
 HOC6H4CH3+R4CH3=OC6H4CH3+CH4 1.8E11 0.0 7.7E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C6H5#=OC6H4CH3+C6H6# 4.9E12 0.0 4.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C5H5#=OC6H4CH3+C5H6# 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C3H5Y=OC6H4CH3+C3H6Y 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+iC4H5=OC6H4CH3+C4H6Z2 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!  
 HOC6H4CH3+C6H5O#=OC6H4CH3+C6H5OH# 4.9E11 0.0 9.4E3 !  
 <estimated(s)>!

HOC6H4CH3+R1H=HOC6H4CH2+H2 1.2E14 0.0 8.4E3 !  
 <estimated(t)>!  
 HOC6H4CH3+B10=HOC6H4CH2+R20H 6.3E11 0.0  
 0.0 !<estimated(t)>!  
 HOC6H4CH3+R20H=HOC6H4CH2+H2O 5.2E9 1.0 0.87E3 !  
 <estimated(t)>!  
 HOC6H4CH3+R300H=HOC6H4CH2+H2O2 4.0E11 0.0 14.0E3 !  
 <estimated(t)>!  
 HOC6H4CH3+R4CH3=HOC6H4CH2+CH4 1.6E12 0.0 11.1E3 !  
 <estimated(t)>!

$\text{HOC6H4CH3} + \text{C3H5Y} = \text{HOC6H4CH2} + \text{C3H6Y}$  1.6E12 0.0 15.1E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C3H3} = \text{HOC6H4CH2} + \text{pC3H4}$  1.6E12 0.0 15.1E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{iC4H5} = \text{HOC6H4CH2} + \text{C4H6Z2}$  1.6E12 0.0 15.1E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{nC4H5} = \text{HOC6H4CH2} + \text{C4H6Z2}$  1.6E12 0.0 11.1E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C5H5\#} = \text{HOC6H4CH2} + \text{C5H6\#}$  1.6E11 0.0 15.1E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C6H5\#} = \text{HOC6H4CH2} + \text{C6H6\#}$  7.9E13 0.0 12.0E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C6H50\#} = \text{HOC6H4CH2} + \text{C6H50H\#}$  1.6E11 0.0 15.1E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C6H4CH3} = \text{HOC6H4CH2} + \text{toluene}$  7.9E13 0.0 12.0E3 !  
 <estimated(t)>!  
 $\text{HOC6H4CH3} + \text{OC6H4CH3} = \text{HOC6H4CH2} + \text{HOC6H4CH3}$  1.6E11 0.0  
 15.1E3 !<estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C6H5CH200} = \text{HOC6H4CH2} + \text{C6H5CH200H}$  4.0E11 0.0  
 14.0E3 !<estimated(t)>!  
 $\text{HOC6H4CH3} + \text{C6H5CH20} = \text{HOC6H4CH2} + \text{C6H5CH20H}$  1.6E11 0.0  
 11.1E3 !<estimated(t)>!  
  
 $\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH200}$  4.6E11 0.0 -377.0 !  
 <estimated(u)>!  
 $\text{HOC6H4CH2} + \text{O2} = \text{HOC6H4CH20} + \text{B10}$  6.3E12 0.0 40.0E3 !  
 <estimated(u)>!  
 $\text{HOC6H4CH2} + \text{R300H} = \text{HOC6H4CH20} + \text{R20H}$  5.0E12 0.0 0.0 !  
 <estimated(u)>!  
 !(u) : Rate constant taken equal to that of the same reaction for benzyl  
 radicals !  
  
 $\text{HOC6H4CH2} + \text{R1H} = \text{HOC6H4CH3}$  1.0E14 0.0 0.0 !  
 <estimated(g)>!  
 $\text{HOC6H4CH2} + \text{R4CH3} = \text{C6H50H\#} + \text{C2H4Z}$  5.0E12 0.0 0.0 !  
 <estimated(g)>!  
  
 $\text{HOC6H4CH200} = \text{C6H40HCHO} + \text{R20H}$  3.4E9 1.0 37.5E3 !<estimated(v)>!  
 !(v) : Rate constant taken equal to that of the same reaction for benzyl  
 peroxy radicals !  
  
 $\text{HOC6H4CH20} = \text{R1H} + \text{C6H40HCHO}$  2.0E13 0.0 27.5E3 !  
 <estimated(w)>!  
 $\text{HOC6H4CH20} = \text{C6H40H\#} + \text{HCHO}$  2.0E13 0.0 27.5E3 !  
 <estimated(w)>!  
 $\text{HOC6H4CH20} + \text{O2} = \text{R300H} + \text{C6H40HCHO}$  6.0E10 0.0 1.6E3 !  
 <estimated(w)>!  
 !(w) : Rate constant taken equal to that of the same reaction for benzyl  
 alcoxy radicals !  
  
 $\text{C6H40HCHO} + \text{R1H} = \text{C6H40HCO} + \text{H2}$  4.0E13 0.0 3.2E3 !<estimated(x)>!  
 $\text{C6H40HCHO} + \text{B10} = \text{C6H40HCO} + \text{R20H}$  6.0E12 0.0 1.8E3 !  
 <estimated(x)>!

$C_6H_4OHC_6H_4O + R_2OH = C_6H_4OHC_6H_4O + H_2O$       7.8E12      0.0      0.0      !  
 <estimated(x)>!  
 $C_6H_4OHC_6H_4O + R_3OOH = C_6H_4OHC_6H_4O + H_2O_2$       3.0E12      0.0      11.0E3      !  
 <estimated(x)>!  
 $C_6H_4OHC_6H_4O + R_4CH_3 = C_6H_4OHC_6H_4O + CH_4$       2.0E-6      5.6      1.5E3      !  
 <estimated(x)>!  
 !(x) : Rate constant taken equal to that of the same reaction for  
 benzaldehyde !

$C_6H_4OHC_6H_4O = C_6H_4OH\# + B_2CO$       2.0E13      0.0      30.5E3      !  
 <estimated(y)>  
 !(y) : Rate constant taken equal to that of the same reaction for  $C_6H_5CO$   
 radicals !

!\*\*\*\*\*!  
 !\*REACTIONS OF BENZYLALCOOL AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

$C_6H_5CH_2OH + O_2 = R_3OOH + C_6H_5CHOH$       1.4E12      0.0      34.0E3      !RODA  
 <estimated(aaa)>!  
 $C_6H_5CH_2OH + O_2 = C_6H_5CH_2O + R_3OOH$       2.0E14      0.0      41.4E3      !  
 <EMDEE92>!

$C_6H_5CH_2OH + R_1H = C_6H_6\# + R_6CH_2OH$       5.8E13      0.0      8.1E3      !  
 <estimated(t)>!

$C_6H_5CH_2OH + R_1H = C_6H_5CHOH + H_2$       8.0E13      0.0      6.4E3      !<estimated(t')>!  
 $C_6H_5CH_2OH + B_{10} = C_6H_5CHOH + R_{20H}$       4.2E11      0.0      -2.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + R_{20H} = C_6H_5CHOH + H_2O$       3.5E9      1.0      -1.13E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + R_3OOH = C_6H_5CHOH + H_2O_2$       2.7E11      0.0      12.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + R_4CH_3 = C_6H_5CHOH + CH_4$       1.1E12      0.0      9.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_3H_5Y = C_6H_5CHOH + C_3H_6Y$       1.1E12      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + iC_4H_5 = C_6H_5CHOH + C_4H_6Z_2$       1.1E12      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + nC_4H_5 = C_6H_5CHOH + C_4H_6Z_2$       1.1E12      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_6H_5\# = C_6H_5CHOH + C_6H_6\#$       5.2E13      0.0      10.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_6H_4CH_3 = C_6H_5CHOH + toluene$       5.2E13      0.0      10.0E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + C_6H_5O\# = C_6H_5CHOH + C_6H_5O\#$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + benzyl = C_6H_5CHOH + toluene$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + OC_6H_4CH_3 = C_6H_5CHOH + HOC_6H_4CH_3$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!  
 $C_6H_5CH_2OH + HOC_6H_4CH_2 = C_6H_5CHOH + HOC_6H_4CH_3$       1.1E11      0.0      13.1E3      !  
 <estimated(t')>!

C6H5CH2OH+C5H5#=C6H5CHOH+C5H6# 1.1E11 0.0 13.1E3 !  
 <estimated(t')>!  
 !t': estimated as toluene with A x(2/3) to take into account the number  
 of abstractable !  
 !H atoms and Ea -2 kcal/mol due to the OH substitution!

C6H5CHOH=C6H5CHO+R1H 2.0E13 0. 36.373E3 !MF  
 DHR=36.79 correlation baptiste E=0.6\*DHR+14.3  
 !R15C2H5O=CH3CHO+R1H 2.0E14 0. 23.3E3 !(243,-  
 243)<HEICKLEN88NIST>!

!\*\*\*\*\*!  
 !\*REACTIONS OF ETHYLBENZENE AND DERIVED RADICALS\*!  
 !\*\*\*\*\*!

!\*\* Amorзages monomolйculaires

etC6H5 = R1H + C8H9# 4.3E14 0.0 83.6E3 !<kingas>!

!\*\* Amorзages bimolйculaires

etC6H5+O2=C8H9#+R300H 1.4E12 0.0 34.0E3 !  
 <estimated(aaa)>!  
 etC6H5+O2=C8H9#-1+R300H 1.2E13 0.0 49.0E3 !  
 <exgas>!

!\*\* Additions ipso

etC6H5+R1H=C6H6#+R11C2H5 5.8E13 0.0 8.1E3 !  
 <estimated(t)>!

!\*\* Metatheses

etC6H5+R1H=C8H9#+H2 8.0E13 0.0 6.4E3  
 !<estimated(t'')>!  
 etC6H5+B10=C8H9#+R20H 4.2E11 0.0 -2.0 !  
 <estimated(t'')>!  
 etC6H5+R20H=C8H9#+H20 3.5E9 1.0 -1.13E3 !  
 <estimated(t'')>!  
 etC6H5+R300H=C8H9#+H202 2.7E11 0.0 12.0E3  
 !<estimated(t'')>!  
 etC6H5+R4CH3=C8H9#+CH4 1.1E12 0.0 9.1E3 !  
 <estimated(t'')>!  
 etC6H5+C3H5Y=C8H9#+C3H6Y 1.1E12 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+iC4H5=C8H9#+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+nC4H5=C8H9#+C4H6Z2 1.1E12 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+C6H5O#=#C8H9#+C6H5OH# 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+benzyl=C8H9#+toluene 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+OC6H4CH3=C8H9#+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!  
 etC6H5+HOC6H4CH2=C8H9#+HOC6H4CH3 1.1E11 0.0 13.1E3 !  
 <estimated(t'')>!

etC6H5+C5H5#=C8H9#+C5H6# 1.1E11 0.0 13.1E3 !  
<estimated(t")>!

!t": estimated as toluene with A x(2/3) to take into account the number  
of abstractable !

!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

etC6H5+R1H=C8H9#-1+H2 7.2E8 1.5 6.79E3 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+B10=C8H9#-1+R20H 5.1E8 1.5 5.05E3 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+R20H=C8H9#-1+H2O 3.6E6 2.0 4.82E2 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+R300H=C8H9#-1+H2O2 4.2E4 2.69 1.85E4 !MF  
correlation Dean-Bozzelli 2000  
etC6H5+R4CH3=C8H9#-1+CH4 2.43E6 1.87 1.03E4 !MF correlation  
Dean-Bozzelli 2000

!mfetC6H5+C6H5#=C6H6#+C8H9# 5.27E13 0.0 12.0E3 !ajout MF as  
2/3 toluene <HECKMANN96>!

etC6H5+C6H5#=C6H6#+C8H9# 5.27E13 0.0 9.0E3 !test mf

etC6H5+C6H5#=C6H6#+C8H9#-1 5.85E10 0.0 3.83E3 !ajout MF as  
C5H12/4 <Park, Int J. Chem. Kinet.33(2001)64-69>

! Ajout ipso MF

etC6H5+B10=C6H5O#+R11C2H5 1.7E13 0.0 3.6E3 !MF as toluene !  
<TAPPE89>!

etC6H5+R20H=C6H5O#+R11C2H5 1.3E13 0.0 10.6E3 !MF as toluene  
<BAULCH94>as benzene

!etC6H5+R4CH3=toluene+R11C2H5 1.2E12 0.0 1.59E4 !MF as benzene  
<Robaugh, J. Phys. Chem.90(1986)4159 - 4163>

etC6H5+R4CH3=toluene+R11C2H5 1.2E12 0.0 1.24E4 ! MF as benzene-  
kcal <Robaugh, J. Phys. Chem.90(1986)4159 - 4163>

! \*\* Decompositions

C8H9#-1=C2H4Z+C6H5# 2.0E13 0.0 35.5E3 !MF correlation exgas  
C8H9# =R1H+styrene 3.1e13 0.0 50670 !<MULLER88>  
C8H9#-1=R1H+styrene 4.0E13 0.0 33.58E3 !MF <Sirjean,  
J.Phys.Chem.A 2008>

! \*\* Reactions of derived radicals

C8H9#+O2=R300H+styrene 6.90E11 0.0  
15.2E3 !<est (exgas-sylvain)>!

!C8H9#+R300H=R20H+R4CH3+C6H5CHO 3.27E12 0.0  
0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

!C8H9#+R300H=R20H+R1H+C6H5COCH3 7.80E10 0.0  
0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>

!C8H9#+R300H=>R20H+C6H5#+CH3CHO 2.54E11 0.0  
0.0 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>



C8H9#+R300H=C8H9#00H	3.60E12	0.0	
0.0 !MF KINGAS			
C8H9#00H=R20H+C8H9#0	5.00E15		
0.0 42500 !MF			
C8H9#0=R4CH3+C6H5CHO	2.69E13	0.0	
12117 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>			
C8H9#0=C6H5#+CH3CHO	1.74E14		
0.0 20458 !MF as but-3-en-1-oxy <Rauk, Can.J.Chem 81(2003)431-442>			
C8H9#-1+O2=R300H+styrene	2.60E11	0.0	
2.5E3			
C8H9#-1+R300H=R20H+HCHO+benzyl	5.00E12	0.0	
0.0 !<kingas>!			
!*****!			
!*REACTIONS OF STYRENE AND DERIVED RADICALS*!			
!*****!			
styrene+O2=R300H+C6H5C2H2	2.0E13	0.0	57.9E3 !
<asbutadiene/2>!			
!C4H6Z2+O2=iC4H5+R300H	4.0E13	0.0	57.9E3 !
<LEUNG95>!			
!styrene+B10=C6H5#+R13CH2CHO	3.0E08	1.45	0.9E3 !
<asbutadiene/2>! ! ENLEVE PAR BENOIT ET PAG			
styrene+R20H=benzyl+HCHO	1.4E12	0.0	-0.9E3 !<as
butadiene/2!			
styrene+R20H=C6H5CHO+R4CH3	1.4E12	0.0	-0.9E3 !MF
idem rñaction pñçñdente as C3H6Y <TSAnG91>			
!C4H6Z2+B10=C3H5Y+R1H+B2C0	6.0E08	1.45	0.9E3 !
<LEUNG95, BREZINSKY84>!			
!C4H6Z2+R20H=C3H5Y+HCHO	2.8E12	0.0	-0.9E3 !
<LINSTEDT96>!			
!C4H6Z2+R20H=CH3CHO+R10C2H3V	5.6E12	0.0	-0.9E3 !
<fromLINSTEDT96>!			
styrene+R1H=C6H5C2H2+H2	3.3E5	2.53	9.2E3 !MF<as
butadiene/2>!			
styrene+R20H=C6H5C2H2+H2O	1.5E6	2.0	0.4E3 !<as
butadiene/2>!			
styrene+R4CH3=C6H5C2H2+CH4	3.5E13	0.0	15.5E3 !<as
butadiene/2>			
!C4H6Z2+R1H=iC4H5+H2	6.6E5	2.53	9.2E3 !
<WANG97>!			
!C4H6Z2+R20H=iC4H5+H2O	3.1E6	2.0	0.4E3 !
<WANG97>!			
!C4H6Z2+R4CH3=iC4H5+CH4	7.0E13	0.0	15.5E3 !
<WU87-3kcal>!			

C6H5C2H2+O2=C6H5CO+HCHO 4.5E16 -1.39 1.0E3 !  
<asMebel C2H3+O2>! \*\*

!\*Addition Zhenyu\*!

C6H5C2H2+R1H=C6H5#C2H+H2 1.0E13 0.0  
0.0 !in Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and  
Tech. 120 (1996) 119-167.

C6H5C2H2+R2OH=C6H5#C2H+H2O 1.0E13 0.0 0.0 !in  
Slavinskaya09, R.P. Lindstedt, L.Q. Maurice, Comb. Sci. and Tech. 120  
(1996) 119-167.

! ajout d'un amorcage Roda

C6H5#C2H => C6H5# + R9C2H 2.2e16 0.0 98.0e3 ! MF  
as toluene

!\*\*\*\*\*!  
!\*REACTIONS OF C5H5CCH AND DERIVED RADICALS\*!  
!\*\*\*\*\*!

!\*Addition Zhenyu\*!

!C5H5CCH=C5H5#+R9C2H 4.2E15 0.0 125.0E3 !  
<KInGAS1500>! pC3H4=R9C2H+R4CH3  
!C5H5CCH+R1H=C5H5#+C2H2 2.0E10 0.0 0.0  
!Lindstedt96  
!C5H5CCH+R1H=C3H3+C4H4 6.0E10 0.0 0.0  
!Lindstedt96  
!C5H5CCH+R2OH=C5H5#+CH2COZ 4.3E11 0.0 -0.8E3  
!<BOODAGHIANs87>! pC3H4+R2OH=CH2COZ+R4CH3  
!C5H4CCH2=C5H5CCH 2.5E12 0.0 59.0E3 !  
<HIDAKA89>! aC3H4=pC3H4  
!C5H4CCH2+R1H=C5H5CCH+R1H 8.5E12 0.0 2.0E3 !  
<WAGnER72>! aC3H4+R1H(+M)=tC3H5(+M)  
!C5H4CCH2+R2OH=C5H5#+CH2COZ 2.0E12 0.0 -0.2E3 !<LIU88>!  
aC3H4+R2OH=CH2COZ+R4CH3

!\*\*\*\*\*!  
!\*REACTIONS OF BIBENZYL AND DERIVED RADICALS\*!  
!\*\*\*\*\*!

bibenzyl=C14H13#+R1H 1.0E16 0.0 83.66E3 !  
<Oehlschlaeger05>! in Sakai07 Zhenyu  
bibenzyl+O2=C14H13#+R30OH 2.8E12 0.0 35.0E3 !<est  
aaaa!  
bibenzyl+R1H=C14H13#+H2 5.4E4 2.5 -1.9E3 !  
Table A-I-21 Zhenyu

bibenzyl+B10=C14H13#+R2OH 8.4E11 0.0 -2.0 !  
<estimated(t'')>!  
bibenzyl+R2OH=C14H13#+H2O 7.0E9 1.0 -1.13E3 !  
<estimated(t'')>!

```

bibenzyl+R300H=C14H13#+H2O2          5.4E11      0.0  12.0E3  !
<estimated(t'')>!
bibenzyl+R4CH3=C14H13#+CH4           2.2E12      0.0    9.1E3  !
<estimated(t'')>!
bibenzyl+C6H5O#=#C14H13#+C6H5OH#     2.2E12      0.0   13.1e3  !
<estimated(t'')>!
bibenzyl+benzyl=C14H13#+toluene      2.2E12      0.0   9.1E3  !
<Oehlschlaeger05>! in Sakai07 Zhenyu

bibenzyl+C3H5Y=C14H13#+C3H6Y         2.2E12      0.0  13.1E3  !
<estimated(t'')>!
!t'': estimated as toluene with A x(4/3) to take into account the number
of abstractable !
!H atoms and Ea -2 kcal/mol due secondary H atoms instead of primary!

!Ajout ipso MF
bibenzyl+R1H=C6H6#+C8H9#-1           5.67E8     1.43  5.65E3  !Calcul CBS-
QB3 Fournet as toluene
bibenzyl+R20H=C6H5OH#+C8H9#-1       7.83E2     2.884  3.2193E3 !Seta V
Nakajima V Miyoshi JPCA 2006
C14H13#=stilbene+R1H                 7.94E15    0.0   51.864E3 !
<Oehlschlaeger05>! in Sakai07 Zhenyu
C14H13#+O2= stilbene+R300H           1.6E12    0.00  15200 !as allylique
C14H13#+R300H=>R20H+C6H5CHO+benzyl  8.21E4     2.20  -5.13E3 ! as benzyl

!*****!
!*REACTIONS OF STILBENE *!
!*****!

!Ajout Ipso MF
stilbene+R1H=>C6H6#+C2H2+C6H5#       5.67E8     1.43  5.65E3  !Calcul CBS-
QB3 Fournet as toluene
stilbene+R20H=C6H5OH#+C6H5C2H2      7.83E2     2.884  3.2193E3 !Seta V
Nakajima V Miyoshi JPCA 2006

! ajout MF
stilbene+R20H=C6H5CHO+benzyl         1.0E13      0.0    5.94E3  !
<Baulch05> as C2H4

!*****!
!* Reactions of naphthalene *!
!*****!
2C5H5#=naphthalene+H2                 4.3E36    -6.3  22.835E3 ! A.M. Dean, J.
Phys. Chem. 94 (1990) 1432-1439.
C6H5#+iC4H3=naphthalene               3.18E23   -3.2  2.13E3  ! H.Y. Zhang, J.T.
McKinnon, CST 107 (1995) 261-300.
C6H5#+C4H4=naphthalene+R1H            3.3E33    -5.7  12.75E3 ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.
benzyl+C3H3=>naphthalene+R1H+R1H      6.0E11    0.0  0.0      ! M.B. Colket,
D.J. Seery, Proc. Combust. Inst. 25 (1994) 883-891.
C6H5C2H2+C2H2=naphthalene+R1H        1.6E16    -1.33  3.3E3   ! J. Appel, H.
Bockhorn, M. Frenklach, Combust. Flame 121 (2000) 122-136.

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naphthalene+O2=R300H+naphthyl like benzene <ALZUETA00>A*8/6!	8.0E13	0.0	63.4E3	!
naphthalene+B10=>indenyl+B2C0+R1H benzene <Nicovich82>A*8/6!	2.7E13	0.0	3.6E3	!like
naphthalene+R1H=naphthyl+H2 benzene <MEBEL97>A*8/6!	8.0E8	1.8	16.8E3	!like
naphthalene+B10=naphthyl+R20H benzene <LINDSTEDT94>A*8/6!	2.7E13	0.0	14.7E3	!like
naphthalene+R20H=naphthyl+H2O benzene <BAULCH92>A*8/6!	2.1E8	1.42	1.45E3	!like
naphthalene+R300H=naphthyl+H2O2 benzene <BAULCH94>A*8/6!	7.3E12	0.0	28.9E3	!like
naphthalene+R4CH3=naphthyl+CH4 benzene <ZHANG89>A*8/6!	2.7E12	0.0	15.0E3	!like

naphthyl+R1H=naphthalene buthylbenzene	1.0E14	0.0	0.0E3	!as n-
naphthyl+O2=>indenyl+B2C0+B10 buthylbenzene	2.6E13	0.0	6.1E3	!as n-
naphthyl+B10=>indenyl+B2C0 buthylbenzene	1.0E14	0.0	0.0	!as n-
naphthyl+R300H=>indenyl+B2C0+R20H buthylbenzene	5.0E12	0.0	0.0	!as n-
naphthyl+R20H=>indenyl+B2C0+R1H buthylbenzene	1.0E13	0.0	0.0	!as n-

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!*****!
!* Reactions of indene and derived radicals *!
! Indene C6H4#/CH2/CH//CH/ *!
! Indenyl C6H4#/CH/CH//CH/ *!
! ph#C3H2 C6H5#/CH(./)/C///CH *!
!*****!

```

indene+R20H=>C2H4Z+C6H5C0	1.37E12	0.0	-1.04E3	!Slavinskaya
indene+R20H=>R10C2H3V+B2C0+C6H6#	1.37E12	0.0	-1.04E3	!Est.
!indene+R20H=>o-methylbenzyl+B2C0	1.37E12	0.0	-1.04E3	

indene+O2=R300H+indenyl buthylbenzene mais E = DH de reaction	1.4E12	0.0	31.03E3	! as n-
indene+B10=indenyl+R20H secondary A*2	1.76E11	0.7	3.25E3	! A-I-21
indene+R1H=indenyl+H2 secondary A*2	1.08E5	2.5	-1.9E3	! A-I-21
indene+R20H=indenyl+H2O secondary A*2	6.0E6	2.0	-1.52E3	! A-I-21
indene+R4CH3=indenyl+CH4 secondary A*2	2.0E11	0.0	7.3E3	! A-I-21
indene+R300H=H2O2+indenyl secondary A*2	1.28E4	2.6	12.4E3	! A-I-21

!indene+R1H=ph#C3H4Y	5.8E13	0.0	8.1E3	!ipso-addition
!indene+R1H=ph#C3H4-1	5.8E13	0.0	8.1E3	!ipso-addition
indene+R1H=>C2H2+benzyl	1.16E14	0.0	8.1E3	!mf 2x ipso-addition

indenyl=>C5H5#+C4H2 5.0E13 0.0 75.0E3 !Slavinskaya09  
5.0E13 0.0 37.5E3  
indenyl+R1H=indene 1.0E14 0.0 0.0 !as n-buthylbenzene  
C6H5#+C3H3=indene 6.46E12 0.0 0.0 !Slavinskaya09  
!indenyl+R300H=>C6H6#+B2CO+R9C2H+R20H 3.0E12 0.0 0.0 ! Est.!  
similar to C5H5#+H02  
indenyl+R300H=>C6H5#C2H+R5CHO+R20H 3.0E12 0.0 0.0 ! Est.!  
similar to C5H5#+H02

indenyl+B10=>C6H6#+B2CO+R9C2H 5.8E13 -0.02 0.02E3 !Est.  
C5H5#+B10=C5H40#+R1H  
indenyl+B10=>C6H5#C2H+R5CHO 5.8E13 -0.02 0.02E3 !Est.  
C5H5#+B10=C5H40#+R1H

indenyl+R20H=>styrene+B2CO 4.0E14 0.0 4.5E3 !Est.  
C5H5#+0H=C4H6Z2+C0

!C9H70#=C9H60#+R1H 2.0E13 0.0 27.5E3 ! Est.like ph#CH20  
!C9H70#=>C6H6#+B2CO+R9C2H 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+C0  
!C9H70#=C6H5#C2H+R5CHO 2.8E13 0.0 17.1E3 ! Est.CH3CO=CH3+C0

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

!\*\*\*\*\*Reactions for Ethyl  
Esters\*\*\*\*\*

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

EF=HC00H+C2H4Z 2.000E+12 0.00 4.729E+04  
!EF(+m)=HC00H+C2H4Z(+m) 4.000E+12 0.00 5.000E+04  
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /  
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troe Fall-off  
reaction  
C2H50CO+R1H(+m)=EF(+m) 1.000E+14 0.00 0.000E+00  
LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /  
TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off  
reaction  
EFEJ+R1H(+m)=EF(+m) 1.000E+14 0.00 0.000E+00  
LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /  
TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off  
reaction  
EFMJ+R1H(+m)=EF(+m) 1.000E+14 0.00 0.000E+00  
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
reaction  
EF(+m)=R5CHO+R15C2H50(+m) 1.650E+24 -2.04 1.002E+05  
LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /  
TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off  
reaction  
EF(+m)=HC02+R11C2H5 (+m) 5.734E+25 -2.76 9.211E+04  
LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /  
TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off  
reaction  
EF(+m)=CH20CHO+R4CH3(+m) 3.388E+21 -1.58 9.209E+04

LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /  
 TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !TroE Fall-off  
 reaction

EF+O2=C2H5OCO+R300H -3kcal	2.000E+13	0.00	4.130E+04	!as ep
EF+O2=EFEJ+R300H	2.000E+13	0.00	4.820E+04	!as ep
EF+O2=EFMJ+R300H	3.000E+13	0.00	5.229E+04	!as ep
EF+R1H=C2H5OCO+H2 et al.	2.720e+07	1.94	7880.0	!Good
EF+R1H=EFEJ+H2 C2H5OH Park et al., J.Chem.Phys. 118 (2003) 9990-9996	1.790E+05	2.53	3.420E+03	!as
EF+R1H=EFMJ+H2 anc7, primARy f	9.400e+04	2.75	6.280e+03	!2
EF+B10=C2H5OCO+R20H Westbrook et al.,	5.510e+05	2.5	2.830e+03	!
EF+B10=EFEJ+R20H C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703	1.450E+05	2.47	8.800E+02	!as
EF+B10=EFMJ+R20H anc7, primARy f	9.650e+04	2.68	3.716e+03	!2
EF+R20H=C2H5OCO+H2O et al.	1.610e+06	1.87	30.0	!Good
EF+R20H=EFEJ+H2O Lin pci 2007 31 159-166	1.306E+05	2.43	-1457.0	! Xu
EF+R20H=EFMJ+H2O rnc7, primARy;	5.250e+09	0.97	1.590e+03	!2
EF+R4CH3=C2H5OCO+CH4 et al.	6.564e+01	3.32	10010.0	!Good
EF+R4CH3=EFEJ+CH4 Xu, PARK, Lin, JcP 120, 6593-6599 (2004)	1.990E+01	3.37	7635.0	!
EF+R4CH3=EFMJ+CH4 anc7, primARy f	4.520e-01	3.65	7.154e+03	!2
EF+R300H=C2H5OCO+H2O2 Westbrook et al.,	9.640e+03	2.6	1.391e+04	!
!EF+R300H=EFEJ+H2O2 MARinov 1998	8.200E+03	2.55	10750.0	!
EF+R300H=EFEJ+H2O2	3.610E+03	2.55	1.053E+04	
EF+R300H=EFMJ+H2O2 anc7, primARy f	8.400e+12	0.00	2.044e+04	!2
EF+R8CH300=C2H5OCO+CH300H Westbrook et al.,	4.820E+03	2.6	1.391E+04	!
EF+R8CH300=EFEJ+CH300H	7.220E+03	2.55	1.053E+04	
EF+R8CH300=EFMJ+CH300H anc7, primARy f	8.400e+12	0.00	2.044e+04	!2
EF+R7CH30 =C2H5OCO+CH30H Herron	1.620e+12	0.00	8190.0	!
EF+R7CH30 =EFEJ+CH30H	4.580E+10	0.00	2.873E+03	
EF+R7CH30 =EFMJ+CH30H rnc7, primARy;	1.581e+11	0.00	7.000e+03	!2
!EFEJ+O2=EFfoo al., Combust Flame, 142 (2005) 170-186 (ks+kq)	1.200e+10	0.00	-2300.0	!Buda et
!EFMJ+O2=EFmoo al., Combust Flame, 142 (2005) 170-186 (ks)	9.000e+18	-2.50	0.000e+00	!Buda et

!EFeo=EFED+R300H	5.075E+42	-9.410	4.249E+04	!Donato et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EFmoo=EFED+R300H	5.044E+38	-8.110	4.149E+04	!Donato et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
C2H5OC0=R15C2H50+B2C0	4.840E+10	1.11	15887.0	!Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
	rev / 3.570E+04	2.485	37247.0 /	
C2H5OC0=R11C2H5 +C02	8.020E+11	0.65	21123.0 !	Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
	rev / 1.350E+04	2.31	7883.0 /	
EFEJ=CH3CHO+R5CHO	1.127E+21	-1.73	4.055E+04	
EFMJ=C2H4Z+HC02	1.340E+13	-0.40	2.461E+04 !	Westbrook et al., (2009)
EFEJ=EFED+R1H	3.000E+13	0.00	3.900E+04	!ST
EFMJ=EFED+R1H	3.000E+13	0.00	3.800E+04	!ST
!EFEJ+02=EFED+R300H	1.580E+12	0.00	5.000E+03	!Battin-
Leclerc, Prog Energy Combust Sci,	34 (2008) 440-498			
!EFMJ+02=EFED+R300H	1.580E+12	0.00	5.000E+03	!Battin-
Leclerc, Prog Energy Combust Sci,	34 (2008) 440-498			
EFEJ+R300H=EFED+H2O2	2.410E+13	0.0	0.0 !	(=R19C3H7/TSA88)
EFMJ+R300H=EFED+H2O2	2.410E+13	0.0	0.0 !	(=R19C3H7/TSA88)
HCHO+R20H=HCOOH+R1H	4.450E+07	1.18	-447.0 !	(TSANG HAMPSON 86)
HCOOH+M=B2CO+H2O+M	2.300E+13	0.0	50000.0 !	(82HSU/SHA)
HCOOH+M=C02+H2+M	1.500E+16	0.0	57000.0 !	(82HSU/SHA)
HCOOH+R20H=HC02+H2O	2.710E+11	0.0	0.0 !	(92ATK/BAU)
HC02=>R1H+C02	1.740E+12	0.31	32928.0 !	(88LAR/STE)
EFED+R20H=>HCHO+CH2OCHO	1.370E+12	0.00	-1.040E+03 !	Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EFED+R20H=>CH3CHO+HC02	1.370E+12	0.00	-1.040E+03 !	Heyberger et al., Combust Flame, 126 (2001) 1780-1802
EA=CH3C0OH+C2H4Z	2.000E+12	0.00	4.729E+04	
!EA(+m)=CH3C0OH+C2H4Z(+m)	4.000E+12	0.00	5.000E+04	
!LOW / 1.3100E+17	-9.9000E-01	1.1880E+04	/	
!TROE / 2.4323E-01	1.0000E+00	1.0000E+10	6.7101E+09 /	!Troee Fall-off reaction
EA2J+R1H(+m)=EA(+m)	1.000E+14	0.00	0.000E+00	
LOW / 4.4360+125	-3.0800E+01	1.1395E+05	/	
TROE / 9.6000E-01	9.9996E+09	1.3439E+00	6.6987E+08 /	!Troee Fall-off reaction
EAEJ+R1H(+m)=EA(+m)	1.000E+14	0.00	0.000E+00	
LOW / 1.3250+113	-2.7260E+01	1.1413E+05	/	

TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off  
 reaction  
 EAMJ+R1H(+m)=EA(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
 TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EA(+m)=C2H5OC0+R4CH3(+m) 2.627E+27 -3.23 9.769E+04 !as ep  
 +3kcal  
 LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /  
 TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off  
 reaction  
 EA(+m)=R14CH3C0+R15C2H50(+m) 1.650E+24 -2.04 1.002E+05  
 LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /  
 TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off  
 reaction  
 EA(+m)=CH3C02+R11C2H5 (+m) 5.734E+25 -2.76 9.211E+04  
 LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /  
 TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off  
 reaction  
 EA(+m)=MEMJ+R4CH3(+m) 3.388E+21 -1.58 9.209E+04  
 LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /  
 TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off  
 reaction  
 EA+O2=EA2J+R300H 2.000E+13 0.00 4.730E+04 !as ep  
 +3kcal  
 EA+O2=EAEJ+R300H 2.000E+13 0.00 4.820E+04 !as ep  
 EA+O2=EAMJ+R300H 3.000E+13 0.00 5.229E+04 !as ep  
  
 EA+R1H=EA2J+H2 9.400e+04 2.75 6.280e+03 !2  
 anc7, primARy f  
 EA+R1H=EAEJ+H2 1.790E+05 2.53 3.420E+03 !as  
 C2H5OH Park et al., J.Chem.Phys. 118 (2003) 9990-9996  
 EA+R1H=EAMJ+H2 9.400e+04 2.75 6.280e+03 !2  
 anc7, primARy f  
 !EA+R1H=EAMJ+H2 6.660E+05 2.54 6.756E+03  
 EA+B10=EA2J+R20H 9.650e+04 2.68 3.716e+03 !2  
 anc7, primARy f  
 EA+B10=EAEJ+R20H 1.450E+05 2.47 8.800E+02 !as  
 C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703  
 EA+B10=EAMJ+R20H 9.650e+04 2.68 3.716e+03 !2  
 anc7, primARy f  
 !EA+B10=EAMJ+R20H 9.810E+05 2.43 4.750E+03  
 EA+R20H=EA2J+H20 5.250e+09 0.97 1.590e+03 !2  
 rnc7, primARy;  
 EA+R20H=EAEJ+H20 1.306E+05 2.43 -1457.0 !as  
 C2H5OH Xu Lin pci 2007 31 159-166  
 EA+R20H=EAMJ+H20 5.250e+09 0.97 1.590e+03 !2  
 rnc7, primARy;  
 !EA+R20H=EAMJ+H20 5.280E+09 0.97 1.586E+03  
 EA+R4CH3=EA2J+CH4 4.520e-01 3.65 7.154e+03 !2  
 anc7, primARy f  
 EA+R4CH3=EAEJ+CH4 1.990E+01 3.37 7635.0 !as  
 C2H5OH Xu et al., J.Chem.Phys. 120, 6593-6599 (2004)



EA+R4CH3=EAMJ+CH4	4.520e-01	3.65	7.154e+03	!2
anc7, primARy f				
!EA+R4CH3=EAMJ+CH4	4.530E-01	3.65	7.154E+03	
EA+R300H=EA2J+H2O2	8.400e+12	0.00	2.044e+04	!2
anc7, primARy f				
!EA+R300H=EAEJ+H2O2	8.200E+03	2.55	10750.0	!
MARinov 1998				
EA+R300H=EAEJ+H2O2	3.610E+03	2.55	1.053E+04	
EA+R300H=EAMJ+H2O2	8.400e+12	0.00	2.044e+04	!2
anc7, primARy f				
!EA+R300H=EAMJ+H2O2	2.379E+04	2.55	1.649E+04	
EA+R8CH300=EA2J+CH300H	8.400e+12	0.00	2.044e+04	!2
anc7, primARy f				
EA+R8CH300=EAEJ+CH300H	7.220E+03	2.55	1.053E+04	
EA+R8CH300=EAMJ+CH300H	8.400e+12	0.00	2.044e+04	!2
anc7, primARy f				
!EA+R8CH300=EAMJ+CH300H	2.379E+04	2.55	1.649E+04	
EA+R7CH30 =EA2J+CH30H	1.581e+11	0.00	7.000e+03	!2
rnc7, primARy;				
EA+R7CH30 =EAEJ+CH30H	4.580E+10	0.00	2.873E+03	
EA+R7CH30 =EAMJ+CH30H	1.581e+11	0.00	7.000e+03	!2
rnc7, primARy;				
!EA+R7CH30 =EAMJ+CH30H	2.169E+11	0.00	6.458E+03	
!EAMJ=EA2J	9.900E+07	1.00	12000.0	! IS 26 KB
!EAEJ=EA2J	5.700E+08	1.00	21300.0	! IS 28 KB
EA2J=EAMJ	1.481e+08	1.00	2.450e+04	!(cyc
lact sat a 6 + 3Hp)				
EA2J=EAEJ	5.746e+08	1.00	1.800e+04	!(cyc
lact sat a 5 + 2Hs - 2kcal/0)				
!!EA2J+O2=EA2oo	9.000e+18	-2.50	0.000e+00	!Buda
et al., Combust Flame, 142 (2005) 170-186 (ks)				
!EA2J+O2=EA2oo	1.200e+10	0.00	-2300.0	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EAEJ+O2=EAeoo	1.200e+10	0.00	-2300.0	!Buda et
al., Combust Flame, 142 (2005) 170-186 (all)				
!EAMJ+O2=eamoo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!				
!eaeoo=EAED+R300H	5.075E+42	-9.410	4.249E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!eamoo=EAED+R300H	5.044E+38	-8.110	4.149E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EA2J=CH2COZ +R15C2H5O	1.280E+12	0.6584	49255.0	!
Huynh and Violi J.Org.Chem. 73 (2008) 94-101				
EA2J=CH2COZ +R15C2H5O	1.460E+12	0.61	53276.0	!
Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!EA2J=CH2COZ +R15C2H5O	9.364E+19	-1.88	5.642E+04	
!EAEJ=CH3CHO+R14CH3CO	1.127E+21	-1.73	4.055E+04	
EAEJ=CH3CHO+R14CH3CO	1.127E+21	-1.73	4.255E+04	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!EAMJ=C2H4Z+CH3CO2	2.325E+14	-0.20	3.297E+04	

EAMJ=C2H4Z+CH3C02	1.340E+13	-0.40	2.461E+04	!
Westbrook et al., (2009)				
!EA2J*o=>C2H50C0+B2C0	1.834e+15	-0.73	1.291e+04	!
Glaude et al., DMC C2H5C0				
EAEJ=EAED+R1H	3.000e+13	0.00	3.900e+04	!ST
EAMJ=EAED+R1H	3.000e+13	0.00	3.800e+04	!ST
!EAEJ+02=EAED+R300H	1.580E+12	0.00	5.000e+03	!Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				
!EAMJ+02=EAED+R300H	1.580E+12	0.00	5.000e+03	!Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				
!EAEJ+R300H=EAED+H202	2.410E+13	0.0	0.0	!
(=R19C3H7/TSA88)				
!EAMJ+R300H=EAED+H202	2.410E+13	0.0	0.0	!
(=R19C3H7/TSA88)				
!eaeoo=eaeooH2j	1.696e+07	1.00	2.270e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 2Hs - 2kcal/0)				
!eaeooH2j+02=eaeooH2oo	1.700e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)				
!eaeooH2oo=>ea2oohe*o+R20H	8.480e+06	1.00	2.350e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 1Ht - 2kcal/0)				
!ea2oohe*o=>HCH0+B2C0+CH3C02+R20H	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!eaeooH2j=>eacy2oe+R20H	3.630e+10	0.00	1.300e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)				
CH3C00H=CH2C0Z +H20	4.470E+14	0.00	7.989E+04	!Duan
et Page, J.Am.Chem.Soc. 117 (1995) 5114-5119				
CH3C00H=CH4+C02	7.080E+13	0.00	7.452E+04	!Duan et
Page, J.Am.Chem.Soc. 117 (1995) 5114-5119				
CH3C00H=>R14CH3C0+R20H	1.4E+0017	0.000	105815.7	! UI
8 KB				
CH3C00H=>CH3C02+R1H	2.3E+0014	0.000	106345.3	! UI 9
KB				
CH3C00H=>R4CH3+H0C0	8.2E+0016	0.000	88817.0	! UI 10
KB				
CH3C00H+R1H=CH2C00H+H2	9.400e+04	2.75	6.280e+03	!2
anc7, primARy f				
!CH3C00H+R1H=CH3C02+H2	4.200E+06	2.00	2400.0	! ME
96 CN				
CH3C00H+R1H=CH3C02+H2	5.550E-23	10.60	-4459.0	!
PARK,Zhu,Lin, JcP 118, 9990-9996 (2003)				
CH3C00H+B10=CH2C00H+R20H	9.650e+04	2.68	3.716e+03	!2
anc7, primARy f				
!CH3C00H+B10=CH3C02+R20H	1.000E+13	0.00	3280.0	! ME
87 CW				
CH3C00H+B10=CH3C02+R20H	1.460E-03	4.73	1727.0	! Wu,
Lee, Xu, Lin, JPcA 2007				
CH3C00H+R20H=CH2C00H+H20	5.250e+09	0.97	1.590e+03	!2
rnc7, primARy;				

!CH3C00H+R20H=CH3C02+H2O 105 CW	1.100E+06	2.00	-1865.0	! ME
CH3C00H+R20H=CH3C02+H2O Lin pci 2007 31 159-166	2.810E+02	2.97	-580.0	! Xu
CH3C00H+R4CH3=CH2C00H+CH4 anc7, primARy f	4.520e-01	3.65	7.154e+03	!2
CH3C00H+R4CH3=CH3C02+CH4 Xu, PARK, Lin, JcP 120, 6593-6599 (2004)	2.035E+00	3.57	7722.0	!
CH3C00H+R300H=>CH2C00H+H2O2 anc7, primARy f	8.400e+12	0.00	2.044e+04	!2
!CH3C00H+R300H=CH3C02+H2O2 96 CN	2.110E+06	0.00	1.400E+04	! ME
CH3C00H+R300H=CH3C02+H2O2 1998	2.500E+12	0.00	24000.0	! MARinov
CH3C00H+R8CH300=CH2C00H+CH300H anc7, primARy f	8.400e+12	0.00	2.044e+04	!2
CH3C00H+R7CH30 =CH2C00H+CH30H rnc7, primARy;	1.581e+11	0.00	7.000e+03	!2
!CH2C00H=CH2COZ +R20H	4.638E+18	-1.28	5.386E+04	
CH2C00H=CH2COZ +R20H	4.000E+13	0.00	5.821E+04	
CH2C00H=>C02+R4CH3	1.700E+09	1.0	38640.0	
!C2H50C0=R15C2H50+B2C0	5.059E+14	0.17	2.552E+04	
!C2H50C0=R11C2H5 +C02	1.805E+16	-0.56	2.017E+04	
!CH3C02+m=R4CH3+C02+m	4.400E+15	0.00	1.050E+04	
EAED+R20H=>HCHO+MEMJ Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!
EAED+R20H=>CH3CHO+CH3C02 Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!
HOCO=B2C0+R20H	1.186E+14	0.13	3.646E+04	
HOCO=C02+R1H	8.220E+11	0.41	3.534E+04	
!ea2*o+R1H=>EA2J*o+H2 Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102	1.200E+14	0.00	7000.0	!
!ea2*o+B10=>EA2J*o+R20H (BAULch92)	5.850E+12	0.00	1808.0	!
!ea2*o+R20H=>EA2J*o+H2O Atkinson et al., 2001	2.650E+12	0.00	-730.0	!
!ea2*o+R300H=>EA2J*o+H2O2 (COLKET 77; CH3CHO)	1.700E+12	0.00	10700.0	!
	3.100E+12	0.00	11920.0	!(BAULch92)
EP=C2H5C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
!EP(+m)=C2H5C00H+C2H4Z(+m)	4.000E+12	0.00	5.000E+04	
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 / !TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !TroE Fall-off reaction				
EP3J+R1H(+m)=EP(+m)	1.000E+14	0.00	0.000E+00	
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 / TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !TroE Fall-off reaction				
EP2J+R1H(+m)=EP(+m)	1.000E+14	0.00	0.000E+00	
LOW / 4.4360+125 -3.0800E+01 1.1395E+05 / TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !TroE Fall-off reaction				
EPEJ+R1H(+m)=EP(+m)	1.000E+14	0.00	0.000E+00	

LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /  
 TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off  
 reaction  
 EPMJ+R1H(+m)=EP(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
 TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EP(+m)=EA2J+R4CH3(+m) 5.732E+23 -2.33 8.774E+04  
 LOW / 4.3520E+14 8.2000E-01 6.3570E+04 /  
 TROE / 1.6900E-01 5.7129E+03 4.0466E+01 6.7101E+09 / !Troe Fall-off  
 reaction  
 EP(+m)=C2H50C0+R11C2H5 (+m) 2.627E+27 -3.23 9.469E+04  
 LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /  
 TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off  
 reaction  
 EP(+m)=R25C2H5C0+R15C2H50(+m) 1.650E+24 -2.04 1.002E+05  
 LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /  
 TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off  
 reaction  
 EP(+m)=C2H50C2+R11C2H5 (+m) 5.734E+25 -2.76 9.211E+04  
 LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /  
 TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off  
 reaction  
 EP(+m)=MPMJ+R4CH3(+m) 3.388E+21 -1.58 9.209E+04  
 LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /  
 TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off  
 reaction  
 EP+O2=EP3J+R300H 3.000E+13 0.00 5.229E+04  
 EP+O2=EP2J+R300H 2.000E+13 0.00 4.430E+04  
 EP+O2=EPEJ+R300H 2.000E+13 0.00 4.820E+04  
 EP+O2=EPMJ+R300H 3.000E+13 0.00 5.229E+04  
  
 EP+R1H=EP3J+H2 9.400e+04 2.75 6.280e+03 !2  
 anc7, primARy f  
 !EP+R1H=EP2J+H2 5.400e+04 2.5 -1.900e+03 !  
 EP+R1H=EP2J+H2 1.300E+06 2.4 4.471E+03 !2  
 anc7, secondARy  
 EP+R1H=EPEJ+H2 1.790E+05 2.53 3.420E+03 !as  
 C2H50H Park et al., J.Chem.Phys. 118 (2003) 9990-9996  
 EP+R1H=EPMJ+H2 9.400e+04 2.75 6.280e+03 !2  
 anc7, primARy f  
 EP+B10=EP3J+R20H 9.650e+04 2.68 3.716e+03 !2  
 anc7, primARy f  
 !EP+B10=EP2J+R20H 8.800e+10 0.70 3.250e+03 !  
 EP+B10=EP2J+R20H 4.770E+04 2.71 2.106E+03 !2  
 anc7, secondARy  
 EP+B10=EPEJ+R20H 1.450E+05 2.47 8.800E+02 !as  
 C2H50H Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703  
 EP+B10=EPMJ+R20H 9.650e+04 2.68 3.716e+03 !2  
 anc7, primARy f  
 EP+R20H=EP3J+H2O 5.250e+09 0.97 1.590e+03 !2  
 rnc7, primARy;  
 !EP+R20H=EP2J+H2O 3.000e+06 2.00 -1.520e+03 !

EP+R20H=EP2J+H20 rnc7, secondARY	4.680E+07	1.61	-3.500E+01	!2
EP+R20H=EPEJ+H20 C2H50H Xu Lin pci 2007 31 159-166	1.306E+05	2.43	-1457.0	!as
EP+R20H=EPMJ+H20 rnc7, primARY;	5.250e+09	0.97	1.590e+03	!2
EP+R4CH3=EP3J+CH4 anc7, primARY f	4.520e-01	3.65	7.154e+03	!2
!EP+R4CH3=EP2J+CH4	1.000e+11	0.00	7.300e+03	!
EP+R4CH3=EP2J+CH4 anc7, secondARY	2.705E+04	2.26	7.287E+03	!2
EP+R4CH3=EPEJ+CH4 C2H50H Xu, PARK, Lin, JcP 120, 6593-6599 (2004)	1.990E+01	3.37	7635.0	!as
EP+R4CH3=EPMJ+CH4 anc7, primARY f	4.520e-01	3.65	7.154e+03	!2
EP+R300H=EP3J+H202 anc7, primARY f	8.400e+12	0.00	2.044e+04	!2
!EP+R300H=EP2J+H202	6.400e+03	2.60	1.240e+04	!
EP+R300H=EP2J+H202 anc7, secondARY	5.600E+12	0.00	1.769E+04	!2
!EP+R300H=EPEJ+H202 MARinov 1998	8.200E+03	2.55	10750.0	!
EP+R300H=EPEJ+H202	3.610E+03	2.55	1.053E+04	
EP+R300H=EPMJ+H202 anc7, primARY f	8.400e+12	0.00	2.044e+04	!2
EP+R7CH30 =EP3J+CH30H rnc7, primARY;	1.581e+11	0.00	7.000e+03	!2
!EP+R7CH30 =EP2J+CH30H	1.780e+12	0.00	1.200e+03	!
EP+R7CH30 =EP2J+CH30H anc7, secondARY	1.095E+11	0.00	5.000E+03	!2
EP+R7CH30 =EPEJ+CH30H	4.580E+10	0.00	2.873E+03	
EP+R7CH30 =EPMJ+CH30H rnc7, primARY;	1.581e+11	0.00	7.000e+03	!2
EP+R8CH300=EP3J+CH300H corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EP+R8CH300=EP2J+CH300H	6.400e+03	2.60	1.240e+04	!
EP+R8CH300=EP2J+CH300H corrected to ag	5.600E+12	0.00	1.769E+04	!2
EP+R8CH300=EPEJ+CH300H	7.220E+03	2.55	1.053E+04	
EP+R8CH300=EPMJ+CH300H corrected to ag	8.400e+12	0.00	2.044e+04	!2
EP3J=EPEJ lact sat a 6 + 2Hs - 2kcal/0)	9.872e+07	1.00	2.000e+04	!(cyc
EP2J=EPMJ lact sat a 6 + 3Hp)	1.481e+08	1.00	2.450e+04	!(cyc
EP2J=EPEJ lact sat a 5 + 2Hs - 2kcal/0)	5.746e+08	1.00	1.800e+04	!(cyc
!EPMJ=EP2J	9.9E+0007	1.000	12000.0	! IS 26 KB
!EPMJ=EP3J	1.7E+0007	1.000	17400.0	! IS 27 KB
!EPEJ=EP2J	5.7E+0008	1.000	21300.0	! IS 28 KB
!EPEJ=EP3J	9.9E+0007	1.000	18000.0	! IS 29 KB

!EP3J+O2=EP3oo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!!EP2J+O2=EP2oo	1.000e+19	-2.50	0.000e+00	!Buda
et al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EP2J+O2=EP2oo	1.200e+10	0.00	-2300.0	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EPEJ+O2=EPEoo	1.200e+10	0.00	-2300.0	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EPMJ+O2=EPmoo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!				
!EP3oo=EP2d+R300H	5.044E+38	-8.110	4.149E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EP2oo=EP2d+R300H	5.075E+42	-9.410	4.249E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPEoo=EPED+R300H	5.075E+42	-9.410	4.249E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPmoo=EPED+R300H	5.044E+38	-8.110	4.149E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EP3J=C2H4Z+C2H5OC0	8.827E+15	-0.67	3.555E+04	
EP3J=C2H4Z+C2H5OC0	3.030E+13	0.27	34667.0	!Huynh
and Violi J.Org.Chem. 73 (2008) 94-101				
!EP2J=CH3CHCO+R15C2H5O	2.786E+22	-2.31	4.566E+04	
EP2J=CH3CHCO+R15C2H5O	1.460E+12	0.61	53276.0	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!EPEJ=CH3CHO+R25C2H5CO	1.127E+21	-1.73	4.255E+04	!
+2kcal				
EPEJ=CH3CHO+R25C2H5CO	1.127E+21	-1.73	4.255E+04	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!EPMJ=C2H4Z+C2H5CO2	2.325E+14	-0.20	3.297E+04	
EPMJ=C2H4Z+C2H5CO2	1.340E+13	-0.40	2.461E+04	!
Westbrook et al., (2009)				
MPMJ=HCHO+R25C2H5CO	1.230E+13	0.375	36714.0	!Huynh
and Violi J.Org.Chem. 73 (2008) 94-101				
!EP3J*o=>EA2J+B2CO	1.834e+15	-0.73	1.291e+04	!
Glaude et al., DMC C2H5CO				
!EP3J2*o=CH2COZ +C2H5OC0	1.230E+13	0.375	36714.0	!
Huynh and Violi J.Org.Chem. 73 (2008) 94-101				
EP3J=EP2d+R1H	3.000e+13	0.00	3.800e+04	!ST
EP2J=EP2d+R1H	3.000e+13	0.00	3.900e+04	!ST
EPEJ=EPED+R1H	3.000e+13	0.00	3.900e+04	!ST
EPMJ=EPED+R1H	3.000e+13	0.00	3.800e+04	!ST
!EP3J+O2=EP2d+R300H	2.600E+11	0.00	2.500E+03	!Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				
!EP2J+O2=EP2d+R300H	1.580E+12	0.00	1.520E+04	!Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				
!EP3J+O2=EP2d+R300H	1.580E+12	0.00	5.000E+03	!Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				
!EP2J+O2=EP2d+R300H	1.580E+12	0.00	5.000E+03	!Battin-
Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				

!EPEJ+O2=EPED+R300H Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498	1.580E+12	0.00	5.000e+03	!Battin-
!EPMJ+O2=EPED+R300H Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498	1.580E+12	0.00	5.000e+03	!Battin-
!EP3J+R300H=EP2d+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EP2J+R300H=EP2d+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPEJ+R300H=EPED+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPMJ+R300H=EPED+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!C2H5C00H=CH2C00H+R4CH3 Doolan et al., Int.J.Chem.Kinet. 18 (1986) 575-596	3.981E+15	0.00	8.852E+04	!
!C2H5C00H=HOCO+R11C2H5 et al., Int.J.Chem.Kinet. 18 (1986) 575-596	1.995E+15	0.00	8.612E+04	!Doolan
!C2H5C00H=CH3CHCO+H2O et al., Int.J.Chem.Kinet. 18 (1986) 575-596	7.079E+12	0.00	7.057E+04	!Doolan
!C2H5C00H=C2H6+CO2 et al., Int.J.Chem.Kinet. 18 (1986) 575-596	5.012E+12	0.00	7.177E+04	!Doolan
C2H5C00H=CH3CHCO+H2O Page, J.Am.Chem.Soc. 117 (1995) 5114-5119	4.470E+14	0.00	7.989E+04	!Duan et
C2H5C00H=C2H6+CO2 Page, J.Am.Chem.Soc. 117 (1995) 5114-5119	7.080E+13	0.00	7.452E+04	!Duan et
C2H5C00H=>R25C2H5CO+R2OH 8 KB	1.4E+0017	0.000	105815.7	! UI
C2H5C00H=>C2H5CO2+R1H KB	2.3E+0014	0.000	106345.3	! UI 9
C2H5C00H=>R11C2H5 +HOCO 10 KB	8.2E+0016	0.000	88817.0	! UI
C2H5C00H=>R4CH3+CH2C00H KB +3kcal	2.9E+0016	0.000	81917.1	! UI 11
C2H5C00H+R1H=CH2CH2C00H+H2 anc7, primARy f	9.400e+04	2.75	6.280e+03	!2
C2H5C00H+R1H=CH3CHC00H+H2 anc7, secondARy	1.300E+06	2.4	4.471E+03	!2
!C2H5C00H+R1H=CH3CHC00H+H2	5.400e+04	2.5	-1.900e+03	!
!C2H5C00H+R1H=C2H5CO2+H2 96 CN	4.2E+0006	2.000	2400.0	! ME
C2H5C00H+R1H=C2H5CO2+H2 PARK,Zhu,Lin, JcP 118, 9990-9996 (2003)	5.550E-23	10.60	-4459.0	!
C2H5C00H+B10=CH2CH2C00H+R2OH anc7, primARy f	9.650e+04	2.68	3.716e+03	!2
C2H5C00H+B10=CH3CHC00H+R2OH anc7, secondARy	4.770E+04	2.71	2.106E+03	!2
!C2H5C00H+B10=CH3CHC00H+R2OH	8.800e+10	0.70	3.250e+03	!
!C2H5C00H+B10=C2H5CO2+R2OH 87 CW	1.0E+0013	0.000	3280.0	! ME
C2H5C00H+B10=C2H5CO2+R2OH Lee, Xu, Lin, JPCa 2007	1.460E-03	4.73	1727.0	! Wu,
C2H5C00H+R2OH=CH2CH2C00H+H2 rnc7, primARy;	5.250e+09	0.97	1.590e+03	!2

C2H5C00H+R20H=CH3CHC00H+H2O rnc7, secondARY	4.680E+07	1.61	-3.500E+01	!2
!C2H5C00H+R20H=CH3CHC00H+H2O	3.000e+06	2.00	-1.520e+03	!
!C2H5C00H+R20H=C2H5C02+H2O 105 CW	1.1E+0006	2.000	-1865.0	! ME
C2H5C00H+R20H=C2H5C02+H2O Lin pci 2007 31 159-166	2.810E+02	2.97	-580.0	! Xu
C2H5C00H+R4CH3=CH2CH2C00H+CH4 anc7, primARY f	4.520e-01	3.65	7.154e+03	!2
C2H5C00H+R4CH3=CH3CHC00H+CH4 anc7, secondARY	2.705E+04	2.26	7.287E+03	!2
!C2H5C00H+R4CH3=CH3CHC00H+CH4	1.000e+11	0.00	7.300e+03	!
C2H5C00H+R4CH3=C2H5C02+CH4 Xu, PARK, Lin, JcP 120, 6593-6599 (2004)	2.035E+00	3.57	7722.0	!
C2H5C00H+R300H=CH2CH2C00H+H2O2 anc7, primARY f	8.400e+12	0.00	2.044e+04	!2
C2H5C00H+R300H=>CH3CHC00H+H2O2 anc7, secondARY	5.600E+12	0.00	1.769E+04	!2
!C2H5C00H+R300H=CH3CHC00H+H2O2	6.400e+03	2.60	1.240e+04	!
!C2H5C00H+R300H=C2H5C02+H2O2 96 CN	2.11E+0006	0.000	14000.0	! ME
C2H5C00H+R300H=C2H5C02+H2O2 1998	2.500E+12	0.00	24000.0	! MARinov
C2H5C00H+R8CH300=CH2CH2C00H+CH300H anc7, primARY f	8.400e+12	0.00	2.044e+04	!2
C2H5C00H+R8CH300=CH3CHC00H+CH300H corrected to ag	5.600E+12	0.00	1.769E+04	!2
!C2H5C00H+R8CH300=CH3CHC00H+CH300H	6.400e+03	2.60	1.240e+04	!
C2H5C00H+R7CH30 =CH2CH2C00H+CH30H rnc7, primARY;	1.581e+11	0.00	7.000e+03	!2
C2H5C00H+R7CH30 =CH3CHC00H+CH30H anc7, secondARY	1.095E+11	0.00	5.000E+03	!2
!C2H5C00H+R7CH30 =CH3CHC00H+CH30H	1.780e+12	0.00	1.200e+03	!
CH2CH2C00H=C2H4Z+HOCO and Violi J.Org.Chem. 73 (2008) 94-101	3.030E+13	0.27	34667.0	!Huynh
!CH2CH2C00H=C2H4Z+HOCO	4.217E+14	-0.32	3.486E+04	
CH2CH2C00H=C2H3C00H+R1H	3.200E+13	0.00	34800.0	!ST
CH3CHC00H=CH3CHCO+R20H	3.046E+21	-1.61	5.730E+04	
CH3CHC00H=C2H3C00H+R1H	3.000E+13	0.00	5.150E+04	!ST
CH3CHC00H=>CO2+R11C2H5	1.700E+09	1.0	38640.0	
C2H3C00H+R20H=>HCHO+CH2C00H Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!
C2H3C00H+R20H=>R4CH3+R5CHO+HOCO Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!
C2H3C00H=R10C2H3V+HOCO	3.752E+21	-1.89	1.129E+05	
C2H3C00H=CH2CHCO+R20H	5.206E+20	-1.16	1.009E+05	
C2H3C00H=C2H4Z+CO2 Page, J.Am.Chem.Soc. 117 (1995) 5114-5119	7.080E+13	0.00	7.452E+04	!Duan et
!C2H3C00H=C2H4Z+CO2	5.012E+12	0.00	7.177E+04	!Doolan
et al., Int.J.Chem.Kinet. 18 (1986) 575-596				
C2H3C00H+R1H=>H2+CO2+R10C2H3V 483	4.2E+0006	2.100	6900.0	! MZB



C2H3COOH+R2OH=>H2O+CO2+R10C2H3V 484	5.4E+0004	2.000	-340.0	!	MZB
C2H3COOH+R300H=>H2O2+CO2+R10C2H3V 485	1.0E+0011	0.000	11500.0	!	MZB
C2H3COOH+R4CH3=>CH4+CO2+R10C2H3V 486	1.4E+0001	3.100	9940.0	!	MZB
C2H3COOH+R11C2H5 =>C2H6+CO2+R10C2H3V MZB 487	1.4E+0001	3.100	8940.0	!	
!C2H5CO2+m=R11C2H5 +CO2+m	4.400E+15	0.00	1.050E+04		
CH3CHCO+R20H=CH3CHO+R5CHO et al., Int.J.Chem.Kinet. 18 (1986) 575-596	1.000E+12	0.00	0.0	!	Doolan
EP2d+R20H=>HCHO+EA2J Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!	
EPED+R20H=>HCHO+MPMJ Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!	
EPED+R20H=>CH3CHO+C2H5CO2 Heyberger et al., Combust Flame, 126 (2001) 1780-1802	1.370e+12	0.00	-1.040e+03	!	
EP2d=C2H3COOH+C2H4Z	2.000E+12	0.00	4.729E+04		
!EP2d(+m)=C2H3COOH+C2H4Z(+m)	1.000E+13	0.00	5.000E+04		
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /					
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troee Fall-off reaction					
!end					
!EP3*o+R1H=EP3J*o+H2 Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102	1.200E+14	0.00	7000.0	!	
!EP3*o+B10=EP3J*o+R20H (BAULch92)	5.850E+12	0.00	1808.0	!	
!EP3*o+R20H=EP3J*o+H2O Atkinson et al., 2001	2.650E+12	0.00	-730.0	!	
!EP3*o+R300H=EP3J*o+H2O2 (COLKET 77; CH3CHO)	1.700E+12	0.00	10700.0	!	
!EP3*o=choCH2COOH+C2H4Z	3.100E+12	0.00	11920.0	!	(BAULch92)
!choCH2COOH+R1H=coCH2COOH+H2	2.000E+12	0.00	4.729E+04		
!Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102	1.200E+14	0.00	7000.0		
!choCH2COOH+B10=coCH2COOH+R20H (BAULch92)	5.850E+12	0.00	1808.0		
!choCH2COOH+R20H=coCH2COOH+H2O Atkinson et al., 2001	2.650E+12	0.00	-730.0		
!choCH2COOH+R300H=coCH2COOH+H2O2 (COLKET 77; CH3CHO)	1.700E+12	0.00	10700.0		
!(COLKET 77; CH3CHO)	3.100E+12	0.00	11920.0	!	(BAULch92)
!coCH2COOH=>CH2co+B2CO+R20H	3.046E+21	-1.61	5.730E+04		
EB=C3H7COOH+C2H4Z	2.000E+12	0.00	4.729E+04		
!EB(+m)=C3H7COOH+C2H4Z(+m)	4.000E+12	0.00	5.000E+04		
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /					
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !Troee Fall-off reaction					
EB4J+R1H(+m)=EB(+m)	1.000E+14	0.00	0.000E+00		
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /					
TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troee Fall-off reaction					
EB3J+R1H(+m)=EB(+m)	1.000E+14	0.00	0.000E+00		
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /					

TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EB2J+R1H(+m)=EB(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /  
 TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off  
 reaction  
 EBEJ+R1H(+m)=EB(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /  
 TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off  
 reaction  
 EBMJ+R1H(+m)=EB(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
 TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EB(+m)=EP3J+R4CH3(+m) 7.213E+18 -0.89 8.721E+04 !asMB  
 LOW / 1.3080E+70 -1.5160E+01 8.4910E+04 /  
 TROE / 1.5409E-01 3.3770E+02 5.6730E+09 6.7100E+09 / !Troe Fall-off  
 reaction  
 EB(+m)=EA2J+R11C2H5 (+m) 2.700E+22 -1.86 8.568E+04 !  
 asMB  
 LOW / 3.9100E+74 -1.6420E+01 8.3700E+04 /  
 TROE / 8.6980E-01 7.4990E+09 1.6303E+00 7.5960E+07 / !Troe Fall-off  
 reaction  
 EB(+m)=C2H5OC0+R19C3H7(+m) 2.627E+27 -3.23 9.469E+04  
 LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /  
 TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off  
 reaction  
 EB(+m)=NC3H7CO+R15C2H50(+m) 1.650E+24 -2.04 1.002E+05  
 LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /  
 TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off  
 reaction  
 EB(+m)=C3H7CO2+R11C2H5 (+m) 5.734E+25 -2.76 9.211E+04  
 LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /  
 TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off  
 reaction  
 EB(+m)=MBMJ+R4CH3(+m) 3.388E+21 -1.58 9.209E+04  
 LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /  
 TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off  
 reaction  
 EB+O2=EB4J+R300H 3.000E+13 0.00 5.229E+04  
 EB+O2=EB3J+R300H 4.000E+13 0.00 4.769E+04 !Tsang et  
 al., J. Phys. Chem. REF. Data 17 (1988) 887-  
 EB+O2=EB2J+R300H 2.000E+13 0.00 4.430E+04  
 EB+O2=EBEJ+R300H 2.000E+13 0.00 4.820E+04  
 EB+O2=EBMJ+R300H 3.000E+13 0.00 5.229E+04  
  
 EB+R1H=EB4J+H2 9.400e+04 2.75 6.280e+03 !2  
 anc7, primARy f  
 EB+R1H=EB3J+H2 1.300E+06 2.4 4.471E+03 !2  
 anc7, secondARy  
 EB+R1H=EB2J+H2 1.300E+06 2.4 4.471E+03 !2  
 anc7, secondARy  
 !EB+R1H=EB2J+H2 5.400e+04 2.5 -1.900e+03 !

EB+R1H=EBEJ+H2	1.790E+05	2.53	3.420E+03	!as
C2H5OH Park et al., J.Chem.Phys. 118 (2003) 9990-9996				
EB+R1H=EBMJ+H2	9.400e+04	2.75	6.280e+03	!2
anc7, primARy f				
EB+B10=EB4J+R20H	9.650e+04	2.68	3.716e+03	!2
anc7, primARy f				
EB+B10=EB3J+R20H	4.770E+04	2.71	2.106E+03	!2
anc7, secondARy				
EB+B10=EB2J+R20H	4.770E+04	2.71	2.106E+03	!2
anc7, secondARy				
!EB+B10=EB2J+R20H	8.800e+10	0.70	3.250e+03	!
EB+B10=EBEJ+R20H	1.450E+05	2.47	8.800E+02	!as
C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703				
EB+B10=EBMJ+R20H	9.650e+04	2.68	3.716e+03	!2
anc7, primARy f				
EB+R20H=EB4J+H2O	5.250e+09	0.97	1.590e+03	!2
rnc7, primARy;				
EB+R20H=EB3J+H2O	4.680E+07	1.61	-3.500E+01	!2
rnc7, secondARy				
EB+R20H=EB2J+H2O	4.680E+07	1.61	-3.500E+01	!2
rnc7, secondARy				
!EB+R20H=EB2J+H2O	3.000e+06	2.00	-1.520e+03	!
EB+R20H=EBEJ+H2O	1.306E+05	2.43	-1457.0	!as
C2H5OH Xu Lin pci 2007 31 159-166				
EB+R20H=EBMJ+H2O	5.250e+09	0.97	1.590e+03	!2
rnc7, primARy;				
EB+R4CH3=EB4J+CH4	4.520e-01	3.65	7.154e+03	!2
anc7, primARy f				
EB+R4CH3=EB3J+CH4	2.705E+04	2.26	7.287E+03	!2
anc7, secondARy				
EB+R4CH3=EB2J+CH4	2.705E+04	2.26	7.287E+03	!2
anc7, secondARy				
!EB+R4CH3=EB2J+CH4	1.000e+11	0.00	7.300e+03	!
EB+R4CH3=EBEJ+CH4	1.990E+01	3.37	7635.0	!as
C2H5OH Xu, PARK, Lin, JcP 120, 6593-6599 (2004)				
EB+R4CH3=EBMJ+CH4	4.520e-01	3.65	7.154e+03	!2
anc7, primARy f				
EB+R300H=EB4J+H2O2	8.400e+12	0.00	2.044e+04	!2
anc7, primARy f				
EB+R300H=EB3J+H2O2	5.600E+12	0.00	1.769E+04	!2
anc7, secondARy				
EB+R300H=EB2J+H2O2	5.600E+12	0.00	1.769E+04	!2
anc7, secondARy				
!EB+R300H=EB2J+H2O2	6.400e+03	2.60	1.240e+04	!
!EB+R300H=EBEJ+H2O2	8.200E+03	2.55	10750.0	!
MARinov 1998				
EB+R300H=EBEJ+H2O2	3.610E+03	2.55	1.053E+04	
EB+R300H=EBMJ+H2O2	8.400e+12	0.00	2.044e+04	!2
anc7, primARy f				
EB+R8CH300=EB4J+CH300H	8.400e+12	0.00	2.044e+04	!2
corrected to ag				
EB+R8CH300=EB3J+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				

EB+R8CH300=EB2J+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
!EB+R8CH300=EB2J+CH300H	6.400e+03	2.60	1.240e+04	!
EB+R8CH300=EBEJ+CH300H	7.220E+03	2.55	1.053E+04	
EB+R8CH300=EBMJ+CH300H	8.400e+12	0.00	2.044e+04	!2
corrected to ag				
EB+R7CH30 =EB4J+CH30H	1.581e+11	0.00	7.000e+03	!2
rnc7, primARY;				
EB+R7CH30 =EB3J+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
EB+R7CH30 =EB2J+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
!EB+R7CH30 =EB2J+CH30H	1.780e+12	0.00	1.200e+03	!
EB+R7CH30 =EBEJ+CH30H	4.580E+10	0.00	2.873E+03	
EB+R7CH30 =EBMJ+CH30H	1.581e+11	0.00	7.000e+03	!2
rnc7, primARY;				
EB3J=EBEJ	9.872e+07	1.00	2.000e+04	!(cyc
lact sat a 6 + 2Hs - 2kcal/0)				
EB2J=EBMJ	1.481e+08	1.00	2.450e+04	!(cyc
lact sat a 6 + 3Hp)				
EB2J=EBEJ	5.746e+08	1.00	1.800e+04	!(cyc
lact sat a 5 + 2Hs - 2kcal/0)				
!EB4J=EB2J	3.3E+0009	1.000	35000.0	! IS 23 KB
!EB4J=EBEJ	1.7E+0007	1.000	15400.0	! IS 24 KB
!EB4J=EBMJ	4.4E+0006	1.000	23400.0	! IS 25 KB
!rev/ 4.4E+0006	1.000	23400.0/	! IS 25 KB	
!EBMJ=EB2J	9.9E+0007	1.000	12000.0	! IS 26 KB
!EBMJ=EB3J	1.7E+0007	1.000	17400.0	! IS 27 KB
!EBEJ=EB2J	5.7E+0008	1.000	21300.0	! IS 28 KB
!EBEJ=EB3J	9.9E+0007	1.000	18000.0	! IS 29 KB
!EB4J+02=EB4oo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!EB3J+02=EB3oo	1.700e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)				
!!EB2J+02=EB2oo	1.000e+19	-2.50	0.000e+00	!Buda
et al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EB2J+02=EB2oo	1.200e+10	0.00	-2300.0	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EBEJ+02=EBeoo	1.200e+10	0.00	-2300.0	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EBMJ+02=EBmoo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!				
!EB4oo=EB3D+R300H	5.044E+38	-8.110	4.149E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EB3oo=EB3D+R300H	5.075E+42	-9.410	4.249E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EB3oo=EB2D+R300H	5.044E+38	-8.110	4.149E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EB2oo=EB2D+R300H	5.044E+38	-8.110	4.149E+04	!Donato et
al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				

!EBeoo=EBed+R300H	5.075E+42	-9.410	4.249E+04	!Donato et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
!EBmoo=EBed+R300H	5.044E+38	-8.110	4.149E+04	!Donato et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal
EB4J=C2H4Z+EA2J	5.250E+11	0.50	26591.0	!Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB4J=C2H4Z+EA2J	2.100E+13	0.00	27800.0	!
EB3J=C3H6Y+C2H50CO	4.530E+12	0.335	34269.0	!Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB3J=C3H6Y+C2H50CO	8.827E+15	-0.67	3.555E+04	
!EB3J=C3H6Y+C2H50CO	2.100E+13	0.00	31200.0	!
!EB2J=C2H5CHCO+R15C2H5O	2.786E+22	-2.31	4.566E+04	
!EB2J=C2H5CHCO+R15C2H5O	2.100E+13	0.00	49000.0	!
EB2J=C2H5CHCO+R15C2H5O	1.460E+12	0.61	53276.0	!Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB2J=EP2d+R4CH3	2.000E+13	0.00	3.700E+04	!Dayma et al., Int J Chem Kinet, 35 (2003) 273-285 +6kcal
EB2J=EP2d+R4CH3	1.330E+11	0.97	34882.0	!Huynh and Violi J.Org.Chem. 73 (2008) 94-101
!EBEJ=CH3CHO+NC3H7CO	1.127E+21	-1.73	4.055E+04	
!EBEJ=CH3CHO+NC3H7CO	2.100E+13	0.00	31900.0	!
EBEJ=CH3CHO+NC3H7CO	1.127E+21	-1.73	4.255E+04	!Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
EBMJ=C2H4Z+C3H7CO2	2.325E+14	-0.20	3.297E+04	
!EBMJ=C2H4Z+C3H7CO2	2.100E+13	0.00	2.510E+04	
MBMJ=HCHO+NC3H7CO	1.230E+13	0.375	36714.0	!Huynh and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101
!EB4J*o=>EP3J+B2CO	1.834e+15	-0.73	1.291e+04	!
Glaude et al., DMC C2H5co				
!EB4J3*o=CH2COZ +EA2J	1.230E+13	0.375	36714.0	!
Huynh and Violi J.Org.Chem. 73 (2008) 94-101				
!EB4J2*o=>C2H4Z+EA2J*o	1.230E+13	0.375	36714.0	!Huynh and Violi J.Org.Chem. 73 (2008) 94-101
EB4J=EB3D+R1H	3.000e+13	0.00	3.800e+04	!ST
EB3J=EB3D+R1H	3.000e+13	0.00	3.900e+04	!ST
EB3J=EB2D+R1H	3.000e+13	0.00	3.800e+04	!ST
EB2J=EB2D+R1H	3.000e+13	0.00	3.800e+04	!ST
EBEJ=EBed+R1H	3.000e+13	0.00	3.900e+04	!ST
EBMJ=EBed+R1H	3.000e+13	0.00	3.800e+04	!ST
!EB4J+02=EB3D+R300H	1.580E+12	0.00	5.000e+03	!Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB3J+02=EB3D+R300H	1.580E+12	0.00	5.000e+03	!Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB3J+02=EB2D+R300H	2.600E+11	0.00	2.500E+03	!Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!EB2J+02=EB2D+R300H	1.580E+12	0.00	1.520E+04	!Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498
!!EB3J+02=EB2D+R300H	1.580E+12	0.00	5.000E+03	!
Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				
!!EB2J+02=EB2D+R300H	1.580E+12	0.00	5.000E+03	!
Battin-Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498				

!EBEJ+O2=EBed+R300H Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498	1.580E+12	0.00	5.000e+03	!Battin-
!EBMJ+O2=EBed+R300H Leclerc, Prog Energy Combust Sci, 34 (2008) 440-498	1.580E+12	0.00	5.000e+03	!Battin-
!EB4J+R300H=EB3D+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EB3J+R300H=EB3D+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EB3J+R300H=EB2D+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EB2J+R300H=EB2D+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EBEJ+R300H=EBed+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EBMJ+R300H=EBed+H2O2 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
C3H7C00H=C2H5CHCO+H2O Page, J.Am.Chem.Soc. 117 (1995) 5114-5119	4.470E+14	0.00	7.989E+04	!Duan et
C3H7C00H=C3H8+CO2 Page, J.Am.Chem.Soc. 117 (1995) 5114-5119	7.080E+13	0.00	7.452E+04	!Duan et
C3H7C00H=>NC3H7CO+R2OH KB	1.4E+0017	0.000	105815.7	! UI 8
C3H7C00H=>C3H7CO2+R1H KB	2.3E+0014	0.000	106345.3	! UI 9
C3H7C00H=>R19C3H7+HOCO KB	8.2E+0016	0.000	88817.0	! UI 10
C3H7C00H=>R11C2H5 +CH2C00H 11 KB	2.9E+0016	0.000	78917.1	! UI
C3H7C00H=>R4CH3+CH2CH2C00H KB	1.7E+0017	0.000	87662.1	! UI 12
C3H7C00H+R1H=PRC00H-4+H2 anc7, primARY f	9.400e+04	2.75	6.280e+03	!2
C3H7C00H+R1H=PRC00H-3+H2 anc7, secondARY	1.300E+06	2.4	4.471E+03	!2
C3H7C00H+R1H=PRC00H-2+H2 anc7, secondARY	1.300E+06	2.4	4.471E+03	!2
!C3H7C00H+R1H=PRC00H-2+H2	5.400e+04	2.5	-1.900e+03	!
!C3H7C00H+R1H=C3H7CO2+H2 96 CN	4.2E+0006	2.000	2400.0	! ME
C3H7C00H+R1H=C3H7CO2+H2 PARK,Zhu,Lin, JcP 118, 9990-9996 (2003)	5.550E-23	10.60	-4459.0	!
C3H7C00H+B10=PRC00H-4+R2OH anc7, primARY f	9.650e+04	2.68	3.716e+03	!2
C3H7C00H+B10=PRC00H-3+R2OH anc7, secondARY	4.770E+04	2.71	2.106E+03	!2
C3H7C00H+B10=PRC00H-2+R2OH anc7, secondARY	4.770E+04	2.71	2.106E+03	!2
!C3H7C00H+B10=PRC00H-2+R2OH	8.800e+10	0.70	3.250e+03	!
!C3H7C00H+B10=C3H7CO2+R2OH 87 CW	1.0E+0013	0.000	3280.0	! ME
C3H7C00H+B10=C3H7CO2+R2OH Lee, Xu, Lin, JPCa 2007	1.460E-03	4.73	1727.0	! Wu,

C3H7C00H+R20H=PRC00H-4+H20 rnc7, primARy;	5.250e+09	0.97	1.590e+03	!2
C3H7C00H+R20H=PRC00H-3+H20 rnc7, secondARy	4.680E+07	1.61	-3.500E+01	!2
C3H7C00H+R20H=PRC00H-2+H20 rnc7, secondARy	4.680E+07	1.61	-3.500E+01	!2
!C3H7C00H+R20H=PRC00H-2+H20	3.000e+06	2.00	-1.520e+03	!
!C3H7C00H+R20H=C3H7C02+H20 105 CW	1.1E+0006	2.000	-1865.0	! ME
C3H7C00H+R20H=C3H7C02+H20 Lin pci 2007 31 159-166	2.810E+02	2.97	-580.0	! Xu
C3H7C00H+R4CH3=PRC00H-4+CH4 anc7, primARy f	4.520e-01	3.65	7.154e+03	!2
C3H7C00H+R4CH3=PRC00H-3+CH4 anc7, secondARy	2.705E+04	2.26	7.287E+03	!2
C3H7C00H+R4CH3=PRC00H-2+CH4 anc7, secondARy	2.705E+04	2.26	7.287E+03	!2
!C3H7C00H+R4CH3=PRC00H-2+CH4	1.000e+11	0.00	7.300e+03	!
C3H7C00H+R4CH3=C3H7C02+CH4 Xu, PARK, Lin, JcP 120, 6593-6599 (2004)	2.035E+00	3.57	7722.0	!
C3H7C00H+R300H=PRC00H-4+H202 anc7, primARy f	8.400e+12	0.00	2.044e+04	!2
C3H7C00H+R300H=PRC00H-3+H202 anc7, secondARy	5.600E+12	0.00	1.769E+04	!2
C3H7C00H+R300H=>PRC00H-2+H202 anc7, secondARy	5.600E+12	0.00	1.769E+04	!2
!C3H7C00H+R300H=PRC00H-2+H202	6.400e+03	2.60	1.240e+04	!
!C3H7C00H+R300H=C3H7C02+H202 96 CN	2.11E+0006	0.000	14000.0	! ME
C3H7C00H+R300H=C3H7C02+H202 1998	2.500E+12	0.00	24000.0	! MARinov
C3H7C00H+R8CH300=PRC00H-4+CH300H anc7, primARy f	8.400e+12	0.00	2.044e+04	!2
C3H7C00H+R8CH300=PRC00H-3+CH300H corrected to ag	5.600E+12	0.00	1.769E+04	!2
C3H7C00H+R8CH300=PRC00H-2+CH300H corrected to ag	5.600E+12	0.00	1.769E+04	!2
!C3H7C00H+R8CH300=PRC00H-2+CH300H	6.400e+03	2.60	1.240e+04	!
C3H7C00H+R7CH30 =PRC00H-4+CH30H rnc7, primARy;	1.581e+11	0.00	7.000e+03	!2
C3H7C00H+R7CH30 =PRC00H-3+CH30H anc7, secondARy	1.095E+11	0.00	5.000E+03	!2
C3H7C00H+R7CH30 =PRC00H-2+CH30H anc7, secondARy	1.095E+11	0.00	5.000E+03	!2
!C3H7C00H+R7CH30 =PRC00H-2+CH30H	1.780e+12	0.00	1.200e+03	!
PRC00H-4=C2H4Z+CH2C00H and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101	5.250E+11	0.50	26591.0	!Huynh
PRC00H-3=C3H6Y+HOCO and Violi J.Org.Chem. 73 (2008) 94-101	3.030E+13	0.27	34667.0	!Huynh
!PRC00H-3=C3H6Y+HOCO	4.217E+14	-0.32	3.486E+04	
PRC00H-2=C2H3C00H+R4CH3 and Violi J.Org.Chem. 73 (2008) 94-101	1.330E+11	0.97	34882.0	!Huynh
PRC00H-2=C2H5CHCO+R20H	3.046E+21	-1.61	5.730E+04	

PRC00H-2=>C02+R19C3H7	1.700E+09	1.0	38640.0	
!PRC00H-4=C2H4Z+CH2C00H	2.000E+13	0.00	28700.0	!
!PRC00H-3=C3H6Y+H0C0	2.000E+13	0.00	28700.0	!
!PRC00H-2=C2H3C00H+R4CH3	2.000E+13	0.00	31000.0	!
!PRC00H-2=C2H5CHC0+R20H	2.000E+13	0.00	49000.0	!
C3H7C02+m=R19C3H7+C02+m	4.400E+15	0.00	1.050E+04	
!C3H7C02=R19C3H7+C02	2.000E+13	0.00	5.100E+03	
PRC00H-4=C3H5C00H+R1H	3.000E+13	0.00	38000.0	!ST
PRC00H-3=C3H5C00H+R1H	3.200E+13	0.00	34800.0	!ST
PRC00H-2=C3H5C00H+R1H	3.000E+13	0.00	5.150E+04	!ST
C3H5C00H+R20H=>HCH0+CH2CH2C00H	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
C3H5C00H+R20H=>CH3CH0+CH2C00H	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
C3H5C00H+R1H=>H2+C02+sC3H5	4.2E+0006	2.100	6900.0	! MZB 483
C3H5C00H+R20H=>H20+C02+sC3H5	5.4E+0004	2.000	-340.0	! MZB 484
C3H5C00H+R300H=>H202+C02+sC3H5	1.0E+0011	0.000	11500.0	! MZB 485
C3H5C00H+R4CH3=>CH4+C02+sC3H5	1.4E+0001	3.100	9940.0	! MZB 486
C3H5C00H+R11C2H5 =>C2H6+C02+sC3H5	1.4E+0001	3.100	8940.0	! MZB 487
EB3D+R20H=>HCH0+EP3J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EB3D+R20H=>CH3CH0+EA2J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EB2D+R20H=>CH3CH0+EA2J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EBed+R20H=>HCH0+MBMJ	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EBed+R20H=>CH3CH0+C3H7C02	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EB3D=C3H5C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
EB2D=C3H5C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
!EB3D(+m)=C3H5C00H+C2H4Z(+m)	4.000E+12	0.00	5.000E+04	
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /				
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !TroE Fall-off reaction				
!EB4*o+R1H=EB4J*o+H2	1.200E+14	0.00	7000.0	!
Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102				
!EB4*o+B10=EB4J*o+R20H	5.850E+12	0.00	1808.0	!
(BAULch92)				
!EB4*o+R20H=EB4J*o+H20	2.650E+12	0.00	-730.0	!
Atkinson et al., 2001				
!EB4*o+R300H=EB4J*o+H202	1.700E+12	0.00	10700.0	!
(COLKET 77; CH3CH0)	3.100E+12	0.00	11920.0	!(BAULch92)
EPE=C4H9C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
!EPE(+m)=C4H9C00H+C2H4Z(+m)	4.000E+12	0.00	5.000E+04	
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /				
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !TroE Fall-off reaction				
EPE5J+R1H(+m)=EPE(+m)	1.000E+14	0.00	0.000E+00	
LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /				



TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EPE4J+R1H(+m)=EPE(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
 TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EPE3J+R1H(+m)=EPE(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
 TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EPE2J+R1H(+m)=EPE(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 4.4360+125 -3.0800E+01 1.1395E+05 /  
 TROE / 9.6000E-01 9.9996E+09 1.3439E+00 6.6987E+08 / !Troe Fall-off  
 reaction  
 EPEEJ+R1H(+m)=EPE(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 1.3250+113 -2.7260E+01 1.1413E+05 /  
 TROE / 8.4076E-02 3.6151E+00 9.9997E+09 6.7101E+09 / !Troe Fall-off  
 reaction  
 EPEMJ+R1H(+m)=EPE(+m) 1.000E+14 0.00 0.000E+00  
 LOW / 9.7420+103 -2.4610E+01 1.1538E+05 /  
 TROE / 8.7200E-01 9.9900E+09 2.9264E+01 7.5961E+07 / !Troe Fall-off  
 reaction  
 EPE(+m)=EB4J+R4CH3(+m) 7.213E+18 -0.89 8.721E+04 !asMB  
 LOW / 1.3080E+70 -1.5160E+01 8.4910E+04 /  
 TROE / 1.5409E-01 3.3770E+02 5.6730E+09 6.7100E+09 / !Troe Fall-off  
 reaction  
 EPE(+m)=EP3J+R11C2H5 (+m) 5.732E+23 -2.33 8.774E+04  
 LOW / 4.3520E+14 8.2000E-01 6.3570E+04 /  
 TROE / 1.6900E-01 5.7129E+03 4.0466E+01 6.7101E+09 / !Troe Fall-off  
 reaction  
 EPE(+m)=EA2J+R19C3H7(+m) 2.700E+22 -1.86 8.568E+04 !asMB  
 LOW / 3.9100E+74 -1.6420E+01 8.3700E+04 /  
 TROE / 8.6980E-01 7.4990E+09 1.6303E+00 7.5960E+07 / !Troe Fall-off  
 reaction  
 EPE(+m)=C2H5OC0+R20C4H9(+m) 2.627E+27 -3.23 9.469E+04  
 LOW / 7.7180E+18 -2.7000E-01 7.1920E+04 /  
 TROE / 6.3200E-01 8.8245E+09 1.6237E+03 7.5961E+07 / !Troe Fall-off  
 reaction  
 EPE(+m)=NC4H9C0+R15C2H50(+m) 1.650E+24 -2.04 1.002E+05  
 LOW / 1.3610E+16 7.6000E-01 7.8320E+04 /  
 TROE / 7.4000E-01 7.3301E+09 2.1169E+03 6.7101E+09 / !Troe Fall-off  
 reaction  
 EPE(+m)=C4H9C02+R11C2H5 (+m) 5.734E+25 -2.76 9.211E+04  
 LOW / 9.7120E+16 2.8000E-01 6.8840E+04 /  
 TROE / 4.4800E-01 1.2624E+03 4.6756E+09 1.7861E+09 / !Troe Fall-off  
 reaction  
 EPE(+m)=MPEMJ+R4CH3(+m) 3.388E+21 -1.58 9.209E+04  
 LOW / 5.6740E+12 1.4600E+00 6.8820E+04 /  
 TROE / 4.0600E-01 1.5235E+03 4.8431E+09 9.3301E+09 / !Troe Fall-off  
 reaction  
 EPE+02=EPE5J+R300H 3.000E+13 0.00 5.229E+04  
 EPE+02=EPE4J+R300H 4.000E+13 0.00 4.769E+04 !Tsang et  
 al., J. Phys. Chem. REF. Data 17 (1988) 887-

EPE+O2=EPE3J+R300H al., J. Phys. Chem. REF. Data 17 (1988) 887-	4.000E+13	0.00	4.769E+04	!Tsang et
EPE+O2=EPE2J+R300H	2.000E+13	0.00	4.430E+04	
EPE+O2=EPEEJ+R300H	2.000E+13	0.00	4.820E+04	
EPE+O2=EPEMJ+R300H	3.000E+13	0.00	5.229E+04	
EPE+R1H=EPE5J+H2 anc7, primARY f	9.400e+04	2.75	6.280e+03	!2
EPE+R1H=EPE4J+H2 anc7, secondARY	1.300E+06	2.4	4.471E+03	!2
EPE+R1H=EPE3J+H2 anc7, secondARY	1.300E+06	2.4	4.471E+03	!2
EPE+R1H=EPE2J+H2 anc7, secondARY	1.300E+06	2.4	4.471E+03	!2
!EPE+R1H=EPE2J+H2	5.400e+04	2.5	-1.900e+03	
EPE+R1H=EPEEJ+H2 C2H5OH Park et al., J.Chem.Phys. 118 (2003) 9990-9996	1.794E+05	2.53	3.420E+03	!as
EPE+R1H=EPEMJ+H2 anc7, primARY f	9.400e+04	2.75	6.280e+03	!2
EPE+B10=EPE5J+R20H anc7, primARY f	9.650e+04	2.68	3.716e+03	!2
EPE+B10=EPE4J+R20H anc7, secondARY	4.770E+04	2.71	2.106E+03	!2
EPE+B10=EPE3J+R20H anc7, secondARY	4.770E+04	2.71	2.106E+03	!2
EPE+B10=EPE2J+R20H anc7, secondARY	4.770E+04	2.71	2.106E+03	!2
!EPE+B10=EPE2J+R20H	8.800e+10	0.70	3.250e+03	
EPE+B10=EPEEJ+R20H C2H5OH Wu et al., J.Phys.Chem.A 111 (2007) 6693-6703	1.450E+05	2.41	8.760E+02	!as
EPE+B10=EPEMJ+R20H anc7, primARY f	9.650e+04	2.68	3.716e+03	!2
EPE+R20H=EPE5J+H2 rnc7, primARY;	5.250e+09	0.97	1.590e+03	!2
EPE+R20H=EPE4J+H2 rnc7, secondARY	4.680E+07	1.61	-3.500E+01	!2
EPE+R20H=EPE3J+H2 rnc7, secondARY	4.680E+07	1.61	-3.500E+01	!2
EPE+R20H=EPE2J+H2 rnc7, secondARY	4.680E+07	1.61	-3.500E+01	!2
!EPE+R20H=EPE2J+H2	3.000e+06	2.00	-1.520e+03	
EPE+R20H=EPEEJ+H2 C2H5OH Xu et al., Proc.Combust.Inst., 31 (2007) 159-166	1.306E+05	2.43	-1457.0	!as
EPE+R20H=EPEMJ+H2 rnc7, primARY;	5.250e+09	0.97	1.590e+03	!2
EPE+R4CH3=EPE5J+CH4 anc7, primARY f	4.520e-01	3.65	7.154e+03	!2
EPE+R4CH3=EPE4J+CH4 anc7, secondARY	2.705E+04	2.26	7.287E+03	!2
EPE+R4CH3=EPE3J+CH4 anc7, secondARY	2.705E+04	2.26	7.287E+03	!2
EPE+R4CH3=EPE2J+CH4 anc7, secondARY	2.705E+04	2.26	7.287E+03	!2
!EPE+R4CH3=EPE2J+CH4	1.000e+11	0.00	7.300e+03	

EPE+R4CH3=EPEEJ+CH4	1.990E+01	3.37	7635.0	!as
C2H5OH Xu et al., J.Chem.Phys., 120 (2004) 6593-6599				
EPE+R4CH3=EPEMJ+CH4	4.520e-01	3.65	7.154e+03	!2
anc7, primARY f				
EPE+R300H=EPE5J+H2O2	8.400e+12	0.00	2.044e+04	!2
anc7, primARY f				
EPE+R300H=EPE4J+H2O2	5.600E+12	0.00	1.769E+04	!2
anc7, secondARY				
EPE+R300H=EPE3J+H2O2	5.600E+12	0.00	1.769E+04	!2
anc7, secondARY				
EPE+R300H=EPE2J+H2O2	5.600E+12	0.00	1.769E+04	!2
anc7, secondARY				
!EPE+R300H=EPE2J+H2O2	6.400e+03	2.60	1.240e+04	
!EPE+R300H=EPEEJ+H2O2	8.200E+03	2.55	10750.0	!
MARinov 1998				
EPE+R300H=EPEEJ+H2O2	3.610E+03	2.55	1.053E+04	
EPE+R300H=EPEMJ+H2O2	8.400e+12	0.00	2.044e+04	!2
anc7, primARY f				
EPE+R8CH300=EPE5J+CH300H	8.400e+12	0.00	2.044e+04	!2
corrected to ag				
EPE+R8CH300=EPE4J+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
EPE+R8CH300=EPE3J+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
EPE+R8CH300=EPE2J+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
!EPE+R8CH300=EPE2J+CH300H	6.400e+03	2.60	1.240e+04	
EPE+R8CH300=EPEEJ+CH300H	5.600e+12	0.00	1.769e+04	!2
corrected to ag				
!EPE+R8CH300=EPEEJ+CH300H	7.220E+03	2.55	1.053E+04	
EPE+R8CH300=EPEMJ+CH300H	8.400e+12	0.00	2.044e+04	!2
corrected to ag				
EPE+R7CH30 =EPE5J+CH30H	1.581e+11	0.00	7.000e+03	!2
rnc7, primARY;				
EPE+R7CH30 =EPE4J+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
EPE+R7CH30 =EPE3J+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
EPE+R7CH30 =EPE2J+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
!EPE+R7CH30 =EPE2J+CH30H	1.780e+12	0.00	1.200e+03	
EPE+R7CH30 =EPEEJ+CH30H	4.580E+10	0.00	2.873E+03	
EPE+R7CH30 =EPEMJ+CH30H	1.581e+11	0.00	7.000e+03	!2
rnc7, primARY;				
!EPE+EPE500=EPE5J+EPE500h	8.400e+12	0.00	2.044e+04	!2
corrected to ag				
!EPE+EPE500=EPE4J+EPE500h	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
!EPE+EPE500=EPE3J+EPE500h	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
!EPE+EPE500=EPE2J+EPE500h	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
!EPE+EPE500=EPEEJ+EPE500h	5.600E+12	0.00	1.769E+04	!2
corrected to ag				

!EPE+EPE500=EPEMJ+EPE500h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPE400=EPE5J+EPE400h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPE400=EPE4J+EPE400h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE400=EPE3J+EPE400h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE400=EPE2J+EPE400h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE400=EPEEJ+EPE400h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE400=EPEMJ+EPE400h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPE300=EPE5J+EPE300h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPE300=EPE4J+EPE300h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE300=EPE3J+EPE300h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE300=EPE2J+EPE300h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE300=EPEEJ+EPE300h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE300=EPEMJ+EPE300h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPE200=EPE5J+EPE200h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPE200=EPE4J+EPE200h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE200=EPE3J+EPE200h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE200=EPE2J+EPE200h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE200=EPEEJ+EPE200h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPE200=EPEMJ+EPE200h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPEe00=EPE5J+EPEe00h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPEe00=EPE4J+EPEe00h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEe00=EPE3J+EPEe00h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEe00=EPE2J+EPEe00h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEe00=EPEEJ+EPEe00h corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEe00=EPEMJ+EPEe00h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPEm00=EPE5J+EPEm00h corrected to ag	8.400e+12	0.00	2.044e+04	!2
!EPE+EPEm00=EPE4J+EPEm00h corrected to ag	5.600E+12	0.00	1.769E+04	!2

!EPE+EPEmoo=EPE3J+EPEmooh corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEmoo=EPE2J+EPEmooh corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEmoo=EPEEJ+EPEmooh corrected to ag	5.600E+12	0.00	1.769E+04	!2
!EPE+EPEmoo=EPEMJ+EPEmooh corrected to ag	8.400e+12	0.00	2.044e+04	!2
EPE2J=EPE5J a 5 + 3Hp)	8.619e+08	1.00	1.980e+04	!(cyc sat
EPE3J=EPEEJ lact sat a 6 + 2Hs - 2kcal/0)	9.872e+07	1.00	2.000e+04	!(cyc
EPE2J=EPEMJ lact sat a 6 + 3Hp)	1.481e+08	1.00	2.450e+04	!(cyc
EPE2J=EPEEJ lact sat a 5 + 2Hs - 2kcal/0)	5.746e+08	1.00	1.800e+04	!(cyc
!EPE4J=EPE2J	3.3E+0009	1.000	35000.0	! IS 23 KB
!EPE4J=EPEEJ	1.7E+0007	1.000	15400.0	! IS 24 KB
!EPE4J=EPEMJ	4.4E+0006	1.000	23400.0	! IS 25 KB
!EPEMJ=EPE2J	9.9E+0007	1.000	12000.0	! IS 26 KB
!EPEMJ=EPE3J	1.7E+0007	1.000	17400.0	! IS 27 KB
!EPEEJ=EPE2J	5.7E+0008	1.000	21300.0	! IS 28 KB
!EPEEJ=EPE3J	9.9E+0007	1.000	18000.0	! IS 29 KB
!EPE5J+02=EPE4D+R300H Leclerc, Prog Energy Combust Sci,	1.580e+12	0.00	4.700e+03	!Battin-
34 (2008) 440-498				
!EPE4J+02=EPE4D+R300H Leclerc, Prog Energy Combust Sci,	6.900e+11	0.00	4.700e+03	!Battin-
34 (2008) 440-498				
!EPE4J+02=EPE3D+R300H Leclerc, Prog Energy Combust Sci,	1.580e+12	0.00	4.700e+03	!Battin-
34 (2008) 440-498				
!EPE3J+02=EPE3D+R300H Leclerc, Prog Energy Combust Sci,	1.580e+12	0.00	4.700e+03	!Battin-
34 (2008) 440-498				
!EPE3J+02=EPE2D+R300H Leclerc, Prog Energy Combust Sci,	2.600E+11	0.00	2.500E+03	!Battin-
34 (2008) 440-498				
!EPE2J+02=EPE2D+R300H Leclerc, Prog Energy Combust Sci,	1.580E+12	0.00	1.520E+04	!Battin-
34 (2008) 440-498				
!EPE3J+02=EPE2D+R300H Leclerc, Prog Energy Combust Sci,	1.580E+12	0.00	5.000E+03	!Battin-
34 (2008) 440-498				
!EPE2J+02=EPE2D+R300H Leclerc, Prog Energy Combust Sci,	1.580E+12	0.00	5.000E+03	!Battin-
34 (2008) 440-498				
!EPEEJ+02=EPEED+R300H Leclerc, Prog Energy Combust Sci,	6.900e+11	0.00	5.000e+03	!Battin-
34 (2008) 440-498				
!EPEMJ+02=EPEED+R300H Leclerc, Prog Energy Combust Sci,	1.580e+12	0.00	5.000e+03	!Battin-
34 (2008) 440-498				
!EPE5J+R300H=EPE4D+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPE4J+R300H=EPE4D+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPE4J+R300H=EPE3D+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPE3J+R300H=EPE3D+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!

!EPE3J+R300H=EPE2D+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPE2J+R300H=EPE2D+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPEEJ+R300H=EPEED+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPEMJ+R300H=EPEED+H202 (=R19C3H7/TSA88)	2.410E+13	0.0	0.0	!
!EPE5J+O2=EPE5oo al., Combust Flame, 142 (2005) 170-186 (ks)	9.000e+18	-2.50	0.000e+00	!Buda et
!EPE4J+O2=EPE4oo al., Combust Flame, 142 (2005) 170-186 (kp+ks)	1.700e+19	-2.50	0.000e+00	!Buda et
!EPE3J+O2=EPE3oo al., Combust Flame, 142 (2005) 170-186 (2ks)	1.800e+19	-2.50	0.000e+00	!Buda et
!!EPE2J+O2=EPE2oo et al., Combust Flame, 142 (2005) 170-186 (ks+kq)	1.000e+19	-2.50	0.000e+00	!Buda
!EPE2J+O2=EPE2oo al., Combust Flame, 142 (2005) 170-186 (ks+kq)	1.200e+10	0.00	-2300.0	!Buda et
!!EPEEJ+O2=EPEeoo et al., Combust Flame, 142 (2005) 170-186 (kp+ks)	1.700e+19	-2.50	0.000e+00	!Buda
!EPEEJ+O2=EPEeoo al., Combust Flame, 142 (2005) 170-186 (ks+kq)	1.200e+10	0.00	-2300.0	!Buda et
!EPEMJ+O2=EPEmoo al., Combust Flame, 142 (2005) 170-186 (ks)	9.000e+18	-2.50	0.000e+00	!Buda et
!				
!EPE5oo=EPE5ooH4j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)	5.746e+08	1.00	3.250e+04	!Buda et
!EPE5oo=EPE5ooH3j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs)	9.872e+07	1.00	2.500e+04	!Buda et
!EPE5oo=EPE5ooH2j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 2Hs)	1.696e+07	1.00	2.200e+04	!Buda et
!EPE4oo=EPE4ooH5j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 3Hp)	8.619e+08	1.00	3.550e+04	!Buda et
!EPE4oo=EPE4ooH3j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)	5.746e+08	1.00	3.250e+04	!Buda et
!EPE4oo=EPE4ooH2j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs)	9.872e+07	1.00	2.500e+04	!Buda et
!EPE3oo=EPE3ooH5j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 3Hp)	1.481e+08	1.00	2.800e+04	!Buda et
!EPE3oo=EPE3ooH4j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)	5.746e+08	1.00	3.250e+04	!Buda et
!EPE3oo=EPE3ooH2j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)	5.746e+08	1.00	3.250e+04	!Buda et
!EPE2oo=EPE2ooH5j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 3Hp)	2.544e+07	1.00	2.500e+04	!Buda et
!EPE2oo=EPE2ooH4j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs)	9.872e+07	1.00	2.500e+04	!Buda et
!EPE2oo=EPE2ooH3j al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs)	5.746e+08	1.00	3.250e+04	!Buda et
!EPE2oo=EPE2oohej al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 2Hs - 2kcal/O)	1.696e+07	1.00	2.270e+04	!Buda et
!EPEeoo=EPEeooH2j al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 2Hs)	1.696e+07	1.00	2.550e+04	!Buda et

!EPEeoo=EPEeooHmj	8.619e+08	1.00	3.550e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 3Hp)				
!EPEmoo=EPEmoohej	5.746e+08	1.00	3.050e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs - 2kcal/O)				
!				
!EPE5ooH4j+O2=EPE5ooH4oo	1.800e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)				
!EPE5ooH3j+O2=EPE5ooH3oo	1.800e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)				
!EPE5ooH2j+O2=EPE5ooH2oo	1.000e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EPE4ooH5j+O2=EPE4ooH5oo	1.500e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kt)				
!EPE4ooH3j+O2=EPE4ooH3oo	1.050e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kt)				
!EPE4ooH2j+O2=EPE4ooH2oo	1.000e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EPE3ooH5j+O2=EPE3ooH5oo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!EPE3ooH4j+O2=EPE3ooH4oo	9.500e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+kt)				
!EPE3ooH2j+O2=EPE3ooH2oo	2.500e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kt+kq)				
!EPE2ooH5j+O2=EPE2ooH5oo	9.000e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks)				
!EPE2ooH4j+O2=EPE2ooH4oo	1.700e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)				
!EPE2ooH3j+O2=EPE2ooH3oo	1.050e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kt)				
!EPE2oohej+O2=EPE2ooheoo	1.700e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kp+ks)				
!EPEeooH2j+O2=EPEeooH2oo	1.050e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (ks+kq)				
!EPEeooHmj+O2=EPEeooHmoo	1.500e+18	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (kt)				
!EPEmoohej+O2=EPEmooheoo	1.800e+19	-2.50	0.000e+00	!Buda et
al., Combust Flame, 142 (2005) 170-186 (2ks)				
!				
!EPE5ooH4oo=>EPE4ooH5*o+R2OH	5.746e+08	1.00	3.050e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs - 2kcal/O)				
!EPE5ooH3oo=>EPE3ooH5*o+R2OH	9.872e+07	1.00	2.300e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 2Hs - 2kcal/O)				
!EPE5ooH2oo=>EPE2ooH5*o+R2OH	1.696e+07	1.00	2.000e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 2Hs - 2kcal/O)				
!EPE4ooH5oo=>EPE5ooH4*o+R2OH	2.873e+08	1.00	2.750e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)				
!EPE4ooH3oo=>EPE3ooH4*o+R2OH	2.873e+08	1.00	2.750e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)				
!EPE4ooH2oo=>EPE2ooH4*o+R2OH	4.936e+07	1.00	2.000e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 1Ht - 2kcal/O)				
!EPE3ooH5oo=>EPE5ooH3*o+R2OH	4.936e+07	1.00	2.000e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 1Ht - 2kcal/O)				
!EPE3ooH4oo=>EPE4ooH3*o+R2OH	2.873e+08	1.00	2.750e+04	!Buda et
al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)				

!EPE3ooH2O=>EPE2ooh3*o+R2OH	2.873e+08	1.00	2.750e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)				
!EPE2ooh5oo=>EPE5ooH2*o+R2OH	8.480e+06	1.00	1.700e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 7 + 1Ht - 2kcal/O)				
!EPE2ooh4oo=>EPE4ooH2*o+R2OH	4.936e+07	1.00	2.000e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 6 + 1Ht - 2kcal/O)				
!EPE2ooh3oo=>EPE3ooH2*o+R2OH	2.873e+08	1.00	2.750e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 2kcal/O)				
!EPE2ooheoo=>EPEeooH2*o+R2OH	8.480e+06	1.00	2.350e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 1Ht - 2kcal/O)				
!EPEeooH2O=>EPE2oohe*o+R2OH	8.480e+06	1.00	1.770e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc lact sat a 7 + 1Ht - 4kcal/O)				
!EPEeooHmoo=>EPEmoohe*o+R2OH	2.873e+08	1.00	2.550e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 1Ht - 4kcal/O)				
!EPEmooheoo=>EPEeooHm*o+R2OH	5.746e+08	1.00	3.050e+04	!Buda
et al., Combust Flame, 142 (2005) 170-186 (cyc sat a 5 + 2Hs - 2kcal/O)				
!				
!EPE4ooh5*o=>CHOCHO+EP3J+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE3ooh5*o=>R13CH2CHO+EP3*o+R2OH	5.000e+15	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE3ooh5*o=>chocH2cho+EA2J+R2OH	5.000e+15	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE2ooh5*o=>choC2h4cho+C2H5OC0+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE5ooh4*o=>HCHO+EB4J*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE3ooh4*o=>R14CH3C0+EP3*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE2ooh4*o=>c4ald3oxo+C2H5OC0+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE5ooh3*o=>HCHO+EB4J3*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE4ooh3*o=>CH3CHO+EP3J*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE2ooh3*o=>c4ald2oxo+C2H5OC0+R2OH	5.000e+15	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE2ooh3*o=>ea2*o+R25C2H5C0+R2OH	5.000e+15	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE5ooH2*o=>HCHO+EB4J2*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE4ooH2*o=>CH3CHO+EP3J2*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE3ooH2*o=>C2H5CHO+EA2J*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPEeooH2*o=>CH3CHO+C3H7COC02+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPE2oohe*o=>NC3H7CHO+CH3COC02+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!EPEmoohe*o=>HCHO+MPEMJ*o+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				



!EPEeooHm*o=>C4H9CO2+CHOCHO+R2OH	1.000e+16	0.00	4.300e+04	!
Curran et al., Combust Flame, 114 (1998) 149-177				
!				
!EPE5ooH4j=>EPEcy5o4+R2OH	1.380e+12	0.00	1.590e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)				
!EPE5ooH3j=>EPEcy5o3+R2OH	2.042e+11	0.00	1.950e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cs)				
!EPE5ooH2j=>EPEcy5O2+R2OH	3.630e+10	0.00	1.300e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)				
!EPE4ooH5j=>EPEcy5o4+R2OH	3.981e+12	0.00	1.700e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cp)				
!EPE4ooH3j=>EPEcy4o3+R2OH	1.380e+12	0.00	1.590e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)				
!EPE4ooH2j=>EPEcy4O2+R2OH	2.042e+11	0.00	1.950e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cs)				
!EPE3ooH5j=>EPEcy5o3+R2OH	4.467e+11	0.00	2.190e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cp)				
!EPE3ooH4j=>EPEcy4o3+R2OH	1.380e+12	0.00	1.590e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)				
!EPE3ooH2j=>EPEcy3O2+R2OH	1.380e+12	0.00	1.590e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)				
!EPE2ooH5j=>EPEcy5O2+R2OH	5.130e+10	0.00	1.480e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cp)				
!EPE2ooH4j=>EPEcy4O2+R2OH	2.042e+11	0.00	1.950e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 4+Cs)				
!EPE2ooH3j=>EPEcy3O2+R2OH	1.380e+12	0.00	1.590e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)				
!EPE2oohej=>EPEcy2oe+R2OH	3.630e+10	0.00	1.300e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)				
!EPEeooH2j=>EPEcy2oe+R2OH	3.630e+10	0.00	1.300e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 5+Cs)				
!EPEeooHmj=>EPEcyeom+R2OH	3.981e+12	0.00	1.700e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cp)				
!EPEmoohj=>EPEcyeom+R2OH	1.380e+12	0.00	1.590e+04	!
Wijaya et al., J. Phys. Chem. A, 107 (2003) 4908-4920 (cycle 3+Cs)				
!				
!EPEcy5o4+R1H=>H2+C2H3CHOZ+EA2J	9.600E+08	1.50	2785.0	!25
dbr, see shee				
!EPEcy5o4+R1H=>H2+CH2COZ +EP3J	4.800E+08	1.50	2005.0	!
25 dbr, see shee				
!EPEcy5o3+R1H=>H2+R5CHO+EB3D	9.600E+08	1.50	2785.0	!25
dbr, see shee				
!EPEcy5o3+R1H=>H2+C2H4Z+EP3J*o	4.800E+08	1.50	2005.0	!25
dbr, see shee				
!EPEcy5O2+R1H=>H2+R13CH2CHO+EP2d	9.600E+08	1.50	2785.0	!25
dbr, see shee				
!EPEcy5O2+R1H=>H2+C2H4Z+EP3J2*o	4.800E+08	1.50	2005.0	!25
dbr, see shee				
!EPEcy4o3+R1H=>H2+C2H3COCH3+C2H5OCO	4.800E+08	1.50	2005.0	!25
dbr, see shee				
!EPEcy4o3+R1H=>H2+CH3CHCO+EA2J	4.800E+08	1.50	2005.0	!25
dbr, see shee				
!EPEcy4O2+R1H=>H2+R14CH3CO+EP2d	4.800E+08	1.50	2005.0	!25
dbr, see shee				

!EPEcy402+R1H=>H2+C3H6Y+EA2J*o dbr, see shee	4.800E+08	1.50	2005.0	!25
!EPEcy302+R1H=>H2+C2H50C0+C2H5CHC0 dbr, see shee	9.600E+08	1.50	2005.0	!25
!EPEcy20e+R1H=>H2+B2C0+R14CH3C0+NC3H7CH0 2005.0 !25 dbr, see shee	4.800E+08	1.50		
!EPEcy20e+R1H=>H2+CH3C02+C4H8C0 dbr, see shee	4.800E+08	1.50	2005.0	!25
!EPEcy20e+R1H=>H2+CH3CH0+prcoco dbr, see shee	4.800E+08	1.50	2005.0	!25
!EPEcyeom+R1H=>H2+CH0CH0+NC4H9C0 dbr, see shee	9.600E+08	1.50	2785.0	!25
!EPEcyeom+R1H=>H2+CH2C0Z +C4H9C02 25 dbr, see shee	4.800E+08	1.50	2005.0	!
!EPEcy504+R20H=>H20+C2H3CH0Z+EA2J dbr, see shee	4.800E+06	2.00	-1192.0	!25
!EPEcy504+R20H=>H20+CH2C0Z +EP3J 25 dbr, see shee	2.400E+06	2.00	-1192.0	!
!EPEcy503+R20H=>H20+R5CH0+EB3D dbr, see shee	4.800E+06	2.00	-1192.0	!25
!EPEcy503+R20H=>H20+C2H4Z+EP3J*o dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy502+R20H=>H20+R13CH2CH0+EP2d dbr, see shee	4.800E+06	2.00	-1192.0	!25
!EPEcy502+R20H=>H20+C2H4Z+EP3J2*o dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy403+R20H=>H20+C2H3C0CH3+C2H50C0 dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy403+R20H=>H20+CH3CHC0+EA2J dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy402+R20H=>H20+R14CH3C0+EP2d dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy402+R20H=>H20+C3H6Y+EA2J*o dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy302+R20H=>H20+C2H50C0+C2H5CHC0 dbr, see shee	4.800E+06	2.00	-1192.0	!25
!EPEcy20e+R20H=>H20+B2C0+R14CH3C0+NC3H7CH0 -1192.0 !25 dbr, see shee	2.400E+06	2.00		
!EPEcy20e+R20H=>H20+CH3C02+C4H8C0 dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcy20e+R20H=>H20+CH3CH0+prcoco dbr, see shee	2.400E+06	2.00	-1192.0	!25
!EPEcyeom+R20H=>H20+CH0CH0+NC4H9C0 dbr, see shee	4.800E+06	2.00	-1192.0	!25
!EPEcyeom+R20H=>H20+CH2C0Z +C4H9C02 25 dbr, see shee	2.400E+06	2.00	-1192.0	!
!EPEcy504+R300H=>H202+C2H3CH0Z+EA2J my evans-po	8.000E+12	0.00	14400.0	!25
!EPEcy504+R300H=>H202+CH2C0Z +EP3J 25 my evans-po	4.000E+12	0.00	13260.0	!
!EPEcy503+R300H=>H202+R5CH0+EB3D my evans-po	8.000E+12	0.00	14400.0	!25
!EPEcy503+R300H=>H202+C2H4Z+EP3J*o my evans-po	4.000E+12	0.00	13260.0	!25

!EPEcy502+R300H=>H202+R13CH2CHO+EP2d my evans-po	8.000E+12	0.00	14400.0	!25
!EPEcy502+R300H=>H202+C2H4Z+EP3J2*o my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcy4o3+R300H=>H202+C2H3COCH3+C2H5OCO my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcy4o3+R300H=>H202+CH3CHCO+EA2J my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcy402+R300H=>H202+R14CH3CO+EP2d my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcy402+R300H=>H202+C3H6Y+EA2J*o my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcy302+R300H=>H202+C2H5OCO+C2H5CHCO my evans-po	8.000E+12	0.00	13260.0	!25
!EPEcy2oe+R300H=>H202+B2CO+R14CH3CO+NC3H7CHO !25 my evans-po	4.000E+12	0.00	13260.0	
!EPEcy2oe+R300H=>H202+CH3CO2+C4H8CO my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcy2oe+R300H=>H202+CH3CHO+prcoco my evans-po	4.000E+12	0.00	13260.0	!25
!EPEcyeom+R300H=>H202+CHOCHO+NC4H9CO my evans-po	8.000E+12	0.00	14400.0	!25
!EPEcyeom+R300H=>H202+CH2COZ +C4H9CO2 25 my evans-po	4.000E+12	0.00	13260.0	!
!				
!EPE5oo+R300H=EPE5ooh+02 Anglada et al.,	2.110e+10	0.00	-3640.0	!
!EPE4oo+R300H=EPE4ooh+02 Anglada et al.,	2.110e+10	0.00	-3640.0	!
!EPE3oo+R300H=EPE3ooh+02 Anglada et al.,	2.110e+10	0.00	-3640.0	!
!EPE2oo+R300H=EPE2ooh+02 Anglada et al.,	2.110e+10	0.00	-3640.0	!
!EPEeoo+R300H=EPEeooH+02 Anglada et al.,	2.110e+10	0.00	-3640.0	!
!EPEmoo+R300H=EPEmooH+02 Anglada et al.,	2.110e+10	0.00	-3640.0	!
!EPE5ooh=EPE5o+R20H Baulch et al., (1994)	4.000e+15	0.00	42920.0	!
!EPE4ooh=EPE4o+R20H Baulch et al., (1994)	4.000e+15	0.00	42920.0	!
!EPE3ooh=EPE3o+R20H Baulch et al., (1994)	4.000e+15	0.00	42920.0	!
!EPE2ooh=EPE2o+R20H Baulch et al., (1994)	4.000e+15	0.00	42920.0	!
!EPEeooH=EPEeo+R20H Baulch et al., (1994)	4.000e+15	0.00	42920.0	!
!EPEmooH=EPEmo+R20H Baulch et al., (1994)	4.000e+15	0.00	42920.0	!
!EPE5o=HCHO+EB4J et al., Int.J.Chem.Kinet. 38(2006)250-275	5.890e+13	0.00	13890.0	!Curran
!EPE4o=R4CH3+EB4*o Curran et al., Int.J.Chem.Kinet. 38(2006)250-275	1.780e+13	0.00	14890.0	!

!EPE4o=CH3CHO+EP3J	5.250e+13	0.00	11690.0	!Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPE3o=R11C2H5 +EP3*o	5.250e+13	0.00	11690.0	!
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPE3o=C2H5CHO+EA2J	5.250e+13	0.00	11690.0	!Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPE2o=>R19C3H7+ea2*o	5.250e+13	0.00	11690.0	!
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPE2o=NC3H7CHO+C2H5OCO	5.250e+13	0.00	11690.0	!Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPEeo=C4H9CO2+CH3CHO	5.250e+13	0.00	11690.0	!Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPEeo=mpem*o+R4CH3	1.780e+13	0.00	14890.0	!
Curran et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPEmo=MPEMJ+HCHO	5.890e+13	0.00	13890.0	!Curran
et al., Int.J.Chem.Kinet. 38(2006)250-275				
!EPE4D+R300H=EPE5ooh4j	2.470e+04	2.13	1.216e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPE4D+R300H=EPE4ooh5j	7.740e+03	2.29	1.108e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPE3D+R300H=EPE4ooh3j	7.740e+03	2.29	1.108e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPE3D+R300H=EPE3ooh4j	7.740e+03	2.29	1.108e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPE2D+R300H=EPE3ooh2j	7.740e+03	2.29	1.108e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPE2D+R300H=EPE2ooh3j	7.740e+03	2.29	1.108e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPEED+R300H=EPEeooHmj	7.740e+03	2.29	1.108e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!EPEED+R300H=EPEmoohj	2.470e+04	2.13	1.216e+04	!Chen
et al., J.Phys.Chem.A, 104 (2000) 4997-5012				
!				
!EPE5ooh3j=>EB3D+HCHO+R2OH	2.000e+13	0.00	2.870e+04	!
!EPE5ooh3j=>C2H5OCO+c4h81ooh3d	2.000e+13	0.00	2.870e+04	!
!EPE5ooh2j=>EP2d+R16C2H400H	2.000e+13	0.00	2.870e+04	!
!EPE4ooh2j=>EP2d+CH3CHO+R2OH	2.000e+13	0.00	2.870e+04	!
!EPE3ooh5j=>C2H4Z+EP3*o+R2OH	2.000e+13	0.00	2.870e+04	!
!EPE2ooh5j=>C2H4Z+EP2d+R300H	2.000e+13	0.00	2.870e+04	!
!EPE2ooh4j=>C3H6Y+ea2*o+R2OH	2.000e+13	0.00	2.870e+04	!
!EPE2oohej=>CH3CHO+C4H8CO+R300H	2.000e+13	0.00	2.870e+04	!
!EPEeooH2j=>CH3CHO+C4H8CO+R300H	2.000e+13	0.00	2.870e+04	!
!				
!EPE5oo=EPE4D+R300H	5.044E+38	-8.110	4.149E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPE4oo=EPE4D+R300H	5.075E+42	-9.410	4.249E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPE4oo=EPE3D+R300H	5.044E+38	-8.110	4.149E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPE3oo=EPE3D+R300H	5.044E+38	-8.110	4.149E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPE3oo=EPE2D+R300H	5.044E+38	-8.110	4.149E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				

!EPE2oo=EPE2D+R300H	5.044E+38	-8.110	4.149E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPEeoo=EPEED+R300H	5.075E+42	-9.410	4.249E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!EPEmoo=EPEED+R300H	5.044E+38	-8.110	4.149E+04	!Donato
et al., J.Eng.GasTurbines and Power, 132 (2010) 051502 +1kcal				
!				
EPE5J=C2H4Z+EP3J	2.000E+13	0.00	2.870E+04	!Dayma
et al., Int J Chem Kinet, 35 (2003) 273-285				
EPE4J=C3H6Y+EA2J	5.250E+11	0.50	26591.0	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!EPE4J=C3H6Y+EA2J	2.000E+13	0.00	2.870E+04	!Dayma
et al., Int J Chem Kinet, 35 (2003) 273-285				
!EPE3J=C4H8Y+C2H5OC0	4.530E+12	0.335	34269.0	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
EPE3J=C4H8Y+C2H5OC0	2.000E+13	0.00	3.100E+04	!Dayma et
al., Int J Chem Kinet, 35 (2003) 273-285				
EPE3J=EB3D+R4CH3	2.000E+13	0.00	3.100E+04	!Dayma
et al., Int J Chem Kinet, 35 (2003) 273-285				
!EPE2J=C4H8CO+R15C2H5O	2.786E+22	-2.31	4.566E+04	
EPE2J=C4H8CO+R15C2H5O	1.460E+12	0.61	53276.0	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
EPE2J=R11C2H5 +EP2d	2.000E+13	0.00	3.470E+04	!
Dayma et al., Int J Chem Kinet, 35 (2003) 273-285 (+6kcal)				
!EPE2J=R11C2H5 +EP2d	1.330E+11	0.97	34882.0	!Huynh
and Violi J. Org. Chem. 73 (2008) 94-101				
!EPEEJ=CH3CHO+NC4H9CO	1.127E+21	-1.73	4.055E+04	
EPEEJ=CH3CHO+NC4H9CO	1.127E+21	-1.73	4.255E+04	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!EPEMJ=C2H4Z+C4H9CO2	2.325E+14	-0.20	3.297E+04	
EPEMJ=C2H4Z+C4H9CO2	2.000E+13	0.00	2.800E+04	
MPEMJ=HCHO+NC4H9CO	1.230E+13	0.375	36714.0	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
EPE5J=EPE4D+R1H	3.000E+13	0.00	3.800E+04	!ST
EPE4J=EPE4D+R1H	3.000E+13	0.00	3.900E+04	!ST
EPE4J=EPE3D+R1H	3.000E+13	0.00	3.800E+04	!ST
EPE3J=EPE3D+R1H	3.000E+13	0.00	3.800E+04	!ST
EPE3J=EPE2D+R1H	3.000E+13	0.00	3.800E+04	!ST
EPE2J=EPE2D+R1H	3.000E+13	0.00	3.800E+04	!ST
EPEEJ=EPEED+R1H	3.000E+13	0.00	3.900E+04	!ST
EPEMJ=EPEED+R1H	3.000E+13	0.00	3.800E+04	!ST
C4H9C00H=>C4H8CO+H2O	4.470E+14	0.00	7.989E+04	!Duan et
Page, J. Am. Chem. Soc. 117 (1995) 5114-5119				
C4H9C00H=>C4H10+CO2	7.080E+13	0.00	7.452E+04	!Duan et
Page, J. Am. Chem. Soc. 117 (1995) 5114-5119				
C4H9C00H=>NC4H9CO+R20H	1.4E+0017	0.000	105815.7	! UI 8
KB				
C4H9C00H=>C4H9CO2+R1H	2.3E+0014	0.000	106345.3	! UI 9
KB				
C4H9C00H=>R20C4H9+HOCO	8.2E+0016	0.000	88817.0	! UI 10
KB				

C4H9C00H=>R19C3H7+CH2C00H KB	2.9E+0016	0.000	78917.1	! UI 11
C4H9C00H=>R11C2H5 +CH2CH2C00H 12 KB	1.7E+0017	0.000	87662.1	! UI
C4H9C00H+R1H=BUC00H-5+H2 anc7, primARy f	9.400e+04	2.75	6.280e+03	!2
C4H9C00H+R1H=BUC00H-4+H2 anc7, secondARy	1.300E+06	2.4	4.471E+03	!2
C4H9C00H+R1H=BUC00H-3+H2 anc7, secondARy	1.300E+06	2.4	4.471E+03	!2
C4H9C00H+R1H=BUC00H-2+H2 anc7, secondARy	1.300E+06	2.4	4.471E+03	!2
!C4H9C00H+R1H=BUC00H-2+H2	5.400e+04	2.5	-1.900e+03	!
!C4H9C00H+R1H=C4H9C02+H2 96 CN	4.2E+0006	2.000	2400.0	! ME
C4H9C00H+R1H=C4H9C02+H2 PARK,Zhu,Lin, JcP 118, 9990-9996 (2003)	5.550E-23	10.60	-4459.0	!
C4H9C00H+B10=BUC00H-5+R20H anc7, primARy f	9.650e+04	2.68	3.716e+03	!2
C4H9C00H+B10=BUC00H-4+R20H anc7, secondARy	4.770E+04	2.71	2.106E+03	!2
C4H9C00H+B10=BUC00H-3+R20H anc7, secondARy	4.770E+04	2.71	2.106E+03	!2
C4H9C00H+B10=BUC00H-2+R20H anc7, secondARy	4.770E+04	2.71	2.106E+03	!2
!C4H9C00H+B10=BUC00H-2+R20H	8.800e+10	0.70	3.250e+03	!
!C4H9C00H+B10=C4H9C02+R20H 87 CW	1.0E+0013	0.000	3280.0	! ME
C4H9C00H+B10=C4H9C02+R20H Lee, Xu, Lin, JPcA 2007	1.460E-03	4.73	1727.0	! Wu,
C4H9C00H+R20H=BUC00H-5+H20 rnc7, primARy;	5.250e+09	0.97	1.590e+03	!2
C4H9C00H+R20H=BUC00H-4+H20 rnc7, secondARy	4.680E+07	1.61	-3.500E+01	!2
C4H9C00H+R20H=BUC00H-3+H20 rnc7, secondARy	4.680E+07	1.61	-3.500E+01	!2
C4H9C00H+R20H=BUC00H-2+H20 rnc7, secondARy	4.680E+07	1.61	-3.500E+01	!2
!C4H9C00H+R20H=BUC00H-2+H20	3.000e+06	2.00	-1.520e+03	!
!C4H9C00H+R20H=C4H9C02+H20 105 CW	1.1E+0006	2.000	-1865.0	! ME
C4H9C00H+R20H=C4H9C02+H20 Lin pci 2007 31 159-166	2.810E+02	2.97	-580.0	! Xu
C4H9C00H+R4CH3=BUC00H-5+CH4 anc7, primARy f	4.520e-01	3.65	7.154e+03	!2
C4H9C00H+R4CH3=BUC00H-4+CH4 anc7, secondARy	2.705E+04	2.26	7.287E+03	!2
C4H9C00H+R4CH3=BUC00H-3+CH4 anc7, secondARy	2.705E+04	2.26	7.287E+03	!2
C4H9C00H+R4CH3=BUC00H-2+CH4 anc7, secondARy	2.705E+04	2.26	7.287E+03	!2
!C4H9C00H+R4CH3=BUC00H-2+CH4	1.000e+11	0.00	7.300e+03	!

C4H9C00H+R4CH3=C4H9C02+CH4	2.035E+00	3.57	7722.0	!
Xu, PARK, Lin, JcP 120, 6593-6599 (2004)				
C4H9C00H+R300H=BUC00H-5+H202	8.400E+12	0.00	2.044E+04	!2
anc7, primARY f				
C4H9C00H+R300H=BUC00H-4+H202	5.600E+12	0.00	1.769E+04	!2
anc7, secondARY				
C4H9C00H+R300H=BUC00H-3+H202	5.600E+12	0.00	1.769E+04	!2
anc7, secondARY				
C4H9C00H+R300H=>BUC00H-2+H202	5.600E+12	0.00	1.769E+04	!2
anc7, secondARY				
!C4H9C00H+R300H=BUC00H-2+H202	6.400E+03	2.60	1.240E+04	!
!C4H9C00H+R300H=C4H9C02+H202	2.11E+0006	0.000	14000.0	! ME
96 CN				
C4H9C00H+R300H=C4H9C02+H202	2.500E+12	0.00	24000.0	! MARinov
1998				
C4H9C00H+R8CH300=BUC00H-5+CH300H	8.400E+12	0.00	2.044E+04	!2
anc7, primARY f				
C4H9C00H+R8CH300=BUC00H-4+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
C4H9C00H+R8CH300=BUC00H-3+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
C4H9C00H+R8CH300=BUC00H-2+CH300H	5.600E+12	0.00	1.769E+04	!2
corrected to ag				
!C4H9C00H+R8CH300=BUC00H-2+CH300H	6.400E+03	2.60	1.240E+04	!
C4H9C00H+R7CH30 =BUC00H-5+CH30H	1.581E+11	0.00	7.000E+03	!2
rnc7, primARY;				
C4H9C00H+R7CH30 =BUC00H-4+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
C4H9C00H+R7CH30 =BUC00H-3+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
C4H9C00H+R7CH30 =BUC00H-2+CH30H	1.095E+11	0.00	5.000E+03	!2
anc7, secondARY				
!C4H9C00H+R7CH30 =BUC00H-2+CH30H	1.780E+12	0.00	1.200E+03	!
BUC00H-5=C2H4Z+CH2CH2C00H	2.000E+13	0.00	2.870E+04	!Dayma
et al., Int J Chem Kinet, 35 (2003) 273-285				
BUC00H-4=C3H6Y+CH2C00H	5.250E+11	0.50	26591.0	!Huynh
and Violi J. Org. Chem. 2008 vol. 73 pp. 94-101				
!BUC00H-4=C3H6Y+CH2C00H	2.000E+13	0.00	2.870E+04	!Dayma
et al., Int J Chem Kinet, 35 (2003) 273-285				
BUC00H-3=C4H8Y+HOC0	3.030E+13	0.27	34667.0	!Huynh and
Violi J. Org. Chem. 73 (2008) 94-101				
!BUC00H-3=C4H8Y+HOC0	4.217E+14	-0.32	3.486E+04	
BUC00H-3=>C3H5C00H+R4CH3	2.000E+13	0.00	3.100E+04	!Dayma
et al., Int J Chem Kinet, 35 (2003) 273-285				
BUC00H-2=C4H8C0+R20H	3.046E+21	-1.61	5.730E+04	
BUC00H-2=R11C2H5 +C2H3C00H	2.000E+13	0.00	3.270E+04	!
Dayma et al., Int J Chem Kinet, 35 (2003) 273-285 (+4kcal)				
BUC00H-2=>C02+R20C4H9	1.700E+09	1.0	38640.0	
C4H9C02+m=R20C4H9+C02+m	4.400E+15	0.00	1.050E+04	
C3H7C0C02+m=>NC3H7C0+C02+m	4.400E+15	0.00	10500.0	
CH3C0C02+m=>R14CH3C0+C02+m	4.400E+15	0.00	10500.0	
NC4H9C0=>R20C4H9+B2C0	1.834E+15	-0.73	1.291E+04	!
Glaude et al., DMC C2H5C0				

BUC00H-5=C4H7C00H+R1H	3.000E+13	0.00	38000.0	!ST
BUC00H-4=C4H7C00H+R1H	3.000E+13	0.00	38000.0	!ST
BUC00H-3=C4H7C00H+R1H	3.200E+13	0.00	34800.0	!ST
BUC00H-2=C4H7C00H+R1H	3.000E+13	0.00	5.150E+04	!ST
C4H7C00H+R20H=>HCHO+PRC00H-4	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
C4H7C00H+R20H=>CH3CHO+CH2CH2C00H	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
C4H7C00H+R20H=>C2H5CHO+CH2C00H	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
C4H7C00H+R1H=>H2+C02+C4H7-1	4.2E+0006	2.100	6900.0	! MZB
483				
C4H7C00H+R20H=>H2O+C02+C4H7-1	5.4E+0004	2.000	-340.0	! MZB
484				
C4H7C00H+R300H=>H2O2+C02+C4H7-1	1.0E+0011	0.000	11500.0	! MZB
485				
C4H7C00H+R4CH3=>CH4+C02+C4H7-1	1.4E+0001	3.100	9940.0	! MZB
486				
C4H7C00H+R11C2H5 =>C2H6+C02+C4H7-1	1.4E+0001	3.100	8940.0	!
MZB 487				
EPE4D+R20H=>HCHO+EB4J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPE4D+R20H=>CH3CHO+EP3J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPE3D+R20H=>CH3CHO+EP3J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPE3D+R20H=>C2H5CHO+EA2J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPE2D+R20H=>C2H5CHO+EA2J	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPEED+R20H=>HCHO+MPEMJ	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPEED+R20H=>CH3CHO+C4H9C02	1.370e+12	0.00	-1.040e+03	!
Heyberger et al., Combust Flame, 126 (2001) 1780-1802				
EPE4D=C4H7C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
EPE3D=C4H7C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
EPE2D=C4H7C00H+C2H4Z	2.000E+12	0.00	4.729E+04	
!EPE2D(+m)=C4H7C00H+C2H4Z(+m)	4.000E+12	0.00	5.000E+04	
!LOW / 1.3100E+17 -9.9000E-01 1.1880E+04 /				
!TROE / 2.4323E-01 1.0000E+00 1.0000E+10 6.7101E+09 / !TroE Fall-off				
reaction				
!END				
!!				
CH3C02+M=R4CH3+C02+M	4.400E+15	0.00	10500.0	
!!				
!C2H5CHO=R13CH2CHO+R4CH3	1.000e+17	0.0	8.465e+04	!
asC4H10 Dean, J.Phys.Chem. 89 (1985) 4600-4608				
!C4H8Y+R20H=R4CH3+C2H5CHO	6.800E+11	0.0	-928.0	!(89ATK*RTi)
!metathesis same as n-butanal				
C2H5CHO+R300H=R25C2H5CO+H2O2	1.700E+12	0.00	10700.0	!
(COLKET 77; C				
C2H5CHO+R20H=CH3CHCHO+H2O	4.680e+07	1.61	-3.500e+01	!2
rnc7, se				



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!C2H5CHO+R2OH=R25C2H5CO+H2O          2.650E+12   0.00   -730.0   !
Atkinson et
!C2H5CHO+R1H=R25C2H5CO+H2            1.200E+14   0.00   7000.0   !
Yasunaga et
!decomposition
R25C2H5CO=CH3CHCO+R1H                 4.658E+10   0.79   4.255E+04   !
rev / 2.000
R25C2H5CO=CH2COZ +R4CH3                2.745E+09   1.41
3.583E+04 !rev / 1.
!R25C2H5CO=>R11C2H5+B2CO              1.834e+15  -0.73   1.291e+04
!Glaude et a
CH3CHCHO=CH3CHCO+R1H 1.345E+13 -0.17 3.346E+04
rev / 5.000E+12 0.00 1.200E+03 /
!!!!!!!!!!!!Reactions of butanal!!!!!!!!!!!!
!initiation
NC3H7CHO=R11C2H5+R13CH2CHO            1.580e+17   0.0    8.028e+04   !asC4H10
Dean, J.Phys.Chem. 89 (1985) 4600-4608
!metathesis
NC3H7CHO+R1H=NC3H7CO+H2               1.200E+14   0.00   7000.0   !
Yasunaga et al., Int.J.chem.Kinet., 40 (2008) 73-102
!decomposition
NC3H7CO+M=R19C3H7+B2CO+M              8.640E+15   0.00
14400.0 !(WILK89) idem R14CH3CO+M
NC3H7CO=CH2COZ +R11C2H5               2.745E+09   1.41   3.583E+04 !
rev / 1.000E+04 2.48 6.130E+03 /
END

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